



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:38 AM GMT

PDB ID : 2RHS  
Title : PheRS from Staphylococcus haemolyticus- rational protein engineering and inhibitor studies  
Authors : Evdokimov, A.G.; Mekel, M.  
Deposited on : 2007-10-09  
Resolution : 2.20 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](mailto: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.

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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

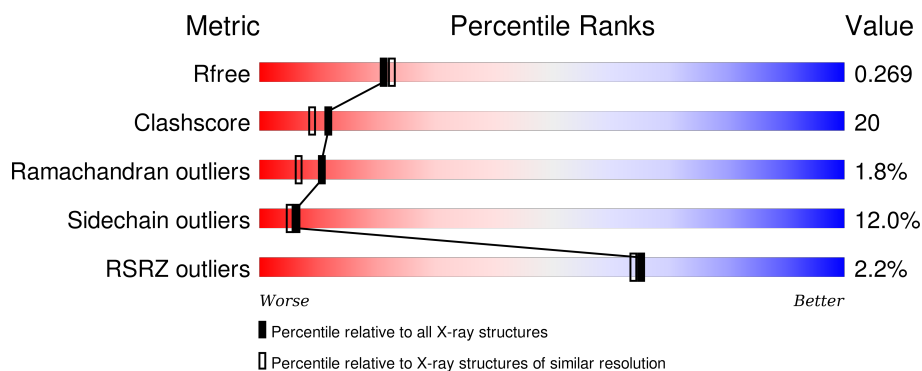
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

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  $\geq 3$ , 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	294	<div> <div>54%</div> <div>28%</div> <div>•</div> <div>15%</div> </div>
1	C	294	<div> <div>%</div> <div>59%</div> <div>28%</div> <div>5%</div> <div>•</div> <div>8%</div> </div>
2	B	800	<div> <div>%</div> <div>68%</div> <div>26%</div> <div>5%</div> <div>•</div> </div>
2	D	800	<div> <div>5%</div> <div>55%</div> <div>33%</div> <div>10%</div> <div>••</div> </div>

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 17461 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 Phenylalanyl-tRNA synthetase alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	249	Total	C	N	O	S	0	3	0
			2006	1270	337	389	10			
1	C	271	Total	C	N	O	S	0	4	0
			2181	1381	367	418	15			

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	58	MET	-	EXPRESSION TAG	UNP Q4L5E3
A	59	GLY	-	EXPRESSION TAG	UNP Q4L5E3
A	60	SER	-	EXPRESSION TAG	UNP Q4L5E3
A	61	SER	-	EXPRESSION TAG	UNP Q4L5E3
A	62	HIS	-	EXPRESSION TAG	UNP Q4L5E3
A	63	HIS	-	EXPRESSION TAG	UNP Q4L5E3
A	64	HIS	-	EXPRESSION TAG	UNP Q4L5E3
A	65	HIS	-	EXPRESSION TAG	UNP Q4L5E3
A	66	HIS	-	EXPRESSION TAG	UNP Q4L5E3
A	67	HIS	-	EXPRESSION TAG	UNP Q4L5E3
A	68	SER	-	EXPRESSION TAG	UNP Q4L5E3
A	69	SER	-	EXPRESSION TAG	UNP Q4L5E3
A	70	GLY	-	EXPRESSION TAG	UNP Q4L5E3
A	71	LEU	-	EXPRESSION TAG	UNP Q4L5E3
A	72	VAL	-	EXPRESSION TAG	UNP Q4L5E3
A	73	PRO	-	EXPRESSION TAG	UNP Q4L5E3
A	74	ARG	-	EXPRESSION TAG	UNP Q4L5E3
A	75	GLY	-	EXPRESSION TAG	UNP Q4L5E3
A	76	SER	-	EXPRESSION TAG	UNP Q4L5E3
A	77	HIS	-	EXPRESSION TAG	UNP Q4L5E3
A	78	MET	-	EXPRESSION TAG	UNP Q4L5E3
A	79	GLY	-	EXPRESSION TAG	UNP Q4L5E3
A	80	THR	-	EXPRESSION TAG	UNP Q4L5E3
A	81	GLU	-	EXPRESSION TAG	UNP Q4L5E3
A	82	LEU	-	EXPRESSION TAG	UNP Q4L5E3

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Chain	Residue	Modelled	Actual	Comment	Reference
A	83	MET	-	EXPRESSION TAG	UNP Q4L5E3
C	58	MET	-	EXPRESSION TAG	UNP Q4L5E3
C	59	GLY	-	EXPRESSION TAG	UNP Q4L5E3
C	60	SER	-	EXPRESSION TAG	UNP Q4L5E3
C	61	SER	-	EXPRESSION TAG	UNP Q4L5E3
C	62	HIS	-	EXPRESSION TAG	UNP Q4L5E3
C	63	HIS	-	EXPRESSION TAG	UNP Q4L5E3
C	64	HIS	-	EXPRESSION TAG	UNP Q4L5E3
C	65	HIS	-	EXPRESSION TAG	UNP Q4L5E3
C	66	HIS	-	EXPRESSION TAG	UNP Q4L5E3
C	67	HIS	-	EXPRESSION TAG	UNP Q4L5E3
C	68	SER	-	EXPRESSION TAG	UNP Q4L5E3
C	69	SER	-	EXPRESSION TAG	UNP Q4L5E3
C	70	GLY	-	EXPRESSION TAG	UNP Q4L5E3
C	71	LEU	-	EXPRESSION TAG	UNP Q4L5E3
C	72	VAL	-	EXPRESSION TAG	UNP Q4L5E3
C	73	PRO	-	EXPRESSION TAG	UNP Q4L5E3
C	74	ARG	-	EXPRESSION TAG	UNP Q4L5E3
C	75	GLY	-	EXPRESSION TAG	UNP Q4L5E3
C	76	SER	-	EXPRESSION TAG	UNP Q4L5E3
C	77	HIS	-	EXPRESSION TAG	UNP Q4L5E3
C	78	MET	-	EXPRESSION TAG	UNP Q4L5E3
C	79	GLY	-	EXPRESSION TAG	UNP Q4L5E3
C	80	THR	-	EXPRESSION TAG	UNP Q4L5E3
C	81	GLU	-	EXPRESSION TAG	UNP Q4L5E3
C	82	LEU	-	EXPRESSION TAG	UNP Q4L5E3
C	83	MET	-	EXPRESSION TAG	UNP Q4L5E3

- Molecule 2 is a protein called Phenylalanyl-tRNA synthetase beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	786	Total	C	N	O	S	0	3	0
			6141	3864	1037	1223	17			
2	D	785	Total	C	N	O	S	0	2	0
			6116	3846	1031	1222	17			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	34	ASN	ASP	ENGINEERED	UNP Q4L5E4
B	144	PRO	GLN	ENGINEERED	UNP Q4L5E4
B	661	GLY	GLU	ENGINEERED	UNP Q4L5E4

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Chain	Residue	Modelled	Actual	Comment	Reference
B	663	ALA	GLN	ENGINEERED	UNP Q4L5E4
B	664	GLY	ASP	ENGINEERED	UNP Q4L5E4
D	34	ASN	ASP	ENGINEERED	UNP Q4L5E4
D	144	PRO	GLN	ENGINEERED	UNP Q4L5E4
D	661	GLY	GLU	ENGINEERED	UNP Q4L5E4
D	663	ALA	GLN	ENGINEERED	UNP Q4L5E4
D	664	GLY	ASP	ENGINEERED	UNP Q4L5E4

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).

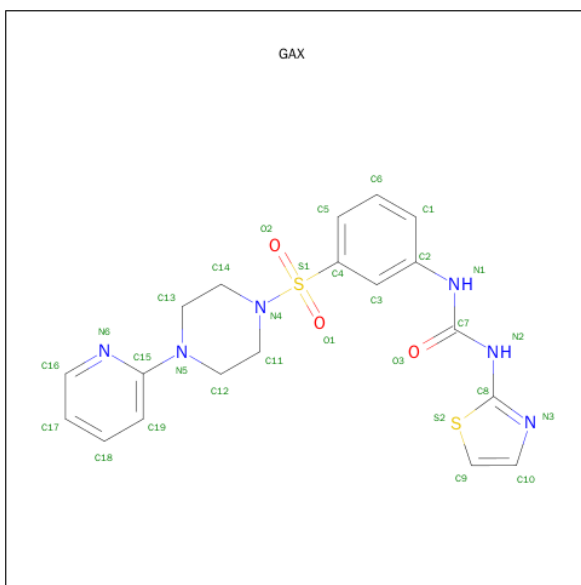


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	1	Total	Zn	0	0
			1	1		

- Molecule 5 is 1-{3-[(4-PYRIDIN-2-YLPIPERAZIN-1-YL)SULFONYL]PHENYL}-3-(1,3-T HIAZOL-2-YL)UREA (three-letter code: GAX) (formula: C<sub>19</sub>H<sub>20</sub>N<sub>6</sub>O<sub>3</sub>S<sub>2</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total 30	C 19	N 6	O 3	S 2	0	0
5	C	1	Total 30	C 19	N 6	O 3	S 2	0	0

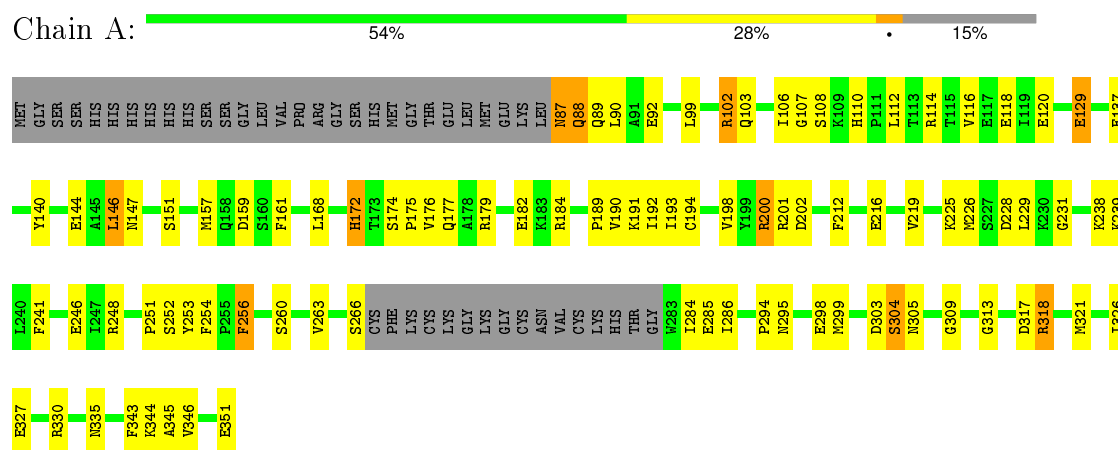
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	110	Total O 110 110	0	0
6	B	403	Total O 403 403	0	0
6	C	119	Total O 119 119	0	0
6	D	314	Total O 314 314	0	0

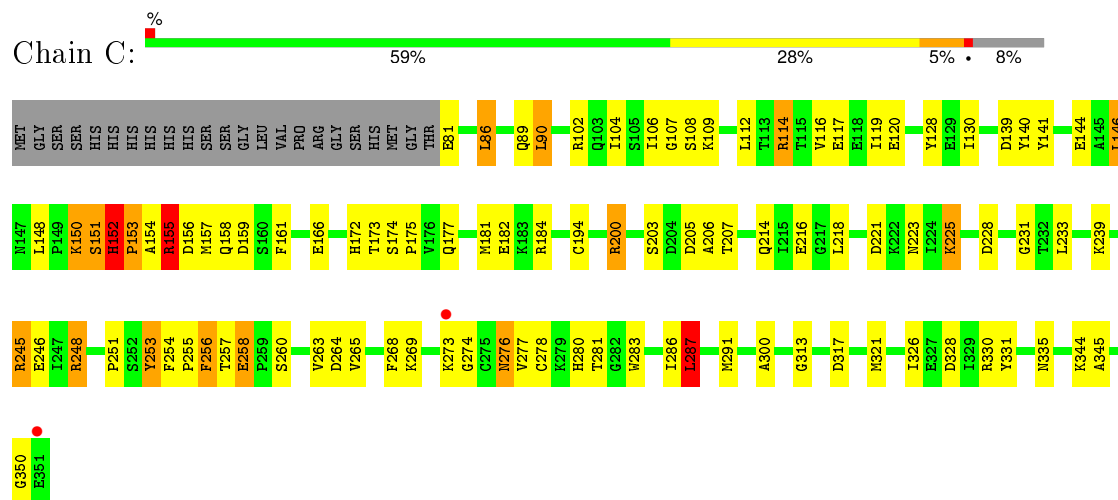
### 3 Residue-property plots

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.

