



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:03 AM GMT

PDB ID : 2F5Z
Title : Crystal Structure of Human Dihydrolipoamide Dehydrogenase (E3) Complexed to the E3-Binding Domain of Human E3-Binding Protein
Authors : Brautigam, C.A.; Chuang, J.L.; Wynn, R.M.; Tomchick, D.R.; Machius, M.; Chuang, D.T.
Deposited on : 2005-11-28
Resolution : 2.18 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

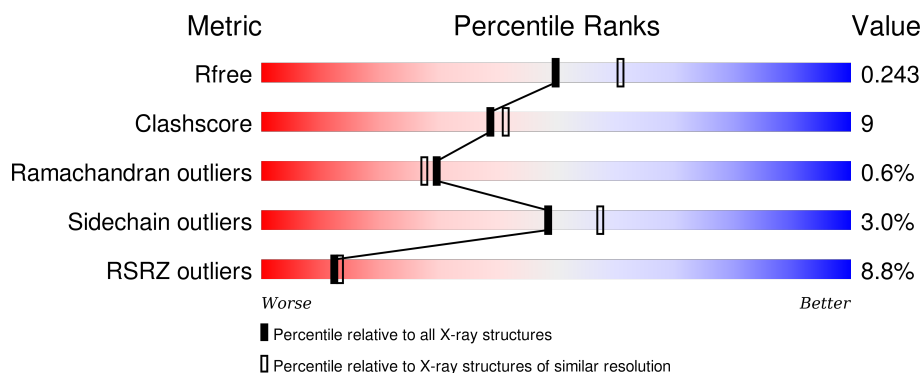
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.18 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	5130 (2.20-2.16)
Clashscore	102246	5965 (2.20-2.16)
Ramachandran outliers	100387	5863 (2.20-2.16)
Sidechain outliers	100360	5864 (2.20-2.16)
RSRZ outliers	91569	5142 (2.20-2.16)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	474	<div> <div>5%</div> <div>81%</div> <div>18%</div> </div>
1	B	474	<div> <div>17%</div> <div>73%</div> <div>25%</div> <div>..</div> </div>
1	C	474	<div> <div>4%</div> <div>81%</div> <div>17%</div> <div>.</div> </div>
1	D	474	<div> <div>5%</div> <div>87%</div> <div>12%</div> <div>..</div> </div>
1	E	474	<div> <div>7%</div> <div>85%</div> <div>14%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	474	
1	G	474	
1	H	474	
1	I	474	
1	J	474	
2	K	64	
2	L	64	
2	M	64	
2	N	64	
2	O	64	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	SO4	B	2489	-	-	X	-
3	SO4	C	2490	-	-	-	X
3	SO4	E	2499	-	-	X	-
3	SO4	H	2510	-	-	X	-
3	SO4	H	2511	-	-	X	-
3	SO4	I	2515	-	-	X	-
3	SO4	J	2520	-	-	X	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 40176 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Dihydrolipoyl dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	472	Total	C	N	O	S	0	0	0
			3505	2208	606	672	19			
1	B	471	Total	C	N	O	S	0	0	0
			3496	2203	604	670	19			
1	C	472	Total	C	N	O	S	0	0	0
			3505	2208	606	672	19			
1	D	471	Total	C	N	O	S	0	0	0
			3496	2203	604	670	19			
1	E	472	Total	C	N	O	S	0	0	0
			3505	2208	606	672	19			
1	F	471	Total	C	N	O	S	0	0	0
			3496	2203	604	670	19			
1	G	472	Total	C	N	O	S	0	0	0
			3505	2208	606	672	19			
1	H	472	Total	C	N	O	S	0	0	0
			3505	2208	606	672	19			
1	I	470	Total	C	N	O	S	0	0	0
			3496	2204	604	669	19			
1	J	472	Total	C	N	O	S	0	0	0
			3505	2208	606	672	19			

- Molecule 2 is a protein called Pyruvate dehydrogenase protein X component.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	K	43	Total	C	N	O	0	0	0
			301	186	57	58			
2	L	43	Total	C	N	O	0	43	0
			590	364	112	114			
2	M	43	Total	C	N	O	0	43	0
			590	364	112	114			
2	N	43	Total	C	N	O	0	43	0
			590	364	112	114			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	O	43	Total	C	N	O	0	43	0
			590	364	112	114			

There are 40 discrepancies between the modelled and reference sequences:

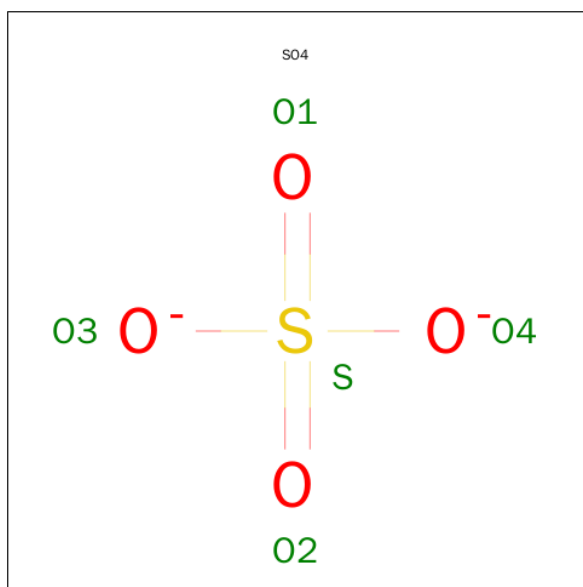
Chain	Residue	Modelled	Actual	Comment	Reference
K	120	GLY	LYS	ENGINEERED	UNP O00330
K	176	LEU	THR	ENGINEERED	UNP O00330
K	178	HIS	-	EXPRESSION TAG	UNP O00330
K	179	HIS	-	EXPRESSION TAG	UNP O00330
K	180	HIS	-	EXPRESSION TAG	UNP O00330
K	181	HIS	-	EXPRESSION TAG	UNP O00330
K	182	HIS	-	EXPRESSION TAG	UNP O00330
K	183	HIS	-	EXPRESSION TAG	UNP O00330
L	120	GLY	LYS	ENGINEERED	UNP O00330
L	176	LEU	THR	ENGINEERED	UNP O00330
L	178	HIS	-	EXPRESSION TAG	UNP O00330
L	179	HIS	-	EXPRESSION TAG	UNP O00330
L	180	HIS	-	EXPRESSION TAG	UNP O00330
L	181	HIS	-	EXPRESSION TAG	UNP O00330
L	182	HIS	-	EXPRESSION TAG	UNP O00330
L	183	HIS	-	EXPRESSION TAG	UNP O00330
M	120	GLY	LYS	ENGINEERED	UNP O00330
M	176	LEU	THR	ENGINEERED	UNP O00330
M	178	HIS	-	EXPRESSION TAG	UNP O00330
M	179	HIS	-	EXPRESSION TAG	UNP O00330
M	180	HIS	-	EXPRESSION TAG	UNP O00330
M	181	HIS	-	EXPRESSION TAG	UNP O00330
M	182	HIS	-	EXPRESSION TAG	UNP O00330
M	183	HIS	-	EXPRESSION TAG	UNP O00330
N	120	GLY	LYS	ENGINEERED	UNP O00330
N	176	LEU	THR	ENGINEERED	UNP O00330
N	178	HIS	-	EXPRESSION TAG	UNP O00330
N	179	HIS	-	EXPRESSION TAG	UNP O00330
N	180	HIS	-	EXPRESSION TAG	UNP O00330
N	181	HIS	-	EXPRESSION TAG	UNP O00330
N	182	HIS	-	EXPRESSION TAG	UNP O00330
N	183	HIS	-	EXPRESSION TAG	UNP O00330
O	120	GLY	LYS	ENGINEERED	UNP O00330
O	176	LEU	THR	ENGINEERED	UNP O00330
O	178	HIS	-	EXPRESSION TAG	UNP O00330
O	179	HIS	-	EXPRESSION TAG	UNP O00330

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Chain	Residue	Modelled	Actual	Comment	Reference
O	180	HIS	-	EXPRESSION TAG	UNP O00330
O	181	HIS	-	EXPRESSION TAG	UNP O00330
O	182	HIS	-	EXPRESSION TAG	UNP O00330
O	183	HIS	-	EXPRESSION TAG	UNP O00330

- Molecule 3 is SULFATE ION (three-letter code: SO₄) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		

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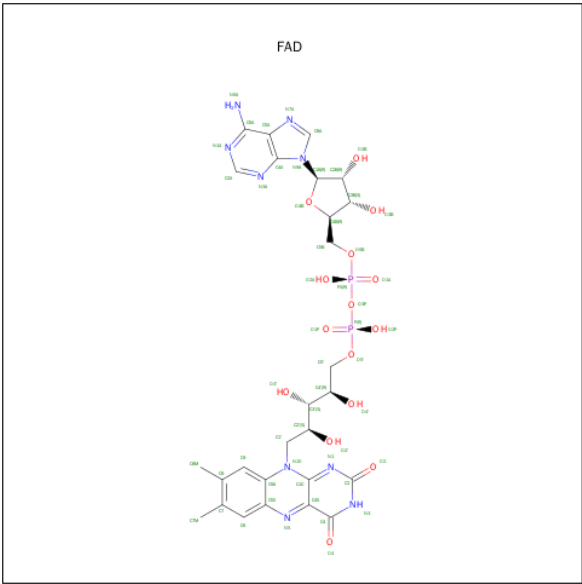
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	D	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	F	1	Total	O	S	0	0
			5	4	1		
3	F	1	Total	O	S	0	0
			5	4	1		
3	F	1	Total	O	S	0	0
			5	4	1		
3	F	1	Total	O	S	0	0
			5	4	1		
3	G	1	Total	O	S	0	0
			5	4	1		
3	G	1	Total	O	S	0	0
			5	4	1		
3	G	1	Total	O	S	0	0
			5	4	1		
3	G	1	Total	O	S	0	0
			5	4	1		
3	H	1	Total	O	S	0	0
			5	4	1		
3	H	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	H	1	Total	O	S	0	0
			5	4	1		
3	H	1	Total	O	S	0	0
			5	4	1		
3	I	1	Total	O	S	0	0
			5	4	1		
3	I	1	Total	O	S	0	0
			5	4	1		
3	I	1	Total	O	S	0	0
			5	4	1		
3	J	1	Total	O	S	0	0
			5	4	1		
3	J	1	Total	O	S	0	0
			5	4	1		
3	J	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 53	C 27	N 9	O 15	P 2	0	0
4	B	1	Total 53	C 27	N 9	O 15	P 2	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
4	D	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
4	E	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
4	F	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
4	G	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
4	H	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
4	I	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
4	J	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	183	Total	O	0	0
			183	183		
5	B	101	Total	O	0	0
			101	101		
5	C	172	Total	O	0	0
			172	172		
5	D	243	Total	O	0	0
			243	243		
5	E	150	Total	O	0	0
			150	150		
5	F	217	Total	O	0	0
			217	217		
5	G	188	Total	O	0	0
			188	188		
5	H	315	Total	O	0	0
			315	315		
5	I	73	Total	O	0	0
			73	73		
5	J	132	Total	O	0	0
			132	132		
5	N	1	Total	O	0	0
			1	1		

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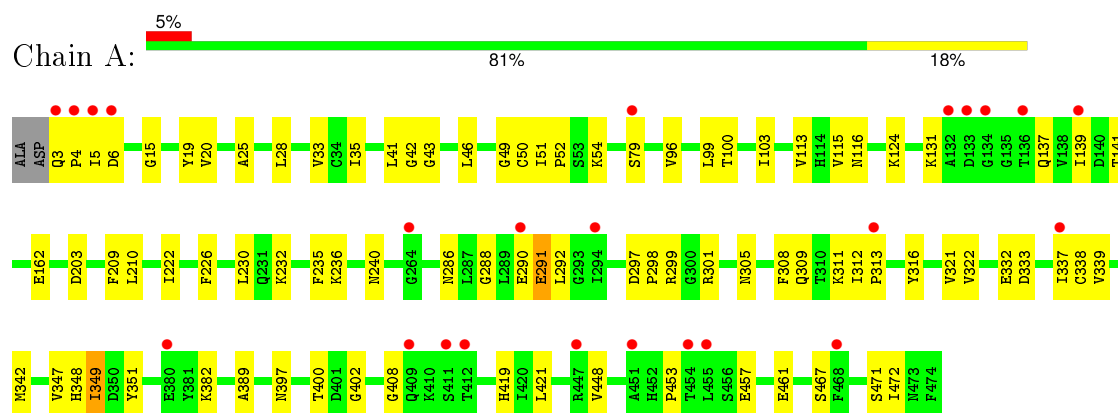
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	O	1	Total	O	0	0
			1	1		

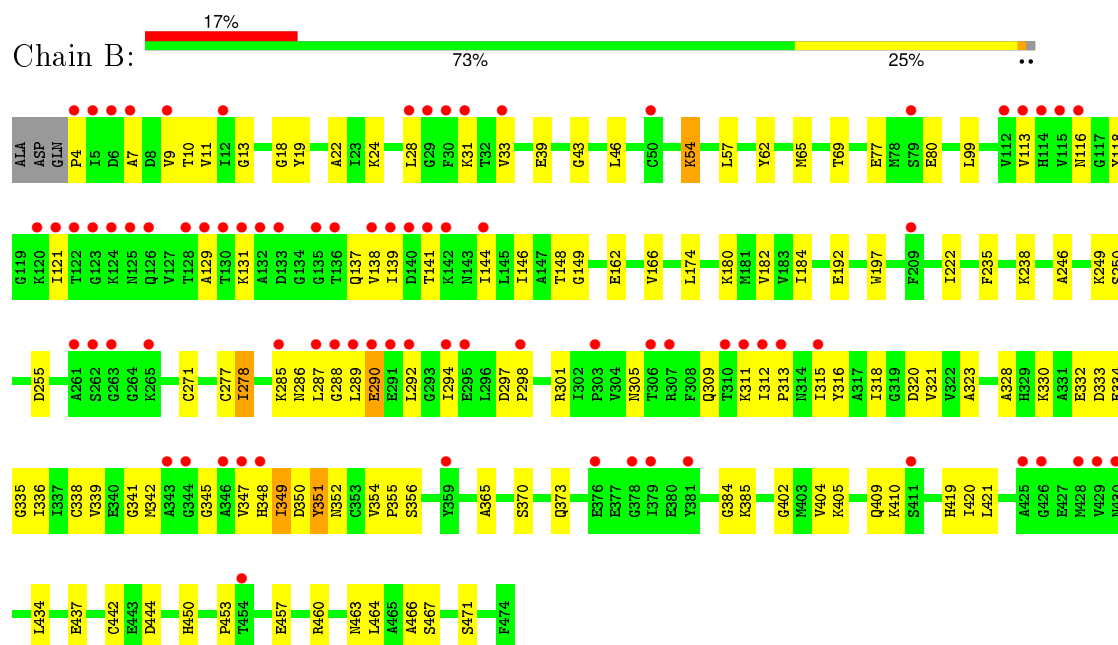
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

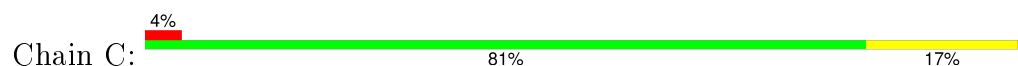
• Molecule 1: Dihydrolipoyl dehydrogenase

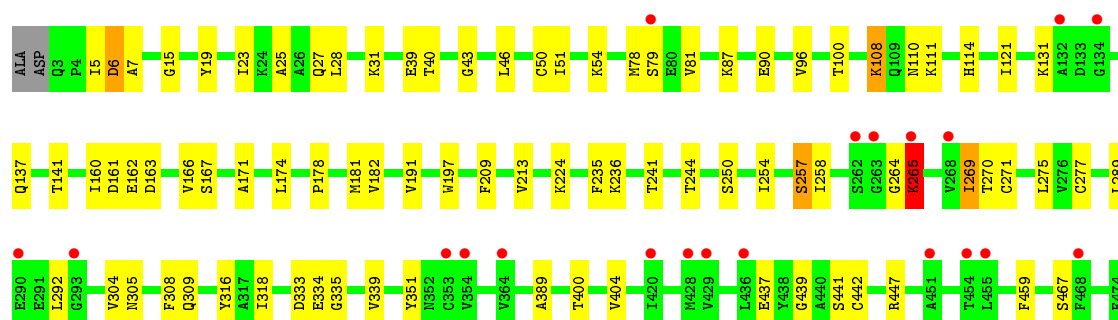


• Molecule 1: Dihydrolipoyl dehydrogenase

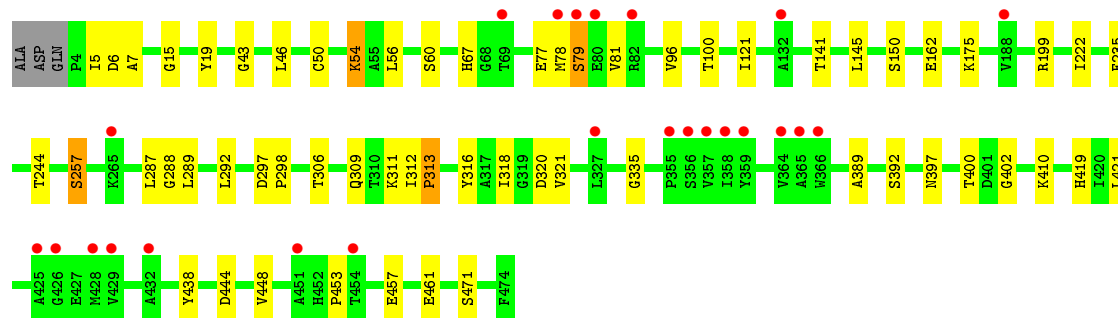
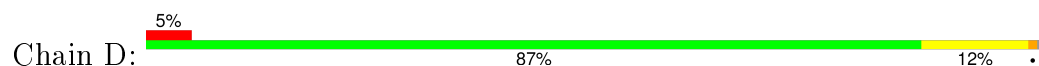


