



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:06 PM GMT

PDB ID : 1E0T
Title : R292D MUTANT OF E. COLI PYRUVATE KINASE
Authors : Fortin, R.; Mattevi, A.
Deposited on : 2000-04-10
Resolution : 1.80 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

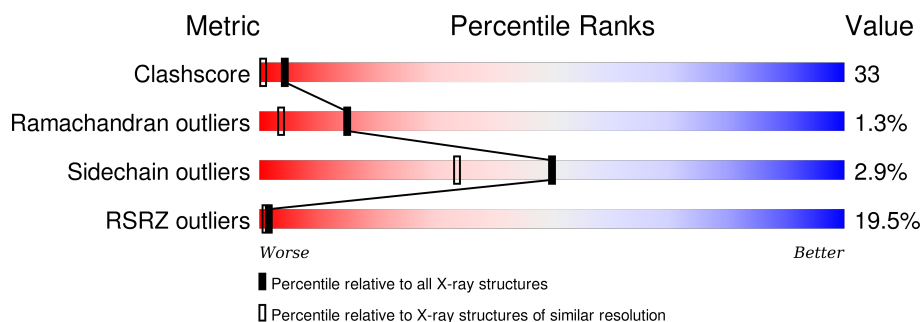
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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))
Clashscore	102246	5383 (1.80-1.80)
Ramachandran outliers	100387	5320 (1.80-1.80)
Sidechain outliers	100360	5319 (1.80-1.80)
RSRZ outliers	91569	4547 (1.80-1.80)

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	470	
1	B	470	
1	C	470	
1	D	470	

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
2	SO4	A	701	-	X	-	-
2	SO4	B	702	-	X	X	-
2	SO4	C	703	-	X	X	-
2	SO4	D	704	-	X	-	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 13374 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 PYRUVATE KINASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	446	Total	C	N	O	S	0	0	0
			3307	2060	568	657	22			
1	B	446	Total	C	N	O	S	0	0	0
			3307	2060	568	657	22			
1	C	446	Total	C	N	O	S	0	0	0
			3307	2060	568	657	22			
1	D	446	Total	C	N	O	S	0	0	0
			3307	2060	568	657	22			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	292	ASP	ARG	ENGINEERED MUTATION	UNP P14178
B	292	ASP	ARG	ENGINEERED MUTATION	UNP P14178
C	292	ASP	ARG	ENGINEERED MUTATION	UNP P14178
D	292	ASP	ARG	ENGINEERED MUTATION	UNP P14178
A	279	MET	GLN	CONFLICT	UNP P14178
B	279	MET	GLN	CONFLICT	UNP P14178
C	279	MET	GLN	CONFLICT	UNP P14178
D	279	MET	GLN	CONFLICT	UNP P14178

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

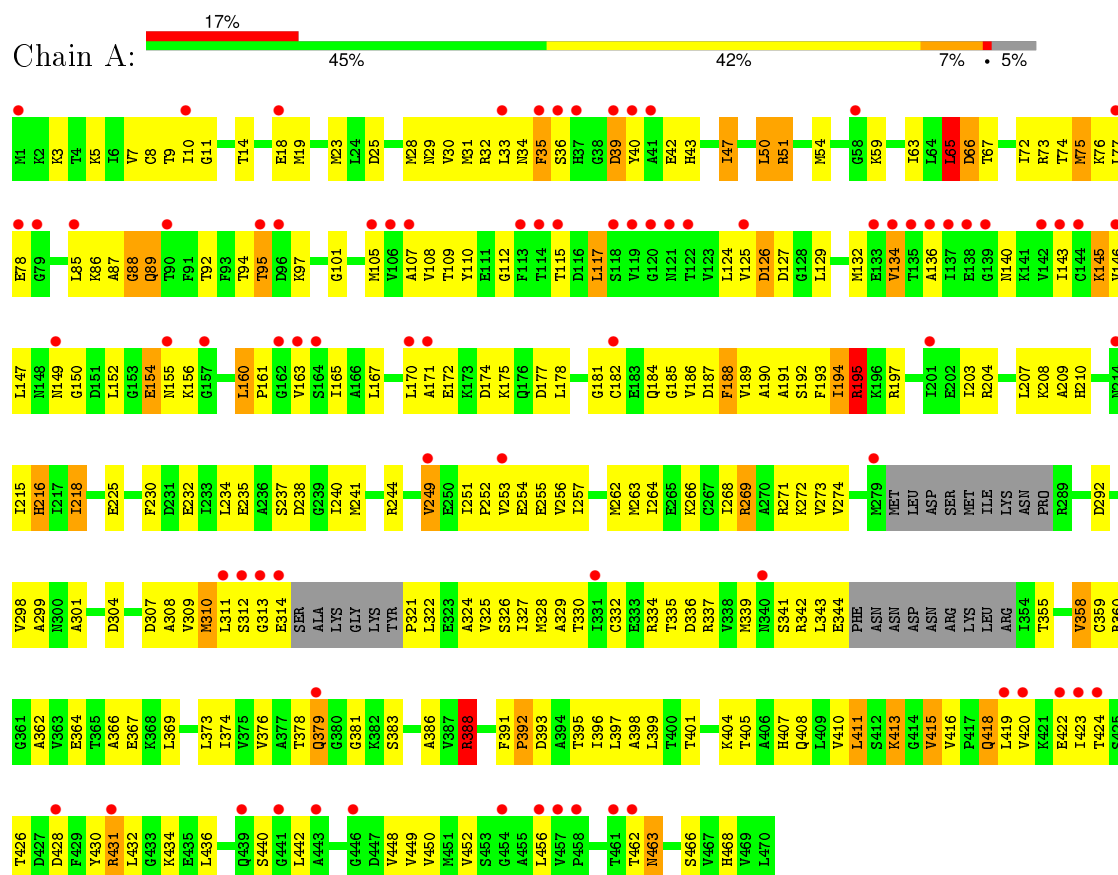
- Molecule 3 is water.

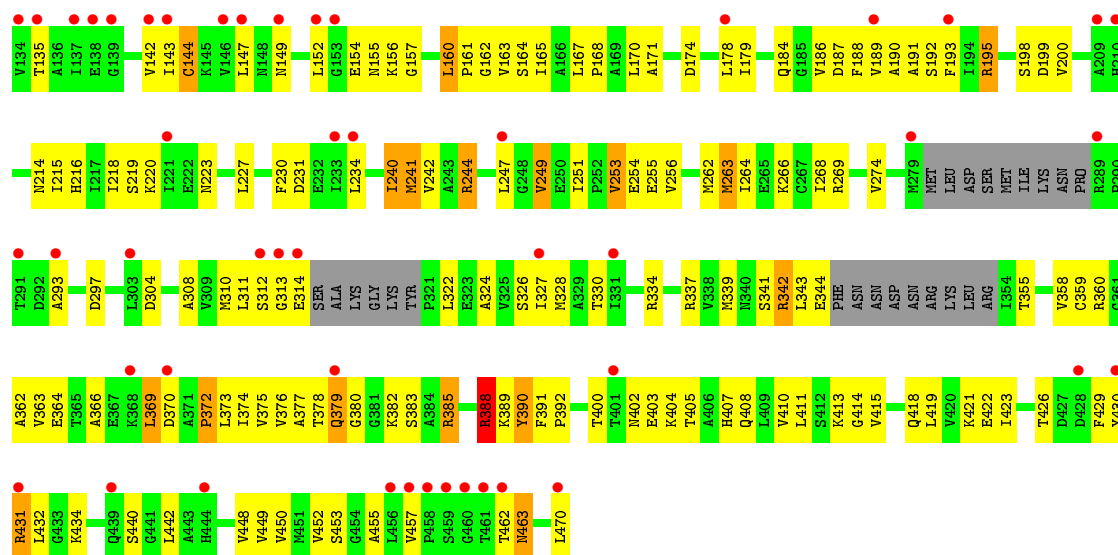
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	24	Total	O	0	0
			24	24		
3	B	35	Total	O	0	0
			35	35		
3	C	29	Total	O	0	0
			29	29		
3	D	38	Total	O	0	0
			38	38		

3 Residue-property plots

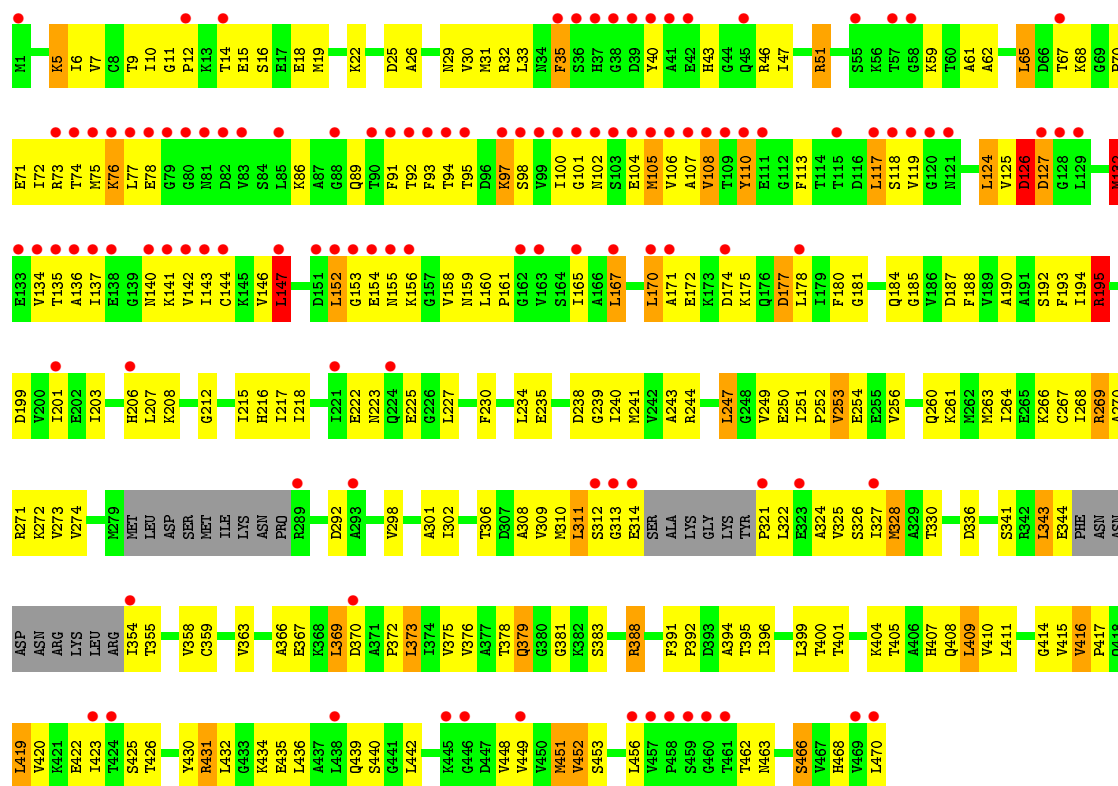
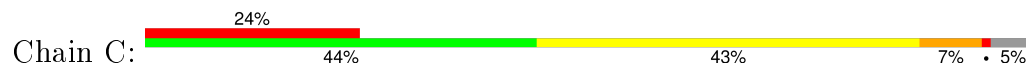
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: PYRUVATE KINASE

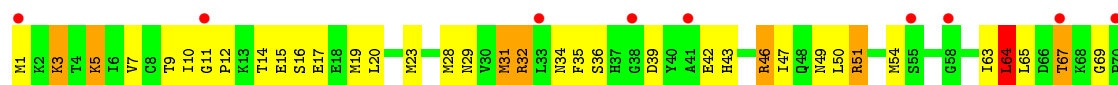


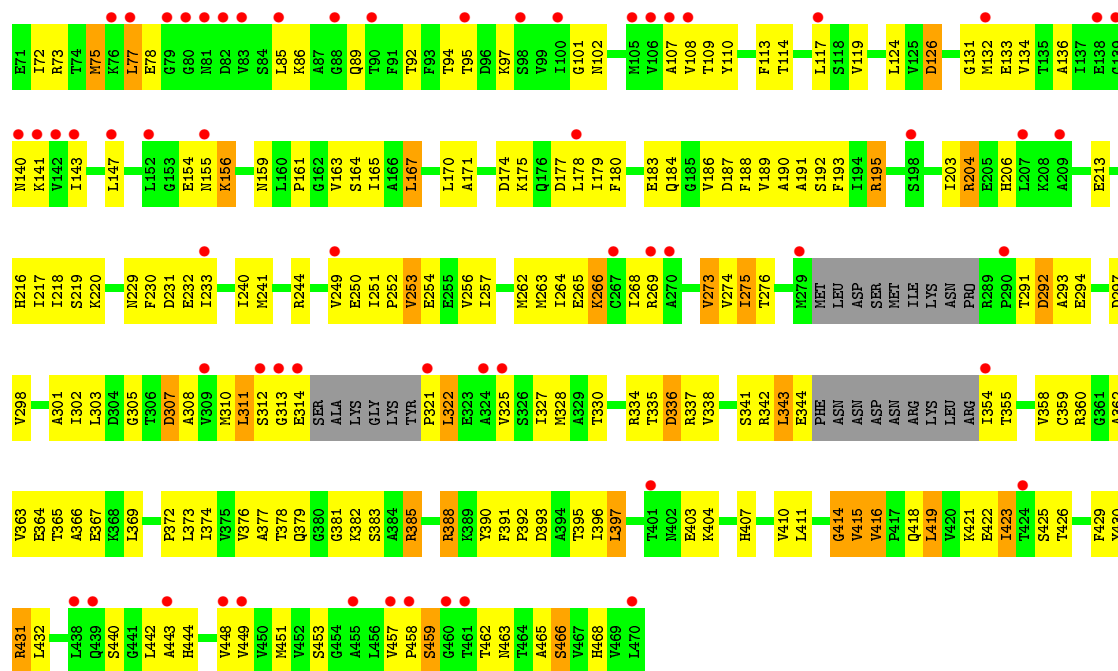


• Molecule 1: PYRUVATE KINASE



• Molecule 1: PYRUVATE KINASE





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	74.47Å 129.34Å 240.37Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 1.80 14.97 – 2.80	Depositor EDS
% Data completeness (in resolution range)	96.3 (15.00-1.80) 96.3 (14.97-2.80)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	8.88 (at 2.81Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.246 , 0.315 0.242 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	25.1	Xtriage
Anisotropy	0.776	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 77.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	3 of 55542 reflections (0.005%)	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	13374	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 40.41 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 2.7480e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² 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: SO4

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	0.65	0/3337	1.66	50/4507 (1.1%)
1	B	0.67	0/3337	1.65	46/4507 (1.0%)
1	C	0.68	0/3337	1.70	52/4507 (1.2%)
1	D	0.67	0/3337	1.68	44/4507 (1.0%)
All	All	0.66	0/13348	1.67	192/18028 (1.1%)

There are no bond length outliers.