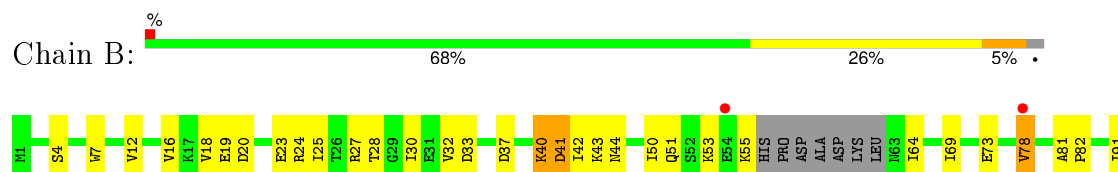
#### • Molecule 1: Phenylalanyl-tRNA synthetase alpha chain

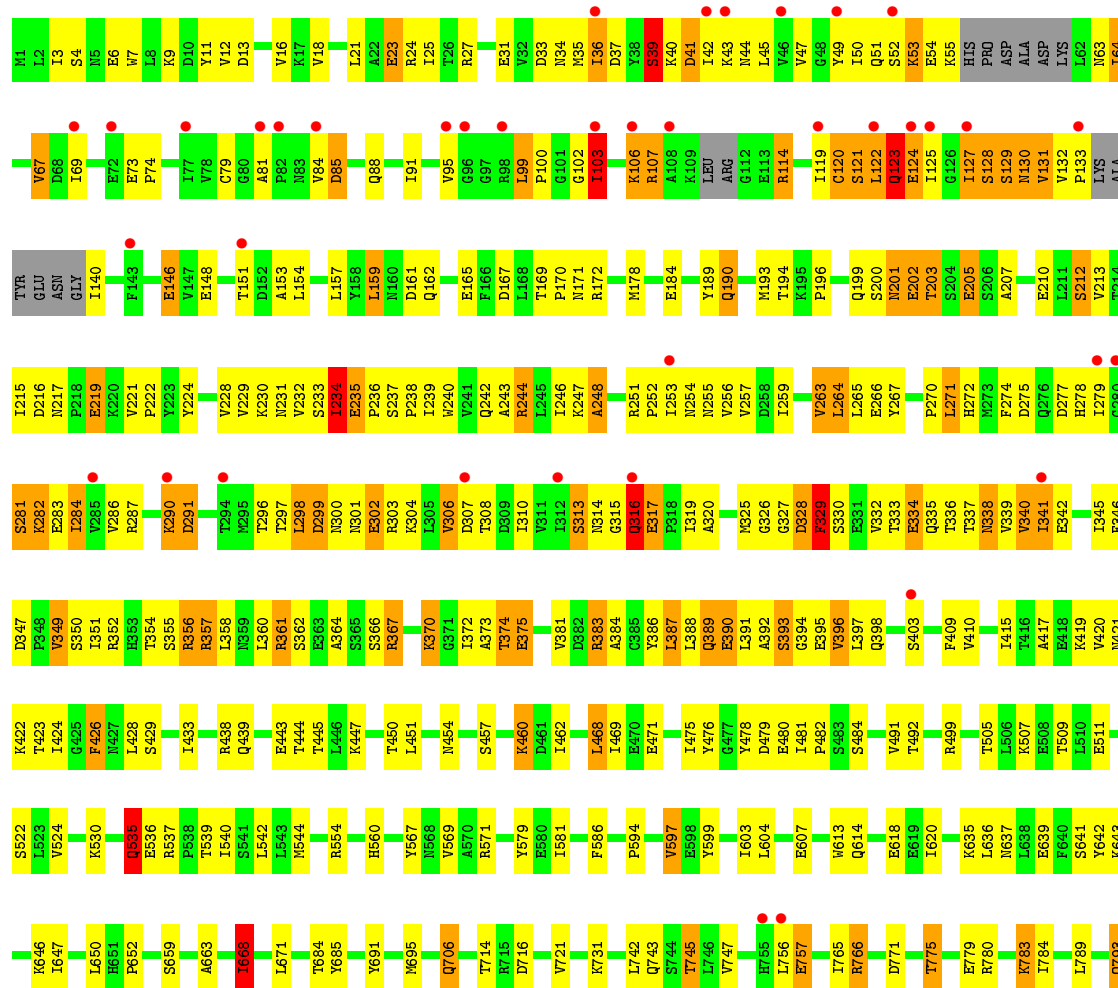


#### • Molecule 1: Phenylalanyl-tRNA synthetase alpha chain



#### • Molecule 2: Phenylalanyl-tRNA synthetase beta chain









## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	60.71Å 87.86Å 234.04Å 90.00° 90.59° 90.00°	Depositor
Resolution (Å)	57.30 – 2.20 49.95 – 2.20	Depositor EDS
% Data completeness (in resolution range)	89.3 (57.30-2.20) 89.3 (49.95-2.20)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.02 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.193 , 0.271 0.192 , 0.269	Depositor DCC
$R_{free}$ test set	5602 reflections (5.28%)	DCC
Wilson B-factor (Å <sup>2</sup> )	32.8	Xtriage
Anisotropy	0.127	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 47.0	EDS
Estimated twinning fraction	0.047 for h,-k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	1 of 111707 reflections (0.001%)	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	17461	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.14% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: ZN, SO4, GAX

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	0/2051	0.94	1/2771 (0.0%)
1	C	0.43	0/2233	0.88	2/3012 (0.1%)
2	B	0.43	0/6241	0.89	6/8452 (0.1%)
2	D	0.39	0/6212	0.81	3/8415 (0.0%)
All	All	0.42	0/16737	0.87	12/22650 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	3
2	B	0	4
2	D	0	7
All	All	0	14

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	330	ARG	NE-CZ-NH1	-6.27	117.16	120.30
2	B	504	ARG	NE-CZ-NH2	-6.08	117.26	120.30
2	D	742	LEU	CA-CB-CG	-6.04	101.40	115.30
2	B	400	ARG	NE-CZ-NH2	-5.97	117.32	120.30
2	B	504	ARG	NE-CZ-NH1	5.85	123.23	120.30
2	B	554	ARG	NE-CZ-NH1	-5.74	117.43	120.30
2	B	742	LEU	CB-CG-CD2	-5.58	101.51	111.00
2	B	742	LEU	CA-CB-CG	-5.38	102.93	115.30
1	C	152	HIS	N-CA-C	5.24	125.13	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	668	ILE	CB-CA-C	-5.21	101.19	111.60
2	D	668	ILE	N-CA-C	-5.21	96.95	111.00
1	C	221	ASP	CB-CG-OD1	5.20	122.98	118.30

There are no chirality outliers.

All (14) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	298	LEU	Peptide
2	B	534	LEU	Peptide
2	B	740	ASP	Peptide
2	B	752	GLU	Peptide
1	C	273	LYS	Peptide
1	C	287	LEU	Peptide
1	C	335	ASN	Peptide
2	D	102	GLY	Peptide
2	D	120	CYS	Peptide
2	D	122	LEU	Peptide
2	D	123	GLN	Peptide
2	D	372	ILE	Peptide
2	D	535	GLN	Peptide
2	D	67	VAL	Peptide

## 5.2 Too-close contacts [i](#)

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	2006	0	1949	66	0
1	C	2181	0	2130	96	0
2	B	6141	0	6121	188	0
2	D	6116	0	6088	349	0
3	B	5	0	0	0	0
3	D	5	0	0	1	0
4	C	1	0	0	0	0
5	A	30	0	20	2	0
5	C	30	0	20	3	0
6	A	110	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	403	0	0	17	0
6	C	119	0	0	5	0
6	D	314	0	0	9	0
All	All	17461	0	16328	663	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 20.