• Molecule 1: Dihydrolipoyl dehydrogenase

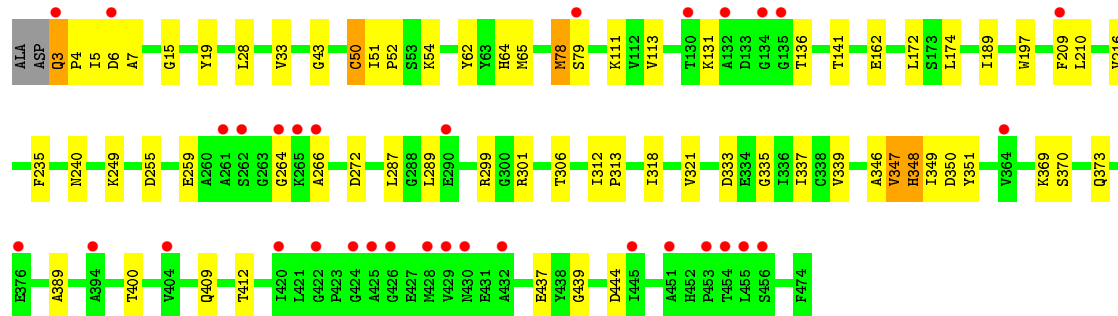
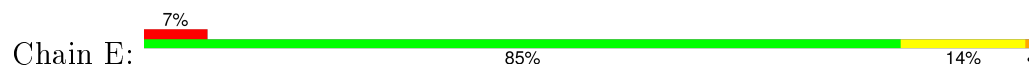




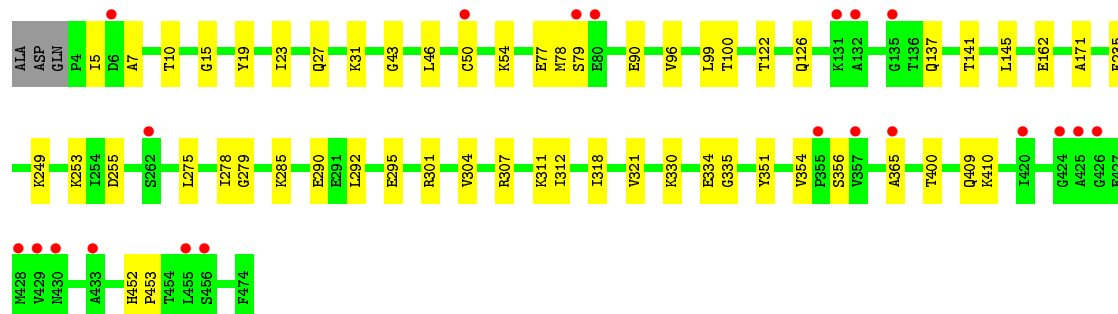
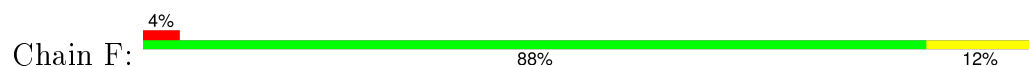
• Molecule 1: Dihydrolipoyl dehydrogenase



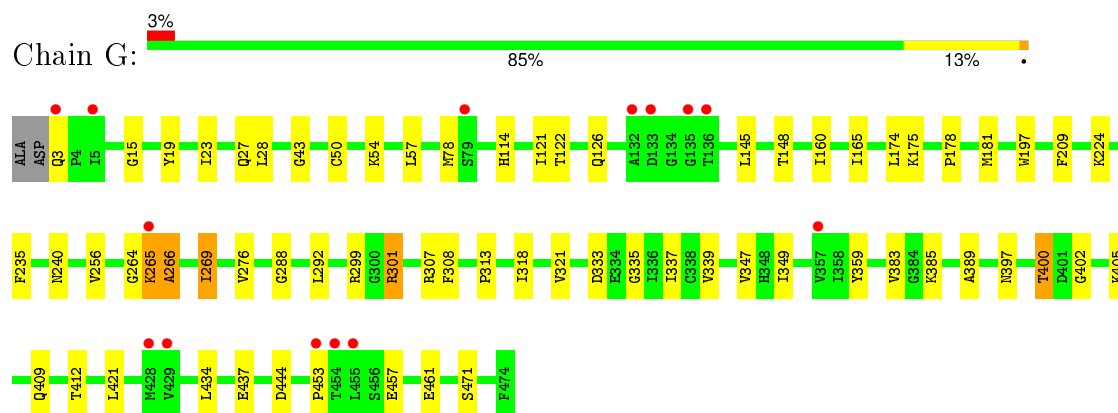
• Molecule 1: Dihydrolipoyl dehydrogenase



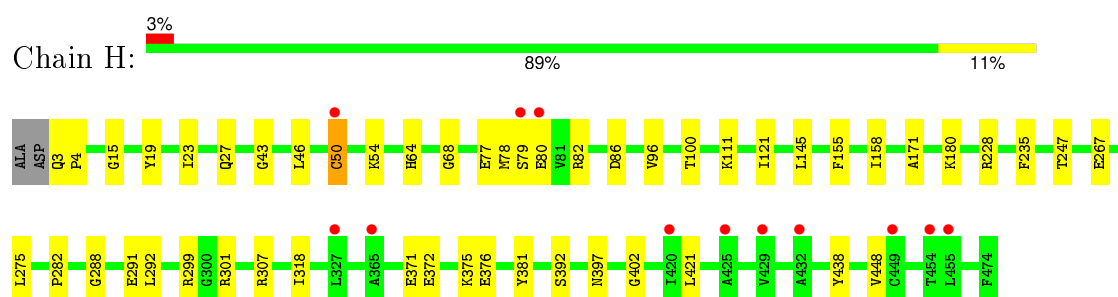
• Molecule 1: Dihydrolipoyl dehydrogenase



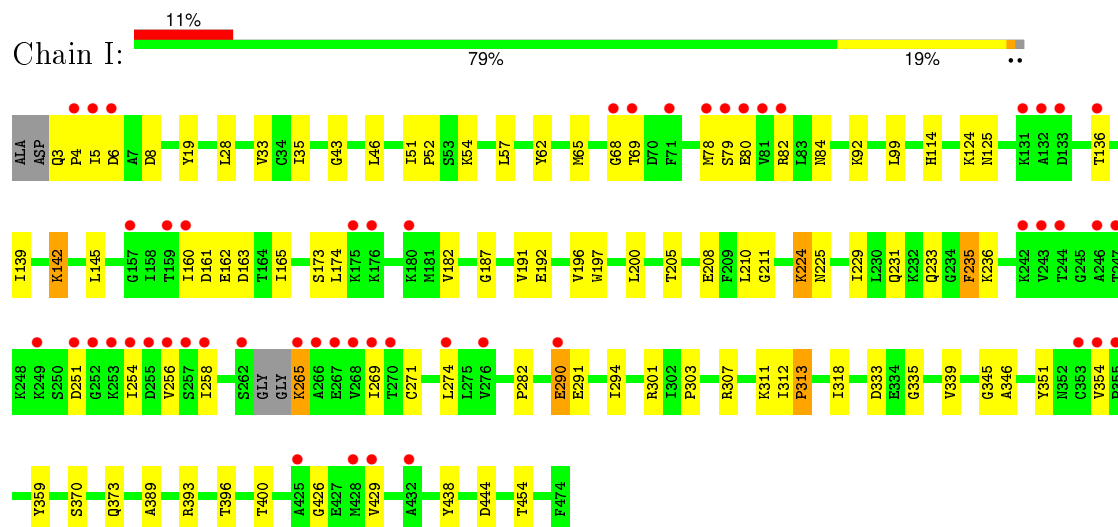
• Molecule 1: Dihydrolipoyl dehydrogenase



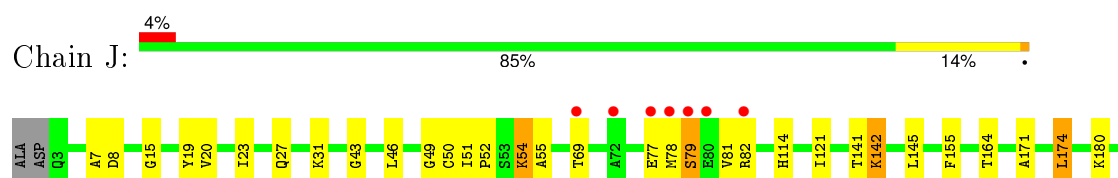
• Molecule 1: Dihydrolipoyl dehydrogenase

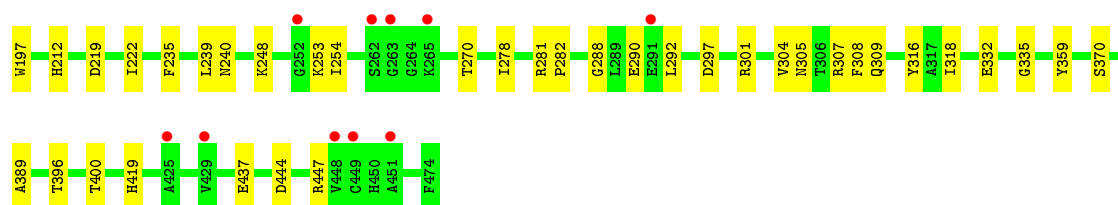


• Molecule 1: Dihydrolipoyl dehydrogenase

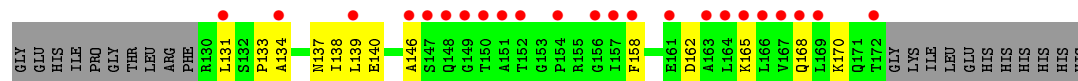


• Molecule 1: Dihydrolipoyl dehydrogenase

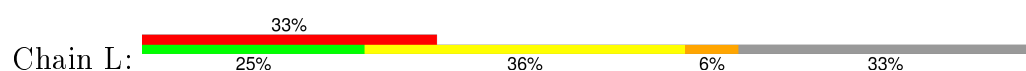




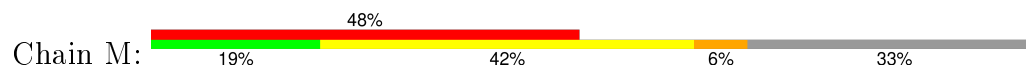
• Molecule 2: Pyruvate dehydrogenase protein X component



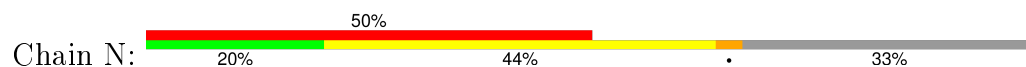
• Molecule 2: Pyruvate dehydrogenase protein X component



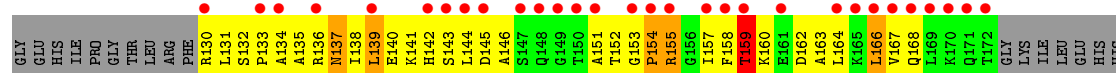
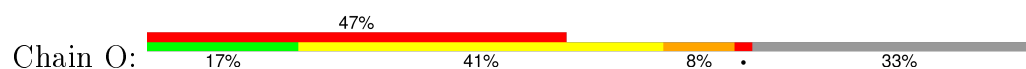
• Molecule 2: Pyruvate dehydrogenase protein X component



• Molecule 2: Pyruvate dehydrogenase protein X component



• Molecule 2: Pyruvate dehydrogenase protein X component



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4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	171.15Å 187.73Å 224.39Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.40 – 2.18 46.92 – 2.18	Depositor EDS
% Data completeness (in resolution range)	98.1 (37.40-2.18) 98.3 (46.92-2.18)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.79 (at 2.18Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.205 , 0.242 0.207 , 0.243	Depositor DCC
R_{free} test set	4517 reflections (1.23%)	DCC
Wilson B-factor (Å ²)	35.9	Xtriage
Anisotropy	0.311	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 48.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 367467 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	40176	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.16% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, FAD

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.46	0/3560	0.70	1/4809 (0.0%)
1	B	0.42	0/3551	0.67	0/4796
1	C	0.52	0/3560	0.74	1/4809 (0.0%)
1	D	0.55	0/3551	0.75	1/4796 (0.0%)
1	E	0.51	0/3560	0.70	1/4809 (0.0%)
1	F	0.55	0/3551	0.74	3/4796 (0.1%)
1	G	0.52	0/3560	0.73	2/4809 (0.0%)
1	H	0.62	0/3560	0.77	1/4809 (0.0%)
1	I	0.46	0/3550	0.69	0/4796
1	J	0.50	0/3560	0.72	1/4809 (0.0%)
2	K	0.37	0/304	0.70	0/411
2	L	0.31	0/596	0.62	0/808
2	M	0.34	0/596	0.65	0/808
2	N	0.35	0/596	0.70	0/808
2	O	0.32	0/596	0.63	0/808
All	All	0.50	0/38251	0.72	11/51681 (0.0%)