All (192) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	292	ASP	CB-CG-OD1	13.34	130.31	118.30
1	D	117	LEU	CA-CB-CG	9.33	136.75	115.30
1	D	459	SER	N-CA-CB	8.94	123.91	110.50
1	D	311	LEU	CB-CG-CD2	-8.91	95.86	111.00
1	B	75	MET	CA-CB-CG	-8.81	98.33	113.30
1	B	117	LEU	CA-CB-CG	8.62	135.12	115.30
1	B	244	ARG	NE-CZ-NH1	8.57	124.58	120.30
1	A	413	LYS	CD-CE-NZ	8.25	130.67	111.70
1	A	262	MET	CA-CB-CG	8.23	127.29	113.30
1	C	269	ARG	NE-CZ-NH2	8.14	124.37	120.30
1	A	51	ARG	NE-CZ-NH1	8.07	124.34	120.30
1	A	456	LEU	CB-CG-CD2	7.97	124.55	111.00
1	A	216	HIS	N-CA-CB	7.59	124.27	110.60
1	C	311	LEU	CB-CG-CD2	-7.53	98.20	111.00
1	C	409	LEU	CA-CB-CG	7.49	132.52	115.30
1	A	39	ASP	CB-CG-OD1	7.43	124.99	118.30
1	A	336	ASP	CB-CG-OD2	-7.42	111.62	118.30
1	D	117	LEU	CB-CA-C	7.42	124.30	110.20
1	B	227	LEU	CB-CG-CD2	-7.42	98.39	111.00
1	D	466	SER	N-CA-CB	-7.38	99.43	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	35	PHE	CB-CA-C	7.30	125.01	110.40
1	D	322	LEU	CB-CG-CD2	-7.29	98.60	111.00
1	B	241	MET	CG-SD-CE	7.28	111.85	100.20
1	B	32	ARG	NE-CZ-NH1	7.17	123.89	120.30
1	C	177	ASP	CB-CG-OD2	-7.17	111.84	118.30
1	C	336	ASP	CB-CG-OD1	7.16	124.74	118.30
1	C	247	LEU	CB-CG-CD2	-7.10	98.93	111.00
1	B	262	MET	CA-CB-CG	7.09	125.35	113.30
1	A	411	LEU	CB-CG-CD2	7.08	123.03	111.00
1	A	334	ARG	NE-CZ-NH1	7.07	123.83	120.30
1	A	35	PHE	CB-CA-C	7.07	124.53	110.40
1	B	195	ARG	NE-CZ-NH1	-7.05	116.77	120.30
1	D	167	LEU	CB-CG-CD2	-7.05	99.02	111.00
1	A	182	CYS	CA-CB-SG	6.99	126.58	114.00
1	C	271	ARG	NE-CZ-NH2	-6.98	116.81	120.30
1	C	373	LEU	N-CA-CB	-6.95	96.50	110.40
1	B	342	ARG	NE-CZ-NH2	-6.91	116.85	120.30
1	C	199	ASP	CB-CG-OD1	6.91	124.51	118.30
1	B	8	CYS	CA-CB-SG	-6.89	101.60	114.00
1	A	160	LEU	CB-CG-CD2	-6.88	99.30	111.00
1	B	334	ARG	NE-CZ-NH1	6.88	123.74	120.30
1	B	253	VAL	CB-CA-C	-6.87	98.36	111.40
1	B	160	LEU	CB-CG-CD1	-6.85	99.35	111.00
1	A	51	ARG	NE-CZ-NH2	-6.83	116.89	120.30
1	B	66	ASP	CB-CG-OD2	-6.75	112.22	118.30
1	B	199	ASP	CB-CG-OD2	-6.74	112.24	118.30
1	C	167	LEU	CB-CG-CD2	-6.73	99.57	111.00
1	A	195	ARG	N-CA-C	6.72	129.14	111.00
1	D	292	ASP	N-CA-CB	-6.67	98.60	110.60
1	C	451	MET	CA-CB-CG	-6.66	101.97	113.30
1	B	322	LEU	CB-CG-CD2	-6.64	99.71	111.00
1	A	269	ARG	NE-CZ-NH2	6.57	123.59	120.30
1	C	110	TYR	N-CA-C	6.55	128.68	111.00
1	B	373	LEU	N-CA-CB	-6.50	97.40	110.40
1	C	328	MET	CG-SD-CE	6.44	110.50	100.20
1	A	89	GLN	CB-CA-C	-6.41	97.58	110.40
1	D	64	LEU	CA-CB-CG	6.39	129.99	115.30
1	D	343	LEU	CA-CB-CG	-6.38	100.62	115.30
1	C	271	ARG	CB-CA-C	6.31	123.03	110.40
1	C	98	SER	CB-CA-C	-6.30	98.14	110.10
1	D	253	VAL	CB-CA-C	-6.30	99.44	111.40
1	A	195	ARG	NE-CZ-NH1	-6.27	117.16	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	250	GLU	N-CA-C	6.27	127.92	111.00
1	C	194	ILE	CB-CA-C	-6.25	99.09	111.60
1	C	147	LEU	CA-CB-CG	6.25	129.67	115.30
1	C	167	LEU	C-N-CD	-6.25	106.86	120.60
1	B	54	MET	CG-SD-CE	6.24	110.18	100.20
1	B	144	CYS	CA-CB-SG	6.23	125.21	114.00
1	A	30	VAL	CB-CA-C	-6.17	99.67	111.40
1	C	126	ASP	CB-CG-OD2	-6.14	112.78	118.30
1	C	71	GLU	CB-CA-C	-6.13	98.14	110.40
1	C	170	LEU	CA-CB-CG	6.11	129.34	115.30
1	A	456	LEU	CD1-CG-CD2	-6.10	92.21	110.50
1	A	50	LEU	CB-CG-CD2	-6.07	100.67	111.00
1	B	73	ARG	NE-CZ-NH2	-6.02	117.29	120.30
1	A	388	ARG	NE-CZ-NH1	-6.02	117.29	120.30
1	C	132	MET	CG-SD-CE	-6.02	90.57	100.20
1	A	249	VAL	CB-CA-C	-6.00	99.99	111.40
1	D	177	ASP	CB-CG-OD1	6.00	123.70	118.30
1	C	456	LEU	CB-CG-CD1	5.99	121.19	111.00
1	B	39	ASP	CB-CG-OD1	5.97	123.67	118.30
1	C	419	LEU	CB-CG-CD2	-5.96	100.86	111.00
1	D	31	MET	CA-CB-CG	-5.96	103.17	113.30
1	A	415	VAL	CB-CA-C	-5.95	100.09	111.40
1	D	385	ARG	NE-CZ-NH2	-5.93	117.33	120.30
1	C	369	LEU	CA-CB-CG	-5.91	101.70	115.30
1	A	310	MET	CG-SD-CE	-5.90	90.76	100.20
1	D	233	ILE	CG1-CB-CG2	5.89	124.37	111.40
1	A	271	ARG	CB-CA-C	5.89	122.17	110.40
1	C	124	LEU	CB-CG-CD1	-5.86	101.05	111.00
1	D	51	ARG	NE-CZ-NH2	5.83	123.22	120.30
1	B	369	LEU	CB-CG-CD2	-5.82	101.11	111.00
1	C	343	LEU	CA-CB-CG	-5.82	101.92	115.30
1	D	419	LEU	CB-CG-CD1	5.80	120.86	111.00
1	A	75	MET	CA-CB-CG	-5.78	103.47	113.30
1	C	466	SER	N-CA-CB	-5.76	101.86	110.50
1	B	339	MET	CG-SD-CE	5.76	109.41	100.20
1	D	32	ARG	NE-CZ-NH1	5.75	123.18	120.30
1	D	266	LYS	CD-CE-NZ	-5.75	98.47	111.70
1	C	416	VAL	CB-CA-C	-5.70	100.58	111.40
1	D	265	GLU	CA-CB-CG	5.68	125.89	113.40
1	A	65	LEU	CB-CG-CD1	-5.67	101.36	111.00
1	A	145	LYS	CB-CG-CD	5.67	126.33	111.60
1	B	385	ARG	NE-CZ-NH1	-5.66	117.47	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	77	LEU	CB-CG-CD2	-5.64	101.40	111.00
1	A	154	GLU	OE1-CD-OE2	5.64	130.07	123.30
1	D	307	ASP	CB-CA-C	-5.62	99.16	110.40
1	A	188	PHE	CB-CA-C	-5.54	99.31	110.40
1	A	418	GLN	N-CA-CB	5.54	120.57	110.60
1	A	65	LEU	N-CA-C	-5.52	96.09	111.00
1	A	210	HIS	CB-CA-C	-5.52	99.36	110.40
1	D	416	VAL	CB-CA-C	-5.52	100.92	111.40
1	A	342	ARG	N-CA-C	-5.51	96.11	111.00
1	D	1	MET	CA-CB-CG	5.50	122.66	113.30
1	C	132	MET	N-CA-CB	5.49	120.48	110.60
1	A	309	VAL	CA-CB-CG1	5.49	119.13	110.90
1	B	223	ASN	N-CA-CB	-5.48	100.74	110.60
1	C	167	LEU	CB-CG-CD1	5.47	120.30	111.00
1	D	423	ILE	N-CA-C	-5.47	96.24	111.00
1	C	269	ARG	NE-CZ-NH1	-5.45	117.57	120.30
1	C	6	ILE	CB-CA-C	-5.45	100.71	111.60
1	D	3	LYS	CD-CE-NZ	-5.43	99.20	111.70
1	B	231	ASP	CB-CG-OD1	5.43	123.19	118.30
1	C	311	LEU	CB-CG-CD1	-5.42	101.78	111.00
1	D	415	VAL	CB-CA-C	-5.42	101.10	111.40
1	B	249	VAL	CB-CA-C	-5.42	101.10	111.40
1	A	145	LYS	N-CA-C	-5.42	96.37	111.00
1	B	73	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	B	304	ASP	CB-CA-C	-5.38	99.63	110.40
1	A	218	ILE	CB-CA-C	-5.38	100.85	111.60
1	D	204	ARG	NE-CZ-NH1	-5.38	117.61	120.30
1	B	125	VAL	CG1-CB-CG2	-5.36	102.32	110.90
1	A	66	ASP	O-C-N	5.36	131.28	122.70
1	B	116	ASP	CB-CG-OD1	5.36	123.12	118.30
1	D	46	ARG	N-CA-CB	-5.34	100.98	110.60
1	D	393	ASP	CB-CG-OD2	5.34	123.10	118.30
1	C	250	GLU	OE1-CD-OE2	5.33	129.70	123.30
1	C	5	LYS	CD-CE-NZ	5.33	123.95	111.70
1	C	195	ARG	N-CA-C	5.32	125.37	111.00
1	B	372	PRO	C-N-CA	-5.32	108.41	121.70
1	A	419	LEU	CB-CG-CD2	-5.31	101.97	111.00
1	C	308	ALA	CA-C-N	-5.29	105.55	117.20
1	B	263	MET	CG-SD-CE	-5.29	91.73	100.20
1	B	240	ILE	CG1-CB-CG2	5.29	123.04	111.40
1	A	8	CYS	CB-CA-C	-5.29	99.83	110.40
1	B	35	PHE	CB-CA-C	5.28	120.97	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	234	LEU	CB-CG-CD1	5.27	119.96	111.00
1	A	117	LEU	CA-CB-CG	5.25	127.38	115.30
1	A	134	VAL	CB-CA-C	-5.25	101.42	111.40
1	B	99	VAL	CB-CA-C	-5.25	101.43	111.40
1	D	303	LEU	CB-CG-CD1	5.23	119.89	111.00
1	A	369	LEU	CA-CB-CG	-5.23	103.27	115.30
1	A	195	ARG	CB-CA-C	-5.23	99.94	110.40
1	A	311	LEU	CB-CG-CD1	-5.22	102.12	111.00
1	C	110	TYR	CA-C-N	-5.22	105.72	117.20
1	C	195	ARG	CB-CA-C	-5.22	99.96	110.40
1	C	126	ASP	CB-CG-OD1	5.22	123.00	118.30
1	C	452	VAL	CB-CA-C	-5.21	101.50	111.40
1	C	292	ASP	CB-CG-OD2	-5.20	113.62	118.30
1	C	227	LEU	CB-CG-CD2	-5.19	102.18	111.00
1	B	388	ARG	NE-CZ-NH1	-5.17	117.72	120.30
1	C	261	LYS	CD-CE-NZ	5.17	123.58	111.70
1	A	292	ASP	CB-CG-OD1	5.16	122.95	118.30
1	D	275	ILE	O-C-N	5.16	130.96	122.70
1	B	19	MET	CG-SD-CE	-5.16	91.94	100.20
1	A	47	ILE	CB-CA-C	-5.15	101.30	111.60
1	B	253	VAL	CA-CB-CG2	-5.14	103.19	110.90
1	D	273	VAL	N-CA-C	5.14	124.88	111.00
1	A	304	ASP	CB-CA-C	-5.13	100.14	110.40
1	C	309	VAL	C-N-CA	-5.13	108.88	121.70
1	C	234	LEU	CB-CG-CD1	5.13	119.72	111.00
1	D	5	LYS	CD-CE-NZ	5.13	123.49	111.70
1	B	198	SER	N-CA-CB	-5.12	102.81	110.50
1	B	337	ARG	CA-CB-CG	5.12	124.67	113.40
1	C	193	PHE	CB-CA-C	5.12	120.65	110.40
1	B	1	MET	CB-CG-SD	5.11	127.73	112.40
1	D	75	MET	CG-SD-CE	5.11	108.38	100.20
1	D	419	LEU	CB-CA-C	5.11	119.91	110.20
1	B	418	GLN	N-CA-CB	5.10	119.78	110.60
1	C	451	MET	CG-SD-CE	-5.10	92.05	100.20
1	D	336	ASP	CB-CG-OD1	-5.10	113.71	118.30
1	C	292	ASP	CB-CA-C	-5.09	100.22	110.40
1	D	397	LEU	CB-CA-C	-5.08	100.54	110.20
1	C	425	SER	CB-CA-C	-5.08	100.45	110.10
1	D	189	VAL	N-CA-C	-5.07	97.30	111.00
1	B	390	TYR	CA-CB-CG	-5.06	103.78	113.40
1	B	339	MET	CA-CB-CG	-5.06	104.70	113.30
1	D	85	LEU	CB-CG-CD2	5.05	119.59	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	418	GLN	N-CA-CB	5.05	119.68	110.60
1	A	216	HIS	CB-CA-C	-5.04	100.31	110.40
1	D	425	SER	CB-CA-C	-5.02	100.56	110.10
1	A	358	VAL	CA-CB-CG2	-5.02	103.38	110.90