All (663) 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)
2:D:91:ILE:CD1	2:D:153:ALA:HB1	1.74	1.17
2:B:424:ILE:HD11	2:B:469:ILE:HG23	1.26	1.15
1:A:87:ASN:HD22	1:A:87:ASN:N	1.44	1.14
2:D:53:LYS:HB3	2:D:53:LYS:NZ	1.65	1.11
2:B:464:ILE:HG13	2:B:466:GLU:HG2	1.22	1.10
2:D:21:LEU:O	2:D:25:ILE:HG13	1.55	1.06
2:D:367:ARG:HH11	2:D:367:ARG:HG3	1.17	1.05
2:B:333:THR:H	2:B:336:THR:CG2	1.69	1.05
2:D:279:ILE:HD11	2:D:340:VAL:HG11	1.37	1.04
2:D:99:LEU:HD11	2:D:103:ILE:HB	1.00	0.99
2:D:91:ILE:HD13	2:D:153:ALA:HB1	1.42	0.99
2:B:534:LEU:N	2:B:535:GLN:HB2	1.78	0.98
2:D:99:LEU:CD1	2:D:103:ILE:HB	1.93	0.97
2:D:259:ILE:O	2:D:263:VAL:HG23	1.65	0.95
2:D:325:MET:HG3	2:D:326:GLY:H	1.27	0.94
2:B:424:ILE:HD11	2:B:469:ILE:CG2	1.97	0.94
1:A:146:LEU:HD11	1:A:174:SER:CB	1.98	0.93
2:D:235:GLU:HB2	2:D:236:PRO:CD	1.99	0.93
2:D:129:SER:O	2:D:131:VAL:N	2.01	0.93
2:D:99:LEU:HD11	2:D:103:ILE:CB	1.96	0.93
2:D:264:LEU:HD22	2:D:270:PRO:HA	1.51	0.91
2:B:464:ILE:CG1	2:B:466:GLU:HG2	2.01	0.90
2:D:283:GLU:HG2	2:D:314:ASN:O	1.69	0.90
2:B:98:ARG:HH11	2:B:98:ARG:HG3	1.33	0.90
2:D:34:ASN:ND2	2:D:165:GLU:OE1	2.04	0.89
2:D:40:LYS:O	2:D:41:ASP:HB2	1.68	0.89
2:D:53:LYS:HB3	2:D:53:LYS:HZ2	1.32	0.89
2:B:18:VAL:HG12	2:B:19:GLU:OE2	1.73	0.89
2:D:130:ASN:HA	2:D:251:ARG:NH1	1.88	0.88
2:B:332:VAL:HA	2:B:336:THR:HG21	1.55	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:346:PHE:HB3	2:D:351:ILE:HD11	1.56	0.88
1:C:251:PRO:HG3	2:D:478:TYR:CE2	2.09	0.88
1:C:86:LEU:CD1	1:C:90:LEU:HD22	2.04	0.87
2:D:36:ILE:HD12	2:D:37:ASP:N	1.88	0.87
2:D:230:LYS:O	2:D:395:GLU:HG2	1.74	0.87
1:A:87:ASN:N	1:A:87:ASN:ND2	2.21	0.86
2:B:299:ASP:O	2:B:300:ASN:HB2	1.73	0.86
2:D:346:PHE:CB	2:D:351:ILE:HD11	2.05	0.86
1:C:251:PRO:HG3	2:D:478:TYR:CD2	2.10	0.86
1:C:146:LEU:HD21	1:C:174:SER:HB3	1.57	0.86
2:D:279:ILE:CD1	2:D:340:VAL:HG11	2.06	0.85
1:C:214:GLN:HG3	6:C:410:HOH:O	1.75	0.85
2:D:127:ILE:CD1	2:D:132:VAL:HG21	2.06	0.84
1:A:146:LEU:HD11	1:A:174:SER:HB3	1.58	0.84
2:D:366:SER:O	2:D:370:LYS:HE3	1.76	0.84
2:B:466:GLU:HA	2:B:469:ILE:HD12	1.58	0.84
2:D:370:LYS:N	2:D:370:LYS:HD3	1.92	0.83
2:D:297:THR:HB	2:D:325:MET:HG2	1.60	0.83
2:D:389:GLN:HG2	2:D:390:GLU:OE1	1.78	0.83
2:D:6:GLU:OE1	2:D:247:LYS:NZ	2.12	0.82
2:D:297:THR:O	2:D:299:ASP:N	2.12	0.82
2:B:18:VAL:HG11	2:B:162:GLN:HG3	1.60	0.81
1:A:129:GLU:HG3	1:A:192:ILE:HG22	1.63	0.80
2:D:259:ILE:O	2:D:263:VAL:CG2	2.29	0.80
2:B:98:ARG:NH1	2:B:98:ARG:HG3	1.92	0.80
2:D:274:PHE:HB2	2:D:340:VAL:HG13	1.64	0.80
2:D:325:MET:HG3	2:D:326:GLY:N	1.97	0.79
2:D:361:ARG:HH12	2:D:366:SER:HB3	1.47	0.79
2:D:127:ILE:CD1	2:D:132:VAL:CG2	2.61	0.79
2:B:705:GLU:HG2	6:B:1166:HOH:O	1.82	0.79
2:B:424:ILE:CD1	2:B:469:ILE:HG23	2.11	0.78
2:D:235:GLU:HB2	2:D:236:PRO:HD3	1.65	0.78
2:D:91:ILE:HD12	2:D:153:ALA:HB1	1.64	0.77
2:B:698:ALA:HB1	1:C:350:GLY:HA2	1.66	0.77
2:D:314:ASN:OD1	2:D:317:GLU:HB2	1.85	0.77
2:D:130:ASN:HA	2:D:251:ARG:HH12	1.46	0.77
2:D:36:ILE:C	2:D:36:ILE:HD12	2.04	0.76
2:B:210:GLU:O	2:B:282:LYS:HG3	1.85	0.76
2:D:586:PHE:HE2	2:D:597:VAL:CG1	1.98	0.76
2:D:279:ILE:HD11	2:D:340:VAL:CG1	2.15	0.76
1:A:159:ASP:HB3	1:A:200:ARG:NH1	2.02	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:714:THR:HG21	2:D:766:ARG:HD2	1.68	0.75
2:D:731:LYS:HE3	2:D:745:THR:HG22	1.68	0.74
2:B:78:VAL:HG23	2:B:115:SER:HB2	1.68	0.74
1:A:176:VAL:HB	1:A:194[B]:CYS:SG	2.27	0.74
2:B:375:GLU:HB2	2:B:457:SER:OG	1.87	0.74
1:A:146:LEU:HD11	1:A:174:SER:HB2	1.69	0.74
2:D:299:ASP:HB2	2:D:325:MET:HE3	1.69	0.73
1:C:159:ASP:HA	1:C:200:ARG:HH11	1.54	0.73
2:D:264:LEU:CD2	2:D:270:PRO:HA	2.18	0.73
2:D:53:LYS:HB3	2:D:53:LYS:HZ3	1.48	0.72
2:B:429:SER:O	2:B:433:ILE:HG13	1.88	0.72
2:D:361:ARG:NH1	2:D:366:SER:HB3	2.04	0.72
2:D:438:ARG:NH2	2:D:444:THR:O	2.23	0.72
1:C:281:THR:HG22	1:C:283:TRP:H	1.55	0.72
2:B:341:ILE:HD11	2:B:388:LEU:HD12	1.73	0.71
2:B:123:GLN:HG3	2:B:132:VAL:HG21	1.71	0.71
2:D:522:SER:O	2:D:554:ARG:HG2	1.89	0.71
1:A:159:ASP:HB3	1:A:200:ARG:HH12	1.55	0.71
1:C:265:VAL:HG23	1:C:286:ILE:HG12	1.71	0.71
2:B:534:LEU:H	2:B:535:GLN:HB2	1.53	0.71
2:D:162:GLN:HG3	6:D:947:HOH:O	1.89	0.71
2:B:18:VAL:HG11	2:B:162:GLN:CG	2.20	0.71
2:D:37:ASP:O	2:D:40:LYS:HB3	1.91	0.70
2:D:230:LYS:HD2	2:D:397:LEU:HD11	1.72	0.70
2:B:335:GLN:HG3	6:B:1117:HOH:O	1.91	0.70
2:D:255:ASN:ND2	2:D:392:ALA:HB2	2.06	0.70
1:C:205:ASP:HA	1:C:330:ARG:NH1	2.06	0.70
2:D:328:ASP:O	2:D:329:PHE:HB3	1.89	0.69
2:D:229:VAL:HG13	2:D:339:VAL:HG22	1.72	0.69
2:B:40:LYS:O	2:B:41:ASP:HB2	1.91	0.69
2:D:290:LYS:NZ	2:D:291:ASP:HB2	2.07	0.69
1:C:148:LEU:HD11	1:C:255:PRO:HG2	1.75	0.68
2:D:277:ASP:OD2	2:D:338:ASN:ND2	2.26	0.68
2:D:127:ILE:HD12	2:D:132:VAL:CG2	2.22	0.68
2:D:37:ASP:OD1	2:D:162:GLN:HG2	1.93	0.68
2:D:374:THR:HG23	2:D:409:PHE:CE2	2.29	0.68
2:B:777:THR:OG1	2:B:780:ARG:HB2	1.94	0.68
2:D:410:VAL:CG1	2:D:454:ASN:HB3	2.24	0.67
2:B:749:ASP:OD2	6:B:1201:HOH:O	2.11	0.67
1:C:184:ARG:HD2	6:C:415:HOH:O	1.93	0.67
1:C:154:ALA:C	1:C:156:ASP:H	1.98	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:131:VAL:HA	2:D:251:ARG:HB2	1.76	0.67
2:D:127:ILE:HD12	2:D:132:VAL:HB	1.76	0.67
2:D:358:LEU:O	2:D:360:LEU:HG	1.95	0.67
2:B:333:THR:N	2:B:336:THR:CG2	2.52	0.67
2:B:289:ALA:O	2:B:307:ASP:HA	1.95	0.67
2:D:317:GLU:O	2:D:319:ILE:HG23	1.95	0.66
2:D:9:LYS:HA	2:D:12:VAL:O	1.94	0.66
2:D:216:ASP:HB2	2:D:287:ARG:HB3	1.77	0.66
2:D:35:MET:HB3	6:D:1059:HOH:O	1.94	0.66
2:D:367:ARG:HH11	2:D:367:ARG:CG	2.00	0.66
2:B:299:ASP:O	2:B:300:ASN:CB	2.44	0.66
2:B:275:ASP:OD1	2:B:336:THR:HB	1.94	0.66
2:D:196:PRO:HD2	2:D:267:TYR:OH	1.95	0.66
2:D:313:SER:HA	2:D:317:GLU:O	1.95	0.66
2:D:314:ASN:CG	2:D:317:GLU:HB2	2.15	0.66
2:D:731:LYS:HE3	2:D:745:THR:CG2	2.25	0.66
2:B:424:ILE:CG2	2:B:481:ILE:HD12	2.25	0.66
2:D:73:GLU:HG3	2:D:74:PRO:HD2	1.76	0.66
2:D:793:GLN:OE1	2:D:799:ILE:HG12	1.96	0.66
2:B:44:ASN:HB3	2:B:94:LYS:HB2	1.79	0.65
2:D:40:LYS:O	2:D:41:ASP:CB	2.44	0.65
1:C:245:ARG:HG3	1:C:265:VAL:CG1	2.26	0.65
2:D:421:ASN:HB3	2:D:426:PHE:O	1.96	0.65
2:B:322:ALA:HB1	2:B:346:PHE:CE1	2.31	0.65
2:D:299:ASP:OD2	2:D:303:ARG:NH2	2.30	0.65
2:D:716:ASP:OD1	2:D:766:ARG:HD3	1.96	0.65
2:D:410:VAL:HG11	2:D:454:ASN:HB3	1.78	0.65
2:B:534:LEU:HB2	2:B:535:GLN:HG2	1.79	0.64
2:B:98:ARG:HH11	2:B:98:ARG:CG	2.07	0.64
2:D:148:GLU:O	2:D:151:THR:OG1	2.12	0.64
2:D:50:ILE:HG12	2:D:67:VAL:HG22	1.79	0.64
2:D:367:ARG:NH1	2:D:367:ARG:HG3	1.97	0.64
1:A:174:SER:N	1:A:216:GLU:OE2	2.30	0.64
1:C:278:CYS:O	1:C:281:THR:HB	1.97	0.64
2:D:233:SER:O	2:D:235:GLU:HG2	1.97	0.64
2:B:43:LYS:HG2	2:B:98:ARG:HB2	1.79	0.64
2:D:375:GLU:HB2	2:D:457:SER:OG	1.97	0.64
2:D:386:TYR:O	2:D:389:GLN:HB3	1.99	0.63
2:B:333:THR:H	2:B:336:THR:HG23	1.59	0.63
2:D:424:ILE:HG23	2:D:481:ILE:HG12	1.80	0.63
2:D:586:PHE:CE2	2:D:597:VAL:CG1	2.82	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:341:ILE:HD11	2:B:388:LEU:CD1	2.27	0.63
1:A:106:ILE:HG22	1:A:107:GLY:O	1.98	0.63
2:B:33:ASP:OD1	2:B:167:ASP:HB2	1.98	0.63
2:D:43:LYS:HG2	2:D:44:ASN:HD22	1.63	0.63
2:D:122:LEU:O	2:D:127:ILE:HG12	1.99	0.62
1:C:106:ILE:O	1:C:344:LYS:HE2	1.98	0.62
2:B:234:ILE:HD13	2:B:333:THR:O	2.00	0.62
2:D:234:ILE:HG21	2:D:334:GLU:HB3	1.80	0.62
1:A:298:GLU:OE2	1:A:304:SER:OG	2.16	0.62
2:B:366:SER:O	2:B:370:LYS:HD2	2.00	0.62
2:D:714:THR:CG2	2:D:766:ARG:HD2	2.29	0.62
2:D:357:ARG:HB3	2:D:357:ARG:HH11	1.65	0.62
2:D:299:ASP:HB3	2:D:301:ASN:H	1.64	0.62
2:D:45:LEU:HD11	2:D:91:ILE:CG2	2.30	0.61
2:D:53:LYS:HD2	2:D:63:ASN:HB3	1.81	0.61
2:B:78:VAL:HG23	2:B:115:SER:CB	2.30	0.61
2:B:616:LYS:NZ	2:D:618:GLU:OE2	2.25	0.61
2:D:267:TYR:HE2	2:D:383:ARG:HG3	1.64	0.61
2:B:418:GLU:O	2:B:422:LYS:HB2	2.01	0.61
2:D:219[B]:GLU:CD	2:D:219[B]:GLU:H	2.04	0.61
2:B:333:THR:O	2:B:336:THR:HG23	2.01	0.61
2:D:212:SER:O	2:D:284:ILE:N	2.29	0.61
1:A:175:PRO:O	1:A:179:ARG:HG3	2.00	0.61
2:B:264:LEU:HD11	2:B:367:ARG:HD2	1.81	0.61
2:D:278:HIS:O	2:D:330:SER:HA	2.01	0.60
2:B:53:LYS:HA	2:B:64:ILE:O	2.01	0.60
2:D:328:ASP:O	2:D:329:PHE:CB	2.49	0.60
2:D:374:THR:HG23	2:D:409:PHE:HE2	1.66	0.60
1:C:141:TYR:O	1:C:146:LEU:HD12	2.01	0.60
2:D:586:PHE:HE2	2:D:597:VAL:HG13	1.64	0.60
2:B:392:ALA:O	2:B:393:SER:HB2	2.00	0.60
2:B:741:ILE:O	2:B:769:TYR:HA	2.01	0.60
1:A:99:LEU:HD22	2:D:747:VAL:HG21	1.84	0.60
2:D:540:ILE:HD11	2:D:594:PRO:HB3	1.82	0.60
2:D:231:ASN:N	2:D:337:THR:O	2.34	0.59
1:C:148:LEU:O	1:C:155:ARG:NH1	2.34	0.59
2:D:283:GLU:CG	2:D:314:ASN:O	2.48	0.59
1:C:177:GLN:HG2	1:C:194[A]:CYS:SG	2.43	0.59
2:D:314:ASN:ND2	2:D:317:GLU:HB2	2.16	0.59
2:D:352:ARG:O	2:D:356:ARG:HB2	2.02	0.59
1:C:251:PRO:CG	2:D:478:TYR:CE2	2.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:691:TYR:OH	2:D:695:MET:HE1	2.03	0.59
2:B:91:ILE:HD11	2:B:157:LEU:HD11	1.83	0.59
1:C:269:LYS:HG3	1:C:277:VAL:HG21	1.84	0.59
2:D:255:ASN:HD21	2:D:392:ALA:HB2	1.66	0.59
2:D:127:ILE:HD12	2:D:132:VAL:CB	2.32	0.59
2:B:589:GLY:O	2:B:592:GLU:HG3	2.02	0.58
2:B:352:ARG:O	2:B:356:ARG:HG3	2.03	0.58
2:D:297:THR:O	2:D:300:ASN:N	2.36	0.58
2:D:85:ASP:H	2:D:88:GLN:CD	2.06	0.58
2:D:333:THR:O	2:D:336:THR:HG23	2.03	0.58
2:D:91:ILE:HD13	2:D:153:ALA:CB	2.26	0.58
2:B:771:ASP:HB3	2:B:776:LEU:HD13	1.85	0.58
2:D:54:GLU:C	2:D:55:LYS:CG	2.72	0.58
2:D:84:VAL:HA	2:D:88:GLN:HE22	1.69	0.58
2:D:254:ASN:ND2	2:D:257:VAL:HG23	2.18	0.58
5:C:2:GAX:S2	5:C:2:GAX:O3	2.62	0.58
2:D:315:GLY:O	2:D:316:GLN:HB2	2.04	0.57
2:D:524:VAL:HG12	2:D:560:HIS:CE1	2.39	0.57
2:D:793:GLN:OE1	2:D:799:ILE:CD1	2.52	0.57
2:B:786:ASP:O	2:B:790:GLU:HG3	2.04	0.57
2:D:272:HIS:HB3	2:D:342:GLU:HB3	1.87	0.57
2:D:146:GLU:HG3	2:D:146:GLU:O	2.04	0.57
2:D:647:ILE:HB	2:D:650:LEU:HD12	1.85	0.57
1:A:99:LEU:CD2	2:D:747:VAL:HG21	2.34	0.57
2:B:714:THR:HG22	6:B:934:HOH:O	2.03	0.57
1:C:253[A]:TYR:CD2	2:D:171:ASN:OD1	2.58	0.57
2:D:264:LEU:HD22	2:D:270:PRO:CA	2.30	0.57