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	50	CYS	CA-CB-SG	7.22	127.00	114.00
1	F	50	CYS	CA-CB-SG	6.26	125.27	114.00
1	J	50	CYS	CA-CB-SG	6.15	125.07	114.00
1	G	50	CYS	CA-CB-SG	6.04	124.86	114.00
1	E	50	CYS	CA-CB-SG	5.96	124.72	114.00
1	A	50	CYS	CA-CB-SG	5.91	124.64	114.00
1	D	50	CYS	CA-CB-SG	5.72	124.31	114.00
1	G	400	THR	N-CA-C	5.54	125.97	111.00
1	F	400	THR	N-CA-C	5.32	125.36	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	50	CYS	CA-CB-SG	5.18	123.32	114.00
1	F	31	LYS	N-CA-C	-5.02	97.45	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3505	0	3556	62	0
1	B	3496	0	3549	100	0
1	C	3505	0	3556	55	0
1	D	3496	0	3549	41	0
1	E	3505	0	3556	58	0
1	F	3496	0	3549	35	0
1	G	3505	0	3556	43	0
1	H	3505	0	3556	39	0
1	I	3496	0	3549	71	0
1	J	3505	0	3556	55	0
2	K	301	0	289	15	0
2	L	590	0	546	37	0
2	M	590	0	546	35	0
2	N	590	0	546	44	0
2	O	590	0	546	55	0
3	A	20	0	0	2	0
3	B	20	0	0	4	0
3	C	20	0	0	1	0
3	D	20	0	0	0	0
3	E	20	0	0	3	0
3	F	20	0	0	2	0
3	G	20	0	0	1	0
3	H	20	0	0	4	0
3	I	15	0	0	3	0
3	J	20	0	0	4	0
4	A	53	0	31	2	0
4	B	53	0	31	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	53	0	31	3	0
4	D	53	0	31	2	0
4	E	53	0	31	3	0
4	F	53	0	31	4	0
4	G	53	0	31	2	0
4	H	53	0	31	5	0
4	I	53	0	31	1	0
4	J	53	0	31	3	0
5	A	183	0	0	0	0
5	B	101	0	0	3	0
5	C	172	0	0	2	0
5	D	243	0	0	1	0
5	E	150	0	0	2	0
5	F	217	0	0	4	0
5	G	188	0	0	1	0
5	H	315	0	0	5	0
5	I	73	0	0	3	0
5	J	132	0	0	0	0
5	N	1	0	0	1	0
5	O	1	0	0	0	0
All	All	40176	0	38315	692	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (692) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:290:GLU:HB3	3:I:2516:SO4:O4	1.54	1.07
1:A:461:GLU:HG2	1:A:471:SER:HB2	1.37	1.02
1:G:337:ILE:HG12	1:G:349:ILE:HD11	1.37	1.02
1:B:144:ILE:HB	1:B:315:ILE:HD13	1.39	1.01
2:O:158[B]:PHE:O	2:O:162[B]:ASP:HB2	1.71	0.90
1:A:308:PHE:HE2	1:A:337:ILE:HD11	1.33	0.89
2:N:142[B]:HIS:HB3	2:N:144[B]:LEU:HD13	1.54	0.89
2:O:157[B]:ILE:HG22	2:O:159[B]:THR:H	1.38	0.89
1:I:80:GLU:HG2	1:J:79:SER:HB3	1.58	0.85
1:B:370:SER:H	1:B:373:GLN:NE2	1.75	0.85
1:H:307:ARG:NH1	5:H:2731:HOH:O	2.08	0.85
2:O:154[B]:PRO:HG2	2:O:157[B]:ILE:HD13	1.59	0.84
1:E:78:MET:HG2	1:F:78:MET:HG2	1.59	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:67:HIS:HA	1:D:81:VAL:HG11	1.59	0.82
2:N:132[B]:SER:HB3	2:N:157[B]:ILE:HD11	1.63	0.81
2:O:159[B]:THR:HG23	2:O:162[B]:ASP:H	1.45	0.80
2:M:138[B]:ILE:HD11	2:M:163[B]:ALA:HB3	1.64	0.79
1:B:288:GLY:O	1:B:292:LEU:HD13	1.82	0.79
1:E:79:SER:HB2	1:F:79:SER:OG	1.83	0.79
1:F:307:ARG:NH1	5:F:2714:HOH:O	2.16	0.78
1:E:370:SER:H	1:E:373:GLN:NE2	1.82	0.78
1:B:11:VAL:HG11	1:B:22:ALA:HB2	1.64	0.78
2:N:130[B]:ARG:O	2:N:157[B]:ILE:HD12	1.84	0.78
1:A:308:PHE:CE2	1:A:337:ILE:HD11	2.19	0.77
1:I:79:SER:HB2	1:J:79:SER:OG	1.85	0.76
1:A:5:ILE:HG22	1:A:137:GLN:HE21	1.51	0.76
1:J:447:ARG:NE	2:O:137[A]:ASN:ND2	2.34	0.76
2:N:166[A]:LEU:HD13	2:N:166[A]:LEU:O	1.86	0.76
1:B:250:SER:HB3	1:J:304:VAL:HG23	1.67	0.76
1:H:438:TYR:O	2:N:130[B]:ARG:HD2	1.86	0.75
2:M:157[A]:ILE:HG22	2:M:159[A]:THR:H	1.50	0.75
2:K:162:ASP:O	2:K:165:LYS:HG2	1.87	0.75
2:N:159[B]:THR:OG1	2:N:161[B]:GLU:HG2	1.87	0.75
2:O:130[A]:ARG:NH2	2:O:155[A]:ARG:HD2	2.03	0.72
1:C:305:ASN:HD21	1:C:309:GLN:HE21	1.37	0.72
1:C:79:SER:HB2	1:D:79:SER:OG	1.89	0.72
1:B:10:THR:OG1	1:B:141:THR:HG21	1.90	0.72
1:E:216:VAL:HG23	5:E:2646:HOH:O	1.88	0.72
1:J:20:VAL:HG21	1:J:332:GLU:HG2	1.69	0.72
1:E:249:LYS:HD2	1:E:255:ASP:CG	2.10	0.72
2:N:140[B]:GLU:OE2	5:N:1791:HOH:O	2.08	0.71
2:O:159[B]:THR:HG22	2:O:162[B]:ASP:OD2	1.90	0.71
2:M:133[B]:PRO:O	2:M:134[B]:ALA:HB3	1.91	0.70
2:L:164[A]:LEU:O	2:L:167[A]:VAL:HG22	1.91	0.70
1:E:28:LEU:HD12	1:E:339:VAL:HG12	1.72	0.70
1:G:397:ASN:HB3	5:H:2648:HOH:O	1.92	0.70
2:M:164[B]:LEU:O	2:M:167[B]:VAL:HG12	1.92	0.70
2:K:162:ASP:HA	2:K:165:LYS:HD3	1.72	0.70
1:F:122:THR:OG1	1:F:126:GLN:HG2	1.91	0.70
1:G:308:PHE:HE1	1:G:337:ILE:HD11	1.55	0.70
2:O:138[B]:ILE:HD11	2:O:163[B]:ALA:HB3	1.73	0.70
1:I:258:ILE:HD13	1:I:269:ILE:HD11	1.73	0.69
1:H:301:ARG:NH1	3:H:2510:SO4:O1	2.25	0.69
1:I:35:ILE:HD11	1:I:139:ILE:HD12	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:297:ASP:HB2	1:A:298:PRO:HD2	1.74	0.69
2:O:157[B]:ILE:H	2:O:157[B]:ILE:HD12	1.58	0.69
2:L:164[B]:LEU:O	2:L:167[B]:VAL:HG22	1.91	0.69
2:O:133[B]:PRO:O	2:O:134[B]:ALA:HB3	1.93	0.68
2:O:140[A]:GLU:HG2	2:O:141[A]:LYS:H	1.57	0.68
1:G:409:GLN:HG2	1:G:412:THR:OG1	1.93	0.68
1:I:182:VAL:HG12	1:I:271:CYS:SG	2.33	0.68
1:H:288:GLY:O	1:H:292:LEU:HD13	1.94	0.68
1:I:62:TYR:CD1	1:I:65:MET:HE3	2.29	0.68
2:L:144[A]:LEU:HD21	2:L:166[A]:LEU:HG	1.75	0.67
2:M:131[A]:LEU:HD11	2:M:146[A]:ALA:HB2	1.75	0.67
2:O:135[A]:ALA:O	2:O:139[A]:LEU:HB2	1.95	0.67
1:E:51:ILE:HB	1:E:52:PRO:HD3	1.77	0.66
1:J:248:LYS:HD2	1:J:254:ILE:HG12	1.77	0.65
1:J:121:ILE:HG21	1:J:292:LEU:HD21	1.77	0.65
1:D:60:SER:OG	1:D:199:ARG:HD2	1.96	0.65
1:D:96:VAL:O	1:D:100:THR:HG23	1.95	0.65
1:E:370:SER:H	1:E:373:GLN:HE21	1.42	0.65
1:H:121:ILE:HG21	1:H:292:LEU:HD21	1.78	0.65
2:L:159[A]:THR:HG22	2:L:162[A]:ASP:OD2	1.96	0.64
2:N:139[A]:LEU:HD21	2:N:146[A]:ALA:HB2	1.79	0.64
2:N:158[A]:PHE:O	2:N:162[A]:ASP:HB2	1.98	0.64
1:I:444:ASP:OD2	2:O:133[B]:PRO:O	2.16	0.64
2:L:158[A]:PHE:HE1	2:L:163[A]:ALA:HB2	1.62	0.64
1:E:64:HIS:CE1	3:E:2499:SO4:O4	2.50	0.64
2:O:133[A]:PRO:O	2:O:134[A]:ALA:HB3	1.98	0.64
1:I:307:ARG:NH1	5:I:2581:HOH:O	2.31	0.64
1:B:62:TYR:HD1	1:B:65:MET:HE3	1.62	0.64
1:E:79:SER:HB2	1:F:79:SER:HG	1.61	0.64
1:D:297:ASP:HB2	1:D:298:PRO:HD2	1.80	0.63
1:I:318:ILE:HD13	1:I:335:GLY:HA2	1.80	0.63
2:O:160[B]:LYS:O	2:O:164[B]:LEU:HD23	1.98	0.63
1:I:265:LYS:O	1:I:265:LYS:HD2	1.99	0.63
1:G:121:ILE:HG21	1:G:292:LEU:HD11	1.81	0.63
1:I:69:THR:HG22	5:I:2522:HOH:O	1.99	0.62
2:O:130[A]:ARG:HH21	2:O:155[A]:ARG:HD2	1.63	0.62
1:I:211:GLY:N	3:I:2515:SO4:O2	2.31	0.62
2:L:133[A]:PRO:O	2:L:134[A]:ALA:HB3	1.99	0.62
1:E:249:LYS:HD2	1:E:255:ASP:OD1	2.00	0.62
1:C:5:ILE:HG23	1:C:137:GLN:NE2	2.14	0.62
2:K:133:PRO:O	2:K:134:ALA:HB3	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:382:LYS:HG2	1:A:408:GLY:O	1.99	0.62
1:A:288:GLY:O	1:A:292:LEU:HG	2.00	0.62
1:E:369:LYS:HA	1:E:373:GLN:NE2	2.15	0.61
1:I:84:ASN:HB2	1:J:77:GLU:OE1	1.99	0.61
1:A:25:ALA:HA	1:A:339:VAL:HG11	1.81	0.61
1:B:312:ILE:HD12	1:B:312:ILE:N	2.15	0.61
2:O:159[B]:THR:CG2	2:O:162[B]:ASP:H	2.13	0.61
2:M:158[A]:PHE:O	2:M:162[A]:ASP:HB2	1.99	0.61
2:L:130[B]:ARG:HB2	2:L:157[B]:ILE:HA	1.83	0.61
1:I:51:ILE:HG23	1:J:396:THR:OG1	2.00	0.61
2:M:143[A]:SER:O	2:M:144[A]:LEU:HB3	2.01	0.61
1:I:33:VAL:HG11	1:I:139:ILE:HD13	1.83	0.60
1:A:290:GLU:OE1	1:A:290:GLU:HA	2.01	0.60
1:A:305:ASN:HD21	1:A:309:GLN:HB2	1.65	0.60
1:I:182:VAL:HG13	1:I:274:LEU:HD12	1.83	0.60
1:I:161:ASP:OD1	1:I:163:ASP:HB3	2.01	0.60
2:N:145[A]:ASP:O	2:N:146[A]:ALA:HB3	2.01	0.60
1:J:15:GLY:HA3	4:J:480:FAD:H52A	1.84	0.60
1:C:277:CYS:HA	5:C:2512:HOH:O	2.01	0.60
2:N:138[A]:ILE:HD11	2:N:163[A]:ALA:HB3	1.83	0.60
1:J:290:GLU:HB3	3:J:2520:SO4:O1	2.00	0.60
1:E:62:TYR:HD1	1:E:65:MET:HE2	1.66	0.60
2:M:134[B]:ALA:HA	2:M:137[B]:ASN:HB3	1.83	0.60
1:B:402:GLY:HA3	1:B:421:LEU:O	2.02	0.60
1:B:182:VAL:HG23	1:B:271:CYS:HB3	1.84	0.60
2:L:156[B]:GLY:O	2:L:157[B]:ILE:HB	2.02	0.60
1:H:292:LEU:CD1	5:H:2814:HOH:O	2.49	0.60
1:C:5:ILE:HG23	1:C:137:GLN:HE22	1.66	0.60
1:B:43:GLY:HA2	4:B:480:FAD:O3B	2.02	0.60
1:H:3:GLN:HB2	1:H:4:PRO:HD3	1.84	0.59
2:N:164[B]:LEU:HA	2:N:167[B]:VAL:HG22	1.84	0.59
1:B:301:ARG:HH11	1:B:323:ALA:HA	1.67	0.59
1:B:9:VAL:HG22	1:B:342:MET:HE1	1.85	0.59
1:B:9:VAL:CG2	1:B:342:MET:HE1	2.32	0.59
1:B:384:GLY:HA3	1:B:466:ALA:HB2	1.85	0.59
1:G:308:PHE:CE1	1:G:337:ILE:HD11	2.36	0.59
1:E:369:LYS:HA	1:E:373:GLN:HE22	1.67	0.59
1:B:328:ALA:O	1:B:332:GLU:HG3	2.03	0.59
1:H:375:LYS:HE3	1:H:381:TYR:OH	2.03	0.59
1:I:57:LEU:HD22	1:I:359:TYR:O	2.03	0.58
1:I:307:ARG:NH2	1:I:345:GLY:O	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:152[B]:THR:HG22	2:M:153[B]:GLY:H	1.69	0.58
2:N:135[A]:ALA:O	2:N:139[A]:LEU:HB2	2.03	0.58
2:M:138[B]:ILE:HD11	2:M:163[B]:ALA:CB	2.32	0.58
2:L:144[B]:LEU:HD11	2:L:167[B]:VAL:HA	1.86	0.58
1:A:51:ILE:HB	1:A:52:PRO:HD3	1.84	0.58
1:I:389:ALA:HA	1:I:400:THR:HB	1.86	0.58
2:O:159[B]:THR:HG22	2:O:162[B]:ASP:CG	2.23	0.58
1:B:370:SER:H	1:B:373:GLN:HE21	1.51	0.58
2:M:167[B]:VAL:HG13	2:M:168[B]:GLN:N	2.19	0.58
1:E:43:GLY:HA2	4:E:480:FAD:O3B	2.03	0.58
1:D:309:GLN:HG2	1:D:316:TYR:CE2	2.39	0.58
1:H:372:GLU:O	1:H:376:GLU:HG3	2.03	0.58
1:B:116:ASN:O	1:B:131:LYS:HG2	2.03	0.58
1:B:144:ILE:HD12	1:B:315:ILE:HD11	1.86	0.58
1:J:8:ASP:HA	1:J:142:LYS:HD3	1.84	0.58
1:E:62:TYR:HD1	1:E:65:MET:CE	2.17	0.57
1:A:96:VAL:O	1:A:100:THR:HG23	2.04	0.57
2:N:134[B]:ALA:O	2:N:138[B]:ILE:HG23	2.03	0.57
2:O:135[B]:ALA:O	2:O:139[B]:LEU:HB2	2.05	0.57
1:E:259:GLU:HB2	1:E:264:GLY:O	2.03	0.57
2:N:131[B]:LEU:HD12	2:N:158[B]:PHE:HB3	1.86	0.57
2:N:146[A]:ALA:C	2:N:148[A]:GLN:H	2.08	0.57
1:I:51:ILE:HB	1:I:52:PRO:HD3	1.86	0.57
1:C:250:SER:HB3	2:K:131:LEU:HD11	1.87	0.57
1:E:349:ILE:O	1:E:350:ASP:HB3	2.04	0.57
1:I:62:TYR:HD1	1:I:65:MET:HE3	1.68	0.57
1:I:294:ILE:HD11	1:I:312:ILE:HD12	1.86	0.57
1:I:229:ILE:O	1:I:233:GLN:HG3	2.05	0.57
1:E:174:LEU:HD12	1:E:197:TRP:CE2	2.40	0.57
1:B:348:HIS:CD2	1:B:349:ILE:H	2.22	0.57
1:B:139:ILE:HD12	1:B:139:ILE:N	2.20	0.57
1:I:231:GLN:HA	1:I:235:PHE:O	2.05	0.57
1:E:209:PHE:O	1:E:240:ASN:HA	2.05	0.56
1:F:301:ARG:HD3	5:F:2713:HOH:O	2.04	0.56
2:O:157[B]:ILE:HD12	2:O:157[B]:ILE:N	2.19	0.56
1:A:5:ILE:HG22	1:A:137:GLN:NE2	2.19	0.56
1:B:289:LEU:HB3	1:B:294:ILE:HB	1.85	0.56
1:G:28:LEU:HD12	1:G:339:VAL:HG12	1.86	0.56
1:F:15:GLY:HA3	4:F:480:FAD:H52A	1.88	0.56
1:J:46:LEU:O	1:J:46:LEU:HD12	2.05	0.56
1:J:318:ILE:HD13	1:J:335:GLY:HA2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:171:ALA:HB2	1:H:275:LEU:HD13	1.88	0.56
1:I:57:LEU:HD13	1:I:359:TYR:HB2	1.88	0.56
1:A:43:GLY:HA2	4:A:480:FAD:O3B	2.05	0.56
2:L:159[A]:THR:HG23	2:L:162[A]:ASP:H	1.70	0.55
2:O:134[B]:ALA:HA	2:O:137[B]:ASN:HB3	1.88	0.55
1:C:182:VAL:HG23	1:C:271:CYS:HB3	1.86	0.55
1:E:33:VAL:HG22	1:E:113:VAL:HB	1.87	0.55
2:L:135[B]:ALA:O	2:L:139[B]:LEU:HG	2.06	0.55
1:H:371:GLU:O	1:H:375:LYS:HG2	2.05	0.55
1:D:402:GLY:HA3	1:D:421:LEU:O	2.05	0.55
2:M:156[B]:GLY:O	2:M:157[B]:ILE:HG23	2.07	0.55
1:G:23:ILE:O	1:G:27:GLN:HG3	2.05	0.55
2:N:133[B]:PRO:O	2:N:134[B]:ALA:HB3	2.07	0.55
1:C:318:ILE:HD13	1:C:335:GLY:HA2	1.88	0.55
2:M:134[B]:ALA:O	2:M:138[B]:ILE:HG23	2.06	0.55
1:I:5:ILE:HD12	1:I:6:ASP:H	1.72	0.55
1:E:62:TYR:CD1	1:E:65:MET:HE2	2.41	0.55
1:G:307:ARG:HG2	1:G:347:VAL:HG21	1.88	0.55
1:D:318:ILE:HD13	1:D:335:GLY:HA2	1.89	0.55
1:B:137:GLN:HG3	1:B:139:ILE:HD11	1.89	0.55
1:G:265:LYS:O	1:G:266:ALA:HB2	2.07	0.55
1:D:444:ASP:OD2	2:L:133[A]:PRO:O	2.24	0.55
1:A:49:GLY:O	1:A:52:PRO:HD2	2.05	0.55
1:A:210:LEU:HB3	3:A:2484:SO4:O2	2.06	0.55
1:C:437:GLU:HG2	1:D:448:VAL:HG22	1.90	0.54
1:J:51:ILE:HB	1:J:52:PRO:HD3	1.89	0.54
2:O:138[B]:ILE:HD11	2:O:163[B]:ALA:CB	2.38	0.54
1:H:77:GLU:C	1:H:78:MET:HG3	2.28	0.54
1:D:56:LEU:O	1:D:60:SER:CB	2.55	0.54
1:D:392:SER:HB2	5:D:2701:HOH:O	2.07	0.54
1:J:49:GLY:O	1:J:52:PRO:HD2	2.06	0.54
1:B:305:ASN:OD1	1:B:309:GLN:HB2	2.07	0.54
1:B:312:ILE:HD12	1:B:312:ILE:H	1.73	0.54
1:C:162:GLU:HA	1:C:166:VAL:HG12	1.90	0.54
2:L:155[A]:ARG:HE	2:L:155[A]:ARG:N	2.06	0.54
1:B:121:ILE:HG21	1:B:292:LEU:HD21	1.87	0.54
2:L:158[A]:PHE:CE1	2:L:163[A]:ALA:HB2	2.42	0.54
1:H:3:GLN:CB	1:H:4:PRO:HD3	2.38	0.53
1:H:43:GLY:HA2	4:H:480:FAD:O3B	2.08	0.53
2:O:136[B]:ARG:HH11	2:O:136[B]:ARG:HG2	1.73	0.53
1:C:15:GLY:HA3	4:C:480:FAD:H52A	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:438:TYR:O	2:N:157[A]:ILE:HD11	2.07	0.53
1:C:305:ASN:HD21	1:C:309:GLN:NE2	2.05	0.53
2:L:131[A]:LEU:HD13	2:L:136[A]:ARG:HG3	1.91	0.53
1:B:349:ILE:O	1:B:349:ILE:HG23	2.08	0.53
1:B:138:VAL:C	1:B:139:ILE:HD12	2.28	0.53
1:C:108:LYS:HB2	1:C:108:LYS:NZ	2.23	0.53
1:G:15:GLY:HA3	4:G:480:FAD:H52A	1.90	0.53
1:D:444:ASP:OD2	2:L:134[A]:ALA:HB3	2.09	0.53
1:C:289:LEU:N	3:C:2493:SO4:O4	2.41	0.53
1:D:43:GLY:HA2	4:D:480:FAD:O3B	2.08	0.53
1:I:438:TYR:O	2:O:130[A]:ARG:HD2	2.09	0.53
1:B:370:SER:N	1:B:373:GLN:NE2	2.54	0.53
1:H:228:ARG:NH1	1:H:228:ARG:HB2	2.24	0.53
1:F:43:GLY:HA2	4:F:480:FAD:O3B	2.09	0.53
2:L:135[A]:ALA:HA	2:L:138[A]:ILE:HD11	1.91	0.53
1:G:43:GLY:HA2	4:G:480:FAD:O3B	2.07	0.53
1:G:145:LEU:HD11	1:G:318:ILE:HG12	1.89	0.53
2:L:159[A]:THR:HG22	2:L:162[A]:ASP:CG	2.29	0.52
1:I:43:GLY:HA2	4:I:480:FAD:O3B	2.10	0.52
1:J:309:GLN:HG2	1:J:316:TYR:CE2	2.45	0.52
1:C:79:SER:HB2	1:D:79:SER:CB	2.40	0.52
1:B:318:ILE:HD13	1:B:335:GLY:HA2	1.91	0.52
1:B:180:LYS:HE3	5:B:2575:HOH:O	2.09	0.52
1:B:149:GLY:HA2	1:B:320:ASP:HB2	1.91	0.52
1:F:23:ILE:O	1:F:27:GLN:HG3	2.10	0.52
1:C:23:ILE:O	1:C:27:GLN:HG3	2.09	0.52
1:I:52:PRO:HB3	1:I:92:LYS:HD3	1.90	0.52
1:A:46:LEU:HD11	1:A:99:LEU:HB2	1.90	0.52
2:L:134[A]:ALA:O	2:L:138[A]:ILE:HG12	2.10	0.52
1:C:121:ILE:HG21	1:C:292:LEU:HD11	1.91	0.52
1:J:23:ILE:O	1:J:27:GLN:HG3	2.09	0.52
1:J:121:ILE:CG2	1:J:292:LEU:HD21	2.38	0.52
1:J:69:THR:OG1	3:J:2518:SO4:O4	2.27	0.52
1:E:318:ILE:HD13	1:E:335:GLY:HA2	1.91	0.52
1:I:351:TYR:HA	1:I:354:VAL:HG23	1.92	0.52
1:A:5:ILE:HG13	1:A:6:ASP:N	2.24	0.52
1:I:311:LYS:HD2	5:I:2563:HOH:O	2.10	0.52
1:C:110:ASN:O	1:C:111:LYS:HB2	2.09	0.52
5:C:2664:HOH:O	1:D:397:ASN:HB3	2.09	0.52
1:H:46:LEU:O	1:H:46:LEU:HD12	2.10	0.52
1:B:464:LEU:HD23	1:B:471:SER:HA	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:7:ALA:O	1:J:141:THR:HA	2.09	0.52
1:H:282:PRO:HG2	1:H:301:ARG:HG3	1.92	0.51
1:D:7:ALA:O	1:D:141:THR:HA	2.10	0.51
1:E:28:LEU:HD12	1:E:339:VAL:CG1	2.41	0.51
1:B:370:SER:OG	1:B:373:GLN:HG3	2.10	0.51
1:E:28:LEU:CD1	1:E:339:VAL:HG12	2.41	0.51
1:F:7:ALA:O	1:F:141:THR:HA	2.11	0.51
1:H:121:ILE:CG2	1:H:292:LEU:HD21	2.39	0.51
1:B:62:TYR:CD1	1:B:65:MET:HE3	2.44	0.51
1:G:461:GLU:OE1	1:G:471:SER:HB2	2.10	0.51
2:O:131[A]:LEU:HD21	2:O:146[A]:ALA:HB2	1.93	0.51
2:N:142[A]:HIS:O	2:N:144[A]:LEU:HD22	2.10	0.51
2:K:134:ALA:HA	2:K:137:ASN:HB3	1.92	0.51
1:J:43:GLY:HA2	4:J:480:FAD:O3B	2.10	0.51
1:D:5:ILE:HG22	1:D:6:ASP:N	2.26	0.51
1:G:434:LEU:HD12	1:H:448:VAL:HG21	1.93	0.51
1:B:69:THR:HG23	3:B:2487:SO4:O2	2.10	0.51
2:O:131[B]:LEU:HD21	2:O:146[B]:ALA:HB2	1.94	0.51
1:J:15:GLY:CA	4:J:480:FAD:H52A	2.40	0.51
1:H:80:GLU:HG3	1:H:82:ARG:HH22	1.76	0.51
1:A:402:GLY:HA3	1:A:421:LEU:O	2.11	0.50
2:O:158[B]:PHE:HZ	2:O:166[B]:LEU:HD12	1.75	0.50
2:M:133[B]:PRO:O	2:M:134[B]:ALA:CB	2.55	0.50
1:C:258:ILE:HD13	1:C:269:ILE:HD13	1.92	0.50
2:N:130[A]:ARG:O	2:N:157[A]:ILE:HA	2.11	0.50
1:E:346:ALA:HB1	2:M:140[A]:GLU:CD	2.32	0.50
1:E:5:ILE:HD12	1:E:6:ASP:H	1.76	0.50
1:I:145:LEU:HD11	1:I:318:ILE:HG12	1.94	0.50
1:G:318:ILE:HD13	1:G:335:GLY:CA	2.42	0.50
1:H:80:GLU:HG3	1:H:82:ARG:NH2	2.25	0.50
1:C:447:ARG:CZ	2:L:137[B]:ASN:ND2	2.75	0.50
1:B:146:ILE:HG12	1:B:316:TYR:O	2.12	0.50
1:C:28:LEU:HD12	1:C:339:VAL:HG12	1.93	0.50
2:M:135[A]:ALA:O	2:M:139[A]:LEU:HB2	2.11	0.50
2:O:133[B]:PRO:O	2:O:134[B]:ALA:CB	2.59	0.50
1:C:162:GLU:HA	1:C:162:GLU:OE2	2.12	0.50
1:C:191:VAL:HG21	1:C:213:VAL:CG1	2.42	0.50
1:I:8:ASP:HA	1:I:142:LYS:HG3	1.93	0.50
1:A:124:LYS:HE2	1:A:312:ILE:HD12	1.94	0.50
1:F:5:ILE:HG12	1:F:137:GLN:NE2	2.26	0.50
1:F:318:ILE:HD13	1:F:335:GLY:CA	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:39:GLU:H	1:B:39:GLU:CD	2.15	0.50
1:D:438:TYR:O	2:L:130[B]:ARG:HD2	2.11	0.50
1:I:5:ILE:HD12	1:I:6:ASP:N	2.27	0.50
1:H:15:GLY:HA3	4:H:480:FAD:H52A	1.93	0.50
1:A:25:ALA:CA	1:A:339:VAL:HG11	2.42	0.49
1:J:389:ALA:HA	1:J:400:THR:HB	1.94	0.49
1:J:444:ASP:OD2	2:O:133[A]:PRO:O	2.30	0.49
1:J:437:GLU:HG3	2:O:133[B]:PRO:HG3	1.94	0.49
1:B:278:ILE:H	1:B:278:ILE:HD13	1.77	0.49
1:G:299:ARG:HB2	1:G:301:ARG:HD3	1.93	0.49
1:A:46:LEU:HD11	1:A:99:LEU:CB	2.42	0.49
1:C:178:PRO:HG3	1:C:181:MET:CE	2.42	0.49
2:M:156[B]:GLY:C	2:M:157[B]:ILE:HG13	2.32	0.49
2:M:158[B]:PHE:HE1	2:M:163[B]:ALA:HB2	1.76	0.49
2:L:139[A]:LEU:HG	2:L:163[A]:ALA:HB1	1.94	0.49
1:B:33:VAL:HG22	1:B:113:VAL:HB	1.95	0.49
1:G:402:GLY:HA3	1:G:421:LEU:O	2.12	0.49
1:F:96:VAL:O	1:F:100:THR:HG23	2.12	0.49
1:D:244:THR:OG1	1:D:257:SER:OG	2.28	0.49
1:J:447:ARG:CD	2:O:137[A]:ASN:ND2	2.75	0.49
1:C:178:PRO:HG3	1:C:181:MET:HE2	1.95	0.49
1:E:437:GLU:HG3	2:M:133[A]:PRO:HB3	1.95	0.49
1:G:264:GLY:O	1:G:265:LYS:O	2.31	0.49
1:B:341:GLY:HA2	1:B:345:GLY:O	2.13	0.49
1:B:285:LYS:HG2	1:B:286:ASN:HD22	1.78	0.49
1:I:205:THR:HA	1:I:236:LYS:O	2.13	0.49
1:B:311:LYS:O	1:B:313:PRO:HD3	2.12	0.49
1:A:305:ASN:ND2	1:A:309:GLN:HB2	2.26	0.49