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	3307	0	3346	223	0
1	B	3307	0	3346	204	0
1	C	3307	0	3346	252	1
1	D	3307	0	3346	206	1
2	A	5	0	0	1	0
2	B	5	0	0	2	0
2	C	5	0	0	3	0
2	D	5	0	0	1	0
3	A	24	0	0	4	0
3	B	35	0	0	11	0
3	C	29	0	0	13	0
3	D	38	0	0	7	0
All	All	13374	0	13384	880	1

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 33.

All (880) 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:A:163:VAL:HG12	1:A:165:ILE:HD12	1.36	1.08
1:B:50:LEU:HD23	1:B:63:ILE:HD11	1.38	1.06
1:C:170:LEU:HD11	1:C:178:LEU:HD12	1.40	1.04
1:C:92:THR:HB	1:C:105:MET:HB2	1.38	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:409:LEU:HB2	3:C:2024:HOH:O	1.57	1.01
1:C:170:LEU:HD13	1:C:175:LYS:HG2	1.43	0.99
1:C:95:THR:HB	1:C:140:ASN:HB2	1.40	0.99
1:A:75:MET:HE2	1:A:97:LYS:HA	1.44	0.96
1:C:355:THR:HG23	1:C:462:THR:HB	1.48	0.95
1:C:132:MET:HA	1:C:147:LEU:HD22	1.52	0.92
1:C:132:MET:CA	1:C:147:LEU:HD22	2.01	0.91
1:B:67:THR:HG22	1:B:192:SER:HB2	1.50	0.90
1:A:193:PHE:CD2	1:A:195:ARG:HD2	2.10	0.86
1:B:268:ILE:HD13	1:B:391:PHE:CZ	2.11	0.85
1:C:170:LEU:CD2	1:C:174:ASP:HB3	2.06	0.85
1:C:14:THR:HA	1:C:19:MET:HG2	1.57	0.85
1:D:86:LYS:O	1:D:89:GLN:HG2	1.76	0.85
1:D:10:ILE:HG22	1:D:46:ARG:HD2	1.59	0.84
1:C:170:LEU:HD22	1:C:174:ASP:HB3	1.60	0.83
1:D:124:LEU:HD12	1:D:161:PRO:HD3	1.61	0.83
1:D:72:ILE:HG23	1:D:110:TYR:HB3	1.58	0.83
1:D:154:GLU:O	1:D:156:LYS:HE2	1.77	0.83
1:C:117:LEU:HD11	1:C:160:LEU:HD22	1.61	0.82
1:B:25:ASP:OD1	1:B:59:LYS:NZ	2.12	0.82
1:C:124:LEU:HD11	1:C:161:PRO:HG3	1.62	0.81
1:A:75:MET:HG3	1:A:107:ALA:O	1.81	0.81
1:A:404:LYS:O	1:A:408:GLN:HG3	1.81	0.81
1:D:230:PHE:CE2	1:D:263:MET:HG2	2.16	0.80
1:C:154:GLU:HA	3:C:2010:HOH:O	1.81	0.80
1:D:264:ILE:O	1:D:268:ILE:HG13	1.81	0.80
1:C:76:LYS:HE3	3:C:2002:HOH:O	1.81	0.80
1:C:326:SER:O	1:C:330:THR:HG23	1.81	0.80
1:C:75:MET:HB2	3:C:2003:HOH:O	1.81	0.80
1:D:355:THR:HG23	1:D:462:THR:HB	1.65	0.79
1:C:411:LEU:HG	3:C:2025:HOH:O	1.82	0.79
1:A:373:LEU:HD12	1:A:395:THR:O	1.83	0.78
1:A:193:PHE:CE2	1:A:195:ARG:HD2	2.19	0.77
1:B:449:VAL:HG21	1:B:470:LEU:HD11	1.64	0.77
1:C:187:ASP:HA	1:C:404:LYS:HE3	1.67	0.77
1:D:10:ILE:HG12	1:D:31:MET:HG3	1.65	0.77
1:A:324:ALA:O	1:A:327:ILE:HG22	1.85	0.76
1:C:132:MET:N	1:C:147:LEU:HD22	2.00	0.76
1:C:78:GLU:HG3	1:C:101:GLY:O	1.84	0.76
1:C:170:LEU:HD11	1:C:178:LEU:CD1	2.15	0.76
1:B:11:GLY:HA2	1:B:46:ARG:NH1	1.99	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:326:SER:O	1:B:330:THR:HG23	1.86	0.76
1:C:134:VAL:HA	1:C:144:CYS:SG	2.26	0.76
1:A:10:ILE:HG12	1:A:31:MET:HG3	1.67	0.76
1:D:124:LEU:HD11	1:D:161:PRO:HG3	1.68	0.76
1:B:167:LEU:HB3	1:B:168:PRO:HD2	1.68	0.75
1:A:165:ILE:HG22	1:A:167:LEU:H	1.51	0.75
1:C:170:LEU:HD21	1:C:178:LEU:HD11	1.67	0.75
1:C:430:TYR:O	1:C:434:LYS:HG3	1.86	0.75
1:B:67:THR:CG2	1:B:192:SER:HB2	2.15	0.75
1:B:230:PHE:CE2	1:B:263:MET:HG2	2.21	0.75
1:A:208:LYS:HD2	3:A:2014:HOH:O	1.88	0.74
1:C:273:VAL:HG12	3:C:2019:HOH:O	1.86	0.74
1:D:167:LEU:O	1:D:195:ARG:NH2	2.21	0.74
1:C:241:MET:HE1	1:C:310:MET:HE1	1.69	0.73
1:C:11:GLY:HA2	1:C:46:ARG:NH1	2.03	0.73
1:B:268:ILE:HD13	1:B:391:PHE:HZ	1.52	0.73
1:C:77:LEU:HG	1:C:154:GLU:HG2	1.70	0.73
1:B:17:GLU:HG2	1:B:49:ASN:HB3	1.70	0.73
1:C:378:THR:OG1	2:C:703:SO4:O1	2.05	0.73
1:B:50:LEU:HD23	1:B:63:ILE:CD1	2.18	0.72
1:D:78:GLU:HG3	1:D:101:GLY:O	1.89	0.72
1:C:264:ILE:O	1:C:268:ILE:HG13	1.88	0.72
1:A:3:LYS:NZ	1:A:393:ASP:O	2.17	0.72
1:C:75:MET:CE	1:C:97:LYS:HG2	2.19	0.72
1:A:254:GLU:N	1:A:254:GLU:OE1	2.22	0.72
1:A:110:TYR:CD1	1:A:167:LEU:HD21	2.24	0.72
1:A:171:ALA:N	1:A:174:ASP:HB2	2.05	0.72
1:A:170:LEU:HD22	1:A:174:ASP:HB3	1.71	0.72
1:D:165:ILE:HG22	1:D:167:LEU:H	1.55	0.71
1:A:167:LEU:O	1:A:195:ARG:NH2	2.23	0.71
1:C:110:TYR:CD1	1:C:167:LEU:HD21	2.25	0.71
1:D:14:THR:HA	1:D:19:MET:HG2	1.70	0.71
1:D:276:THR:HG21	1:D:301:ALA:CB	2.21	0.71
1:D:276:THR:HG21	1:D:301:ALA:HB1	1.73	0.71
1:A:51:ARG:NH2	1:A:184:GLN:O	2.23	0.71
1:B:430:TYR:O	1:B:434:LYS:HG3	1.89	0.70
1:D:426:THR:HG22	1:D:430:TYR:CE2	2.26	0.70
1:B:67:THR:HG22	1:B:192:SER:CB	2.21	0.70
1:C:94:THR:CG2	1:C:107:ALA:HA	2.22	0.70
1:B:49:ASN:O	1:B:53:VAL:HG23	1.92	0.70
1:C:181:GLY:O	1:C:185:GLY:N	2.25	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:431:ARG:HD3	1:A:432:LEU:N	2.07	0.70
1:B:355:THR:HG23	1:B:462:THR:HB	1.72	0.70
1:C:171:ALA:HB3	1:C:174:ASP:CG	2.12	0.70
1:A:273:VAL:HG21	1:A:411:LEU:HD23	1.73	0.70
1:D:383:SER:HB3	1:D:462:THR:OG1	1.92	0.69
1:B:253:VAL:HG23	1:B:254:GLU:H	1.57	0.69
1:D:124:LEU:HB2	1:D:159:ASN:HB2	1.74	0.69
1:B:253:VAL:HG23	1:B:254:GLU:N	2.08	0.69
1:D:193:PHE:CD2	1:D:195:ARG:HD2	2.29	0.68
1:A:203:ILE:O	1:A:207:LEU:HG	1.93	0.68
1:A:204:ARG:NH1	3:A:2012:HOH:O	2.24	0.68
1:C:153:GLY:O	1:C:156:LYS:HG2	1.92	0.68
1:B:70:PRO:HB2	1:B:167:LEU:HD13	1.73	0.68
1:A:189:VAL:HG23	1:A:215:ILE:HG21	1.74	0.68
1:B:358:VAL:HG21	1:B:463:ASN:HA	1.75	0.68
1:B:380:GLY:N	2:B:702:SO4:O2	2.22	0.68
1:C:124:LEU:CD1	1:C:161:PRO:HG3	2.24	0.68
1:D:219:SER:HB2	1:D:240:ILE:HD13	1.75	0.68
1:B:15:GLU:HB3	1:B:46:ARG:HD3	1.76	0.67
1:C:119:VAL:HG13	1:C:134:VAL:O	1.94	0.67
1:D:188:PHE:CD1	1:D:216:HIS:HB2	2.29	0.67
1:B:268:ILE:HG21	1:B:391:PHE:HE1	1.57	0.67
1:A:181:GLY:O	1:A:185:GLY:N	2.28	0.67
1:C:253:VAL:HG23	1:C:254:GLU:OE1	1.95	0.67
1:A:388:ARG:HB2	1:A:396:ILE:CD1	2.25	0.67
1:C:391:PHE:N	1:C:392:PRO:HD3	2.10	0.67
1:C:378:THR:HA	2:C:703:SO4:O1	1.95	0.66
1:A:87:ALA:N	1:A:149:ASN:OD1	2.27	0.66
1:A:440:SER:HB3	1:A:442:LEU:HG	1.77	0.66
1:B:18:GLU:O	1:B:22:LYS:HG3	1.95	0.66
1:D:132:MET:HA	1:D:147:LEU:HG	1.75	0.66
1:D:312:SER:O	1:D:314:GLU:N	2.29	0.66
1:C:321:PRO:HD2	1:C:322:LEU:H	1.59	0.66
1:A:43:HIS:O	1:A:47:ILE:HG13	1.94	0.66
1:D:94:THR:HG23	1:D:107:ALA:HB2	1.78	0.66
1:C:94:THR:HG23	1:C:107:ALA:HA	1.75	0.66
1:D:67:THR:HG22	1:D:192:SER:HB2	1.78	0.66
1:D:360:ARG:NH2	1:D:364:GLU:OE1	2.27	0.66
1:C:170:LEU:HD22	1:C:174:ASP:CB	2.25	0.65
1:C:95:THR:HB	1:C:140:ASN:CB	2.24	0.65
1:A:86:LYS:O	1:A:89:GLN:HG2	1.94	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:11:GLY:O	1:B:15:GLU:N	2.29	0.65
1:C:373:LEU:HD12	1:C:395:THR:O	1.95	0.65
1:B:268:ILE:HD13	1:B:391:PHE:CE1	2.32	0.65
1:D:75:MET:HE2	1:D:97:LYS:HA	1.79	0.65
1:C:207:LEU:O	1:C:212:GLY:N	2.28	0.65
1:A:163:VAL:HG12	1:A:165:ILE:CD1	2.20	0.65
1:A:94:THR:HG23	1:A:107:ALA:HB2	1.79	0.65
1:D:124:LEU:HD12	1:D:161:PRO:CD	2.27	0.65
1:D:47:ILE:O	1:D:51:ARG:HG2	1.97	0.65
1:A:171:ALA:H	1:A:174:ASP:HB2	1.62	0.64
1:B:379:GLN:N	2:B:702:SO4:O2	2.29	0.64
1:A:374:ILE:O	1:A:376:VAL:HG23	1.97	0.64
1:D:39:ASP:OD1	1:D:42:GLU:HG3	1.98	0.64
1:D:69:GLY:HA2	1:D:174:ASP:OD2	1.97	0.64
1:C:93:PHE:HB2	1:C:142:VAL:HB	1.79	0.64
1:A:163:VAL:CG1	1:A:165:ILE:HD12	2.22	0.64
1:D:67:THR:HG21	3:D:2014:HOH:O	1.96	0.64
1:A:253:VAL:HG23	1:A:254:GLU:H	1.62	0.64
1:C:75:MET:HE1	1:C:97:LYS:HG2	1.78	0.64
1:C:373:LEU:HA	1:C:394:ALA:HB1	1.80	0.64
1:C:415:VAL:HG12	1:C:416:VAL:N	2.11	0.64
1:C:117:LEU:HD13	1:C:160:LEU:HD13	1.79	0.64
1:B:117:LEU:HD13	1:B:160:LEU:HD13	1.80	0.64
1:B:372:PRO:HD2	1:B:448:VAL:O	1.97	0.64
1:C:77:LEU:N	1:C:154:GLU:OE2	2.28	0.64
1:A:326:SER:O	1:A:330:THR:HG23	1.98	0.64
1:B:342:ARG:HD2	1:B:391:PHE:CD1	2.33	0.63
1:D:12:PRO:HD3	1:D:46:ARG:HH12	1.61	0.63
1:A:73:ARG:O	1:A:108:VAL:HA	1.98	0.63
1:A:75:MET:CE	1:A:97:LYS:HA	2.24	0.63
1:A:170:LEU:HD11	1:A:178:LEU:HD12	1.80	0.63
1:D:16:SER:OG	1:D:19:MET:HB2	1.99	0.63
1:C:10:ILE:HG22	1:C:11:GLY:N	2.13	0.63
1:C:235:GLU:O	1:C:272:LYS:NZ	2.31	0.63
1:B:114:THR:OG1	1:B:115:THR:N	2.28	0.63
1:A:329:ALA:O	1:A:332:CYS:N	2.30	0.63
1:A:186:VAL:O	1:A:215:ILE:HG12	1.99	0.63
1:B:10:ILE:CD1	1:B:23:MET:HE1	2.28	0.63
1:A:132:MET:HA	1:A:147:LEU:HG	1.80	0.63
1:D:124:LEU:CD1	1:D:161:PRO:HG3	2.29	0.63