2:B:447:LYS:HG3	6:B:1008:HOH:O	2.03	0.57
2:D:346:PHE:HB2	2:D:351:ILE:HD11	1.86	0.57
1:C:161:PHE:CD1	2:D:542:LEU:HD13	2.40	0.57
2:D:39:SER:O	2:D:39:SER:OG	2.20	0.57
2:D:200:SER:HB2	2:D:396:VAL:HG11	1.87	0.57
2:D:264:LEU:HD11	2:D:367:ARG:HD2	1.86	0.57
2:B:333:THR:H	2:B:336:THR:HG22	1.63	0.57
1:C:114:ARG:HB3	1:C:114:ARG:HH21	1.68	0.57
1:C:181:MET:HG3	1:C:218:LEU:HD21	1.86	0.57
1:C:116:VAL:O	1:C:120:GLU:HG3	2.04	0.57
2:B:628:VAL:O	2:B:632:VAL:HG23	2.05	0.57
2:D:36:ILE:CD1	2:D:36:ILE:C	2.68	0.56
2:B:444:THR:HA	2:B:452:THR:O	2.05	0.56
1:A:176:VAL:CB	1:A:194[B]:CYS:SG	2.93	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:506:LEU:HD11	2:B:632:VAL:HG13	1.87	0.56
2:D:95:VAL:HG11	2:D:107:ARG:HG2	1.85	0.56
2:D:207:ALA:HA	2:D:210:GLU:HG3	1.86	0.56
1:A:285:GLU:O	1:A:318:ARG:NH2	2.39	0.56
2:D:235:GLU:HB2	2:D:236:PRO:HD2	1.86	0.56
2:D:49:TYR:H	2:D:67:VAL:HG13	1.71	0.56
2:D:132:VAL:O	2:D:251:ARG:HD2	2.05	0.56
2:D:444:THR:CG2	2:D:451:LEU:HD22	2.35	0.56
1:C:254:PHE:CD2	1:C:260:SER:HB3	2.40	0.56
2:D:428:LEU:HD21	2:D:476:TYR:CE1	2.41	0.56
2:B:420:VAL:O	2:B:424:ILE:HD12	2.06	0.56
2:B:464:ILE:HG12	2:B:467:ASP:CG	2.26	0.56
2:B:42:ILE:HA	2:B:98:ARG:O	2.06	0.56
2:D:392:ALA:O	2:D:394:GLY:N	2.39	0.56
2:D:691:TYR:CE1	2:D:695:MET:HE2	2.41	0.56
2:D:95:VAL:HG13	2:D:106:LYS:HA	1.88	0.56
2:B:742:LEU:HD11	2:B:767:LEU:HB3	1.88	0.56
1:C:251:PRO:HG3	2:D:478:TYR:HE2	1.65	0.56
2:D:100:PRO:HG3	2:D:125:ILE:O	2.06	0.56
1:C:159:ASP:HA	1:C:200:ARG:NH1	2.19	0.56
2:B:414:ASP:OD1	2:B:452:THR:HG23	2.06	0.56
2:D:239:ILE:HD12	2:D:242:GLN:HB2	1.88	0.56
2:D:33:ASP:OD2	2:D:167:ASP:HB2	2.06	0.55
2:B:780:ARG:HG3	2:B:780:ARG:HH11	1.71	0.55
2:B:335:GLN:CG	6:B:1117:HOH:O	2.53	0.55
2:D:297:THR:C	2:D:299:ASP:N	2.58	0.55
2:D:91:ILE:CD1	2:D:157:LEU:HD11	2.36	0.55
2:D:505:THR:HG22	2:D:635:LYS:HD3	1.87	0.55
1:A:90:LEU:HD22	2:D:652:PRO:HD2	1.89	0.55
2:D:275:ASP:OD1	2:D:336:THR:HG22	2.05	0.55
1:A:177:GLN:HG2	1:A:194[A]:CYS:SG	2.47	0.55
2:B:190:GLN:HG3	6:B:1180:HOH:O	2.06	0.55
2:D:157:LEU:HB3	2:D:159:LEU:HD12	1.88	0.55
2:B:264:LEU:HD11	2:B:367:ARG:CD	2.36	0.55
1:C:146:LEU:CD2	1:C:174:SER:HB3	2.32	0.55
1:C:251:PRO:HG3	2:D:478:TYR:HD2	1.66	0.55
2:D:297:THR:C	2:D:299:ASP:H	2.11	0.54
1:C:139:ASP:OD2	1:C:140:TYR:N	2.41	0.54
2:D:290:LYS:HZ1	2:D:291:ASP:HB2	1.70	0.54
1:C:106:ILE:HG22	1:C:107:GLY:O	2.08	0.54
2:D:298:LEU:HD23	6:D:1026:HOH:O	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:267:TYR:CE2	2:D:383:ARG:HG3	2.42	0.54
2:D:121:SER:HB3	2:D:124:GLU:HG3	1.89	0.54
2:D:255:ASN:HD21	2:D:392:ALA:CB	2.21	0.54
2:D:264:LEU:CD1	2:D:367:ARG:HD2	2.39	0.53
2:D:266:GLU:OE2	2:D:383:ARG:HD2	2.08	0.53
2:B:589:GLY:O	2:B:590:GLU:HB2	2.06	0.53
2:D:132:VAL:O	2:D:251:ARG:CD	2.56	0.53
1:C:268:PHE:CE1	1:C:269:LYS:HD3	2.44	0.53
2:B:361:ARG:HB3	2:B:361:ARG:CZ	2.37	0.53
2:D:731:LYS:HG2	2:D:745:THR:CG2	2.39	0.53
1:C:245:ARG:HG3	1:C:265:VAL:HG11	1.90	0.53
2:D:374:THR:CG2	2:D:409:PHE:CE2	2.91	0.53
2:D:47:VAL:HG23	2:D:151:THR:HB	1.91	0.53
2:D:127:ILE:HD13	2:D:132:VAL:CG2	2.37	0.53
1:C:114:ARG:NH1	1:C:345:ALA:O	2.42	0.53
2:D:635:LYS:HG3	2:D:635:LYS:O	2.09	0.53
1:C:173:THR:OG1	1:C:216:GLU:HG3	2.09	0.53
2:D:793:GLN:OE1	2:D:799:ILE:CG1	2.57	0.52
1:A:140:TYR:HA	1:A:144:GLU:HB3	1.90	0.52
1:A:241:PHE:HE2	1:A:286:ILE:HD13	1.72	0.52
2:D:122:LEU:HD23	2:D:127:ILE:HD13	1.91	0.52
6:C:467:HOH:O	2:D:492:THR:HG23	2.09	0.52
2:B:25:ILE:CG2	2:B:30:ILE:HB	2.40	0.52
2:D:215:ILE:HG22	2:D:217:ASN:H	1.74	0.52
1:A:146:LEU:HD12	1:A:172:HIS:CE1	2.45	0.52
2:D:424:ILE:CG2	2:D:481:ILE:HG12	2.39	0.52
2:B:40:LYS:O	2:B:41:ASP:CB	2.56	0.52
2:D:290:LYS:HG3	2:D:291:ASP:N	2.24	0.52
2:D:259:ILE:HD12	2:D:388:LEU:HD23	1.92	0.52
2:D:49:TYR:N	2:D:67:VAL:HG13	2.24	0.52
1:C:276:ASN:H	1:C:276:ASN:HD22	1.58	0.52
2:D:85:ASP:O	2:D:88:GLN:OE1	2.28	0.52
2:D:235:GLU:CB	2:D:236:PRO:CD	2.78	0.52
1:A:107:GLY:HA3	2:B:515:LEU:O	2.10	0.52
2:D:259:ILE:HD13	2:D:387:LEU:HB3	1.92	0.51
1:C:117:GLU:OE1	2:D:507:LYS:NZ	2.42	0.51
1:C:251:PRO:CB	2:D:478:TYR:HE2	2.22	0.51
2:D:263:VAL:HG11	2:D:383:ARG:HB3	1.93	0.51
2:D:54:GLU:HB2	2:D:64:ILE:HB	1.93	0.51
1:C:276:ASN:H	1:C:276:ASN:ND2	2.08	0.51
1:C:231:GLY:HA3	2:D:484:SER:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:42:ILE:HD11	2:D:100:PRO:HD2	1.93	0.51
2:D:127:ILE:HD12	2:D:132:VAL:HG21	1.84	0.51
2:D:367:ARG:NH1	2:D:367:ARG:CG	2.66	0.51
1:C:263:VAL:HB	1:C:287:LEU:HB2	1.91	0.51
1:A:345:ALA:HB1	2:D:637:ASN:HB2	1.93	0.51
1:C:251:PRO:CG	2:D:478:TYR:CD2	2.89	0.51
1:C:152:HIS:CE1	1:C:153:PRO:HG2	2.45	0.51
2:B:506:LEU:HD23	2:B:581:ILE:HD11	1.93	0.51
2:B:276:GLN:HB2	2:B:340:VAL:HG23	1.92	0.51
2:B:224:TYR:O	2:B:402:SER:HA	2.11	0.51
1:C:154:ALA:C	1:C:156:ASP:N	2.64	0.51
2:B:723:HIS:HA	2:B:761:LYS:HG2	1.93	0.51
2:D:224:TYR:OH	2:D:342:GLU:OE2	2.20	0.51
2:D:202:GLU:OE1	2:D:398:GLN:HG2	2.11	0.51
2:D:132:VAL:HG22	2:D:133:PRO:HD2	1.92	0.50
2:D:233:SER:O	2:D:234:ILE:C	2.48	0.50
2:B:634:GLU:HG2	1:C:106:ILE:HD12	1.92	0.50
1:C:114:ARG:CB	1:C:114:ARG:HH21	2.24	0.50
1:A:321:MET:HA	1:A:326:ILE:HB	1.93	0.50
2:D:586:PHE:HE2	2:D:597:VAL:HG11	1.75	0.50
2:D:793:GLN:OE1	2:D:799:ILE:HD11	2.12	0.50
2:D:255:ASN:ND2	2:D:391:LEU:O	2.41	0.50
2:B:219:GLU:HB2	6:B:1016:HOH:O	2.11	0.50
2:D:42:ILE:HD11	2:D:100:PRO:CD	2.42	0.50
1:C:251:PRO:CG	2:D:478:TYR:HE2	2.23	0.50
2:D:586:PHE:CE2	2:D:597:VAL:HG13	2.46	0.50
2:D:511:GLU:OE2	2:D:579:TYR:OH	2.24	0.50
2:D:659:SER:HA	2:D:663:ALA:O	2.11	0.50
1:C:86:LEU:C	1:C:86:LEU:CD1	2.80	0.50
2:D:121:SER:N	2:D:124:GLU:OE1	2.45	0.50
1:A:114:ARG:NH1	1:A:343:PHE:O	2.43	0.50
1:A:231:GLY:HA3	2:B:484:SER:O	2.10	0.50
2:D:567:TYR:O	2:D:571:ARG:HG2	2.11	0.50
2:B:771:ASP:HB3	2:B:776:LEU:CD1	2.41	0.50
2:D:581:ILE:HA	2:D:599:TYR:O	2.12	0.50
2:B:23:GLU:HG3	2:B:27:ARG:HD3	1.94	0.50
2:D:42:ILE:HG21	2:D:154:LEU:HD11	1.93	0.50
2:D:341:ILE:CD1	2:D:384:ALA:HB3	2.41	0.50
2:B:32:VAL:HG22	2:B:166:PHE:CE2	2.47	0.50
2:D:270:PRO:HB3	2:D:364:ALA:HB1	1.93	0.50
1:C:182:GLU:HA	1:C:300:ALA:O	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:229:VAL:HG13	2:D:339:VAL:CG2	2.41	0.50
2:B:749:ASP:HB3	2:B:764:ALA:HB3	1.94	0.50
2:D:202:GLU:OE1	2:D:398:GLN:CG	2.60	0.50
1:C:225:LYS:HD2	6:C:422:HOH:O	2.10	0.50
1:A:118:GLU:O	1:A:239:LYS:HE2	2.12	0.50
2:B:437:PHE:HB2	2:B:444:THR:HG21	1.94	0.50
1:A:248:ARG:CD	2:B:27:ARG:HH11	2.26	0.49
2:D:306:VAL:C	2:D:308:THR:H	2.15	0.49
2:D:771:ASP:OD2	2:D:780:ARG:NH1	2.39	0.49
1:A:252:SER:OG	1:A:253:TYR:N	2.45	0.49
1:A:344:LYS:HE3	6:B:1085:HOH:O	2.12	0.49
2:B:490:GLU:O	2:B:490:GLU:HG3	2.12	0.49
2:D:215:ILE:HD11	2:D:403:SER:HB3	1.95	0.49
1:C:257:THR:O	1:C:258:GLU:HB2	2.13	0.49
1:A:88:GLN:HB2	1:A:92:GLU:OE2	2.12	0.49
2:D:329:PHE:C	2:D:329:PHE:CD2	2.85	0.49
2:B:422:LYS:NZ	6:B:1024:HOH:O	2.24	0.49
2:B:240:TRP:O	2:B:244:ARG:HG3	2.12	0.49
2:B:534:LEU:CA	2:B:535:GLN:HB2	2.42	0.49
2:D:263:VAL:HB	2:D:271:LEU:HD11	1.94	0.49
2:D:47:VAL:CG2	2:D:151:THR:HB	2.43	0.49
2:D:81:ALA:CB	2:D:140:ILE:HG23	2.43	0.49
2:D:756:LEU:O	2:D:757:GLU:C	2.51	0.49
1:C:86:LEU:HD12	1:C:90:LEU:HD22	1.93	0.48
2:D:691:TYR:OH	2:D:695:MET:CE	2.61	0.48
2:D:203:THR:OG1	2:D:205:GLU:HG3	2.12	0.48
1:A:191:LYS:NZ	2:B:492:THR:OG1	2.45	0.48
1:A:161:PHE:CD1	2:B:542:LEU:HD13	2.48	0.48
2:B:464:ILE:HG12	2:B:467:ASP:OD2	2.13	0.48
2:B:157:LEU:HD23	2:B:157:LEU:HA	1.49	0.48
2:B:32:VAL:HG22	2:B:166:PHE:CD2	2.48	0.48
2:D:775:THR:HG22	6:D:852:HOH:O	2.13	0.48
2:B:24:ARG:HG2	2:B:188:LEU:HD13	1.96	0.48
2:D:154:LEU:HA	2:D:157:LEU:HD12	1.96	0.48
2:B:43:LYS:HE3	2:B:96:GLY:O	2.13	0.48
2:D:290:LYS:HZ3	2:D:291:ASP:HB2	1.79	0.48
2:B:352:ARG:HB2	2:B:369:GLU:HG2	1.96	0.48
2:D:444:THR:HG22	2:D:451:LEU:HD22	1.94	0.48
1:C:248:ARG:HD2	1:C:264:ASP:OD2	2.13	0.48
1:C:86:LEU:HD11	1:C:90:LEU:HD22	1.92	0.48
2:D:248:ALA:CB	2:D:265:LEU:HD13	2.42	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:243:ALA:O	2:D:246:ILE:N	2.47	0.48
2:D:91:ILE:HD12	2:D:157:LEU:HD11	1.96	0.48
6:C:467:HOH:O	2:D:492:THR:CG2	2.61	0.48
2:B:18:VAL:CG1	2:B:19:GLU:OE2	2.55	0.47
1:C:152:HIS:HA	1:C:153:PRO:HD2	1.54	0.47
1:A:344:LYS:CE	6:B:1085:HOH:O	2.62	0.47
1:A:295:ASN:O	1:A:299:MET:HG3	2.14	0.47
2:D:479:ASP:HA	6:D:836:HOH:O	2.14	0.47
2:B:648[B]:GLU:HG3	6:B:1182:HOH:O	2.13	0.47
2:B:7:TRP:CE3	2:B:244:ARG:HB3	2.48	0.47
2:D:251:ARG:HA	2:D:252:PRO:HD3	1.73	0.47
2:D:215:ILE:HG21	2:D:221:VAL:HB	1.97	0.47
2:B:360:LEU:HD23	2:B:360:LEU:HA	1.70	0.47
2:B:333:THR:H	2:B:336:THR:HG21	1.71	0.47
2:D:207:ALA:HA	2:D:210:GLU:CG	2.44	0.47
2:D:127:ILE:HD13	2:D:132:VAL:HG23	1.95	0.47
2:D:231:ASN:ND2	2:D:395:GLU:OE2	2.44	0.47
2:D:9:LYS:HE2	2:D:13:ASP:OD2	2.15	0.47
1:C:205:ASP:O	1:C:207:THR:N	2.48	0.47
2:B:25:ILE:HG22	2:B:30:ILE:HB	1.96	0.47
2:B:415:ILE:HG13	2:B:416:THR:N	2.29	0.47
2:D:234:ILE:HG21	2:D:334:GLU:CB	2.43	0.47
2:D:210:GLU:O	2:D:282:LYS:HB3	2.15	0.47
2:D:123:GLN:HA	2:D:127:ILE:H	1.80	0.47
2:D:40:LYS:O	2:D:40:LYS:HG3	2.15	0.47
2:B:332:VAL:CA	2:B:336:THR:HG21	2.37	0.47
2:D:161:ASP:OD2	2:D:247:LYS:HE2	2.15	0.47
2:B:415:ILE:HD12	2:B:465:LYS:HB2	1.97	0.47
2:B:297:THR:HA	2:B:327:GLY:HA2	1.97	0.47
2:D:447:LYS:NZ	2:D:447:LYS:HB2	2.30	0.47
1:C:253[A]:TYR:CG	2:D:171:ASN:OD1	2.67	0.47
1:A:248:ARG:HD2	2:B:27:ARG:HH11	1.80	0.47
2:B:799:ILE:O	2:B:800:ARG:HG3	2.15	0.47
2:D:417:ALA:HA	2:D:433:ILE:CD1	2.45	0.47
2:B:314:ASN:OD1	2:B:316:GLN:HB2	2.15	0.47
2:D:420:VAL:HG22	2:D:469:ILE:HG12	1.97	0.46
2:D:238:PRO:HB2	2:D:240:TRP:CD1	2.50	0.46
1:A:159:ASP:CB	1:A:200:ARG:NH1	2.76	0.46
2:D:278:HIS:HB3	2:D:329:PHE:O	2.14	0.46
2:B:4:SER:HB3	2:B:7:TRP:HB3	1.96	0.46
2:B:799:ILE:O	2:B:800:ARG:C	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:335:ASN:HA	6:A:384:HOH:O	2.14	0.46
1:A:225:LYS:O	1:A:228:ASP:HB2	2.16	0.46
2:D:122:LEU:HB3	2:D:127:ILE:CD1	2.46	0.46