1:B:404:VAL:HG22	1:B:420:ILE:HG23	1.95	0.49
1:E:439:GLY:HA3	2:M:154[B]:PRO:HG3	1.94	0.49
1:I:192:GLU:O	1:I:196:VAL:HG23	2.12	0.49
1:D:145:LEU:HD11	1:D:318:ILE:HG12	1.94	0.49
1:A:162:GLU:HA	1:A:162:GLU:OE1	2.12	0.49
1:E:272:ASP:OD2	5:E:2540:HOH:O	2.20	0.49
1:B:7:ALA:CB	1:B:31:LYS:HD2	2.42	0.48
1:J:288:GLY:O	1:J:292:LEU:HD13	2.12	0.48
1:H:64:HIS:CE1	3:H:2511:SO4:O1	2.66	0.48
1:F:318:ILE:HD13	1:F:335:GLY:HA2	1.94	0.48
2:N:154[B]:PRO:HD2	2:N:157[B]:ILE:CG2	2.43	0.48
1:D:389:ALA:HA	1:D:400:THR:HB	1.95	0.48
1:A:226:PHE:CZ	1:A:230:LEU:HD11	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:144:ILE:HD12	1:B:315:ILE:CD1	2.44	0.48
2:M:164[A]:LEU:O	2:M:167[A]:VAL:HG22	2.13	0.48
1:D:15:GLY:HA3	4:D:480:FAD:H52A	1.96	0.48
1:E:52:PRO:HB2	1:E:172:LEU:HD13	1.95	0.48
1:C:43:GLY:HA2	4:C:480:FAD:O3B	2.13	0.48
2:K:131:LEU:HD21	2:K:146:ALA:CB	2.43	0.48
1:F:301:ARG:NH1	3:F:2502:SO4:O3	2.46	0.48
1:B:162:GLU:OE1	1:B:162:GLU:HA	2.13	0.48
1:G:148:THR:OG1	1:G:321:VAL:HG11	2.14	0.48
1:A:290:GLU:C	1:A:292:LEU:H	2.16	0.48
1:A:337:ILE:HG13	1:A:338:CYS:N	2.29	0.48
1:C:39:GLU:HG2	1:C:40:THR:HG23	1.95	0.48
2:O:132[A]:SER:O	2:O:135[A]:ALA:HB3	2.14	0.48
1:B:7:ALA:HB2	1:B:31:LYS:HD2	1.95	0.48
1:A:46:LEU:HD21	1:A:100:THR:HA	1.96	0.48
1:G:174:LEU:HD12	1:G:197:TRP:CE2	2.49	0.48
1:B:249:LYS:HA	1:J:305:ASN:HA	1.96	0.48
1:F:330:LYS:HD3	1:F:334:GLU:CD	2.35	0.48
1:A:448:VAL:HG21	1:B:434:LEU:HD12	1.95	0.47
2:N:138[B]:ILE:HD11	2:N:163[B]:ALA:CB	2.44	0.47
2:N:164[B]:LEU:O	2:N:167[B]:VAL:HG22	2.14	0.47
1:J:7:ALA:HA	1:J:31:LYS:HD3	1.96	0.47
1:H:402:GLY:HA3	1:H:421:LEU:O	2.15	0.47
1:I:46:LEU:HD11	1:I:99:LEU:HB2	1.95	0.47
1:E:210:LEU:N	1:E:210:LEU:HD12	2.30	0.47
2:L:156[B]:GLY:C	2:L:157[B]:ILE:HD12	2.34	0.47
2:M:131[B]:LEU:HD13	2:M:136[B]:ARG:HA	1.96	0.47
1:D:461:GLU:OE1	1:D:471:SER:HB2	2.14	0.47
1:B:370:SER:CB	1:B:373:GLN:HE21	2.26	0.47
1:B:442:CYS:HB3	1:B:463:ASN:O	2.14	0.47
1:B:118:TYR:O	1:B:129:ALA:HA	2.15	0.47
1:H:96:VAL:O	1:H:100:THR:HG23	2.15	0.47
1:F:311:LYS:HE2	5:F:2545:HOH:O	2.14	0.47
1:B:121:ILE:CG2	1:B:292:LEU:HD21	2.44	0.47
2:O:140[A]:GLU:HG2	2:O:141[A]:LYS:N	2.26	0.47
1:D:56:LEU:O	1:D:60:SER:HB2	2.15	0.47
1:A:3:GLN:N	1:A:4:PRO:CD	2.78	0.47
1:C:389:ALA:HA	1:C:400:THR:HB	1.96	0.47
1:H:155:PHE:CD1	1:H:158:ILE:HD12	2.49	0.47
1:B:350:ASP:C	1:B:352:ASN:H	2.18	0.47
1:E:259:GLU:HB3	1:E:266:ALA:HA	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:318:ILE:HD13	1:G:335:GLY:HA2	1.97	0.47
1:B:13:GLY:O	1:B:18:GLY:HA3	2.15	0.47
1:E:349:ILE:O	1:E:350:ASP:CB	2.62	0.47
1:F:15:GLY:CA	4:F:480:FAD:H52A	2.44	0.47
2:O:134[B]:ALA:HA	2:O:137[B]:ASN:CB	2.45	0.47
1:B:442:CYS:CB	1:B:467:SER:HB2	2.45	0.47
1:I:165:ILE:HD11	1:I:254:ILE:HD12	1.97	0.46
1:E:64:HIS:NE2	3:E:2499:SO4:O4	2.48	0.46
1:A:46:LEU:HD12	1:A:51:ILE:HG13	1.97	0.46
5:G:2556:HOH:O	1:H:397:ASN:HB3	2.15	0.46
1:E:306:THR:O	1:E:347:VAL:HG11	2.15	0.46
1:B:28:LEU:HD12	1:B:339:VAL:HG12	1.97	0.46
1:A:35:ILE:HG12	1:A:115:VAL:HB	1.98	0.46
1:A:461:GLU:CG	1:A:471:SER:HB2	2.27	0.46
2:L:160[B]:LYS:O	2:L:164[B]:LEU:HG	2.15	0.46
1:I:258:ILE:CD1	1:I:269:ILE:HD11	2.44	0.46
1:A:15:GLY:HA3	4:A:480:FAD:H52A	1.97	0.46
1:E:210:LEU:CD1	1:E:210:LEU:N	2.78	0.46
1:A:286:ASN:HA	3:A:2485:SO4:O2	2.15	0.46
1:B:347:VAL:O	1:B:347:VAL:HG23	2.15	0.46
2:M:145[A]:ASP:C	2:M:147[A]:SER:H	2.18	0.46
1:D:287:LEU:HB3	1:D:289:LEU:HG	1.97	0.46
1:H:299:ARG:NH2	3:H:2510:SO4:O4	2.49	0.46
2:N:138[B]:ILE:CD1	2:N:164[B]:LEU:HD22	2.45	0.46
1:E:301:ARG:NH1	3:E:2498:SO4:O4	2.48	0.46
1:A:397:ASN:HB3	5:B:2533:HOH:O	2.14	0.46
2:K:133:PRO:O	2:K:134:ALA:CB	2.64	0.46
1:B:246:ALA:HA	1:B:255:ASP:O	2.16	0.46
1:B:444:ASP:OD1	2:K:134:ALA:HB3	2.14	0.46
1:B:442:CYS:HB2	1:B:467:SER:HB2	1.97	0.46
1:F:351:TYR:HA	1:F:354:VAL:HG13	1.98	0.46
1:A:299:ARG:CZ	1:A:301:ARG:HH12	2.28	0.46
1:C:171:ALA:HB2	1:C:275:LEU:HD13	1.98	0.46
1:I:370:SER:OG	1:I:373:GLN:HG3	2.15	0.46
2:K:139:LEU:CD2	2:K:146:ALA:HB2	2.46	0.46
1:J:212:HIS:ND1	3:J:2519:SO4:O3	2.48	0.46
1:J:155:PHE:CD2	1:J:278:ILE:HD13	2.50	0.46
2:M:167[B]:VAL:CG1	2:M:168[B]:GLN:N	2.79	0.46
1:I:258:ILE:HD13	1:I:269:ILE:CD1	2.45	0.46
1:J:164:THR:HG21	1:J:248:LYS:NZ	2.31	0.46
1:G:122:THR:OG1	1:G:126:GLN:HG2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:62:TYR:CD1	1:E:65:MET:CE	2.98	0.45
1:H:15:GLY:N	4:H:480:FAD:H52A	2.31	0.45
1:E:321:VAL:HG22	1:E:321:VAL:O	2.16	0.45
1:I:290:GLU:HG3	1:I:291:GLU:N	2.31	0.45
2:O:157[A]:ILE:CG2	2:O:159[A]:THR:HG23	2.45	0.45
1:J:290:GLU:CB	3:J:2520:SO4:O1	2.63	0.45
1:F:171:ALA:HB2	1:F:275:LEU:HD13	1.99	0.45
1:G:160:ILE:HA	1:G:165:ILE:HG22	1.98	0.45
1:C:46:LEU:HD12	1:C:46:LEU:O	2.16	0.45
2:O:167[A]:VAL:HG23	2:O:168[A]:GLN:N	2.32	0.45
2:O:157[A]:ILE:HG22	2:O:159[A]:THR:HG23	1.99	0.45
2:O:160[A]:LYS:O	2:O:164[A]:LEU:HD13	2.15	0.45
1:G:160:ILE:HD11	1:G:276:VAL:HB	1.97	0.45
1:I:78:MET:HG2	1:J:81:VAL:HG22	1.98	0.45
1:J:180:LYS:HD3	1:J:270:THR:O	2.16	0.45
1:D:121:ILE:HG21	1:D:292:LEU:HD21	1.97	0.45
2:M:157[B]:ILE:O	2:M:158[B]:PHE:C	2.54	0.45
1:G:265:LYS:HD3	1:G:265:LYS:N	2.32	0.45
1:J:447:ARG:HD2	2:O:137[A]:ASN:ND2	2.31	0.45
1:C:439:GLY:O	2:L:130[A]:ARG:HD2	2.17	0.45
1:B:290:GLU:HB3	3:B:2489:SO4:O1	2.16	0.45
1:C:244:THR:OG1	1:C:257:SER:OG	2.34	0.45
1:E:444:ASP:OD2	2:M:133[B]:PRO:O	2.35	0.45
2:L:154[B]:PRO:C	2:L:156[B]:GLY:H	2.19	0.45
2:K:134:ALA:O	2:K:138:ILE:HG13	2.16	0.45
1:B:338:CYS:O	1:B:342:MET:HG3	2.17	0.45
1:E:189:ILE:HG23	4:E:480:FAD:HM73	1.98	0.45
1:B:250:SER:CB	1:J:304:VAL:HG23	2.43	0.45
1:A:309:GLN:HG2	1:A:316:TYR:CE2	2.52	0.45
1:J:155:PHE:HD2	1:J:278:ILE:HD13	1.81	0.45
1:I:426:GLY:O	1:I:429:VAL:HG12	2.17	0.45
1:A:139:ILE:HD12	1:A:139:ILE:N	2.31	0.45
1:B:444:ASP:OD1	2:K:133:PRO:O	2.35	0.45
2:K:131:LEU:HD21	2:K:146:ALA:HB2	1.99	0.45
1:I:124:LYS:HE2	1:I:125:ASN:OD1	2.17	0.45
1:H:180:LYS:HB3	1:H:180:LYS:HE2	1.85	0.45
1:A:222:ILE:HG13	1:A:419:HIS:HB3	1.98	0.45
1:B:277:CYS:HA	5:B:2547:HOH:O	2.17	0.45
1:C:309:GLN:HG2	1:C:316:TYR:CE2	2.52	0.44
1:E:7:ALA:O	1:E:141:THR:HA	2.17	0.44
1:G:383:VAL:HG11	1:G:385:LYS:HE3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:57:LEU:HD11	1:B:192:GLU:HB3	1.98	0.44
2:N:145[A]:ASP:O	2:N:146[A]:ALA:CB	2.65	0.44
1:C:15:GLY:CA	4:C:480:FAD:H52A	2.47	0.44
1:F:290:GLU:HB3	3:F:2505:SO4:O4	2.17	0.44
1:C:161:ASP:OD1	1:C:163:ASP:HB3	2.18	0.44
2:O:158[B]:PHE:O	2:O:159[B]:THR:O	2.35	0.44
1:G:437:GLU:HG3	2:N:133[A]:PRO:HG3	2.00	0.44
2:L:140[A]:GLU:C	2:L:142[A]:HIS:H	2.21	0.44
1:A:41:LEU:HD23	1:A:103:ILE:HG22	1.99	0.44
1:A:389:ALA:HA	1:A:400:THR:HB	1.99	0.44
2:N:145[A]:ASP:C	2:N:147[A]:SER:H	2.21	0.44
1:C:79:SER:CB	1:D:79:SER:OG	2.62	0.44
2:K:131:LEU:HD23	2:K:158:PHE:HB3	1.98	0.44
1:B:54:LYS:HE3	1:B:54:LYS:N	2.33	0.44
1:I:79:SER:HB2	1:J:79:SER:CB	2.48	0.44
2:M:158[A]:PHE:O	2:M:159[A]:THR:O	2.35	0.44
1:E:370:SER:N	1:E:373:GLN:HE21	2.12	0.44
1:A:42:GLY:HA3	1:A:46:LEU:HD23	2.00	0.44
1:J:8:ASP:HA	1:J:142:LYS:CD	2.48	0.44
1:F:452:HIS:HA	1:F:453:PRO:HA	1.82	0.44
1:C:174:LEU:HD12	1:C:197:TRP:CE2	2.53	0.44
2:L:131[B]:LEU:HD23	2:L:136[B]:ARG:NH1	2.33	0.44
1:H:68:GLY:HA3	3:H:2511:SO4:O2	2.17	0.44
1:I:393:ARG:HD2	1:I:454:THR:HA	1.98	0.44
1:A:33:VAL:HG22	1:A:113:VAL:HB	1.98	0.44
2:N:144[B]:LEU:HD22	2:N:167[B]:VAL:HG12	1.99	0.44
1:B:62:TYR:CD1	1:B:65:MET:CE	3.00	0.44
1:B:148:THR:OG1	1:B:321:VAL:HG11	2.18	0.44
1:F:10:THR:HB	1:F:141:THR:HG21	2.00	0.44
1:F:249:LYS:HD3	1:F:255:ASP:OD2	2.18	0.44
1:E:78:MET:CE	1:F:78:MET:HG2	2.48	0.43
1:G:409:GLN:HG3	1:G:412:THR:H	1.81	0.43
1:B:4:PRO:HB3	1:B:138:VAL:HB	2.00	0.43
1:G:437:GLU:HG2	1:H:448:VAL:HG22	1.99	0.43
2:N:158[B]:PHE:HE1	2:N:163[B]:ALA:HA	1.82	0.43
2:M:160[A]:LYS:HE3	2:M:164[A]:LEU:HD11	2.00	0.43
1:E:15:GLY:HA3	4:E:480:FAD:H52A	2.00	0.43
1:C:87:LYS:HE3	1:C:90:GLU:OE2	2.18	0.43
1:F:292:LEU:HG	1:F:312:ILE:CD1	2.48	0.43
2:N:167[B]:VAL:HG23	2:N:168[B]:GLN:N	2.33	0.43
2:M:158[A]:PHE:O	2:M:162[A]:ASP:OD2	2.37	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:330:LYS:HE2	1:B:334:GLU:OE2	2.18	0.43
1:E:312:ILE:HA	1:E:313:PRO:HD2	1.82	0.43
1:I:173:SER:O	1:I:174:LEU:C	2.55	0.43
1:D:46:LEU:O	1:D:46:LEU:HD12	2.17	0.43
1:I:187:GLY:O	1:I:191:VAL:HG23	2.17	0.43
1:I:197:TRP:CE3	1:I:200:LEU:HD12	2.53	0.43
1:J:318:ILE:HD13	1:J:335:GLY:CA	2.49	0.43
1:C:81:VAL:HG22	1:D:78:MET:HG2	2.00	0.43
1:D:222:ILE:HG13	1:D:419:HIS:HB3	2.01	0.43
1:J:171:ALA:HA	1:J:174:LEU:HD13	2.01	0.43
2:N:164[A]:LEU:O	2:N:167[A]:VAL:HG22	2.19	0.43
2:L:144[B]:LEU:CD1	2:L:167[B]:VAL:HA	2.48	0.43
1:I:28:LEU:HD12	1:I:339:VAL:HG12	2.01	0.43
2:N:159[B]:THR:N	2:N:162[B]:ASP:HB2	2.33	0.43
1:C:121:ILE:CG2	1:C:292:LEU:HD11	2.48	0.43
1:A:301:ARG:HG2	1:A:322:VAL:C	2.39	0.43
1:G:444:ASP:OD1	2:N:133[B]:PRO:O	2.37	0.43
2:M:143[A]:SER:O	2:M:144[A]:LEU:CB	2.66	0.43
4:H:480:FAD:H51A	5:H:2517:HOH:O	2.18	0.43
1:D:288:GLY:O	1:D:292:LEU:HB2	2.19	0.43
1:C:304:VAL:HB	1:C:308:PHE:HA	2.01	0.43
1:B:46:LEU:HD11	1:B:99:LEU:HB2	2.00	0.43
1:G:209:PHE:O	1:G:240:ASN:HA	2.19	0.43
1:G:389:ALA:HA	1:G:400:THR:HB	2.00	0.43
2:O:131[B]:LEU:HD23	2:O:158[B]:PHE:CB	2.48	0.43
2:M:134[A]:ALA:O	2:M:138[A]:ILE:HG23	2.18	0.43
1:B:7:ALA:O	1:B:141:THR:HA	2.19	0.43
2:O:142[B]:HIS:C	2:O:144[B]:LEU:H	2.22	0.43
2:L:159[A]:THR:O	2:L:162[A]:ASP:HB2	2.18	0.43
1:B:287:LEU:HD23	1:B:289:LEU:HD21	2.01	0.43
1:E:3:GLN:N	1:E:4:PRO:CD	2.81	0.43
1:B:354:VAL:HA	1:B:355:PRO:HD3	1.83	0.43
1:A:203:ASP:OD1	1:A:236:LYS:NZ	2.42	0.43
2:O:141[B]:LYS:O	2:O:142[B]:HIS:HD2	2.02	0.43
1:I:182:VAL:HG13	1:I:274:LEU:CD1	2.47	0.43
1:B:162:GLU:HA	1:B:166:VAL:HG12	2.01	0.43
1:F:162:GLU:OE1	1:F:162:GLU:HA	2.19	0.43
1:C:209:PHE:HA	1:C:241:THR:O	2.19	0.43
1:I:346:ALA:HB1	2:O:140[A]:GLU:CD	2.40	0.42
1:I:254:ILE:HG23	1:I:271:CYS:SG	2.59	0.42
1:C:442:CYS:HB2	1:C:467:SER:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:288:GLY:N	3:G:2509:SO4:O4	2.48	0.42
1:I:3:GLN:N	1:I:4:PRO:CD	2.82	0.42
1:A:337:ILE:CD1	1:A:347:VAL:O	2.68	0.42
2:L:157[B]:ILE:O	2:L:158[B]:PHE:HB3	2.19	0.42
1:C:441:SER:CB	2:L:160[B]:LYS:HD3	2.49	0.42
1:C:404:VAL:HG11	1:C:459:PHE:HA	2.01	0.42
1:E:409:GLN:HB3	1:E:412:THR:OG1	2.19	0.42
1:A:116:ASN:O	1:A:131:LYS:HG2	2.20	0.42
2:O:151[A]:ALA:O	2:O:152[A]:THR:HB	2.20	0.42
2:N:146[A]:ALA:C	2:N:148[A]:GLN:N	2.73	0.42
1:B:301:ARG:NH1	3:B:2486:SO4:O4	2.53	0.42
1:D:54:LYS:N	1:D:54:LYS:HE3	2.34	0.42
2:K:168:GLN:C	2:K:170:LYS:H	2.21	0.42
1:J:281:ARG:HB2	1:J:282:PRO:HD2	2.00	0.42
2:L:139[A]:LEU:HD22	2:L:144[A]:LEU:O	2.20	0.42
1:H:145:LEU:HD11	1:H:318:ILE:HG12	2.01	0.42
1:D:162:GLU:OE1	1:D:162:GLU:HA	2.19	0.42
2:N:144[A]:LEU:HD22	2:N:144[A]:LEU:N	2.35	0.42
2:O:133[A]:PRO:O	2:O:135[A]:ALA:N	2.43	0.42
2:N:149[B]:GLY:HA3	2:N:166[B]:LEU:HD11	2.02	0.42
1:I:182:VAL:HG11	1:I:256:VAL:HG21	2.01	0.42
1:F:278:ILE:HD12	1:F:279:GLY:N	2.34	0.42
1:B:356:SER:O	1:B:365:ALA:HA	2.19	0.42
1:B:450:HIS:ND1	1:B:460:ARG:HD2	2.35	0.42
2:N:153[A]:GLY:HA3	2:N:159[A]:THR:CG2	2.49	0.42
2:L:131[B]:LEU:HA	2:L:157[B]:ILE:O	2.20	0.42
1:D:56:LEU:O	1:D:60:SER:HB3	2.19	0.42
1:H:15:GLY:CA	4:H:480:FAD:H52A	2.48	0.42
2:M:170[B]:LYS:C	2:M:172[B]:THR:H	2.23	0.42
1:D:453:PRO:HA	1:D:457:GLU:OE1	2.20	0.42
1:A:209:PHE:O	1:A:240:ASN:HA	2.19	0.42
1:I:162:GLU:HA	1:I:162:GLU:OE2	2.19	0.42
2:O:153[B]:GLY:HA3	2:O:154[B]:PRO:HD2	1.96	0.42
2:O:133[A]:PRO:O	2:O:134[A]:ALA:CB	2.64	0.42
2:L:131[B]:LEU:N	2:L:157[B]:ILE:O	2.52	0.42
1:A:339:VAL:HA	1:A:342:MET:HE3	2.02	0.42
1:A:299:ARG:NH1	1:A:301:ARG:HH12	2.17	0.42
1:D:312:ILE:HA	1:D:313:PRO:HD2	1.75	0.42
2:N:133[B]:PRO:O	2:N:135[B]:ALA:N	2.44	0.42
1:A:348:HIS:HB3	2:K:140:GLU:OE1	2.19	0.42
2:O:134[A]:ALA:O	2:O:138[A]:ILE:HG13	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:301:ARG:NH1	1:B:323:ALA:HA	2.32	0.42
1:G:299:ARG:HB2	1:G:301:ARG:CD	2.50	0.42
1:I:136:THR:O	1:I:136:THR:HG23	2.19	0.42
1:I:225:ASN:O	1:I:229:ILE:HG13	2.20	0.42
1:B:350:ASP:O	1:B:352:ASN:N	2.53	0.42
1:I:282:PRO:HG2	1:I:301:ARG:HG3	2.00	0.42
1:I:301:ARG:O	1:I:303:PRO:HD3	2.20	0.42
1:C:334:GLU:OE2	1:C:351:TYR:OH	2.31	0.42
1:J:239:LEU:O	1:J:240:ASN:C	2.58	0.42
1:B:238:LYS:HD3	1:B:238:LYS:HA	1.86	0.42
1:F:46:LEU:HD12	1:F:46:LEU:O	2.20	0.42
1:D:77:GLU:OE2	1:D:77:GLU:HA	2.21	0.41
1:G:178:PRO:HG3	1:G:181:MET:CE	2.50	0.41
1:J:297:ASP:OD2	1:J:297:ASP:C	2.58	0.41
1:C:265:LYS:HE3	1:C:265:LYS:HB3	1.89	0.41
1:I:396:THR:HG23	1:J:55:ALA:HB2	2.02	0.41
2:O:130[A]:ARG:NH2	2:O:157[A]:ILE:HD11	2.34	0.41
1:A:453:PRO:HA	1:A:457:GLU:OE2	2.20	0.41
1:C:7:ALA:O	1:C:141:THR:HA	2.20	0.41
1:I:438:TYR:O	2:O:154[B]:PRO:HG3	2.20	0.41
1:G:437:GLU:CG	2:N:133[A]:PRO:HG3	2.50	0.41
1:A:339:VAL:HG22	1:A:342:MET:HE1	2.02	0.41
1:H:228:ARG:HB2	1:H:228:ARG:CZ	2.51	0.41
1:C:160:ILE:HD13	1:C:167:SER:HB3	2.01	0.41
1:J:219:ASP:HA	1:J:370:SER:HB2	2.01	0.41
1:F:145:LEU:HD11	1:F:318:ILE:HG12	2.03	0.41
1:J:307:ARG:O	1:J:308:PHE:HB2	2.20	0.41
1:D:150:SER:HB3	1:D:320:ASP:HB3	2.02	0.41
1:J:54:LYS:HE2	1:J:359:TYR:HB2	2.02	0.41
2:L:131[A]:LEU:HB3	2:L:132[A]:SER:H	1.67	0.41
1:B:286:ASN:HA	3:B:2489:SO4:O2	2.21	0.41
1:I:208:GLU:HG3	1:I:210:LEU:H	1.86	0.41
1:E:370:SER:N	1:E:373:GLN:NE2	2.61	0.41
1:B:9:VAL:HG21	1:B:342:MET:HE1	2.01	0.41
1:B:351:TYR:O	1:B:354:VAL:HG12	2.21	0.41
1:H:23:ILE:O	1:H:27:GLN:HG3	2.21	0.41
1:B:174:LEU:HD12	1:B:197:TRP:CE2	2.55	0.41
1:E:162:GLU:OE2	1:E:162:GLU:HA	2.19	0.41
1:E:347:VAL:O	1:E:348:HIS:O	2.39	0.41
1:J:174:LEU:HB2	1:J:197:TRP:CZ2	2.56	0.41
2:M:157[A]:ILE:HG22	2:M:158[A]:PHE:N	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:133[A]:PRO:C	2:O:135[A]:ALA:H	2.22	0.41
2:O:139[A]:LEU:HD22	2:O:139[A]:LEU:HA	1.87	0.41
1:I:312:ILE:HA	1:I:313:PRO:HD3	1.77	0.41
1:B:335:GLY:O	1:B:339:VAL:HG23	2.21	0.41
1:C:87:LYS:HA	1:C:87:LYS:HD2	1.72	0.41
1:B:453:PRO:HA	1:B:457:GLU:OE1	2.21	0.41
1:E:333:ASP:O	1:E:337:ILE:HG12	2.21	0.41
2:O:152[A]:THR:HB	2:O:162[A]:ASP:OD2	2.20	0.41
1:A:290:GLU:O	1:A:292:LEU:N	2.54	0.41
1:A:25:ALA:HA	1:A:339:VAL:CG1	2.49	0.41
1:E:5:ILE:HG13	1:E:6:ASP:N	2.36	0.41
1:D:77:GLU:C	1:D:78:MET:HG3	2.41	0.41
1:A:349:ILE:HD13	1:A:351:TYR:CZ	2.55	0.41
1:E:389:ALA:HA	1:E:400:THR:HB	2.03	0.41
1:J:222:ILE:HG13	1:J:419:HIS:HB3	2.03	0.41
1:F:356:SER:O	1:F:365:ALA:HA	2.21	0.41
1:C:254:ILE:O	1:C:270:THR:HA	2.21	0.41
1:B:297:ASP:HB2	1:B:298:PRO:CD	2.51	0.41
1:B:222:ILE:HG13	1:B:419:HIS:HB3	2.03	0.41
2:M:151[B]:ALA:HB1	2:M:158[B]:PHE:H	1.85	0.41
2:N:149[B]:GLY:HA2	2:N:166[B]:LEU:HD21	2.03	0.41
1:I:211:GLY:CA	3:I:2515:SO4:O2	2.69	0.41
1:B:309:GLN:HG2	1:B:316:TYR:CE2	2.56	0.41
1:H:392:SER:HB2	5:H:2653:HOH:O	2.20	0.41
1:G:57:LEU:HD13	1:G:359:TYR:HB2	2.03	0.41
1:I:224:LYS:HE2	1:I:224:LYS:HA	2.03	0.41
1:A:308:PHE:HE2	1:A:337:ILE:CD1	2.16	0.40
2:N:146[B]:ALA:O	2:N:148[B]:GLN:N	2.54	0.40
1:D:60:SER:OG	1:D:199:ARG:CD	2.68	0.40
1:E:349:ILE:HG23	1:E:351:TYR:CE1	2.56	0.40
1:C:25:ALA:HA	1:C:339:VAL:HG11	2.02	0.40
1:F:253:LYS:HE3	5:F:2587:HOH:O	2.21	0.40
2:N:154[B]:PRO:HD2	2:N:157[B]:ILE:HG21	2.02	0.40
1:B:184:ILE:HG22	1:B:278:ILE:CG2	2.51	0.40
1:B:285:LYS:CG	1:B:286:ASN:HD22	2.34	0.40
1:G:385:LYS:HE2	1:G:405:LYS:HD2	2.04	0.40
1:A:20:VAL:HG21	1:A:332:GLU:HG2	2.02	0.40
1:C:96:VAL:O	1:C:100:THR:HG23	2.20	0.40
1:G:453:PRO:HA	1:G:457:GLU:OE2	2.21	0.40
1:A:311:LYS:O	1:A:313:PRO:HD3	2.21	0.40
1:H:438:TYR:CE1	2:N:132[B]:SER:HB2	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:148:THR:O	4:B:480:FAD:H8A	2.22	0.40
1:B:24:LYS:O	1:B:28:LEU:HG	2.20	0.40
1:E:287:LEU:HD23	1:E:289:LEU:HD21	2.03	0.40
1:I:160:ILE:O	1:I:160:ILE:HG13	2.21	0.40
1:A:337:ILE:HD12	1:A:347:VAL:O	2.22	0.40
2:N:144[B]:LEU:HD21	2:N:167[B]:VAL:HA	2.03	0.40
1:E:78:MET:HE3	1:F:78:MET:CE	2.51	0.40
1:J:447:ARG:HD2	2:O:137[A]:ASN:HD22	1.86	0.40
1:F:15:GLY:N	4:F:480:FAD:H52A	2.36	0.40
1:B:24:LYS:HA	1:B:24:LYS:HD2	1.84	0.40
1:J:78:MET:HG2	1:J:81:VAL:HG22	2.04	0.40
2:L:159[B]:THR:O	2:L:162[B]:ASP:HB2	2.21	0.40
1:J:145:LEU:HD11	1:J:318:ILE:HG12	2.03	0.40
1:G:299:ARG:HG3	1:G:299:ARG:HH11	1.87	0.40
2:M:145[A]:ASP:O	2:M:147[A]:SER:N	2.54	0.40
1:C:46:LEU:HD13	1:C:51:ILE:HG13	2.03	0.40
1:F:46:LEU:HD11	1:F:99:LEU:HB2	2.04	0.40
1:I:208:GLU:HG3	1:I:210:LEU:N	2.37	0.40
1:G:256:VAL:HB	1:G:269:ILE:HG12	2.03	0.40
1:A:472:ILE:CD1	1:B:336:ILE:HD11	2.51	0.40
1:C:6:ASP:O	1:C:31:LYS:HE3	2.21	0.40
1:G:114:HIS:CD2	1:G:114:HIS:C	2.93	0.40
1:B:385:LYS:HE2	1:B:405:LYS:CD	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	470/474 (99%)	445 (95%)	23 (5%)	2 (0%)	39	40
1	B	469/474 (99%)	440 (94%)	27 (6%)	2 (0%)	39	40