1:B:10:ILE:HG12	1:B:31:MET:HG3	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:170:LEU:HD11	1:A:178:LEU:CD1	2.28	0.63
1:B:64:LEU:HD21	1:B:190:ALA:HB2	1.80	0.63
1:D:133:GLU:HG2	3:D:2009:HOH:O	1.99	0.62
1:A:257:ILE:HD11	3:A:2017:HOH:O	1.99	0.62
1:B:240:ILE:O	1:B:274:VAL:HA	2.00	0.62
1:C:170:LEU:CD1	1:C:175:LYS:HG2	2.25	0.62
1:D:72:ILE:HG23	1:D:110:TYR:CB	2.27	0.62
1:A:7:VAL:HG11	1:A:310:MET:HE2	1.80	0.62
1:A:23:MET:HB3	1:A:28:MET:HE2	1.82	0.62
1:B:174:ASP:O	1:B:178:LEU:HG	2.00	0.62
1:B:241:MET:HE2	1:B:310:MET:HE3	1.81	0.62
1:A:78:GLU:HG3	1:A:101:GLY:O	1.99	0.62
1:B:5:LYS:HG3	1:B:410:VAL:O	2.00	0.61
1:C:76:LYS:O	1:C:101:GLY:N	2.29	0.61
1:B:87:ALA:N	1:B:149:ASN:OD1	2.29	0.61
1:C:449:VAL:HG21	1:C:470:LEU:HD11	1.83	0.61
1:B:216:HIS:ND1	3:B:2017:HOH:O	2.24	0.61
1:D:321:PRO:O	1:D:325:VAL:HG23	2.01	0.61
1:B:391:PHE:N	1:B:392:PRO:HD3	2.16	0.61
1:C:312:SER:O	1:C:314:GLU:N	2.34	0.61
1:D:126:ASP:HB2	1:D:156:LYS:HG3	1.82	0.61
1:A:253:VAL:HG23	1:A:254:GLU:N	2.16	0.61
1:A:7:VAL:CG1	1:A:310:MET:HE2	2.31	0.61
1:D:94:THR:HG23	1:D:107:ALA:CB	2.30	0.60
1:D:195:ARG:O	1:D:229:ASN:ND2	2.31	0.60
1:A:171:ALA:HB3	1:A:174:ASP:CG	2.22	0.60
1:A:47:ILE:O	1:A:51:ARG:HG3	2.02	0.60
1:D:373:LEU:HD12	1:D:395:THR:O	2.01	0.60
1:A:92:THR:HG23	1:A:143:ILE:HD13	1.81	0.60
1:B:379:GLN:O	1:B:405:THR:HG21	2.01	0.60
1:D:170:LEU:HD23	3:D:2014:HOH:O	2.02	0.60
1:B:297:ASP:OD1	3:B:2027:HOH:O	2.16	0.60
1:A:321:PRO:HD2	1:A:322:LEU:H	1.65	0.60
1:D:273:VAL:HG12	1:D:307:ASP:CG	2.22	0.60
1:D:342:ARG:HD2	1:D:391:PHE:CD1	2.36	0.60
1:B:10:ILE:HD12	1:B:23:MET:HE1	1.84	0.60
1:D:165:ILE:N	1:D:165:ILE:HD12	2.17	0.60
1:B:244:ARG:HD2	1:B:256:VAL:CG1	2.31	0.60
1:D:65:LEU:HD23	1:D:65:LEU:C	2.22	0.60
1:D:126:ASP:CB	1:D:156:LYS:HG3	2.31	0.60
1:D:244:ARG:HD2	1:D:256:VAL:CG1	2.32	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:132:MET:HB3	1:C:146:VAL:HA	1.83	0.60
1:C:240:ILE:CG2	1:C:241:MET:N	2.65	0.60
1:C:172:GLU:OE1	1:C:172:GLU:HA	2.01	0.60
1:D:297:ASP:OD1	3:D:2029:HOH:O	2.16	0.60
1:B:230:PHE:CE2	1:B:263:MET:CG	2.85	0.59
1:B:171:ALA:O	1:B:174:ASP:N	2.35	0.59
1:D:302:ILE:HB	1:D:335:THR:HG21	1.85	0.59
1:B:312:SER:O	1:B:314:GLU:N	2.36	0.59
1:B:403:GLU:HG2	1:B:419:LEU:HD22	1.84	0.59
1:C:170:LEU:HD23	1:C:174:ASP:HB3	1.81	0.59
1:C:152:LEU:HD12	1:C:153:GLY:O	2.02	0.59
1:D:51:ARG:NH2	1:D:184:GLN:O	2.36	0.59
1:B:67:THR:HG22	1:B:192:SER:H	1.68	0.59
1:B:10:ILE:CG1	1:B:31:MET:HG3	2.33	0.59
1:D:92:THR:HG23	1:D:143:ILE:HD13	1.84	0.59
1:C:77:LEU:HG	1:C:154:GLU:CG	2.32	0.59
1:B:67:THR:CG2	1:B:192:SER:H	2.16	0.58
1:C:136:ALA:HB3	1:C:143:ILE:HB	1.85	0.58
1:A:321:PRO:O	1:A:325:VAL:HG23	2.02	0.58
1:C:195:ARG:O	1:C:225:GLU:HG2	2.02	0.58
1:D:302:ILE:O	1:D:305:GLY:N	2.34	0.58
1:D:422:GLU:HG3	1:D:423:ILE:N	2.19	0.58
1:A:73:ARG:NH1	1:A:155:ASN:O	2.36	0.58
1:B:343:LEU:O	1:B:360:ARG:HD2	2.03	0.58
1:D:253:VAL:HG23	1:D:254:GLU:N	2.18	0.58
1:C:7:VAL:HG11	1:C:310:MET:HE2	1.85	0.58
1:D:231:ASP:OD1	1:D:266:LYS:NZ	2.35	0.58
1:A:422:GLU:HG3	1:A:423:ILE:N	2.19	0.58
1:C:452:VAL:HG12	1:C:453:SER:N	2.18	0.58
1:A:216:HIS:HB3	1:A:238:ASP:CB	2.34	0.58
1:B:449:VAL:CG2	1:B:470:LEU:HD11	2.34	0.58
1:B:171:ALA:O	1:B:174:ASP:HB2	2.04	0.58
1:D:262:MET:SD	1:D:266:LYS:HE3	2.44	0.57
1:C:388:ARG:HB2	1:C:396:ILE:CD1	2.34	0.57
1:A:124:LEU:CD1	1:A:161:PRO:HG3	2.34	0.57
1:C:170:LEU:HD13	1:C:175:LYS:CG	2.29	0.57
1:D:15:GLU:HB3	1:D:46:ARG:HD3	1.85	0.57
1:A:23:MET:CB	1:A:28:MET:HE2	2.34	0.57
1:A:452:VAL:CG1	1:A:462:THR:HG21	2.35	0.57
1:B:391:PHE:N	1:B:392:PRO:CD	2.66	0.57
1:B:117:LEU:HD11	1:B:160:LEU:HD22	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:422:GLU:HG3	1:B:423:ILE:N	2.19	0.57
1:C:230:PHE:CE1	1:C:263:MET:HG2	2.40	0.57
1:A:67:THR:O	1:A:192:SER:OG	2.23	0.57
1:C:67:THR:O	1:C:192:SER:OG	2.21	0.57
1:B:413:LYS:O	1:B:415:VAL:N	2.37	0.57
1:C:10:ILE:CG1	1:C:31:MET:HG3	2.34	0.57
1:B:65:LEU:C	1:B:65:LEU:HD23	2.25	0.57
1:D:159:ASN:CG	1:D:249:VAL:HG11	2.26	0.57
1:A:10:ILE:CG1	1:A:31:MET:HG3	2.35	0.57
1:C:10:ILE:HG13	1:C:31:MET:HG3	1.87	0.57
1:A:388:ARG:HD3	1:A:388:ARG:C	2.25	0.57
1:C:241:MET:CE	1:C:310:MET:HE1	2.33	0.57
1:D:75:MET:CE	1:D:97:LYS:HA	2.35	0.57
1:B:403:GLU:HG2	1:B:419:LEU:CD2	2.35	0.57
1:A:378:THR:OG1	1:A:381:GLY:HA2	2.05	0.57
1:B:132:MET:HA	1:B:147:LEU:HG	1.85	0.57
1:A:195:ARG:HB3	1:A:225:GLU:HG2	1.86	0.57
1:A:187:ASP:HA	1:A:404:LYS:HE3	1.87	0.57
1:C:30:VAL:HG22	1:C:62:ALA:HB3	1.86	0.57
1:A:171:ALA:H	1:A:174:ASP:CB	2.17	0.57
1:C:35:PHE:CZ	1:C:43:HIS:CD2	2.92	0.57
1:C:65:LEU:HD23	1:C:65:LEU:C	2.24	0.57
1:C:274:VAL:HG13	1:C:274:VAL:O	2.03	0.56
1:D:253:VAL:HG23	1:D:254:GLU:H	1.69	0.56
1:D:343:LEU:O	1:D:360:ARG:HD2	2.05	0.56
1:C:431:ARG:HD3	1:C:432:LEU:N	2.21	0.56
1:B:9:THR:HA	1:B:32:ARG:HB3	1.85	0.56
1:B:65:LEU:HD23	1:B:66:ASP:N	2.20	0.56
1:C:417:PRO:HB3	3:C:2024:HOH:O	2.06	0.56
1:A:73:ARG:O	1:A:109:THR:N	2.37	0.56
1:C:400:THR:O	1:C:420:VAL:N	2.36	0.56
1:C:73:ARG:HD3	1:C:155:ASN:OD1	2.06	0.56
1:A:466:SER:OG	1:A:468:HIS:NE2	2.38	0.56
1:B:51:ARG:NH2	1:B:184:GLN:O	2.39	0.56
1:A:72:ILE:HG23	1:A:110:TYR:HB3	1.88	0.55
1:A:360:ARG:NH2	1:A:364:GLU:OE1	2.39	0.55
1:A:341:SER:HA	1:A:391:PHE:O	2.05	0.55
1:D:94:THR:CG2	1:D:107:ALA:HB2	2.35	0.55
1:B:240:ILE:HG23	1:B:241:MET:N	2.21	0.55
1:D:358:VAL:HG21	1:D:463:ASN:HA	1.88	0.55
1:D:359:CYS:O	1:D:363:VAL:HG23	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:388:ARG:C	1:B:388:ARG:HD3	2.27	0.55
1:D:10:ILE:CG1	1:D:31:MET:HG3	2.36	0.55
1:C:369:LEU:O	1:C:370:ASP:HB2	2.06	0.55
1:B:81:ASN:HA	3:B:2004:HOH:O	2.06	0.55
1:D:443:ALA:C	1:D:444:HIS:CD2	2.80	0.55
1:C:195:ARG:N	1:C:195:ARG:HD3	2.22	0.55
1:A:165:ILE:N	1:A:165:ILE:HD12	2.22	0.55
1:C:244:ARG:HD2	1:C:256:VAL:HG12	1.89	0.55
1:A:18:GLU:OE1	1:A:18:GLU:N	2.40	0.55
1:D:19:MET:O	1:D:23:MET:HG2	2.07	0.55
1:A:358:VAL:HG21	1:A:463:ASN:HA	1.88	0.55
1:C:363:VAL:O	1:C:366:ALA:HB3	2.06	0.55
1:B:82:ASP:N	3:B:2004:HOH:O	2.28	0.54
1:B:96:ASP:OD2	1:B:99:VAL:HG23	2.07	0.54
1:D:140:ASN:OD1	1:D:141:LYS:HE2	2.08	0.54
1:B:39:ASP:OD1	1:B:42:GLU:HG3	2.07	0.54
1:A:430:TYR:O	1:A:434:LYS:HG3	2.07	0.54
1:D:327:ILE:HG23	1:D:328:MET:N	2.21	0.54
1:A:14:THR:HA	1:A:19:MET:HG2	1.89	0.54
1:D:178:LEU:HD12	1:D:206:HIS:CD2	2.43	0.54
1:A:379:GLN:O	1:A:405:THR:HG21	2.07	0.54
1:C:70:PRO:HB2	1:C:167:LEU:HD12	1.89	0.54
1:D:190:ALA:HA	1:D:218:ILE:HB	1.89	0.54
1:B:404:LYS:HE2	3:B:2032:HOH:O	2.07	0.54
1:A:312:SER:O	1:A:314:GLU:N	2.40	0.54
1:D:154:GLU:HA	3:D:2011:HOH:O	2.06	0.54
1:A:92:THR:O	1:A:105:MET:HG3	2.07	0.54
1:B:312:SER:C	1:B:314:GLU:H	2.11	0.54
1:B:73:ARG:N	1:B:109:THR:OG1	2.39	0.54
1:A:50:LEU:O	1:A:54:MET:HG3	2.07	0.54
1:C:124:LEU:HD11	1:C:161:PRO:CG	2.34	0.54
1:B:327:ILE:HD11	1:D:253:VAL:HG21	1.89	0.54
1:D:163:VAL:HG12	1:D:164:SER:N	2.22	0.54
1:A:378:THR:OG1	1:A:381:GLY:CA	2.56	0.54
1:C:216:HIS:CD2	1:C:408:GLN:NE2	2.76	0.54
1:C:110:TYR:CE1	1:C:167:LEU:CD2	2.91	0.54
1:A:10:ILE:HG22	1:A:11:GLY:N	2.23	0.54
1:B:383:SER:HB3	1:B:462:THR:OG1	2.08	0.54
1:A:341:SER:HB3	1:A:367:GLU:OE2	2.07	0.54
1:C:105:MET:HG3	1:C:106:VAL:N	2.22	0.54
1:A:448:VAL:HG12	1:A:449:VAL:N	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:161:PRO:O	1:B:163:VAL:N	2.41	0.54
1:D:5:LYS:HA	1:D:29:ASN:OD1	2.08	0.54
1:D:274:VAL:O	1:D:274:VAL:HG13	2.07	0.54
1:B:359:CYS:O	1:B:363:VAL:HG23	2.08	0.54
1:C:463:ASN:O	1:D:466:SER:HA	2.08	0.54
1:B:382:LYS:O	1:B:385:ARG:HB2	2.08	0.54
1:C:73:ARG:O	1:C:108:VAL:HG12	2.07	0.53
1:B:135:THR:OG1	1:B:143:ILE:HG22	2.08	0.53
1:B:12:PRO:HD3	1:B:46:ARG:HH12	1.73	0.53
1:A:39:ASP:OD1	1:A:42:GLU:HG3	2.08	0.53
1:A:422:GLU:CG	1:A:423:ILE:N	2.71	0.53
1:A:216:HIS:HB3	1:A:238:ASP:HB2	1.88	0.53
1:B:426:THR:HG22	1:B:430:TYR:CE2	2.43	0.53