2:B:415:ILE:HG13	2:B:416:THR:H	1.81	0.46
2:B:465:LYS:O	2:B:468:LEU:HB2	2.16	0.46
1:A:313:GLY:HA3	5:A:1:GAX:O2	2.16	0.46
2:B:119:ILE:HG22	2:B:140:ILE:HG21	1.98	0.46
2:B:37:ASP:O	2:B:40:LYS:HB3	2.15	0.46
2:D:410:VAL:HG13	2:D:454:ASN:HB3	1.96	0.46
2:B:529:ALA:O	2:B:555:GLN:HB2	2.15	0.46
2:D:33:ASP:O	2:D:34:ASN:HB3	2.16	0.46
2:D:349:VAL:HA	2:D:352:ARG:HB3	1.98	0.46
2:D:731:LYS:HG2	2:D:745:THR:HG21	1.97	0.46
1:C:265:VAL:CG2	1:C:286:ILE:CD1	2.93	0.46
1:C:150:LYS:HD3	1:C:155:ARG:HH22	1.80	0.46
2:D:429:SER:O	2:D:433:ILE:HG13	2.16	0.46
2:B:375:GLU:HA	2:B:409:PHE:CE1	2.51	0.46
2:D:73:GLU:HG3	2:D:74:PRO:CD	2.45	0.46
2:B:171:ASN:O	2:B:172:ARG:HD2	2.16	0.46
2:D:535:GLN:HB2	2:D:537:ARG:HG2	1.98	0.46
2:D:212:SER:HB3	2:D:283:GLU:HA	1.97	0.46
2:B:282:LYS:HE3	2:B:282:LYS:HB2	1.53	0.46
2:D:604:LEU:N	2:D:685:TYR:O	2.48	0.46
2:B:540:ILE:HD11	2:B:594:PRO:HB3	1.98	0.46
2:D:54:GLU:OE2	2:D:54:GLU:HA	2.16	0.45
1:A:346:VAL:HG22	2:D:636:LEU:HA	1.98	0.45
2:B:191:THR:OG1	2:B:192:GLU:N	2.46	0.45
2:B:283:GLU:O	2:B:283:GLU:HG2	2.17	0.45
1:C:86:LEU:O	1:C:89:GLN:HB2	2.16	0.45
2:D:604:LEU:HB3	2:D:620:ILE:HD13	1.99	0.45
2:B:702:ILE:HG22	2:B:702:ILE:O	2.16	0.45
1:A:327:GLU:HB3	2:D:706:GLN:HE22	1.80	0.45
2:B:666:GLY:HA3	2:B:688:GLU:O	2.16	0.45
2:D:271:LEU:HD22	2:D:341:ILE:HD11	1.98	0.45
2:D:354:THR:HA	2:D:357:ARG:HH12	1.81	0.45
1:C:276:ASN:ND2	1:C:276:ASN:N	2.65	0.45
1:A:172:HIS:HA	1:A:198:VAL:HG11	1.99	0.45
2:D:275:ASP:OD2	2:D:277:ASP:N	2.49	0.45
2:D:603:ILE:HD11	2:D:684:THR:HG21	1.97	0.45
1:C:155:ARG:HG2	1:C:155:ARG:H	1.49	0.45
2:B:224:TYR:CZ	2:B:342:GLU:HG3	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:112:LEU:HD21	1:A:317:ASP:HA	1.97	0.45
2:D:462:ILE:HG21	2:D:468:LEU:HD13	1.98	0.45
2:B:603:ILE:HA	2:B:685:TYR:O	2.16	0.45
1:C:150:LYS:HD3	1:C:155:ARG:NH2	2.32	0.45
2:D:471:GLU:O	2:D:475:ILE:HG12	2.17	0.45
2:D:3:ILE:HD13	2:D:178:MET:SD	2.57	0.45
2:D:745:THR:HG22	3:D:801:SO4:O1	2.17	0.45
2:D:54:GLU:C	2:D:55:LYS:HG2	2.37	0.45
1:C:181:MET:HG3	1:C:218:LEU:CD2	2.47	0.45
2:D:460:LYS:HB2	2:D:460:LYS:HE3	1.53	0.45
2:B:780:ARG:CG	2:B:780:ARG:HH11	2.29	0.45
2:D:7:TRP:O	2:D:7:TRP:CD1	2.70	0.45
1:C:246:GLU:HA	1:C:246:GLU:OE1	2.17	0.45
2:D:23:GLU:HG3	2:D:24:ARG:N	2.32	0.45
2:D:132:VAL:CG2	2:D:133:PRO:HD2	2.47	0.44
2:D:306:VAL:O	2:D:308:THR:N	2.50	0.44
2:B:12:VAL:HG13	2:B:12:VAL:O	2.17	0.44
1:C:206:ALA:HA	1:C:328:ASP:OD1	2.18	0.44
2:B:350:SER:HA	6:B:844:HOH:O	2.18	0.44
1:C:274:GLY:CA	1:C:280:HIS:HA	2.47	0.44
2:D:254:ASN:C	2:D:254:ASN:OD1	2.56	0.44
1:A:192:ILE:O	1:A:193:ILE:HD13	2.17	0.44
2:D:419:LYS:HE2	2:D:423:THR:OG1	2.17	0.44
2:D:613:TRP:CE2	2:D:614:GLN:HG3	2.53	0.44
1:C:174:SER:N	1:C:175:PRO:HD2	2.32	0.44
1:C:153:PRO:HG3	2:D:170:PRO:HG3	2.00	0.44
1:A:116:VAL:O	1:A:120:GLU:HG3	2.17	0.44
2:B:464:ILE:HB	2:B:466:GLU:OE1	2.17	0.44
2:D:259:ILE:CD1	2:D:388:LEU:HD23	2.48	0.44
1:C:321:MET:HG2	1:C:326:ILE:O	2.17	0.44
2:B:220:LYS:CE	6:B:1100:HOH:O	2.66	0.44
2:B:234:ILE:CD1	2:B:333:THR:O	2.64	0.44
2:B:333:THR:N	2:B:336:THR:HG23	2.29	0.44
1:A:146:LEU:O	1:A:147:ASN:CB	2.65	0.44
2:B:43:LYS:CE	2:B:96:GLY:O	2.66	0.44
2:B:426:PHE:HB3	2:B:482:PRO:HD3	2.00	0.44
1:A:102:ARG:HD2	1:A:102:ARG:O	2.17	0.44
2:B:81:ALA:HA	2:B:82:PRO:HD3	1.88	0.44
2:D:481:ILE:HA	2:D:482:PRO:HD2	1.85	0.44
2:D:438:ARG:HH11	2:D:438:ARG:HG2	1.83	0.44
2:B:613:TRP:CE2	2:B:614:GLN:HG3	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:119:ILE:HA	1:C:119:ILE:HD13	1.82	0.44
2:D:361:ARG:CZ	2:D:366:SER:HB3	2.48	0.43
2:D:554:ARG:NH1	6:D:957:HOH:O	2.50	0.43
2:D:172:ARG:NH2	2:D:184:GLU:OE1	2.39	0.43
1:A:246:GLU:HB3	1:A:266:SER:OG	2.18	0.43
1:A:174:SER:OG	1:A:216:GLU:OE2	2.31	0.43
2:B:123:GLN:CG	2:B:132:VAL:HG21	2.46	0.43
2:D:374:THR:CG2	2:D:409:PHE:CD2	3.02	0.43
1:C:161:PHE:HB3	2:D:542:LEU:HD22	1.99	0.43
2:B:572:LYS:HE2	2:B:572:LYS:HB2	1.61	0.43
1:C:291:MET:HB3	1:C:291:MET:HE3	1.67	0.43
2:B:756:LEU:HD23	2:B:757:GLU:H	1.83	0.43
2:B:210:GLU:O	2:B:282:LYS:CG	2.62	0.43
2:D:255:ASN:ND2	2:D:392:ALA:CB	2.78	0.43
2:D:415:ILE:HD11	2:D:420:VAL:HG23	2.00	0.43
2:D:783:LYS:HE2	2:D:784:ILE:HG13	1.99	0.43
2:D:11:TYR:O	2:D:193:MET:HA	2.18	0.43
2:D:36:ILE:O	2:D:36:ILE:HG13	2.17	0.43
2:D:354:THR:O	2:D:355:SER:C	2.57	0.43
2:B:707:ILE:HA	2:B:708:PRO:HD2	1.77	0.43
2:B:721:VAL:HG22	2:B:725:VAL:HG21	1.99	0.43
1:A:238:LYS:HB2	1:A:238:LYS:HE3	1.50	0.43
2:D:131:VAL:O	2:D:131:VAL:CG1	2.67	0.43
1:A:146:LEU:O	1:A:256:PHE:HB3	2.18	0.43
2:B:748:PHE:CZ	2:B:764:ALA:HB1	2.53	0.43
2:D:691:TYR:CZ	2:D:695:MET:HE2	2.53	0.43
2:D:471:GLU:O	2:D:475:ILE:CG1	2.66	0.43
1:C:140:TYR:HA	1:C:144:GLU:HB2	2.01	0.43
2:D:18:VAL:HG12	6:D:981:HOH:O	2.19	0.43
2:D:569:VAL:HG13	6:D:1070:HOH:O	2.19	0.43
2:D:85:ASP:H	2:D:88:GLN:NE2	2.16	0.42
1:C:251:PRO:HA	2:D:478:TYR:CE2	2.54	0.42
2:B:187:ALA:O	2:B:188:LEU:C	2.57	0.42
2:B:471:GLU:CD	2:B:474:ARG:HE	2.21	0.42
2:B:134:LYS:HB2	2:B:134:LYS:HE3	1.65	0.42
1:C:141:TYR:OH	1:C:182:GLU:OE1	2.26	0.42
2:B:327:GLY:O	2:B:331[A]:GLU:HG3	2.19	0.42
1:C:90:LEU:HA	1:C:90:LEU:HD12	1.73	0.42
2:D:119:ILE:HG22	2:D:120:CYS:N	2.34	0.42
2:B:543:LEU:HA	2:B:543:LEU:HD23	1.74	0.42
2:D:127:ILE:HB	2:D:128:SER:H	1.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:226:MET:O	1:A:229:LEU:HB3	2.18	0.42
2:B:162:GLN:N	2:B:162:GLN:CD	2.72	0.42
1:C:120:GLU:OE2	1:C:130:ILE:HG21	2.19	0.42
1:A:219:VAL:O	1:A:309:GLY:HA2	2.19	0.42
2:D:196:PRO:HB2	2:D:383:ARG:CZ	2.49	0.42
2:D:231:ASN:CA	2:D:337:THR:O	2.68	0.42
1:C:139:ASP:OD1	1:C:166:GLU:OE1	2.36	0.42
2:B:574:LYS:CE	6:B:1084:HOH:O	2.68	0.42
1:C:239:LYS:HD2	1:C:239:LYS:HA	1.76	0.42
2:D:296:THR:HA	2:D:302:GLU:HA	2.02	0.42
2:B:721:VAL:CG2	2:B:725:VAL:HG21	2.50	0.42
2:B:298:LEU:C	2:B:298:LEU:HD12	2.40	0.42
2:D:131:VAL:CG1	2:D:246:ILE:HG23	2.49	0.42
1:C:248:ARG:CD	1:C:264:ASP:OD2	2.68	0.42
2:D:213:VAL:HG12	2:D:403:SER:HB2	2.02	0.42
2:B:12:VAL:O	2:B:12:VAL:CG1	2.67	0.42
2:B:250:ILE:O	2:B:252:PRO:HD3	2.19	0.42
1:A:303:ASP:OD1	1:A:305:ASN:HB2	2.20	0.42
2:D:51:GLN:OE1	2:D:74:PRO:HG3	2.20	0.42
1:C:328:ASP:HB3	1:C:331:TYR:CE1	2.55	0.42
1:A:254:PHE:CD2	1:A:260:SER:HB3	2.55	0.42
2:D:642:TYR:HE1	2:D:668:ILE:HD11	1.85	0.42
2:D:743:GLN:HG2	6:D:1015:HOH:O	2.19	0.42
2:D:346:PHE:O	2:D:347:ASP:C	2.58	0.41
1:C:152:HIS:ND1	1:C:154:ALA:N	2.68	0.41
2:D:499:ARG:HG3	2:D:695:MET:HE3	2.02	0.41
1:C:269:LYS:HD2	1:C:269:LYS:HA	1.70	0.41
2:B:716:ASP:OD1	2:B:766:ARG:NH1	2.53	0.41
2:D:530:LYS:NZ	2:D:539:THR:HG23	2.35	0.41
2:D:480:GLU:OE1	2:D:480:GLU:HA	2.20	0.41
2:D:332:VAL:O	2:D:332:VAL:HG12	2.20	0.41
1:C:255:PRO:HD2	1:C:256:PHE:CE1	2.55	0.41
2:D:298:LEU:HB3	2:D:327:GLY:O	2.21	0.41
2:D:222:PRO:HD2	2:D:345:ILE:O	2.20	0.41
1:A:201:ARG:HG2	2:B:546:MET:HE2	2.02	0.41
2:D:40:LYS:HE2	2:D:100:PRO:HB3	2.02	0.41
2:D:478:TYR:HA	2:D:481:ILE:HD12	2.02	0.41
2:D:390:GLU:OE1	2:D:390:GLU:HA	2.20	0.41
1:A:294:PRO:HD3	6:A:428:HOH:O	2.19	0.41
2:D:189:TYR:C	2:D:190:GLN:HG2	2.39	0.41
2:B:709:LYS:HD2	2:B:709:LYS:H	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:254:PHE:CE2	1:C:260:SER:HB3	2.55	0.41
2:D:306:VAL:C	2:D:308:THR:N	2.73	0.41
1:C:225:LYS:O	1:C:228:ASP:HB2	2.21	0.41
2:D:671:LEU:HD23	2:D:671:LEU:HA	1.73	0.41
2:D:388:LEU:HD23	2:D:388:LEU:HA	1.70	0.41
2:B:264:LEU:HD21	2:B:363:GLU:HB3	2.03	0.41
1:C:112:LEU:HD21	1:C:317:ASP:HA	2.02	0.41
2:B:777:THR:OG1	2:B:779:GLU:HG2	2.20	0.41
1:C:181:MET:HE1	5:C:2:GAX:H9	2.03	0.41
1:A:90:LEU:HD13	2:D:652:PRO:HG2	2.01	0.41
2:D:215:ILE:HG23	2:D:217:ASN:OD1	2.21	0.41
1:C:233:LEU:HD13	1:C:263:VAL:HG21	2.01	0.41
2:D:53:LYS:CD	2:D:63:ASN:HB3	2.49	0.41
2:D:228:VAL:HG12	2:D:397:LEU:HD13	2.02	0.41
2:D:275:ASP:OD1	2:D:336:THR:CG2	2.68	0.41
1:C:313:GLY:HA3	5:C:2:GAX:O2	2.21	0.41
2:B:419:LYS:HD2	2:B:419:LYS:HA	1.86	0.41
2:B:631:ARG:NH1	1:C:104:ILE:HG22	2.36	0.41
2:B:42:ILE:CG1	2:B:100:PRO:HD3	2.51	0.40
2:D:347:ASP:OD2	2:D:349:VAL:HG13	2.21	0.40
1:A:110:HIS:O	1:A:114:ARG:HG3	2.21	0.40
2:B:233:SER:O	6:B:1202:HOH:O	2.22	0.40
2:B:487:VAL:HG22	2:D:491:VAL:CG2	2.51	0.40
2:B:558:LEU:O	2:B:559:PRO:C	2.59	0.40
2:B:622:PHE:C	2:B:622:PHE:CD1	2.94	0.40
2:D:84:VAL:O	2:D:84:VAL:HG13	2.21	0.40
2:D:6:GLU:O	2:D:9:LYS:HG3	2.20	0.40
2:D:254:ASN:O	2:D:256:VAL:N	2.55	0.40
2:B:442:PHE:O	2:B:444:THR:HG22	2.22	0.40
2:B:524:VAL:HG23	2:B:525:SER:O	2.21	0.40
1:A:251:PRO:HG2	2:B:28:THR:C	2.42	0.40
2:D:131:VAL:O	2:D:131:VAL:HG13	2.20	0.40
2:D:281:SER:OG	2:D:283:GLU:N	2.46	0.40
2:D:314:ASN:HD21	2:D:317:GLU:HB2	1.85	0.40
1:A:200:ARG:HB2	1:A:212:PHE:HE1	1.86	0.40
1:C:109:LYS:HE2	1:C:117:GLU:OE2	2.22	0.40
5:A:1:GAX:S2	5:A:1:GAX:O3	2.79	0.40
2:B:257:VAL:HG22	6:B:1095:HOH:O	2.21	0.40
2:B:206:SER:OG	2:B:399:ASP:OD2	2.28	0.40
2:D:123:GLN:N	2:D:125:ILE:H	2.19	0.40
2:B:424:ILE:CD1	2:B:469:ILE:CG2	2.84	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:53:LYS:HE3	2:D:85:ASP:HA	2.03	0.40
2:D:263:VAL:CG1	2:D:383:ARG:HB3	2.51	0.40
2:D:6:GLU:OE2	2:D:244:ARG:NH1	2.41	0.40
2:B:274:PHE:HB2	2:B:340:VAL:HB	2.03	0.40
1:A:189:PRO:CD	2:B:490:GLU:HG2	2.51	0.40
2:B:567:TYR:CE1	2:B:571:ARG:CZ	3.05	0.40
1:A:184:ARG:HG3	1:A:190:VAL:HG22	2.02	0.40
2:B:413:ILE:HD12	2:B:455:VAL:HG21	2.03	0.40
2:D:201:ASN:OD1	2:D:201:ASN:N	2.55	0.40
2:D:338:ASN:N	2:D:338:ASN:ND2	2.68	0.40
1:C:253[A]:TYR:CD2	2:D:171:ASN:CG	2.95	0.40
1:A:248:ARG:O	1:A:263:VAL:HA	2.22	0.40
2:B:119:ILE:HG22	2:B:140:ILE:CG2	2.52	0.40
2:B:726:PRO:HD2	2:B:729:GLU:OE2	2.22	0.40
2:B:633:ALA:HB2	2:B:640:PHE:CD1	2.57	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	246/294 (84%)	226 (92%)	20 (8%)	0	100	100
1	C	271/294 (92%)	252 (93%)	13 (5%)	6 (2%)	8	4
2	B	780/800 (98%)	726 (93%)	47 (6%)	7 (1%)	21	19
2	D	778/800 (97%)	674 (87%)	79 (10%)	25 (3%)	5	2
All	All	2075/2188 (95%)	1878 (90%)	159 (8%)	38 (2%)	11	7