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	470/474 (99%)	455 (97%)	13 (3%)	2 (0%)	39	40
1	D	469/474 (99%)	456 (97%)	11 (2%)	2 (0%)	39	40
1	E	470/474 (99%)	451 (96%)	17 (4%)	2 (0%)	39	40
1	F	469/474 (99%)	452 (96%)	17 (4%)	0	100	100
1	G	470/474 (99%)	456 (97%)	11 (2%)	3 (1%)	30	27
1	H	470/474 (99%)	459 (98%)	10 (2%)	1 (0%)	52	57
1	I	466/474 (98%)	438 (94%)	26 (6%)	2 (0%)	39	40
1	J	470/474 (99%)	452 (96%)	16 (3%)	2 (0%)	39	40
2	K	41/64 (64%)	35 (85%)	6 (15%)	0	100	100
2	L	82/64 (128%)	68 (83%)	6 (7%)	8 (10%)	1	0
2	M	82/64 (128%)	64 (78%)	14 (17%)	4 (5%)	3	1
2	N	82/64 (128%)	60 (73%)	16 (20%)	6 (7%)	1	0
2	O	82/64 (128%)	68 (83%)	8 (10%)	6 (7%)	1	0
All	All	5062/5060 (100%)	4799 (95%)	221 (4%)	42 (1%)	30	20