1:A:3:LYS:HZ1	1:A:393:ASP:C	2.07	0.53
1:B:431:ARG:HD3	1:B:432:LEU:N	2.24	0.53
1:B:10:ILE:CD1	1:B:23:MET:CE	2.87	0.53
1:B:64:LEU:HD21	1:B:190:ALA:CB	2.39	0.53
1:B:324:ALA:O	1:B:327:ILE:HG22	2.08	0.53
1:C:324:ALA:O	1:C:327:ILE:HG22	2.08	0.53
1:D:378:THR:OG1	1:D:381:GLY:N	2.41	0.53
1:A:355:THR:HG23	1:A:462:THR:HB	1.89	0.53
1:A:237:SER:O	1:A:272:LYS:NZ	2.31	0.53
1:B:268:ILE:CD1	1:B:391:PHE:HZ	2.22	0.53
1:A:383:SER:HB3	1:A:462:THR:OG1	2.09	0.53
1:A:25:ASP:OD1	1:A:59:LYS:NZ	2.24	0.53
1:A:240:ILE:CG2	1:A:241:MET:N	2.71	0.53
1:C:165:ILE:HG22	1:C:167:LEU:H	1.75	0.52
1:D:34:ASN:OD1	1:D:36:SER:HB2	2.08	0.52
1:B:11:GLY:HA2	1:B:46:ARG:HH11	1.73	0.52
1:D:312:SER:C	1:D:314:GLU:H	2.13	0.52
1:C:422:GLU:HG3	1:C:423:ILE:N	2.25	0.52
1:D:391:PHE:N	1:D:392:PRO:CD	2.71	0.52
1:A:31:MET:CE	1:A:33:LEU:HD21	2.39	0.52
1:A:124:LEU:HD11	1:A:161:PRO:CG	2.40	0.52
1:B:377:ALA:HB2	1:B:429:PHE:CE1	2.45	0.52
1:B:19:MET:O	1:B:23:MET:HG3	2.08	0.52
1:C:383:SER:HB3	1:C:462:THR:OG1	2.08	0.52
1:A:268:ILE:HD13	1:A:391:PHE:CE1	2.44	0.52
1:C:302:ILE:HA	1:C:306:THR:HG22	1.92	0.52
1:D:50:LEU:HD23	1:D:63:ILE:HD11	1.90	0.52
1:A:416:VAL:O	1:A:416:VAL:HG12	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:94:THR:CG2	1:A:107:ALA:HB2	2.40	0.52
1:D:230:PHE:CD2	1:D:263:MET:HG2	2.44	0.52
1:A:388:ARG:HB2	1:A:396:ILE:HD12	1.91	0.52
1:B:241:MET:CE	1:B:310:MET:HE3	2.40	0.52
1:B:411:LEU:HD12	1:B:411:LEU:O	2.09	0.52
1:B:191:ALA:O	1:B:220:LYS:HB2	2.10	0.52
1:A:397:LEU:HD12	1:A:416:VAL:O	2.10	0.52
1:C:241:MET:HE2	1:C:310:MET:HE3	1.92	0.52
1:B:244:ARG:HD2	1:B:256:VAL:HG12	1.92	0.52
1:C:251:ILE:HB	1:C:252:PRO:HD2	1.91	0.52
1:D:431:ARG:HD3	1:D:432:LEU:N	2.25	0.52
1:A:77:LEU:HD23	1:A:101:GLY:HA3	1.91	0.52
1:B:366:ALA:HA	1:B:450:VAL:HG21	1.91	0.52
1:B:253:VAL:HG21	1:D:327:ILE:HD11	1.92	0.51
1:A:359:CYS:SG	1:A:386:ALA:HB1	2.50	0.51
1:D:321:PRO:HD2	1:D:322:LEU:H	1.74	0.51
1:C:372:PRO:HD2	1:C:448:VAL:O	2.10	0.51
1:C:175:LYS:HB3	1:C:206:HIS:CE1	2.46	0.51
1:C:110:TYR:O	1:C:113:PHE:HB2	2.11	0.51
1:D:422:GLU:CG	1:D:423:ILE:N	2.74	0.51
1:A:426:THR:HG22	1:A:430:TYR:CE2	2.46	0.51
1:A:244:ARG:HD2	1:A:256:VAL:CG1	2.40	0.51
1:D:9:THR:HA	1:D:32:ARG:HB3	1.92	0.51
1:C:195:ARG:HB3	1:C:225:GLU:CD	2.30	0.51
1:A:401:THR:HG22	1:A:420:VAL:O	2.11	0.51
1:C:105:MET:CG	1:C:106:VAL:N	2.74	0.51
1:B:363:VAL:HG21	1:B:390:TYR:HB2	1.93	0.51
1:D:43:HIS:O	1:D:46:ARG:HB3	2.10	0.51
1:A:440:SER:HB3	1:A:442:LEU:CG	2.40	0.51
1:D:171:ALA:HB3	1:D:174:ASP:CG	2.31	0.51
1:D:385:ARG:O	1:D:388:ARG:N	2.44	0.51
1:B:264:ILE:O	1:B:268:ILE:HG13	2.10	0.51
1:C:241:MET:CE	1:C:310:MET:CE	2.89	0.51
1:D:430:TYR:HD1	1:D:451:MET:SD	2.34	0.51
1:A:136:ALA:HB3	1:A:143:ILE:HB	1.92	0.51
1:C:388:ARG:C	1:C:388:ARG:HD3	2.31	0.51
1:C:110:TYR:CD1	1:C:167:LEU:CD2	2.94	0.51
1:D:119:VAL:HG13	1:D:134:VAL:O	2.10	0.51
1:A:126:ASP:HB3	1:A:129:LEU:HB3	1.93	0.51
1:B:249:VAL:HG12	1:B:249:VAL:O	2.11	0.51
1:A:95:THR:HB	1:A:140:ASN:HB2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:291:THR:O	1:D:294:GLU:HB2	2.10	0.50
1:B:167:LEU:O	1:B:195:ARG:NH2	2.45	0.50
1:C:10:ILE:CG2	1:C:11:GLY:N	2.74	0.50
1:A:124:LEU:HD11	1:A:161:PRO:HG3	1.94	0.50
1:B:77:LEU:N	1:B:154:GLU:HG2	2.27	0.50
1:A:366:ALA:HA	1:A:450:VAL:HG21	1.93	0.50
1:D:365:THR:HG22	1:D:369:LEU:HD12	1.91	0.50
1:A:89:GLN:HG3	1:A:89:GLN:O	2.12	0.50
1:C:373:LEU:CA	1:C:394:ALA:HB1	2.40	0.50
1:B:5:LYS:HB2	1:B:308:ALA:HB2	1.93	0.50
1:D:94:THR:HG22	1:D:107:ALA:HA	1.93	0.50
1:B:160:LEU:HB2	1:B:165:ILE:HD11	1.94	0.50
1:C:359:CYS:O	1:C:363:VAL:HG23	2.12	0.50
1:B:440:SER:C	1:B:442:LEU:H	2.14	0.50
1:C:426:THR:HG22	1:C:430:TYR:CE2	2.47	0.50
1:A:74:THR:OG1	1:A:156:LYS:N	2.42	0.50
1:B:187:ASP:HA	1:B:404:LYS:HE3	1.92	0.50
1:A:298:VAL:O	1:A:301:ALA:N	2.45	0.50
1:B:62:ALA:HA	3:B:2011:HOH:O	2.11	0.50
1:C:391:PHE:N	1:C:392:PRO:CD	2.75	0.50
1:B:251:ILE:HD11	1:B:256:VAL:HG22	1.94	0.50
1:B:327:ILE:CG2	1:B:328:MET:N	2.75	0.50
1:A:422:GLU:CG	1:A:423:ILE:H	2.25	0.50
1:C:78:GLU:HG3	1:C:100:ILE:HG22	1.93	0.49
1:B:422:GLU:CG	1:B:423:ILE:N	2.75	0.49
1:D:440:SER:C	1:D:442:LEU:H	2.14	0.49
1:A:7:VAL:HG11	1:A:310:MET:CE	2.42	0.49
1:B:67:THR:HG22	1:B:192:SER:N	2.26	0.49
1:A:327:ILE:CG2	1:A:328:MET:N	2.75	0.49
1:C:119:VAL:HG13	1:C:135:THR:CA	2.42	0.49
1:B:241:MET:HE1	1:B:310:MET:HE1	1.93	0.49
1:D:336:ASP:O	1:D:338:VAL:N	2.45	0.49
1:B:214:ASN:O	1:B:408:GLN:NE2	2.44	0.49
1:D:110:TYR:O	1:D:113:PHE:HB2	2.12	0.49
1:C:430:TYR:HD1	1:C:451:MET:SD	2.35	0.49
1:D:293:ALA:O	1:D:297:ASP:HB2	2.12	0.49
1:D:254:GLU:OE1	1:D:254:GLU:N	2.34	0.49
1:B:9:THR:OG1	1:B:32:ARG:HD3	2.12	0.49
1:C:222:GLU:O	1:C:223:ASN:HB3	2.13	0.49
1:C:466:SER:OG	1:C:468:HIS:NE2	2.42	0.49
1:D:377:ALA:HB2	1:D:429:PHE:CE1	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:5:LYS:HB2	1:A:308:ALA:HB2	1.95	0.49
1:C:30:VAL:HG21	1:C:411:LEU:HD13	1.95	0.49
1:C:240:ILE:HG23	1:C:241:MET:N	2.28	0.49
1:B:189:VAL:HG23	1:B:215:ILE:HG21	1.95	0.49
1:C:94:THR:CG2	1:C:107:ALA:CA	2.91	0.49
1:D:415:VAL:HG12	1:D:416:VAL:N	2.27	0.49
1:A:426:THR:CG2	1:A:430:TYR:CE2	2.96	0.49
1:B:74:THR:O	1:B:155:ASN:HA	2.13	0.49
1:B:255:GLU:OE2	1:D:334:ARG:NE	2.39	0.49
1:D:382:LYS:HB2	2:D:704:SO4:O1	2.12	0.49
1:C:171:ALA:N	1:C:174:ASP:HB2	2.28	0.49
1:C:94:THR:HG22	1:C:107:ALA:HA	1.92	0.49
1:A:189:VAL:HG23	1:A:215:ILE:CG2	2.42	0.49
1:C:449:VAL:CG2	1:C:470:LEU:HD11	2.41	0.49
1:A:268:ILE:HD13	1:A:391:PHE:CZ	2.47	0.49
1:A:50:LEU:HD23	1:A:63:ILE:HD11	1.94	0.49
1:D:73:ARG:O	1:D:108:VAL:HA	2.12	0.49
1:C:378:THR:CG2	1:C:381:GLY:HA2	2.43	0.49
1:A:171:ALA:O	1:A:174:ASP:HB2	2.12	0.49
1:D:94:THR:CG2	1:D:107:ALA:HA	2.43	0.49
1:B:274:VAL:HG13	1:B:274:VAL:O	2.13	0.49
1:B:360:ARG:NH2	1:B:364:GLU:OE1	2.42	0.49
1:D:163:VAL:CG1	1:D:164:SER:N	2.76	0.49
1:A:112:GLY:O	1:A:115:THR:HB	2.12	0.49
1:C:75:MET:HE2	1:C:97:LYS:HG2	1.95	0.49
1:C:119:VAL:HG13	1:C:135:THR:HA	1.95	0.49
1:B:421:LYS:O	1:B:422:GLU:HB2	2.13	0.49
1:A:235:GLU:O	1:A:272:LYS:NZ	2.45	0.49
1:A:35:PHE:CE1	1:A:65:LEU:HG	2.48	0.49
1:C:207:LEU:HD13	1:C:215:ILE:HG21	1.95	0.48
1:C:43:HIS:O	1:C:47:ILE:HG13	2.12	0.48
1:D:343:LEU:O	1:D:344:GLU:O	2.32	0.48
1:A:431:ARG:C	1:A:431:ARG:HD3	2.33	0.48
1:B:240:ILE:CG2	1:B:241:MET:N	2.76	0.48
1:A:117:LEU:HG	1:A:134:VAL:HG21	1.95	0.48
1:C:239:GLY:O	1:C:240:ILE:HG12	2.13	0.48
1:B:253:VAL:HG23	1:B:254:GLU:OE1	2.13	0.48
1:D:230:PHE:CE2	1:D:263:MET:CG	2.93	0.48
1:B:86:LYS:O	1:B:89:GLN:HG2	2.13	0.48
1:A:65:LEU:HD23	1:A:66:ASP:N	2.29	0.48
1:C:354:ILE:HD13	1:C:354:ILE:HG21	1.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:10:ILE:HD11	1:B:23:MET:CE	2.43	0.48
1:C:378:THR:CA	2:C:703:SO4:O1	2.60	0.48
1:C:153:GLY:C	1:C:156:LYS:HE2	2.33	0.48
1:D:95:THR:HB	1:D:140:ASN:HB2	1.95	0.48
1:C:327:ILE:CG2	1:C:328:MET:N	2.76	0.48
1:B:83:VAL:HG11	1:B:103:SER:N	2.28	0.48
1:C:51:ARG:NH2	1:C:184:GLN:O	2.44	0.48
1:D:327:ILE:CG2	1:D:328:MET:N	2.76	0.48
1:C:312:SER:C	1:C:314:GLU:H	2.15	0.48
1:C:407:HIS:O	1:C:410:VAL:HG23	2.13	0.48
1:A:88:GLY:N	1:A:146:VAL:O	2.47	0.48
1:A:124:LEU:HD12	1:A:161:PRO:HG3	1.96	0.48
1:C:125:VAL:O	1:C:126:ASP:O	2.30	0.48
1:D:449:VAL:N	1:D:468:HIS:O	2.46	0.48
1:D:7:VAL:HG11	1:D:310:MET:HE2	1.96	0.48
1:A:424:THR:HG23	1:A:428:ASP:OD2	2.14	0.48
1:C:110:TYR:CE1	1:C:167:LEU:HD23	2.49	0.48
1:C:132:MET:N	1:C:147:LEU:CD2	2.75	0.48
1:B:86:LYS:HA	1:B:149:ASN:OD1	2.14	0.48
1:A:251:ILE:HD12	1:A:255:GLU:HB2	1.96	0.48
1:C:158:VAL:HG12	1:C:159:ASN:N	2.29	0.48
1:B:269:ARG:HA	1:B:389:LYS:HE3	1.96	0.48
1:A:327:ILE:HG23	1:A:328:MET:N	2.29	0.47
1:B:193:PHE:CD2	1:B:195:ARG:HD2	2.49	0.47
1:C:35:PHE:HB3	1:C:177:ASP:OD2	2.14	0.47
1:D:251:ILE:HB	1:D:252:PRO:HD2	1.96	0.47
1:D:192:SER:HA	1:D:220:LYS:HD3	1.96	0.47
1:A:73:ARG:HD3	1:A:155:ASN:OD1	2.14	0.47