All (38) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	151	SER
1	C	152	HIS
1	C	155	ARG
2	D	39	SER
2	D	114	ARG
2	D	121	SER
2	D	124	GLU
2	D	130	ASN
2	D	235	GLU
2	D	298	LEU
2	D	316	GLN
2	D	393	SER
2	B	532	PHE
2	B	590	GLU
2	B	799	ILE
1	C	150	LYS
2	D	41	ASP
2	D	103	ILE
2	D	248	ALA
2	D	307	ASP
2	D	329	PHE
2	D	373	ALA
2	D	389	GLN
2	B	299	ASP
2	B	754	GLU
1	C	153	PRO
2	D	190	GLN
2	D	244	ARG
2	D	375	GLU
2	D	159	LEU
2	D	320	ALA
1	C	258	GLU
2	D	234	ILE
2	D	757	GLU
2	B	534	LEU
2	D	381	VAL
2	B	235	GLU
2	D	127	ILE

### 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	220/257 (86%)	199 (90%)	21 (10%)	11	10
1	C	240/257 (93%)	216 (90%)	24 (10%)	9	8
2	B	678/688 (98%)	608 (90%)	70 (10%)	9	8
2	D	676/688 (98%)	571 (84%)	105 (16%)	3	2
All	All	1814/1890 (96%)	1594 (88%)	220 (12%)	6	5