All (42) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	349	ILE
1	D	79	SER
1	E	348	HIS
1	G	265	LYS
1	H	79	SER
1	J	253	LYS
2	L	154[A]	PRO
2	L	154[B]	PRO
2	M	157[A]	ILE
2	M	157[B]	ILE
2	M	158[A]	PHE
2	M	158[B]	PHE
2	N	148[A]	GLN
2	N	148[B]	GLN
2	O	159[A]	THR
2	O	159[B]	THR
1	C	265	LYS
1	G	266	ALA
2	L	147[A]	SER

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Mol	Chain	Res	Type
2	L	147[B]	SER
2	O	154[A]	PRO
2	O	154[B]	PRO
1	A	79	SER
1	A	291	GLU
1	B	351	TYR
2	N	170[A]	LYS
2	N	170[B]	LYS
2	O	143[A]	SER
2	O	143[B]	SER
1	J	79	SER
1	E	347	VAL
1	I	68	GLY
2	L	158[A]	PHE
2	L	158[B]	PHE
1	D	313	PRO
2	N	154[A]	PRO
2	N	154[B]	PRO
1	C	264	GLY
1	G	313	PRO
2	L	157[A]	ILE
2	L	157[B]	ILE
1	I	313	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	372/373 (100%)	361 (97%)	11 (3%)	48	57
1	B	371/373 (100%)	360 (97%)	11 (3%)	48	57
1	C	372/373 (100%)	358 (96%)	14 (4%)	40	46
1	D	371/373 (100%)	362 (98%)	9 (2%)	57	67
1	E	372/373 (100%)	362 (97%)	10 (3%)	52	62
1	F	371/373 (100%)	360 (97%)	11 (3%)	48	57

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	372/373 (100%)	362 (97%)	10 (3%)	52	62
1	H	372/373 (100%)	363 (98%)	9 (2%)	57	67
1	I	372/373 (100%)	361 (97%)	11 (3%)	48	57
1	J	372/373 (100%)	364 (98%)	8 (2%)	60	70
2	K	28/53 (53%)	28 (100%)	0	100	100
2	L	52/53 (98%)	48 (92%)	4 (8%)	16	14
2	M	52/53 (98%)	46 (88%)	6 (12%)	7	5
2	N	52/53 (98%)	50 (96%)	2 (4%)	40	46
2	O	52/53 (98%)	40 (77%)	12 (23%)	1	0
All	All	3953/3995 (99%)	3825 (97%)	128 (3%)	48	55

All (128) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	TYR
1	A	28	LEU
1	A	54	LYS
1	A	141	THR
1	A	232	LYS
1	A	235	PHE
1	A	291	GLU
1	A	321	VAL
1	A	333	ASP
1	A	349	ILE
1	A	467	SER
1	B	19	TYR
1	B	54	LYS
1	B	77	GLU
1	B	80	GLU
1	B	235	PHE
1	B	278	ILE
1	B	290	GLU
1	B	333	ASP
1	B	409	GLN
1	B	410	LYS
1	B	437	GLU
1	C	6	ASP
1	C	19	TYR
1	C	54	LYS

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Mol	Chain	Res	Type
1	C	78	MET
1	C	108	LYS
1	C	114	HIS
1	C	131	LYS
1	C	224	LYS
1	C	235	PHE
1	C	236	LYS
1	C	257	SER
1	C	265	LYS
1	C	269	ILE
1	C	333	ASP
1	D	19	TYR
1	D	54	LYS
1	D	175	LYS
1	D	235	PHE
1	D	257	SER
1	D	306	THR
1	D	311	LYS
1	D	321	VAL
1	D	410	LYS
1	E	3	GLN
1	E	19	TYR
1	E	50	CYS
1	E	54	LYS
1	E	78	MET
1	E	111	LYS
1	E	131	LYS
1	E	136	THR
1	E	235	PHE
1	E	299	ARG
1	F	19	TYR
1	F	54	LYS
1	F	77	GLU
1	F	90	GLU
1	F	235	PHE
1	F	285	LYS
1	F	295	GLU
1	F	304	VAL
1	F	321	VAL
1	F	409	GLN
1	F	410	LYS
1	G	3	GLN

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Mol	Chain	Res	Type
1	G	19	TYR
1	G	54	LYS
1	G	78	MET
1	G	175	LYS
1	G	224	LYS
1	G	235	PHE
1	G	269	ILE
1	G	301	ARG
1	G	333	ASP
1	H	19	TYR
1	H	50	CYS
1	H	54	LYS
1	H	86	ASP
1	H	111	LYS
1	H	235	PHE
1	H	247	THR
1	H	267	GLU
1	H	291	GLU
1	I	19	TYR
1	I	54	LYS
1	I	82	ARG
1	I	114	HIS
1	I	142	LYS
1	I	224	LYS
1	I	235	PHE
1	I	251	ASP
1	I	265	LYS
1	I	290	GLU
1	I	333	ASP
1	J	19	TYR
1	J	54	LYS
1	J	82	ARG
1	J	114	HIS
1	J	142	LYS
1	J	174	LEU
1	J	235	PHE
1	J	301	ARG
2	L	152[A]	THR
2	L	152[B]	THR
2	L	155[A]	ARG
2	L	155[B]	ARG
2	M	130[A]	ARG

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Mol	Chain	Res	Type
2	M	130[B]	ARG
2	M	138[A]	ILE
2	M	138[B]	ILE
2	M	139[A]	LEU
2	M	139[B]	LEU
2	N	155[A]	ARG
2	N	155[B]	ARG
2	O	137[A]	ASN
2	O	137[B]	ASN
2	O	139[A]	LEU
2	O	139[B]	LEU
2	O	145[A]	ASP
2	O	145[B]	ASP
2	O	155[A]	ARG
2	O	155[B]	ARG
2	O	159[A]	THR
2	O	159[B]	THR
2	O	166[A]	LEU
2	O	166[B]	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	GLN
1	A	137	GLN
1	A	227	GLN
1	A	231	GLN
1	A	286	ASN
1	B	125	ASN
1	B	231	GLN
1	B	286	ASN
1	B	348	HIS
1	B	373	GLN
1	C	67	HIS
1	C	137	GLN
1	C	225	ASN
1	C	286	ASN
1	C	309	GLN
1	D	67	HIS
1	E	373	GLN
1	F	137	GLN
1	G	114	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

49 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	SO4	A	2482	-	4,4,4	0.92	0	6,6,6	0.07	0
3	SO4	A	2483	-	4,4,4	0.90	0	6,6,6	0.09	0
3	SO4	A	2484	-	4,4,4	0.90	0	6,6,6	0.07	0
3	SO4	A	2485	-	4,4,4	0.93	0	6,6,6	0.08	0
4	FAD	A	480	-	48,58,58	1.54	9 (18%)	54,89,89	2.16	11 (20%)
3	SO4	B	2486	-	4,4,4	0.94	0	6,6,6	0.09	0
3	SO4	B	2487	-	4,4,4	0.95	0	6,6,6	0.09	0
3	SO4	B	2488	-	4,4,4	0.92	0	6,6,6	0.09	0
3	SO4	B	2489	-	4,4,4	0.94	0	6,6,6	0.09	0
4	FAD	B	480	-	48,58,58	1.47	6 (12%)	54,89,89	2.18	10 (18%)
3	SO4	C	2490	-	4,4,4	0.93	0	6,6,6	0.10	0
3	SO4	C	2491	-	4,4,4	0.93	0	6,6,6	0.12	0
3	SO4	C	2492	-	4,4,4	0.94	0	6,6,6	0.07	0
3	SO4	C	2493	-	4,4,4	0.95	0	6,6,6	0.08	0
4	FAD	C	480	-	48,58,58	1.39	7 (14%)	54,89,89	2.13	10 (18%)
3	SO4	D	2494	-	4,4,4	0.94	0	6,6,6	0.10	0
3	SO4	D	2495	-	4,4,4	0.93	0	6,6,6	0.12	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SO4	D	2496	-	4,4,4	0.93	0	6,6,6	0.08	0
3	SO4	D	2497	-	4,4,4	0.95	0	6,6,6	0.09	0
4	FAD	D	480	-	48,58,58	1.54	9 (18%)	54,89,89	2.14	11 (20%)
3	SO4	E	2498	-	4,4,4	0.94	0	6,6,6	0.09	0
3	SO4	E	2499	-	4,4,4	0.97	0	6,6,6	0.08	0
3	SO4	E	2500	-	4,4,4	0.94	0	6,6,6	0.11	0
3	SO4	E	2501	-	4,4,4	0.93	0	6,6,6	0.09	0
4	FAD	E	480	-	48,58,58	1.50	9 (18%)	54,89,89	2.09	7 (12%)
3	SO4	F	2502	-	4,4,4	0.93	0	6,6,6	0.09	0
3	SO4	F	2503	-	4,4,4	0.91	0	6,6,6	0.09	0
3	SO4	F	2504	-	4,4,4	0.92	0	6,6,6	0.12	0
3	SO4	F	2505	-	4,4,4	0.95	0	6,6,6	0.08	0
4	FAD	F	480	-	48,58,58	1.51	10 (20%)	54,89,89	2.16	8 (14%)
3	SO4	G	2506	-	4,4,4	0.92	0	6,6,6	0.06	0
3	SO4	G	2507	-	4,4,4	0.91	0	6,6,6	0.09	0
3	SO4	G	2508	-	4,4,4	0.93	0	6,6,6	0.08	0
3	SO4	G	2509	-	4,4,4	0.94	0	6,6,6	0.08	0
4	FAD	G	480	-	48,58,58	1.55	8 (16%)	54,89,89	2.15	7 (12%)
3	SO4	H	2510	-	4,4,4	0.96	0	6,6,6	0.11	0
3	SO4	H	2511	-	4,4,4	0.95	0	6,6,6	0.11	0
3	SO4	H	2512	-	4,4,4	0.91	0	6,6,6	0.12	0
3	SO4	H	2513	-	4,4,4	0.96	0	6,6,6	0.07	0
4	FAD	H	480	-	48,58,58	1.34	7 (14%)	54,89,89	2.13	10 (18%)
3	SO4	I	2514	-	4,4,4	0.92	0	6,6,6	0.08	0
3	SO4	I	2515	-	4,4,4	0.94	0	6,6,6	0.09	0
3	SO4	I	2516	-	4,4,4	0.94	0	6,6,6	0.06	0
4	FAD	I	480	-	48,58,58	1.51	8 (16%)	54,89,89	2.07	9 (16%)
3	SO4	J	2517	-	4,4,4	0.94	0	6,6,6	0.11	0
3	SO4	J	2518	-	4,4,4	0.93	0	6,6,6	0.07	0
3	SO4	J	2519	-	4,4,4	0.94	0	6,6,6	0.08	0
3	SO4	J	2520	-	4,4,4	0.93	0	6,6,6	0.10	0
4	FAD	J	480	-	48,58,58	1.41	7 (14%)	54,89,89	2.15	7 (12%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SO4	A	2482	-	-	0/0/0/0	0/0/0/0
3	SO4	A	2483	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SO4	A	2484	-	-	0/0/0/0	0/0/0/0
3	SO4	A	2485	-	-	0/0/0/0	0/0/0/0
4	FAD	A	480	-	-	0/30/50/50	0/6/6/6
3	SO4	B	2486	-	-	0/0/0/0	0/0/0/0
3	SO4	B	2487	-	-	0/0/0/0	0/0/0/0
3	SO4	B	2488	-	-	0/0/0/0	0/0/0/0
3	SO4	B	2489	-	-	0/0/0/0	0/0/0/0
4	FAD	B	480	-	-	0/30/50/50	0/6/6/6
3	SO4	C	2490	-	-	0/0/0/0	0/0/0/0
3	SO4	C	2491	-	-	0/0/0/0	0/0/0/0
3	SO4	C	2492	-	-	0/0/0/0	0/0/0/0
3	SO4	C	2493	-	-	0/0/0/0	0/0/0/0
4	FAD	C	480	-	-	0/30/50/50	0/6/6/6
3	SO4	D	2494	-	-	0/0/0/0	0/0/0/0
3	SO4	D	2495	-	-	0/0/0/0	0/0/0/0
3	SO4	D	2496	-	-	0/0/0/0	0/0/0/0
3	SO4	D	2497	-	-	0/0/0/0	0/0/0/0
4	FAD	D	480	-	-	0/30/50/50	0/6/6/6
3	SO4	E	2498	-	-	0/0/0/0	0/0/0/0
3	SO4	E	2499	-	-	0/0/0/0	0/0/0/0
3	SO4	E	2500	-	-	0/0/0/0	0/0/0/0
3	SO4	E	2501	-	-	0/0/0/0	0/0/0/0
4	FAD	E	480	-	-	0/30/50/50	0/6/6/6
3	SO4	F	2502	-	-	0/0/0/0	0/0/0/0
3	SO4	F	2503	-	-	0/0/0/0	0/0/0/0
3	SO4	F	2504	-	-	0/0/0/0	0/0/0/0
3	SO4	F	2505	-	-	0/0/0/0	0/0/0/0
4	FAD	F	480	-	-	0/30/50/50	0/6/6/6
3	SO4	G	2506	-	-	0/0/0/0	0/0/0/0
3	SO4	G	2507	-	-	0/0/0/0	0/0/0/0
3	SO4	G	2508	-	-	0/0/0/0	0/0/0/0
3	SO4	G	2509	-	-	0/0/0/0	0/0/0/0
4	FAD	G	480	-	-	0/30/50/50	0/6/6/6
3	SO4	H	2510	-	-	0/0/0/0	0/0/0/0
3	SO4	H	2511	-	-	0/0/0/0	0/0/0/0
3	SO4	H	2512	-	-	0/0/0/0	0/0/0/0
3	SO4	H	2513	-	-	0/0/0/0	0/0/0/0
4	FAD	H	480	-	-	0/30/50/50	0/6/6/6
3	SO4	I	2514	-	-	0/0/0/0	0/0/0/0
3	SO4	I	2515	-	-	0/0/0/0	0/0/0/0
3	SO4	I	2516	-	-	0/0/0/0	0/0/0/0
4	FAD	I	480	-	-	0/30/50/50	0/6/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SO4	J	2517	-	-	0/0/0/0	0/0/0/0
3	SO4	J	2518	-	-	0/0/0/0	0/0/0/0
3	SO4	J	2519	-	-	0/0/0/0	0/0/0/0
3	SO4	J	2520	-	-	0/0/0/0	0/0/0/0
4	FAD	J	480	-	-	0/30/50/50	0/6/6/6