1:B:200:VAL:HG22	1:B:219:SER:OG	2.14	0.47
1:B:16:SER:OG	1:B:19:MET:HB2	2.14	0.47
1:B:167:LEU:HB3	1:B:168:PRO:CD	2.41	0.47
1:A:75:MET:HB2	3:A:2010:HOH:O	2.15	0.47
1:D:65:LEU:CD2	1:D:65:LEU:C	2.82	0.47
1:D:175:LYS:O	1:D:179:ILE:HG13	2.14	0.47
1:C:244:ARG:CD	1:C:256:VAL:HG12	2.44	0.47
1:B:343:LEU:O	1:B:344:GLU:O	2.32	0.47
1:B:422:GLU:HG3	1:B:423:ILE:H	1.79	0.47
1:B:7:VAL:CG1	1:B:32:ARG:HB2	2.44	0.47
1:C:273:VAL:HG11	3:C:2025:HOH:O	2.14	0.47
1:A:10:ILE:CG2	1:A:11:GLY:N	2.77	0.47
1:C:378:THR:HG21	1:C:381:GLY:HA2	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:298:VAL:O	1:D:301:ALA:N	2.47	0.47
1:B:422:GLU:CG	1:B:423:ILE:H	2.28	0.47
1:A:249:VAL:HG12	1:A:249:VAL:O	2.13	0.47
1:C:92:THR:HA	1:C:142:VAL:O	2.15	0.47
1:D:391:PHE:N	1:D:392:PRO:HD3	2.29	0.47
1:C:244:ARG:HD2	1:C:256:VAL:CG1	2.44	0.47
1:A:132:MET:HG2	1:A:146:VAL:HA	1.97	0.47
1:B:241:MET:CE	1:B:310:MET:CE	2.92	0.47
1:B:87:ALA:C	1:B:89:GLN:H	2.18	0.47
1:C:401:THR:HA	1:C:420:VAL:O	2.14	0.47
1:C:102:ASN:OD1	1:C:104:GLU:N	2.40	0.47
1:B:452:VAL:HG12	1:B:453:SER:N	2.29	0.47
1:A:399:LEU:HD21	1:A:436:LEU:HD12	1.96	0.47
1:D:266:LYS:HG2	1:D:269:ARG:HH12	1.79	0.47
1:A:312:SER:C	1:A:314:GLU:H	2.18	0.47
1:A:244:ARG:HG3	1:A:244:ARG:HH11	1.80	0.47
1:C:241:MET:HE2	1:C:310:MET:CE	2.44	0.47
1:C:26:ALA:HB3	1:C:325:VAL:HG11	1.96	0.47
1:A:124:LEU:CD1	1:A:161:PRO:CG	2.92	0.47
1:A:415:VAL:HG12	1:A:416:VAL:N	2.29	0.47
1:C:72:ILE:HG12	1:C:110:TYR:HB3	1.96	0.47
1:C:195:ARG:H	1:C:195:ARG:HD3	1.79	0.47
1:B:11:GLY:O	1:B:14:THR:N	2.39	0.47
1:A:440:SER:C	1:A:442:LEU:H	2.18	0.47
1:C:86:LYS:O	1:C:89:GLN:HG2	2.15	0.47
1:C:378:THR:OG1	1:C:381:GLY:CA	2.63	0.46
1:B:5:LYS:HD3	1:B:5:LYS:HA	1.76	0.46
1:C:18:GLU:O	1:C:22:LYS:HG3	2.15	0.46
1:D:342:ARG:HD2	1:D:391:PHE:CE1	2.51	0.46
1:B:293:ALA:O	1:B:297:ASP:HB2	2.15	0.46
1:D:407:HIS:O	1:D:410:VAL:HG23	2.15	0.46
1:B:369:LEU:HA	1:B:369:LEU:HD23	1.71	0.46
1:B:10:ILE:HD11	1:B:23:MET:HE3	1.97	0.46
1:B:67:THR:HG21	3:B:2010:HOH:O	2.15	0.46
1:C:152:LEU:C	1:C:152:LEU:HD12	2.35	0.46
1:C:422:GLU:CG	1:C:423:ILE:N	2.77	0.46
1:D:191:ALA:CB	1:D:203:ILE:CD1	2.93	0.46
1:C:379:GLN:O	1:C:405:THR:HG21	2.15	0.46
1:C:5:LYS:HA	1:C:29:ASN:OD1	2.16	0.46
1:C:165:ILE:O	1:C:195:ARG:NH2	2.49	0.46
1:B:327:ILE:HA	1:B:327:ILE:HD12	1.73	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:125:VAL:HG12	1:A:126:ASP:N	2.29	0.46
1:B:77:LEU:HD11	1:B:152:LEU:HG	1.97	0.46
1:C:375:VAL:HG12	1:C:376:VAL:N	2.29	0.46
1:A:422:GLU:HG3	1:A:423:ILE:H	1.81	0.46
1:D:187:ASP:HA	1:D:404:LYS:HE3	1.97	0.46
1:B:230:PHE:CE2	1:B:263:MET:SD	3.09	0.46
1:B:93:PHE:HB2	1:B:142:VAL:HB	1.98	0.46
1:A:165:ILE:N	1:A:165:ILE:CD1	2.78	0.46
1:A:195:ARG:O	1:A:225:GLU:HG2	2.16	0.46
1:A:75:MET:HE2	1:A:97:LYS:CA	2.30	0.46
1:A:244:ARG:HD2	1:A:256:VAL:HG12	1.98	0.46
1:A:5:LYS:HG3	1:A:410:VAL:O	2.16	0.46
1:D:372:PRO:HD2	1:D:448:VAL:O	2.15	0.46
1:C:78:GLU:OE1	3:C:2004:HOH:O	2.21	0.46
1:B:10:ILE:HG22	1:B:11:GLY:N	2.31	0.46
1:B:15:GLU:CB	1:B:46:ARG:HD3	2.46	0.46
1:B:85:LEU:O	1:B:149:ASN:HA	2.15	0.46
1:D:186:VAL:O	1:D:404:LYS:NZ	2.31	0.46
1:B:104:GLU:O	3:B:2007:HOH:O	2.20	0.46
1:C:11:GLY:CA	1:C:46:ARG:NH1	2.76	0.46
1:B:133:GLU:O	1:B:144:CYS:HB3	2.16	0.46
1:D:156:LYS:HA	1:D:156:LYS:HD3	1.55	0.45
1:B:43:HIS:O	1:B:46:ARG:HB3	2.16	0.45
1:C:31:MET:CE	1:C:33:LEU:HD21	2.45	0.45
1:D:354:ILE:O	1:D:358:VAL:HG23	2.16	0.45
1:D:363:VAL:O	1:D:367:GLU:HG3	2.16	0.45
1:D:253:VAL:HG23	1:D:254:GLU:OE1	2.16	0.45
1:A:5:LYS:HA	1:A:29:ASN:OD1	2.16	0.45
1:A:398:ALA:C	1:A:399:LEU:HD12	2.35	0.45
1:C:254:GLU:OE1	1:C:254:GLU:N	2.33	0.45
1:D:444:HIS:CD2	1:D:444:HIS:N	2.84	0.45
1:C:343:LEU:O	1:C:344:GLU:O	2.35	0.45
1:C:190:ALA:HA	1:C:218:ILE:HB	1.97	0.45
1:B:74:THR:C	1:B:75:MET:HG3	2.30	0.45
1:C:93:PHE:HA	1:C:106:VAL:O	2.16	0.45
1:A:23:MET:CB	1:A:28:MET:CE	2.94	0.45
1:C:358:VAL:HG21	1:C:463:ASN:HA	1.98	0.45
1:C:127:ASP:C	1:C:249:VAL:HG13	2.36	0.45
1:C:266:LYS:HG2	1:C:269:ARG:HH12	1.81	0.45
1:C:154:GLU:O	1:C:155:ASN:HB3	2.17	0.45
1:D:422:GLU:CG	1:D:423:ILE:H	2.29	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:113:PHE:CD2	1:C:142:VAL:HG21	2.51	0.45
1:D:15:GLU:CB	1:D:46:ARG:HD3	2.46	0.45
1:A:171:ALA:O	1:A:175:LYS:HG3	2.17	0.45
1:B:362:ALA:O	1:B:366:ALA:HB2	2.17	0.45
1:D:17:GLU:HG2	1:D:49:ASN:HB3	1.98	0.45
1:B:179:ILE:HG22	1:B:179:ILE:O	2.16	0.45
1:C:16:SER:OG	1:C:19:MET:HB2	2.16	0.45
1:D:10:ILE:HG13	1:D:31:MET:SD	2.57	0.45
1:D:216:HIS:ND1	3:D:2020:HOH:O	2.36	0.45
1:B:310:MET:HG2	1:B:311:LEU:N	2.32	0.45
1:D:416:VAL:O	1:D:416:VAL:HG12	2.16	0.45
1:D:275:ILE:HA	1:D:308:ALA:O	2.17	0.45
1:A:407:HIS:O	1:A:410:VAL:HG23	2.16	0.45
1:C:217:ILE:O	1:C:238:ASP:HB2	2.17	0.45
1:D:124:LEU:CD1	1:D:161:PRO:CG	2.95	0.45
1:A:440:SER:HB3	1:A:442:LEU:CD1	2.47	0.45
1:B:216:HIS:CE1	3:B:2017:HOH:O	2.69	0.45
1:A:240:ILE:HG23	1:A:241:MET:N	2.32	0.45
1:C:344:GLU:N	3:C:2022:HOH:O	2.48	0.45
1:C:12:PRO:HA	1:C:15:GLU:OE2	2.17	0.45
1:C:91:PHE:HE2	1:C:106:VAL:HG12	1.82	0.45
1:D:240:ILE:CG2	1:D:241:MET:N	2.80	0.45
1:C:216:HIS:CD2	1:C:408:GLN:HE22	2.35	0.45
1:A:362:ALA:O	1:A:366:ALA:HB2	2.17	0.45
1:B:70:PRO:O	1:B:71:GLU:HG3	2.17	0.44
1:B:419:LEU:HD12	1:B:419:LEU:HA	1.53	0.44
1:C:35:PHE:HE2	1:C:40:TYR:CE1	2.35	0.44
1:B:47:ILE:O	1:B:51:ARG:HG2	2.16	0.44
1:A:191:ALA:CB	1:A:194:ILE:HD11	2.46	0.44
1:D:219:SER:HB2	1:D:240:ILE:CD1	2.45	0.44
1:A:307:ASP:HA	1:A:413:LYS:HB2	1.99	0.44
1:D:20:LEU:O	1:D:23:MET:HB2	2.17	0.44
1:B:426:THR:CG2	1:B:430:TYR:CE2	3.00	0.44
1:D:50:LEU:O	1:D:54:MET:HG3	2.17	0.44
1:B:366:ALA:HA	1:B:450:VAL:CG2	2.48	0.44
1:C:170:LEU:O	1:C:175:LYS:HE3	2.17	0.44
1:D:422:GLU:HG3	1:D:423:ILE:H	1.83	0.44
1:C:440:SER:C	1:C:442:LEU:H	2.21	0.44
1:A:172:GLU:HA	1:A:172:GLU:OE1	2.17	0.44
1:D:374:ILE:O	1:D:376:VAL:HG23	2.18	0.44
1:A:193:PHE:O	1:A:195:ARG:HD3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:15:GLU:HB3	1:D:46:ARG:CD	2.48	0.44
1:D:77:LEU:N	1:D:154:GLU:HG2	2.32	0.44
1:D:77:LEU:H	1:D:154:GLU:HG2	1.83	0.44
1:C:170:LEU:HD22	1:C:174:ASP:C	2.38	0.44
1:D:42:GLU:O	1:D:46:ARG:HB2	2.17	0.44
1:C:260:GLN:O	1:C:264:ILE:HG13	2.18	0.44
1:A:170:LEU:CD1	1:A:178:LEU:HD12	2.46	0.44
1:A:466:SER:HA	1:B:463:ASN:O	2.17	0.44
1:C:203:ILE:O	1:C:207:LEU:HG	2.18	0.44
1:D:448:VAL:O	1:D:449:VAL:HG23	2.17	0.44
1:A:47:ILE:O	1:A:47:ILE:HG22	2.18	0.44
1:C:188:PHE:CD2	1:C:216:HIS:HB2	2.53	0.44
1:D:9:THR:OG1	1:D:32:ARG:HD3	2.18	0.44
1:C:165:ILE:N	1:C:165:ILE:HD12	2.32	0.44
1:B:311:LEU:HD23	1:B:311:LEU:HA	1.73	0.44
1:B:242:VAL:HG12	1:B:244:ARG:HG2	1.99	0.44
1:D:421:LYS:O	1:D:422:GLU:HB2	2.18	0.44
1:B:132:MET:CA	1:B:147:LEU:HG	2.48	0.44
1:D:114:THR:HG21	1:D:140:ASN:HA	2.00	0.44
1:B:63:ILE:HG22	1:B:186:VAL:HG12	2.00	0.44
1:D:77:LEU:HD23	1:D:77:LEU:HA	1.50	0.44
1:C:74:THR:O	1:C:155:ASN:HA	2.18	0.44
1:A:391:PHE:N	1:A:392:PRO:CD	2.81	0.44
1:D:388:ARG:C	1:D:388:ARG:HD3	2.38	0.44
1:D:204:ARG:HA	1:D:217:ILE:HD11	1.99	0.44
1:A:452:VAL:CG1	1:A:462:THR:CG2	2.96	0.43
1:B:73:ARG:HG2	1:B:157:GLY:HA2	2.00	0.43
1:D:12:PRO:HA	1:D:15:GLU:OE2	2.18	0.43
1:D:10:ILE:CG2	1:D:46:ARG:HD2	2.37	0.43
1:C:253:VAL:H	1:C:253:VAL:HG22	1.42	0.43
1:C:321:PRO:O	1:C:325:VAL:HG23	2.18	0.43
1:D:73:ARG:NH1	1:D:155:ASN:O	2.51	0.43
1:C:140:ASN:OD1	1:C:141:LYS:HE2	2.18	0.43
1:A:191:ALA:HB2	1:A:203:ILE:CD1	2.48	0.43
1:B:190:ALA:HA	1:B:218:ILE:HB	2.00	0.43
1:B:366:ALA:CA	1:B:450:VAL:HG21	2.48	0.43
1:A:5:LYS:HA	1:A:5:LYS:HD3	1.85	0.43
1:C:77:LEU:H	1:C:154:GLU:CD	2.17	0.43
1:C:415:VAL:CG1	1:C:416:VAL:N	2.80	0.43
1:A:378:THR:OG1	2:A:701:SO4:O3	2.32	0.43
1:C:369:LEU:HD23	1:C:369:LEU:HA	1.68	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:170:LEU:CD2	1:C:174:ASP:CB	2.88	0.43
1:C:178:LEU:O	1:C:181:GLY:N	2.51	0.43