All (220) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	87	ASN
1	A	88	GLN
1	A	89	GLN
1	A	102	ARG
1	A	103	GLN
1	A	108	SER
1	A	129	GLU
1	A	137	GLU
1	A	146	LEU
1	A	151	SER
1	A	157	MET
1	A	168	LEU
1	A	172	HIS
1	A	182	GLU
1	A	200	ARG
1	A	202	ASP
1	A	256	PHE
1	A	284	ILE
1	A	304	SER
1	A	318	ARG
1	A	351	GLU
2	B	16	VAL
2	B	20	ASP
2	B	40	LYS
2	B	41	ASP
2	B	50	ILE
2	B	51	GLN
2	B	55	LYS

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Mol	Chain	Res	Type
2	B	69	ILE
2	B	73	GLU
2	B	78	VAL
2	B	98	ARG
2	B	104	LYS
2	B	109	LYS
2	B	114	ARG
2	B	115	SER
2	B	116	GLU
2	B	128	SER
2	B	129	SER
2	B	138	ASN
2	B	162	GLN
2	B	233	SER
2	B	235	GLU
2	B	239	ILE
2	B	264	LEU
2	B	282	LYS
2	B	304	LYS
2	B	305	LEU
2	B	321	LEU
2	B	331[A]	GLU
2	B	331[B]	GLU
2	B	334	GLU
2	B	336	THR
2	B	339	VAL
2	B	349	VAL
2	B	361	ARG
2	B	367	ARG
2	B	400	ARG
2	B	408	SER
2	B	410	VAL
2	B	411	THR
2	B	415	ILE
2	B	416	THR
2	B	418	GLU
2	B	419	LYS
2	B	426	PHE
2	B	443	GLU
2	B	450	THR
2	B	464	ILE
2	B	466	GLU