All (80) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	480	FAD	P-O2P	-2.10	1.46	1.54
4	A	480	FAD	C6-C7	2.01	1.43	1.37
4	F	480	FAD	C8-C7	2.04	1.46	1.41
4	A	480	FAD	C1'-N10	2.05	1.50	1.48
4	E	480	FAD	C5X-N5	2.07	1.38	1.35
4	F	480	FAD	C2A-N3A	2.07	1.35	1.32
4	D	480	FAD	C1'-N10	2.10	1.50	1.48
4	I	480	FAD	C5B-C4B	2.10	1.58	1.51
4	G	480	FAD	O4B-C1B	2.12	1.43	1.41
4	C	480	FAD	C2A-N1A	2.16	1.38	1.33
4	H	480	FAD	C5X-N5	2.18	1.38	1.35
4	J	480	FAD	C2A-N1A	2.20	1.38	1.33
4	A	480	FAD	C2A-N1A	2.20	1.38	1.33
4	I	480	FAD	C2A-N1A	2.22	1.38	1.33
4	H	480	FAD	C5B-C4B	2.24	1.58	1.51
4	C	480	FAD	C5B-C4B	2.24	1.58	1.51
4	E	480	FAD	C5B-C4B	2.25	1.58	1.51
4	G	480	FAD	C2A-N1A	2.26	1.38	1.33
4	F	480	FAD	C5B-C4B	2.31	1.59	1.51
4	I	480	FAD	C1'-N10	2.31	1.50	1.48
4	B	480	FAD	C2A-N3A	2.33	1.36	1.32
4	G	480	FAD	C5B-C4B	2.34	1.59	1.51
4	F	480	FAD	C10-N1	2.35	1.39	1.35
4	F	480	FAD	C2A-N1A	2.37	1.38	1.33
4	D	480	FAD	C2A-N1A	2.42	1.38	1.33
4	C	480	FAD	C2A-N3A	2.47	1.36	1.32
4	A	480	FAD	C10-N10	2.47	1.42	1.39
4	B	480	FAD	C2A-N1A	2.48	1.38	1.33
4	I	480	FAD	C2A-N3A	2.48	1.36	1.32
4	E	480	FAD	O4B-C1B	2.51	1.44	1.41
4	G	480	FAD	C4-N3	2.53	1.37	1.33
4	F	480	FAD	C5X-N5	2.53	1.39	1.35
4	E	480	FAD	C10-N10	2.55	1.42	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	480	FAD	C2A-N1A	2.61	1.38	1.33
4	F	480	FAD	C10-N10	2.62	1.42	1.39
4	D	480	FAD	C2A-N3A	2.63	1.36	1.32
4	G	480	FAD	C2A-N3A	2.63	1.36	1.32
4	A	480	FAD	C2A-N3A	2.70	1.37	1.32
4	E	480	FAD	C2A-N3A	2.72	1.37	1.32
4	H	480	FAD	C4-N3	2.73	1.38	1.33
4	B	480	FAD	C5X-N5	2.78	1.39	1.35
4	C	480	FAD	C5X-N5	2.81	1.39	1.35
4	J	480	FAD	C1'-N10	2.83	1.51	1.48
4	D	480	FAD	C10-N10	2.88	1.42	1.39
4	H	480	FAD	C2A-N3A	2.89	1.37	1.32
4	I	480	FAD	C5X-N5	2.90	1.39	1.35
4	B	480	FAD	C4-N3	2.90	1.38	1.33
4	I	480	FAD	C4-N3	2.90	1.38	1.33
4	D	480	FAD	C5B-C4B	2.90	1.61	1.51
4	J	480	FAD	C9A-N10	2.93	1.42	1.38
4	D	480	FAD	C5X-N5	2.94	1.40	1.35
4	A	480	FAD	C5X-N5	2.94	1.40	1.35
4	J	480	FAD	C5B-C4B	2.95	1.61	1.51
4	D	480	FAD	C9A-N10	2.97	1.42	1.38
4	C	480	FAD	C9A-N10	2.97	1.42	1.38
4	F	480	FAD	C4-N3	3.04	1.38	1.33
4	D	480	FAD	C4-N3	3.10	1.38	1.33
4	J	480	FAD	C4-N3	3.11	1.38	1.33
4	E	480	FAD	C4-N3	3.27	1.39	1.33
4	A	480	FAD	C9A-N10	3.31	1.43	1.38
4	C	480	FAD	C4-N3	3.36	1.39	1.33
4	J	480	FAD	C5X-N5	3.39	1.40	1.35
4	J	480	FAD	C4X-N5	3.42	1.38	1.33
4	H	480	FAD	O4B-C1B	3.48	1.45	1.41
4	E	480	FAD	C9A-N10	3.48	1.43	1.38
4	G	480	FAD	C9A-N10	3.53	1.43	1.38
4	H	480	FAD	C4X-N5	3.54	1.38	1.33
4	F	480	FAD	C9A-N10	3.73	1.43	1.38
4	B	480	FAD	C9A-N10	3.80	1.44	1.38
4	I	480	FAD	C9A-N10	3.85	1.44	1.38
4	A	480	FAD	C4-N3	3.86	1.40	1.33
4	G	480	FAD	C5X-N5	3.86	1.41	1.35
4	F	480	FAD	C4X-N5	3.88	1.39	1.33
4	C	480	FAD	C4X-N5	3.96	1.39	1.33
4	D	480	FAD	C4X-N5	4.15	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	480	FAD	C4X-N5	4.35	1.40	1.33
4	A	480	FAD	C4X-N5	4.38	1.40	1.33
4	I	480	FAD	C4X-N5	4.53	1.40	1.33
4	B	480	FAD	C4X-N5	4.72	1.40	1.33
4	G	480	FAD	C4X-N5	4.90	1.41	1.33

All (90) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	480	FAD	N3A-C2A-N1A	-5.35	124.80	128.89
4	D	480	FAD	N3A-C2A-N1A	-5.26	124.87	128.89
4	E	480	FAD	N3A-C2A-N1A	-5.22	124.90	128.89
4	B	480	FAD	C4B-O4B-C1B	-5.10	104.12	109.72
4	G	480	FAD	C4B-O4B-C1B	-5.07	104.14	109.72
4	A	480	FAD	C4B-O4B-C1B	-5.07	104.15	109.72
4	F	480	FAD	N3A-C2A-N1A	-5.02	125.05	128.89
4	H	480	FAD	N3A-C2A-N1A	-4.94	125.11	128.89
4	G	480	FAD	N3A-C2A-N1A	-4.94	125.11	128.89
4	B	480	FAD	C4X-C4-N3	-4.91	116.88	123.59
4	C	480	FAD	C4X-C4-N3	-4.84	116.97	123.59
4	J	480	FAD	C4X-C4-N3	-4.79	117.04	123.59
4	I	480	FAD	N3A-C2A-N1A	-4.78	125.23	128.89
4	G	480	FAD	C4X-C4-N3	-4.76	117.08	123.59
4	A	480	FAD	N3A-C2A-N1A	-4.70	125.30	128.89
4	I	480	FAD	C4X-C4-N3	-4.65	117.23	123.59
4	H	480	FAD	C4X-C4-N3	-4.60	117.30	123.59
4	J	480	FAD	N3A-C2A-N1A	-4.58	125.39	128.89
4	E	480	FAD	C4X-C4-N3	-4.56	117.36	123.59
4	B	480	FAD	N3A-C2A-N1A	-4.46	125.48	128.89
4	D	480	FAD	C4X-C4-N3	-4.45	117.50	123.59
4	A	480	FAD	C4X-C4-N3	-4.43	117.53	123.59
4	H	480	FAD	C4B-O4B-C1B	-4.29	105.00	109.72
4	F	480	FAD	C4X-C4-N3	-4.26	117.77	123.59
4	J	480	FAD	C4B-O4B-C1B	-4.19	105.12	109.72
4	C	480	FAD	C4B-O4B-C1B	-4.18	105.12	109.72
4	F	480	FAD	C4B-O4B-C1B	-4.11	105.21	109.72
4	D	480	FAD	C4B-O4B-C1B	-3.66	105.70	109.72
4	G	480	FAD	C4-C4X-C10	-3.35	117.80	119.94
4	I	480	FAD	C4-C4X-C10	-3.18	117.91	119.94
4	E	480	FAD	C4B-O4B-C1B	-3.09	106.33	109.72
4	F	480	FAD	C4X-C10-N10	-3.02	118.74	120.52
4	E	480	FAD	C4-C4X-C10	-3.00	118.02	119.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	480	FAD	C4-C4X-C10	-2.99	118.03	119.94
4	B	480	FAD	C4-C4X-C10	-2.98	118.03	119.94
4	D	480	FAD	C4-C4X-C10	-2.83	118.13	119.94
4	A	480	FAD	C4X-C10-N10	-2.81	118.86	120.52
4	A	480	FAD	C4-C4X-C10	-2.79	118.15	119.94
4	J	480	FAD	C4-C4X-C10	-2.79	118.15	119.94
4	H	480	FAD	C4X-C10-N10	-2.75	118.90	120.52
4	E	480	FAD	C4X-C10-N10	-2.66	118.95	120.52
4	F	480	FAD	C4-C4X-C10	-2.43	118.38	119.94
4	H	480	FAD	C4-C4X-C10	-2.42	118.39	119.94
4	I	480	FAD	C4B-O4B-C1B	-2.32	107.17	109.72
4	D	480	FAD	C4X-C10-N10	-2.22	119.21	120.52
4	B	480	FAD	C4X-C10-N10	-2.05	119.31	120.52
4	A	480	FAD	C9A-C5X-N5	-2.03	119.36	122.36
4	H	480	FAD	O2B-C2B-C3B	2.02	118.39	111.83
4	H	480	FAD	C4-C4X-N5	2.04	121.20	118.72
4	D	480	FAD	C5X-C9A-N10	2.08	119.20	117.62
4	C	480	FAD	P-O3P-PA	2.13	138.71	132.73
4	D	480	FAD	C1'-N10-C9A	2.15	121.27	118.86
4	C	480	FAD	C2B-C1B-N9A	2.15	117.58	114.29
4	B	480	FAD	P-O3P-PA	2.16	138.80	132.73
4	A	480	FAD	O3P-P-O5'	2.16	108.67	102.94
4	H	480	FAD	C5X-C9A-N10	2.24	119.32	117.62
4	A	480	FAD	C5X-C9A-N10	2.26	119.33	117.62
4	I	480	FAD	C4-C4X-N5	2.27	121.47	118.72
4	J	480	FAD	C2B-C1B-N9A	2.31	117.82	114.29
4	A	480	FAD	P-O3P-PA	2.32	139.23	132.73
4	B	480	FAD	C4-C4X-N5	2.32	121.54	118.72
4	B	480	FAD	C1'-N10-C9A	2.35	121.50	118.86
4	D	480	FAD	C2B-C1B-N9A	2.35	117.89	114.29
4	C	480	FAD	C4-C4X-N5	2.38	121.60	118.72
4	G	480	FAD	C4-C4X-N5	2.39	121.62	118.72
4	I	480	FAD	C2B-C1B-N9A	2.41	117.97	114.29
4	F	480	FAD	C2B-C1B-N9A	2.41	117.98	114.29
4	C	480	FAD	C1'-N10-C9A	2.52	121.69	118.86
4	I	480	FAD	C1'-N10-C9A	2.58	121.76	118.86
4	D	480	FAD	P-O3P-PA	2.75	140.44	132.73
4	G	480	FAD	C4X-N5-C5X	3.26	120.51	116.76
4	J	480	FAD	C4X-N5-C5X	3.29	120.54	116.76
4	I	480	FAD	C4X-N5-C5X	3.41	120.68	116.76
4	D	480	FAD	C4X-N5-C5X	3.58	120.88	116.76
4	B	480	FAD	C4X-N5-C5X	3.73	121.06	116.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	480	FAD	C4X-N5-C5X	3.76	121.09	116.76
4	F	480	FAD	C4X-N5-C5X	3.82	121.16	116.76
4	A	480	FAD	C4X-N5-C5X	3.84	121.18	116.76
4	H	480	FAD	C4X-N5-C5X	3.98	121.34	116.76
4	C	480	FAD	C4X-N5-C5X	3.98	121.34	116.76
4	C	480	FAD	C4-N3-C2	9.71	123.64	115.25
4	H	480	FAD	C4-N3-C2	9.74	123.67	115.25
4	A	480	FAD	C4-N3-C2	10.09	123.97	115.25
4	E	480	FAD	C4-N3-C2	10.32	124.17	115.25
4	D	480	FAD	C4-N3-C2	10.34	124.19	115.25
4	G	480	FAD	C4-N3-C2	10.38	124.22	115.25
4	I	480	FAD	C4-N3-C2	10.38	124.22	115.25
4	B	480	FAD	C4-N3-C2	10.63	124.44	115.25
4	F	480	FAD	C4-N3-C2	10.64	124.44	115.25
4	J	480	FAD	C4-N3-C2	10.89	124.66	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

28 monomers are involved in 51 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	2484	SO4	1	0
3	A	2485	SO4	1	0
4	A	480	FAD	2	0
3	B	2486	SO4	1	0
3	B	2487	SO4	1	0
3	B	2489	SO4	2	0
4	B	480	FAD	2	0
3	C	2493	SO4	1	0
4	C	480	FAD	3	0
4	D	480	FAD	2	0
3	E	2498	SO4	1	0
3	E	2499	SO4	2	0
4	E	480	FAD	3	0
3	F	2502	SO4	1	0
3	F	2505	SO4	1	0
4	F	480	FAD	4	0
3	G	2509	SO4	1	0
4	G	480	FAD	2	0
3	H	2510	SO4	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	H	2511	SO4	2	0
4	H	480	FAD	5	0
3	I	2515	SO4	2	0
3	I	2516	SO4	1	0
4	I	480	FAD	1	0
3	J	2518	SO4	1	0
3	J	2519	SO4	1	0
3	J	2520	SO4	2	0
4	J	480	FAD	3	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	472/474 (99%)	0.19	24 (5%) 32 34	26, 44, 68, 86	0
1	B	471/474 (99%)	0.73	79 (16%) 2 2	28, 51, 84, 93	0
1	C	472/474 (99%)	0.12	20 (4%) 40 42	23, 36, 61, 79	0
1	D	471/474 (99%)	0.03	24 (5%) 32 34	21, 31, 53, 74	0
1	E	472/474 (99%)	0.19	33 (6%) 19 21	24, 37, 60, 81	0
1	F	471/474 (99%)	0.07	21 (4%) 37 39	20, 32, 54, 73	0
1	G	472/474 (99%)	0.04	14 (2%) 54 56	21, 36, 60, 79	0
1	H	472/474 (99%)	-0.04	12 (2%) 61 62	16, 27, 48, 66	0
1	I	470/474 (99%)	0.52	52 (11%) 7 8	27, 49, 76, 86	0
1	J	472/474 (99%)	0.05	17 (3%) 46 48	25, 38, 60, 82	0
2	K	43/64 (67%)	2.35	23 (53%) 0 0	54, 68, 81, 92	0
2	L	43/64 (67%)	2.52	21 (48%) 0 0	35, 47, 58, 60	0
2	M	43/64 (67%)	3.10	31 (72%) 0 0	33, 49, 56, 58	0
2	N	43/64 (67%)	3.42	32 (74%) 0 0	38, 51, 60, 61	0
2	O	43/64 (67%)	3.11	30 (69%) 0 0	36, 50, 58, 59	0
All	All	4930/5060 (97%)	0.31	433 (8%) 12 13	16, 38, 69, 93	0

All (433) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	N	172[A]	THR	9.3
2	K	172	THR	8.2
1	B	139	ILE	7.2
2	N	171[A]	GLN	7.2
2	O	164[A]	LEU	6.9
2	O	144[A]	LEU	6.9
2	O	166[A]	LEU	6.5

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Mol	Chain	Res	Type	RSRZ
2	N	157[A]	ILE	6.4
2	O	167[A]	VAL	6.1
2	L	169[A]	LEU	5.8
2	N	169[A]	LEU	5.7
1	B	294	ILE	5.7
2	K	152	THR	5.7
2	O	169[A]	LEU	5.7
1	I	79	SER	5.6
2	L	166[A]	LEU	5.6
2	M	157[A]	ILE	5.6
2	M	149[A]	GLY	5.6
1	I	254	ILE	5.5
1	G	265	LYS	5.5
2	L	172[A]	THR	5.5
2	O	172[A]	THR	5.4
1	C	79	SER	5.4
2	N	154[A]	PRO	5.4
2	N	166[A]	LEU	5.3
2	N	150[A]	THR	5.3
2	L	144[A]	LEU	5.3
2	M	144[A]	LEU	5.3
2	K	146	ALA	5.3
2	L	167[A]	VAL	5.3
2	M	169[A]	LEU	5.3
2	M	172[A]	THR	5.2
2	N	155[A]	ARG	5.1
2	N	145[A]	ASP	5.1
1	B	348	HIS	5.1
1	B	79	SER	5.0
2	M	146[A]	ALA	5.0
2	L	170[A]	LYS	5.0
1	B	138	VAL	5.0
2	N	158[A]	PHE	4.9
1	B	5	ILE	4.9
1	I	269	ILE	4.9
2	O	157[A]	ILE	4.9
2	M	154[A]	PRO	4.9
2	L	171[A]	GLN	4.8
1	B	132	ALA	4.8
1	I	268	VAL	4.8
1	G	79	SER	4.7
2	M	153[A]	GLY	4.7