1:C:91:PHE:CE2	1:C:106:VAL:HG12	2.53	0.43
1:D:78:GLU:CD	1:D:102:ASN:HB3	2.38	0.43
1:A:132:MET:CA	1:A:147:LEU:HG	2.48	0.43
1:A:77:LEU:HD11	1:A:152:LEU:HG	1.99	0.43
1:A:422:GLU:CD	1:A:423:ILE:H	2.22	0.43
1:A:298:VAL:O	1:A:301:ALA:HB3	2.17	0.43
1:C:419:LEU:HA	1:C:419:LEU:HD12	1.75	0.43
1:D:131:GLY:C	1:D:132:MET:HG3	2.39	0.43
1:B:241:MET:HE1	1:B:310:MET:CE	2.48	0.43
1:D:403:GLU:HG2	1:D:419:LEU:CD2	2.49	0.43
1:C:9:THR:HA	1:C:32:ARG:HB3	1.99	0.43
1:C:137:ILE:HA	1:C:141:LYS:O	2.19	0.43
1:B:64:LEU:HA	1:B:188:PHE:O	2.19	0.43
1:A:230:PHE:CE2	1:A:263:MET:HG2	2.54	0.43
1:B:455:ALA:H	1:B:457:VAL:HG22	1.83	0.43
1:C:136:ALA:O	1:C:143:ILE:N	2.44	0.43
1:C:207:LEU:HD13	1:C:215:ILE:CG2	2.49	0.43
1:C:440:SER:HB3	1:C:442:LEU:HG	2.01	0.43
1:C:94:THR:HA	1:C:140:ASN:O	2.19	0.43
1:C:77:LEU:H	1:C:154:GLU:HG2	1.84	0.43
1:B:310:MET:CG	1:B:311:LEU:N	2.82	0.43
1:C:40:TYR:HB3	1:C:180:PHE:CE2	2.53	0.43
1:A:244:ARG:HG3	1:A:244:ARG:NH1	2.33	0.43
1:A:298:VAL:HG12	1:A:299:ALA:N	2.34	0.43
1:B:83:VAL:O	1:B:83:VAL:HG23	2.19	0.43
1:C:61:ALA:HA	1:C:410:VAL:HG11	2.01	0.43
1:D:35:PHE:HZ	1:D:180:PHE:CE2	2.37	0.43
1:D:124:LEU:HD11	1:D:161:PRO:CG	2.44	0.43
1:D:154:GLU:O	1:D:156:LYS:CE	2.59	0.43
1:D:390:TYR:C	1:D:392:PRO:HD3	2.40	0.43
1:A:23:MET:HB2	1:A:28:MET:CE	2.49	0.43
1:D:3:LYS:HB3	1:D:414:GLY:CA	2.49	0.43
1:D:396:ILE:HB	1:D:415:VAL:HA	2.01	0.42
1:C:67:THR:CG2	1:C:68:LYS:N	2.78	0.42
1:A:65:LEU:C	1:A:65:LEU:HD23	2.40	0.42
1:A:188:PHE:CD2	1:A:218:ILE:HD11	2.54	0.42
1:A:34:ASN:C	1:A:36:SER:H	2.22	0.42
1:C:77:LEU:N	1:C:154:GLU:HG2	2.34	0.42
1:C:135:THR:OG1	1:C:143:ILE:O	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:244:ARG:CD	1:D:256:VAL:CG1	2.96	0.42
1:A:355:THR:O	1:A:359:CYS:SG	2.77	0.42
1:D:5:LYS:HB2	1:D:308:ALA:HB2	2.00	0.42
1:C:399:LEU:HD21	1:C:436:LEU:HD12	2.00	0.42
1:B:375:VAL:HG12	1:B:376:VAL:N	2.33	0.42
1:A:197:ARG:HB2	1:A:232:GLU:CD	2.40	0.42
1:A:170:LEU:HD23	1:A:170:LEU:HA	1.83	0.42
1:D:188:PHE:CD1	1:D:216:HIS:CB	3.01	0.42
1:B:117:LEU:CD1	1:B:160:LEU:HD13	2.49	0.42
1:D:415:VAL:CG1	1:D:416:VAL:N	2.81	0.42
1:B:247:LEU:O	1:B:251:ILE:HG12	2.19	0.42
1:D:28:MET:HE2	1:D:28:MET:HB3	1.95	0.42
1:D:457:VAL:HA	1:D:458:PRO:HD3	1.84	0.42
1:C:78:GLU:CG	1:C:100:ILE:HG22	2.49	0.42
1:A:378:THR:OG1	1:A:381:GLY:N	2.52	0.42
1:C:65:LEU:C	1:C:65:LEU:CD2	2.88	0.42
1:C:327:ILE:HA	1:C:327:ILE:HD12	1.75	0.42
1:C:298:VAL:O	1:C:301:ALA:N	2.52	0.42
1:C:94:THR:HG22	1:C:106:VAL:O	2.19	0.42
1:C:135:THR:OG1	1:C:136:ALA:N	2.53	0.42
1:C:251:ILE:HB	1:C:252:PRO:CD	2.49	0.42
1:A:126:ASP:O	1:A:129:LEU:N	2.38	0.42
1:A:65:LEU:C	1:A:65:LEU:CD2	2.88	0.42
1:A:436:LEU:HA	1:A:436:LEU:HD23	1.74	0.42
1:C:436:LEU:O	1:C:439:GLN:N	2.52	0.42
1:C:341:SER:HB3	1:C:367:GLU:OE2	2.20	0.42
1:A:234:LEU:O	1:A:234:LEU:HG	2.15	0.42
1:D:311:LEU:HD23	1:D:311:LEU:HA	1.43	0.42
1:C:244:ARG:NH1	1:C:260:GLN:OE1	2.43	0.42
1:A:191:ALA:HB1	1:A:194:ILE:HD11	2.01	0.42
1:D:170:LEU:HD22	1:D:174:ASP:HB3	2.01	0.42
1:C:416:VAL:HG12	1:C:416:VAL:O	2.19	0.42
1:A:76:LYS:HA	1:A:154:GLU:OE2	2.19	0.42
1:A:85:LEU:N	1:A:150:GLY:O	2.41	0.42
1:C:263:MET:HE2	1:C:263:MET:HB2	1.91	0.42
1:B:369:LEU:O	1:B:370:ASP:HB2	2.18	0.42
1:C:94:THR:N	1:C:106:VAL:O	2.51	0.42
1:A:327:ILE:HA	1:A:327:ILE:HD12	1.69	0.42
1:D:64:LEU:HA	1:D:188:PHE:O	2.20	0.42
1:C:253:VAL:HG23	1:C:254:GLU:H	1.84	0.42
1:A:434:LYS:HE2	1:A:434:LYS:HB3	1.89	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:73:ARG:HB2	1:D:109:THR:HG21	2.02	0.42
1:C:267:CYS:O	1:C:270:ALA:HB3	2.19	0.42
1:D:257:ILE:HA	1:D:257:ILE:HD12	1.80	0.42
1:A:195:ARG:N	1:A:195:ARG:HD3	2.34	0.42
1:B:462:THR:O	1:B:463:ASN:HB3	2.20	0.42
1:B:402:ASN:OD1	1:B:404:LYS:N	2.53	0.42
1:A:63:ILE:HG21	1:A:63:ILE:HD13	1.79	0.42
1:B:440:SER:C	1:B:442:LEU:N	2.73	0.42
1:D:7:VAL:HG11	1:D:310:MET:CE	2.50	0.42
1:D:35:PHE:CZ	1:D:43:HIS:CD2	3.07	0.41
1:C:134:VAL:HG22	1:C:144:CYS:SG	2.59	0.41
1:A:388:ARG:HB2	1:A:396:ILE:HD11	1.99	0.41
1:A:5:LYS:O	1:A:308:ALA:HA	2.20	0.41
1:C:73:ARG:O	1:C:108:VAL:HA	2.20	0.41
1:B:10:ILE:HD12	1:B:10:ILE:HG23	1.77	0.41
1:C:327:ILE:HG23	1:C:328:MET:N	2.35	0.41
1:B:266:LYS:HG2	1:B:269:ARG:HH12	1.85	0.41
1:B:126:ASP:CG	1:B:156:LYS:HG3	2.40	0.41
1:B:170:LEU:HD23	3:B:2010:HOH:O	2.19	0.41
1:D:341:SER:HA	1:D:391:PHE:O	2.20	0.41
1:A:31:MET:HE1	1:A:33:LEU:HD21	2.01	0.41
1:C:434:LYS:HE2	1:C:434:LYS:HB3	1.82	0.41
1:D:136:ALA:HB3	1:D:143:ILE:HB	2.02	0.41
1:A:422:GLU:HA	1:A:422:GLU:OE1	2.20	0.41
1:C:77:LEU:H	1:C:154:GLU:CG	2.32	0.41
1:D:268:ILE:HD13	1:D:391:PHE:CZ	2.55	0.41
1:B:30:VAL:HG12	1:B:31:MET:N	2.35	0.41
1:D:165:ILE:N	1:D:165:ILE:CD1	2.83	0.41
1:D:229:ASN:O	1:D:232:GLU:HG2	2.19	0.41
1:C:321:PRO:CD	1:C:322:LEU:H	2.31	0.41
1:D:5:LYS:HG3	1:D:411:LEU:O	2.21	0.41
1:C:422:GLU:CG	1:C:423:ILE:H	2.33	0.41
1:A:163:VAL:CG1	1:A:165:ILE:CD1	2.92	0.41
1:A:75:MET:CE	1:A:97:LYS:CA	2.94	0.41
1:B:10:ILE:CG2	1:B:11:GLY:N	2.84	0.41
1:D:343:LEU:HA	1:D:343:LEU:HD23	1.70	0.41
1:A:23:MET:HB3	1:A:28:MET:CE	2.49	0.41
1:D:5:LYS:HG3	1:D:410:VAL:O	2.19	0.41
1:A:35:PHE:CD1	1:A:65:LEU:HG	2.56	0.41
1:A:252:PRO:HB2	1:A:255:GLU:HG2	2.03	0.41
1:C:435:GLU:HG2	3:C:2028:HOH:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:11:GLY:HA2	1:D:46:ARG:NH1	2.35	0.41
1:D:180:PHE:O	1:D:183:GLU:HB2	2.21	0.41
1:D:451:MET:O	1:D:465:ALA:HA	2.20	0.41
1:C:25:ASP:OD1	1:C:59:LYS:NZ	2.46	0.41
1:D:362:ALA:O	1:D:366:ALA:HB2	2.21	0.41
1:A:335:THR:O	1:A:339:MET:HG3	2.21	0.41
1:D:165:ILE:HD12	1:D:165:ILE:H	1.82	0.41
1:D:373:LEU:HD11	1:D:397:LEU:HB2	2.01	0.41
1:A:343:LEU:O	1:A:344:GLU:O	2.39	0.41
1:B:244:ARG:CD	1:B:256:VAL:HG12	2.51	0.41
1:D:231:ASP:HB2	3:D:2022:HOH:O	2.19	0.41
1:B:73:ARG:HD3	1:B:155:ASN:OD1	2.20	0.41
1:B:163:VAL:CG1	1:B:164:SER:N	2.84	0.41
1:A:125:VAL:CG1	1:A:126:ASP:N	2.82	0.41
1:A:190:ALA:HA	1:A:218:ILE:O	2.21	0.41
1:A:9:THR:OG1	1:A:32:ARG:HD3	2.21	0.41
1:B:28:MET:HE2	1:B:28:MET:HB3	1.74	0.41
1:C:113:PHE:HD2	1:C:142:VAL:HG21	1.85	0.41
1:C:110:TYR:HD1	1:C:167:LEU:HD21	1.80	0.41
1:D:230:PHE:C	1:D:230:PHE:CD1	2.94	0.41
1:C:310:MET:HG2	1:C:311:LEU:N	2.36	0.41
1:A:171:ALA:H	1:A:174:ASP:CG	2.23	0.41
1:B:187:ASP:OD2	3:B:2011:HOH:O	2.21	0.41
1:B:374:ILE:HA	1:B:450:VAL:O	2.21	0.41
1:B:77:LEU:H	1:B:154:GLU:HG2	1.86	0.41
1:D:403:GLU:HG2	1:D:419:LEU:HD22	2.03	0.41
1:C:201:ILE:HG23	1:C:201:ILE:HD12	1.92	0.41
1:A:74:THR:O	1:A:155:ASN:HA	2.21	0.41
1:D:395:THR:HG22	1:D:396:ILE:N	2.35	0.41
1:A:264:ILE:O	1:A:268:ILE:HG13	2.20	0.41
1:B:404:LYS:O	1:B:407:HIS:N	2.47	0.41
1:C:218:ILE:HD12	1:C:218:ILE:HG23	1.75	0.41
1:B:11:GLY:CA	1:B:46:ARG:HH11	2.33	0.40
1:C:243:ALA:O	1:C:247:LEU:HB2	2.21	0.40
1:A:40:TYR:HE1	1:A:177:ASP:OD1	2.04	0.40
1:B:378:THR:O	1:B:400:THR:HB	2.21	0.40
1:B:434:LYS:HE2	1:B:434:LYS:HB3	1.82	0.40
1:C:321:PRO:CD	1:C:322:LEU:N	2.84	0.40
1:A:143:ILE:HD12	1:A:143:ILE:HG23	1.91	0.40
1:A:35:PHE:CD1	1:A:65:LEU:HD21	2.56	0.40
1:B:452:VAL:CG1	1:B:453:SER:N	2.84	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:398:ALA:O	1:A:418:GLN:N	2.54	0.40
1:C:436:LEU:HA	1:C:436:LEU:HD23	1.77	0.40
1:B:101:GLY:HA2	1:B:105:MET:O	2.21	0.40
1:C:70:PRO:HB2	1:C:167:LEU:CD1	2.50	0.40
1:B:341:SER:HA	1:B:391:PHE:O	2.21	0.40
1:C:426:THR:CG2	1:C:430:TYR:CE2	3.04	0.40
1:A:240:ILE:O	1:A:274:VAL:HA	2.21	0.40
1:A:266:LYS:HG2	1:A:269:ARG:HH12	1.87	0.40
1:C:170:LEU:HD21	1:C:178:LEU:CD1	2.44	0.40
1:C:417:PRO:HD3	3:C:2024:HOH:O	2.21	0.40
1:D:124:LEU:CD1	1:D:161:PRO:CD	2.99	0.40
1:C:273:VAL:CG1	3:C:2025:HOH:O	2.68	0.40
1:D:132:MET:N	1:D:147:LEU:HD12	2.36	0.40
1:D:132:MET:CA	1:D:147:LEU:HG	2.47	0.40
1:A:321:PRO:CD	1:A:322:LEU:H	2.30	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:208:LYS:NZ	1:D:213:GLU:OE2[4_446]	2.14	0.06