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Mol	Chain	Res	Type
2	B	484	SER
2	B	490	GLU
2	B	527	ASP
2	B	571	ARG
2	B	572	LYS
2	B	574	LYS
2	B	590	GLU
2	B	607	GLU
2	B	646	LYS
2	B	702	ILE
2	B	709	LYS
2	B	710	PHE
2	B	724	ASP
2	B	754	GLU
2	B	756	LEU
2	B	767	LEU
2	B	771	ASP
2	B	779	GLU
2	B	789	LEU
2	B	798	THR
2	B	800	ARG
1	C	81	GLU
1	C	86	LEU
1	C	90	LEU
1	C	102	ARG
1	C	108	SER
1	C	114	ARG
1	C	128	TYR
1	C	146	LEU
1	C	151	SER
1	C	155	ARG
1	C	157	MET
1	C	158	GLN
1	C	172	HIS
1	C	200	ARG
1	C	203	SER
1	C	223	ASN
1	C	225	LYS
1	C	245	ARG
1	C	248	ARG
1	C	253[A]	TYR
1	C	253[B]	TYR

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Mol	Chain	Res	Type
1	C	256	PHE
1	C	276	ASN
1	C	287	LEU
2	D	4	SER
2	D	16	VAL
2	D	23	GLU
2	D	27	ARG
2	D	31	GLU
2	D	36	ILE
2	D	39	SER
2	D	52	SER
2	D	53	LYS
2	D	64	ILE
2	D	69	ILE
2	D	79	CYS
2	D	85	ASP
2	D	99	LEU
2	D	103	ILE
2	D	106	LYS
2	D	107	ARG
2	D	114	ARG
2	D	123	GLN
2	D	128	SER
2	D	129	SER
2	D	131	VAL
2	D	146	GLU
2	D	169	THR
2	D	194	THR
2	D	199	GLN
2	D	201	ASN
2	D	202	GLU
2	D	203	THR
2	D	205	GLU
2	D	212	SER
2	D	219[A]	GLU
2	D	219[B]	GLU
2	D	232	VAL
2	D	234	ILE
2	D	237	SER
2	D	253	ILE
2	D	263	VAL
2	D	264	LEU

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Mol	Chain	Res	Type
2	D	271	LEU
2	D	281	SER
2	D	282	LYS
2	D	284	ILE
2	D	286	VAL
2	D	290	LYS
2	D	291	ASP
2	D	299	ASP
2	D	302	GLU
2	D	304	LYS
2	D	306	VAL
2	D	310	ILE
2	D	313	SER
2	D	316	GLN
2	D	317	GLU
2	D	328	ASP
2	D	329	PHE
2	D	334	GLU
2	D	335	GLN
2	D	338	ASN
2	D	340	VAL
2	D	341	ILE
2	D	349	VAL
2	D	350	SER
2	D	356	ARG
2	D	357	ARG
2	D	361	ARG
2	D	362	SER
2	D	367	ARG
2	D	370	LYS
2	D	374	THR
2	D	383	ARG
2	D	387	LEU
2	D	390	GLU
2	D	393	SER
2	D	396	VAL
2	D	422	LYS
2	D	426	PHE
2	D	439	GLN
2	D	443	GLU
2	D	445	THR
2	D	450	THR

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Mol	Chain	Res	Type
2	D	460	LYS
2	D	468	LEU
2	D	509	THR
2	D	535	GLN
2	D	536	GLU
2	D	544	MET
2	D	597	VAL
2	D	607	GLU
2	D	639	GLU
2	D	641	SER
2	D	643	LYS
2	D	646	LYS
2	D	668	ILE
2	D	706	GLN
2	D	721	VAL
2	D	745	THR
2	D	765	ILE
2	D	766	ARG
2	D	775	THR
2	D	779	GLU
2	D	783	LYS
2	D	789	LEU
2	D	793	GLN
2	D	799	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	276	ASN
2	D	44	ASN
2	D	338	ASN

### 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 ⓘ

Of 5 ligands modelled in this entry, 1 is monoatomic - leaving 4 for Mogul analysis.

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$
5	GAX	A	1	-	30,33,33	2.16	5 (16%)	40,46,46	2.52	18 (45%)
3	SO4	B	801	-	4,4,4	0.17	0	6,6,6	0.26	0
5	GAX	C	2	-	30,33,33	2.26	5 (16%)	40,46,46	3.01	20 (50%)
3	SO4	D	801	-	4,4,4	0.12	0	6,6,6	0.32	0

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
5	GAX	A	1	-	-	0/22/34/34	0/4/4/4
3	SO4	B	801	-	-	0/0/0/0	0/0/0/0
5	GAX	C	2	-	-	0/22/34/34	0/4/4/4
3	SO4	D	801	-	-	0/0/0/0	0/0/0/0

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	2	GAX	C4-S1	-11.05	1.60	1.76
5	A	1	GAX	C4-S1	-9.92	1.61	1.76
5	A	1	GAX	C2-N1	-3.98	1.34	1.41
5	A	1	GAX	C7-N1	-3.04	1.32	1.37
5	C	2	GAX	C2-N1	-2.90	1.36	1.41
5	C	2	GAX	C7-N2	-2.63	1.32	1.37
5	A	1	GAX	C7-N2	-2.21	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	2	GAX	C7-N1	-2.18	1.33	1.37
5	A	1	GAX	C15-N5	2.18	1.42	1.37
5	C	2	GAX	C15-N5	2.27	1.42	1.37

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	2	GAX	O1-S1-O2	-5.74	109.57	119.47
5	A	1	GAX	C8-N2-C7	-5.55	123.33	130.13
5	A	1	GAX	O1-S1-O2	-5.42	110.11	119.47
5	C	2	GAX	C13-N5-C15	-5.25	107.75	120.22
5	C	2	GAX	C8-N2-C7	-5.09	123.90	130.13
5	C	2	GAX	C4-S1-N4	-4.83	101.36	107.32
5	C	2	GAX	C11-N4-C14	-4.09	107.22	112.20
5	C	2	GAX	C12-N5-C15	-3.94	110.85	120.22
5	A	1	GAX	C12-N5-C15	-3.83	111.12	120.22
5	A	1	GAX	C13-N5-C15	-3.62	111.61	120.22
5	A	1	GAX	C5-C4-C3	-3.27	116.73	120.52
5	C	2	GAX	O3-C7-N2	-3.14	118.81	123.58
5	A	1	GAX	C4-S1-N4	-3.02	103.59	107.32
5	A	1	GAX	C19-C15-N6	-2.95	117.74	123.17
5	C	2	GAX	C19-C15-N6	-2.76	118.08	123.17
5	A	1	GAX	C6-C1-C2	-2.33	116.76	119.72
5	C	2	GAX	C2-N1-C7	2.06	130.62	126.65
5	C	2	GAX	C11-C12-N5	2.09	114.77	110.63
5	A	1	GAX	C1-C2-C3	2.19	122.30	119.69
5	C	2	GAX	C9-C10-N3	2.45	115.67	109.36
5	C	2	GAX	C18-C19-C15	2.47	121.32	117.73
5	A	1	GAX	C14-C13-N5	2.64	115.85	110.63
5	A	1	GAX	C3-C4-S1	2.73	122.77	119.41
5	C	2	GAX	C14-C13-N5	2.75	116.07	110.63
5	A	1	GAX	N6-C15-N5	2.96	121.23	116.96
5	A	1	GAX	C9-C10-N3	2.98	117.02	109.36
5	C	2	GAX	N6-C15-N5	3.02	121.31	116.96
5	A	1	GAX	C6-C5-C4	3.02	122.22	118.95
5	A	1	GAX	O2-S1-N4	3.16	109.81	106.69
5	C	2	GAX	O1-S1-C4	3.30	112.29	108.00
5	A	1	GAX	O1-S1-C4	3.55	112.61	108.00
5	C	2	GAX	O2-S1-N4	3.64	110.28	106.69
5	C	2	GAX	N1-C7-N2	3.74	118.41	112.53
5	A	1	GAX	O1-S1-N4	3.88	110.53	106.69
5	C	2	GAX	C16-N6-C15	4.09	122.22	116.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1	GAX	C16-N6-C15	4.89	123.25	116.92
5	C	2	GAX	C13-C14-N4	5.22	113.26	109.02
5	C	2	GAX	O1-S1-N4	7.73	114.33	106.69

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1	GAX	2	0
5	C	2	GAX	3	0
3	D	801	SO4	1	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	249/294 (84%)	-0.42	0 100 100	16, 29, 51, 83	0
1	C	271/294 (92%)	-0.36	2 (0%) 89 88	13, 31, 59, 83	0
2	B	786/800 (98%)	-0.38	5 (0%) 90 90	17, 34, 56, 83	1 (0%)
2	D	785/800 (98%)	0.08	39 (4%) 32 32	16, 46, 85, 105	1 (0%)
All	All	2091/2188 (95%)	-0.21	46 (2%) 65 64	13, 35, 75, 105	2 (0%)

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	43	LYS	5.2
2	D	103	ILE	4.9
2	D	151	THR	4.7
2	D	316	GLN	4.3
2	B	78	VAL	4.1
2	D	133	PRO	3.8
2	D	84	VAL	3.8
2	D	81	ALA	3.6
2	D	108	ALA	3.4
2	D	279	ILE	3.3
2	D	124	GLU	3.2
2	D	125	ILE	3.0
2	D	122	LEU	3.0
2	D	756	LEU	3.0
2	D	290	LYS	2.9
2	D	280	GLY	2.9
2	D	36	ILE	2.8
2	D	98	ARG	2.8
2	D	119	ILE	2.8
2	D	253	ILE	2.8
2	D	69	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
2	D	307	ASP	2.7
2	D	127	ILE	2.7
2	D	106	LYS	2.6
2	B	103	ILE	2.6
2	D	294	THR	2.6
2	D	77	ILE	2.6
2	D	82	PRO	2.6
2	D	403	SER	2.5
2	B	54	GLU	2.5
2	D	341	ILE	2.4
1	C	273	LYS	2.4
2	B	589	GLY	2.4
2	D	312	ILE	2.4
2	D	143	PHE	2.3
2	D	96	GLY	2.3
2	D	72	GLU	2.2
2	B	114	ARG	2.2
2	D	95	VAL	2.2
2	D	285	VAL	2.1
1	C	351	GLU	2.1
2	D	755	HIS	2.1
2	D	46	VAL	2.1
2	D	42	ILE	2.0
2	D	52	SER	2.0
2	D	49	TYR	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, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
5	GAX	A	1	30/30	0.94	0.13	1.86	21,39,63,65	0
5	GAX	C	2	30/30	0.96	0.10	-0.51	22,40,56,57	0
4	ZN	C	3	1/1	0.97	0.10	-0.52	47,47,47,47	0
3	SO4	B	801	5/5	0.99	0.07	-	44,44,52,53	0
3	SO4	D	801	5/5	0.98	0.10	-	37,41,44,47	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.