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Mol	Chain	Res	Type	RSRZ
2	M	164[A]	LEU	4.7
2	O	171[A]	GLN	4.7
2	K	149	GLY	4.6
2	M	145[A]	ASP	4.6
2	K	166	LEU	4.6
1	B	290	GLU	4.6
2	L	146[A]	ALA	4.6
1	B	312	ILE	4.5
1	B	265	LYS	4.5
2	O	154[A]	PRO	4.5
1	E	262	SER	4.5
2	N	167[A]	VAL	4.4
2	N	130[A]	ARG	4.4
2	M	171[A]	GLN	4.3
2	M	167[A]	VAL	4.3
1	E	135	GLY	4.3
1	I	258	ILE	4.3
2	M	156[A]	GLY	4.3
1	C	132	ALA	4.3
1	B	129	ALA	4.2
2	L	149[A]	GLY	4.2
2	O	159[A]	THR	4.2
2	N	133[A]	PRO	4.2
1	B	123	GLY	4.2
2	O	145[A]	ASP	4.1
1	B	31	LYS	4.1
1	D	429	VAL	4.1
2	N	146[A]	ALA	4.1
1	B	9	VAL	4.1
1	B	113	VAL	4.1
2	N	131[A]	LEU	4.0
2	M	147[A]	SER	4.0
1	A	79	SER	3.9
1	A	411	SER	3.9
2	K	150	THR	3.9
1	E	261	ALA	3.9
2	O	150[A]	THR	3.9
1	A	3	GLN	3.9
2	N	147[A]	SER	3.9
1	E	455	LEU	3.9
2	O	149[A]	GLY	3.9
1	B	121	ILE	3.9

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Mol	Chain	Res	Type	RSRZ
1	B	344	GLY	3.8
1	B	122	THR	3.8
1	J	265	LYS	3.8
2	O	170[A]	LYS	3.8
1	I	80	GLU	3.8
2	M	142[A]	HIS	3.8
1	I	176	LYS	3.8
2	L	147[A]	SER	3.8
2	M	148[A]	GLN	3.7
1	I	244	THR	3.7
1	B	29	GLY	3.7
1	E	454	THR	3.7
2	N	163[A]	ALA	3.7
2	M	168[A]	GLN	3.7
1	I	132	ALA	3.7
1	B	311	LYS	3.7
2	M	166[A]	LEU	3.7
2	O	158[A]	PHE	3.6
2	M	134[A]	ALA	3.6
2	N	149[A]	GLY	3.6
2	O	153[A]	GLY	3.6
1	B	313	PRO	3.6
2	O	143[A]	SER	3.6
2	M	133[A]	PRO	3.6
2	K	163	ALA	3.6
2	O	134[A]	ALA	3.6
2	N	144[A]	LEU	3.6
2	K	165	LYS	3.6
2	N	151[A]	ALA	3.6
1	D	79	SER	3.6
2	O	147[A]	SER	3.6
1	I	160	ILE	3.5
2	K	168	GLN	3.5
1	I	266	ALA	3.5
2	N	153[A]	GLY	3.5
1	F	135	GLY	3.5
1	J	79	SER	3.5
1	B	381	TYR	3.5
1	E	428	MET	3.5
1	B	6	ASP	3.5
1	B	115	VAL	3.4
1	J	252	GLY	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	131	LYS	3.4
1	B	425	ALA	3.4
1	A	451	ALA	3.4
2	M	150[A]	THR	3.4
1	A	132	ALA	3.4
1	B	289	LEU	3.3
2	K	148	GLN	3.3
1	E	79	SER	3.3
1	I	5	ILE	3.3
1	A	133	ASP	3.3
1	I	243	VAL	3.3
2	L	148[A]	GLN	3.3
1	J	80	GLU	3.3
1	B	133	ASP	3.3
2	M	158[A]	PHE	3.3
1	B	347	VAL	3.2
2	L	133[A]	PRO	3.2
1	A	290	GLU	3.2
1	F	429	VAL	3.2
1	C	263	GLY	3.2
1	G	5	ILE	3.2
1	B	262	SER	3.2
1	B	346	ALA	3.2
1	E	420	ILE	3.2
1	B	126	GLN	3.2
1	J	78	MET	3.2
2	N	152[A]	THR	3.2
1	H	79	SER	3.1
1	B	33	VAL	3.1
1	E	429	VAL	3.1
2	K	151	ALA	3.1
1	B	343	ALA	3.1
1	D	132	ALA	3.1
1	B	291	GLU	3.1
1	I	252	GLY	3.1
1	A	134	GLY	3.1
2	L	151[A]	ALA	3.0
1	B	141	THR	3.0
2	N	143[A]	SER	3.0
2	M	155[A]	ARG	3.0
1	E	132	ALA	3.0
1	B	288	GLY	3.0

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Mol	Chain	Res	Type	RSRZ
2	K	158	PHE	3.0
1	J	263	GLY	3.0
2	O	168[A]	GLN	3.0
1	F	420	ILE	2.9
1	B	287	LEU	2.9
1	C	429	VAL	2.9
1	D	357	VAL	2.9
1	B	30	PHE	2.9
2	O	139[A]	LEU	2.9
1	C	265	LYS	2.9
1	B	292	LEU	2.9
1	F	428	MET	2.9
2	K	147	SER	2.9
1	D	358	ILE	2.9
1	I	6	ASP	2.9
2	O	148[A]	GLN	2.9
2	N	134[A]	ALA	2.9
2	N	148[A]	GLN	2.9
2	L	130[A]	ARG	2.9
1	B	378	GLY	2.8
1	J	77	GLU	2.8
1	J	72	ALA	2.8
1	I	136	THR	2.8
1	J	449	CYS	2.8
1	B	376	GLU	2.8
1	B	12	ILE	2.8
1	C	455	LEU	2.8
2	L	164[A]	LEU	2.8
2	O	151[A]	ALA	2.8
1	C	262	SER	2.8
1	G	429	VAL	2.8
1	I	247	THR	2.8
1	B	116	ASN	2.8
2	N	170[A]	LYS	2.8
1	F	425	ALA	2.8
1	E	426	GLY	2.8
2	K	154	PRO	2.8
1	G	132	ALA	2.8
1	G	454	THR	2.8
1	F	455	LEU	2.8
2	N	139[A]	LEU	2.8
1	E	266	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
2	M	163[A]	ALA	2.7
2	K	139	LEU	2.7
2	M	139[A]	LEU	2.7
2	K	167	VAL	2.7
1	A	380	GLU	2.7
1	J	82	ARG	2.7
1	A	6	ASP	2.7
1	E	6	ASP	2.7
1	I	133	ASP	2.7
1	D	426	GLY	2.7
1	G	135	GLY	2.7
1	B	359	TYR	2.7
1	I	249	LYS	2.7
1	I	262	SER	2.7
1	F	80	GLU	2.7
1	E	264	GLY	2.7
1	A	139	ILE	2.7
2	K	157	ILE	2.7
1	D	432	ALA	2.7
1	B	144	ILE	2.6
1	F	6	ASP	2.6
1	H	429	VAL	2.6
2	K	134	ALA	2.6
2	M	143[A]	SER	2.6
1	A	468	PHE	2.6
1	H	420	ILE	2.6
1	F	357	VAL	2.6
1	B	285	LYS	2.6
2	M	159[A]	THR	2.6
2	L	145[A]	ASP	2.6
1	B	307	ARG	2.6
1	H	455	LEU	2.6
1	A	313	PRO	2.6
1	A	5	ILE	2.6
1	F	131	LYS	2.6
1	I	180	LYS	2.6
1	B	28	LEU	2.6
1	B	136	THR	2.6
1	B	298	PRO	2.6
1	I	355	PRO	2.6
1	C	134	GLY	2.6
1	C	451	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	265	LYS	2.6
1	E	432	ALA	2.6
1	B	315	ILE	2.6
2	O	142[A]	HIS	2.6
1	G	133	ASP	2.6
1	A	4	PRO	2.5
1	E	453	PRO	2.5
1	B	295	GLU	2.5
1	A	447	ARG	2.5
1	I	429	VAL	2.5
1	B	125	ASN	2.5
1	H	425	ALA	2.5
2	K	169	LEU	2.5
1	H	50	CYS	2.5
2	N	136[A]	ARG	2.5
2	O	161[A]	GLU	2.5
1	D	425	ALA	2.5
1	F	365	ALA	2.5
1	I	82	ARG	2.5
1	B	135	GLY	2.5
1	F	426	GLY	2.5
1	C	353	CYS	2.5
2	M	138[A]	ILE	2.5
1	I	290	GLU	2.5
1	F	262	SER	2.5
1	I	257	SER	2.5
2	K	156	GLY	2.5
1	B	124	LYS	2.5
1	D	82	ARG	2.5
2	O	165[A]	LYS	2.5
1	E	394	ALA	2.4
1	A	455	LEU	2.4
1	H	454	THR	2.4
1	I	69	THR	2.4
2	N	138[A]	ILE	2.4
1	B	263	GLY	2.4
1	F	430	ASN	2.4
1	A	136	THR	2.4
1	B	429	VAL	2.4
1	D	428	MET	2.4
1	E	265	LYS	2.4
2	L	168[A]	GLN	2.4

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Mol	Chain	Res	Type	RSRZ
2	O	133[A]	PRO	2.4
1	I	71	PHE	2.4
1	I	175	LYS	2.4
1	D	356	SER	2.4
1	B	7	ALA	2.4
1	C	420	ILE	2.4
1	I	131	LYS	2.4
1	I	251	ASP	2.4
2	M	170[A]	LYS	2.4
1	B	209	PHE	2.4
1	H	327	LEU	2.4
2	O	155[A]	ARG	2.4
1	B	454	THR	2.4
1	D	365	ALA	2.4
1	I	265	LYS	2.4
1	C	428	MET	2.4
1	I	78	MET	2.4
2	K	164	LEU	2.4
1	F	433	ALA	2.3
1	I	256	VAL	2.3
1	I	354	VAL	2.3
1	I	253	LYS	2.3
1	I	267	GLU	2.3
1	B	128	THR	2.3
1	B	428	MET	2.3
2	O	136[A]	ARG	2.3
1	B	379	ILE	2.3
1	I	242	LYS	2.3
1	I	68	GLY	2.3
1	I	157	GLY	2.3
1	A	454	THR	2.3
1	B	4	PRO	2.3
1	E	404	VAL	2.3
1	D	69	THR	2.3
1	J	451	ALA	2.3
1	C	354	VAL	2.3
1	D	366	TRP	2.3
1	E	134	GLY	2.3
1	E	456	SER	2.3
1	I	276	VAL	2.3
1	B	142	LYS	2.3
1	F	50	CYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	J	429	VAL	2.3
1	E	290	GLU	2.3
1	G	3	GLN	2.3
1	I	274	LEU	2.3
2	N	164[A]	LEU	2.3
1	B	426	GLY	2.2
1	F	79	SER	2.2
1	I	255	ASP	2.2
2	K	131	LEU	2.2
2	K	161	GLU	2.2
1	C	468	PHE	2.2
1	C	454	THR	2.2
1	I	159	THR	2.2
1	I	353	CYS	2.2
1	B	411	SER	2.2
1	J	291	GLU	2.2
1	J	262	SER	2.2
2	N	156[A]	GLY	2.2
1	A	264	GLY	2.2
1	F	424	GLY	2.2
1	B	112	VAL	2.2
1	E	451	ALA	2.2
1	H	365	ALA	2.2
2	L	163[A]	ALA	2.2
1	B	430	ASN	2.2
1	D	355	PRO	2.2
1	B	114	HIS	2.2
1	E	3	GLN	2.2
2	M	152[A]	THR	2.2
1	F	456	SER	2.2
1	C	364	VAL	2.2
1	B	261	ALA	2.2
1	I	432	ALA	2.2
1	B	310	THR	2.1
1	E	422	GLY	2.1
1	I	425	ALA	2.1
1	J	448	VAL	2.1
1	A	337	ILE	2.1
2	L	156[A]	GLY	2.1
1	C	436	LEU	2.1
1	E	130	THR	2.1
1	J	69	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	209	PHE	2.1
2	O	130[A]	ARG	2.1
1	G	453	PRO	2.1
1	A	412	THR	2.1
1	B	306	THR	2.1
1	I	270	THR	2.1
1	D	327	LEU	2.1
2	L	139[A]	LEU	2.1
1	H	80	GLU	2.1
1	B	50	CYS	2.1
1	B	120	LYS	2.1
1	B	140	ASP	2.1
1	F	132	ALA	2.1
2	L	134[A]	ALA	2.1
1	D	188	VAL	2.1
1	E	424	GLY	2.1
1	E	430	ASN	2.1
1	A	294	ILE	2.1
1	E	445	ILE	2.1
1	G	455	LEU	2.1
1	C	290	GLU	2.1
1	H	449	CYS	2.1
1	C	268	VAL	2.1
2	M	131[A]	LEU	2.1
1	F	355	PRO	2.1
1	I	4	PRO	2.1
1	C	293	GLY	2.1
1	E	425	ALA	2.1
1	G	357	VAL	2.1
1	I	246	ALA	2.0
1	D	80	GLU	2.0
1	E	376	GLU	2.0
1	B	130	THR	2.0
1	D	359	TYR	2.0
1	D	364	VAL	2.0
1	D	454	THR	2.0
1	I	81	VAL	2.0
1	A	409	GLN	2.0
1	D	78	MET	2.0
1	D	451	ALA	2.0
1	H	432	ALA	2.0
1	J	425	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
2	N	135[A]	ALA	2.0
1	G	136	THR	2.0
1	E	364	VAL	2.0
1	B	303	PRO	2.0
1	G	428	MET	2.0
1	I	428	MET	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	SO4	C	2490	5/5	0.94	0.15	2.28	73,77,81,82	0
3	SO4	C	2493	5/5	0.92	0.21	0.89	80,81,84,86	0
3	SO4	I	2514	5/5	0.96	0.16	0.85	72,74,78,80	0
3	SO4	J	2517	5/5	0.96	0.14	0.83	65,68,69,70	0
3	SO4	A	2485	5/5	0.82	0.27	0.65	91,93,94,98	0
4	FAD	J	480	53/53	0.97	0.13	0.36	23,30,37,39	0
4	FAD	C	480	53/53	0.96	0.13	0.31	25,32,39,43	0
4	FAD	I	480	53/53	0.94	0.15	0.31	31,44,56,57	0
4	FAD	G	480	53/53	0.95	0.13	0.31	21,31,46,51	0
3	SO4	B	2489	5/5	0.80	0.33	0.30	100,101,102,106	0
4	FAD	E	480	53/53	0.95	0.13	0.26	26,35,41,43	0
4	FAD	H	480	53/53	0.97	0.15	0.25	14,21,28,38	0
4	FAD	D	480	53/53	0.96	0.14	0.12	21,27,32,36	0
4	FAD	A	480	53/53	0.95	0.13	0.05	28,39,57,58	0
4	FAD	F	480	53/53	0.96	0.13	0.00	21,29,38,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	SO4	H	2513	5/5	0.95	0.12	-0.09	60,61,67,70	0
3	SO4	I	2516	5/5	0.94	0.18	-0.14	84,86,90,91	0
4	FAD	B	480	53/53	0.90	0.15	-0.24	42,55,68,70	0
3	SO4	J	2520	5/5	0.91	0.12	-0.29	72,73,76,76	0
3	SO4	D	2497	5/5	0.94	0.11	-0.41	58,62,66,67	0
3	SO4	G	2509	5/5	0.91	0.13	-0.48	88,88,91,94	0
3	SO4	F	2502	5/5	0.97	0.12	-0.55	54,59,65,66	0
3	SO4	D	2494	5/5	0.98	0.12	-0.73	61,64,65,68	0
3	SO4	F	2505	5/5	0.94	0.09	-0.75	64,65,71,72	0
3	SO4	E	2501	5/5	0.93	0.08	-1.12	79,81,81,84	0
3	SO4	G	2508	5/5	0.89	0.23	-	84,85,88,89	0
3	SO4	H	2511	5/5	0.95	0.22	-	75,79,83,83	0
3	SO4	B	2486	5/5	0.95	0.16	-	87,90,90,92	0
3	SO4	A	2483	5/5	0.80	0.31	-	88,92,93,95	0
3	SO4	B	2487	5/5	0.91	0.25	-	89,91,92,92	0
3	SO4	C	2491	5/5	0.83	0.24	-	86,89,92,92	0
3	SO4	A	2484	5/5	0.92	0.13	-	77,78,79,81	0
3	SO4	H	2510	5/5	0.83	0.18	-	93,93,95,96	0
3	SO4	D	2495	5/5	0.84	0.23	-	83,86,87,87	0
3	SO4	G	2507	5/5	0.92	0.16	-	87,87,89,91	0
3	SO4	G	2506	5/5	0.94	0.12	-	79,80,81,81	0
3	SO4	D	2496	5/5	0.96	0.11	-	74,74,76,79	0
3	SO4	C	2492	5/5	0.97	0.14	-	86,88,88,88	0
3	SO4	I	2515	5/5	0.93	0.25	-	94,94,97,97	0
3	SO4	H	2512	5/5	0.96	0.16	-	58,60,64,69	0
3	SO4	J	2518	5/5	0.87	0.25	-	93,95,96,96	0
3	SO4	B	2488	5/5	0.89	0.28	-	92,93,94,97	0
3	SO4	F	2503	5/5	0.89	0.26	-	80,81,83,84	0
3	SO4	E	2500	5/5	0.93	0.22	-	83,83,85,87	0
3	SO4	J	2519	5/5	0.93	0.21	-	86,86,88,89	0
3	SO4	E	2498	5/5	0.93	0.14	-	77,81,81,85	0
3	SO4	A	2482	5/5	0.94	0.13	-	74,79,83,83	0
3	SO4	E	2499	5/5	0.90	0.26	-	85,87,89,90	0
3	SO4	F	2504	5/5	0.94	0.23	-	76,76,80,80	0

6.5 Other polymers ⓘ

There are no such residues in this entry.