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	438/470 (93%)	398 (91%)	32 (7%)	8 (2%)	11	2
1	B	438/470 (93%)	401 (92%)	32 (7%)	5 (1%)	17	5
1	C	438/470 (93%)	398 (91%)	36 (8%)	4 (1%)	21	7
1	D	438/470 (93%)	405 (92%)	28 (6%)	5 (1%)	17	5

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1752/1880 (93%)	1602 (91%)	128 (7%)	22 (1%)	15 4

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	414	GLY
1	C	313	GLY
1	D	313	GLY
1	D	337	ARG
1	A	88	GLY
1	A	127	ASP
1	A	313	GLY
1	B	162	GLY
1	B	313	GLY
1	B	463	ASN
1	C	126	ASP
1	D	414	GLY
1	A	126	ASP
1	A	463	ASN
1	B	88	GLY
1	C	127	ASP
1	A	337	ARG
1	C	414	GLY
1	D	126	ASP
1	D	453	SER
1	A	209	ALA
1	A	194	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	358/389 (92%)	349 (98%)	9 (2%)	55 39
1	B	358/389 (92%)	352 (98%)	6 (2%)	68 57
1	C	358/389 (92%)	342 (96%)	16 (4%)	34 16

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	358/389 (92%)	348 (97%)	10 (3%)	51	35
All	All	1432/1556 (92%)	1391 (97%)	41 (3%)	50	34

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	65	LEU
1	A	95	THR
1	A	145	LYS
1	A	160	LEU
1	A	195	ARG
1	A	379	GLN
1	A	388	ARG
1	A	392	PRO
1	A	431	ARG
1	B	60	THR
1	B	67	THR
1	B	117	LEU
1	B	379	GLN
1	B	388	ARG
1	B	431	ARG
1	C	51	ARG
1	C	65	LEU
1	C	76	LYS
1	C	97	LYS
1	C	105	MET
1	C	108	VAL
1	C	117	LEU
1	C	118	SER
1	C	132	MET
1	C	147	LEU
1	C	152	LEU
1	C	195	ARG
1	C	253	VAL
1	C	379	GLN
1	C	388	ARG
1	C	431	ARG
1	D	64	LEU
1	D	67	THR
1	D	156	LYS
1	D	195	ARG
1	D	292	ASP

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Mol	Chain	Res	Type
1	D	330	THR
1	D	379	GLN
1	D	388	ARG
1	D	431	ARG
1	D	459	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	81	ASN
1	A	216	HIS
1	A	300	ASN
1	B	81	ASN
1	B	300	ASN
1	B	379	GLN
1	C	43	HIS
1	C	81	ASN
1	C	216	HIS
1	C	408	GLN
1	D	43	HIS
1	D	81	ASN
1	D	206	HIS
1	D	379	GLN
1	D	444	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

4 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	$\# Z > 2$
2	SO4	A	701	-	4,4,4	2.63	2 (50%)	6,6,6	1.57	2 (33%)
2	SO4	B	702	-	4,4,4	2.61	2 (50%)	6,6,6	1.57	2 (33%)
2	SO4	C	703	-	4,4,4	2.63	2 (50%)	6,6,6	1.58	2 (33%)
2	SO4	D	704	-	4,4,4	2.63	2 (50%)	6,6,6	1.57	2 (33%)

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
2	SO4	A	701	-	-	0/0/0/0	0/0/0/0
2	SO4	B	702	-	-	0/0/0/0	0/0/0/0
2	SO4	C	703	-	-	0/0/0/0	0/0/0/0
2	SO4	D	704	-	-	0/0/0/0	0/0/0/0

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	704	SO4	O3-S	3.44	1.59	1.47
2	C	703	SO4	O3-S	3.47	1.59	1.47
2	B	702	SO4	O3-S	3.48	1.59	1.47
2	A	701	SO4	O3-S	3.51	1.60	1.47
2	B	702	SO4	O4-S	3.84	1.61	1.47
2	A	701	SO4	O4-S	3.86	1.61	1.47
2	C	703	SO4	O4-S	3.90	1.61	1.47
2	D	704	SO4	O4-S	3.91	1.61	1.47

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	C	703	SO4	O4-S-O3	-2.13	100.32	108.98
2	D	704	SO4	O4-S-O3	-2.12	100.36	108.98
2	A	701	SO4	O4-S-O3	-2.11	100.40	108.98
2	B	702	SO4	O4-S-O3	-2.11	100.40	108.98
2	B	702	SO4	O2-S-O1	3.06	119.19	109.50
2	A	701	SO4	O2-S-O1	3.06	119.20	109.50
2	C	703	SO4	O2-S-O1	3.07	119.23	109.50
2	D	704	SO4	O2-S-O1	3.07	119.23	109.50

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	701	SO4	1	0
2	B	702	SO4	2	0
2	C	703	SO4	3	0
2	D	704	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, 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	446/470 (94%)	1.11	79 (17%) 2 1	12, 27, 59, 87	0
1	B	446/470 (94%)	1.18	86 (19%) 2 1	12, 27, 59, 87	0
1	C	446/470 (94%)	1.41	113 (25%) 1 0	11, 27, 59, 88	0
1	D	446/470 (94%)	1.17	69 (15%) 3 2	11, 27, 59, 88	0
All	All	1784/1880 (94%)	1.22	347 (19%) 1 1	11, 27, 59, 88	0

All (347) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	100	ILE	7.2
1	D	313	GLY	7.2
1	C	99	VAL	6.9
1	C	37	HIS	6.6
1	C	313	GLY	6.4
1	C	102	ASN	6.1
1	C	153	GLY	6.0
1	C	137	ILE	6.0
1	D	314	GLU	5.9
1	C	155	ASN	5.9
1	C	98	SER	5.8
1	B	12	PRO	5.8
1	C	77	LEU	5.7
1	C	80	GLY	5.7
1	D	424	THR	5.6
1	C	314	GLU	5.6
1	D	1	MET	5.4
1	B	313	GLY	5.3
1	C	36	SER	5.3
1	B	1	MET	5.3
1	B	11	GLY	5.3

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Mol	Chain	Res	Type	RSRZ
1	C	152	LEU	5.2
1	A	134	VAL	5.1
1	D	58	GLY	5.0
1	A	171	ALA	5.0
1	C	134	VAL	5.0
1	B	135	THR	4.9
1	A	458	PRO	4.9
1	C	103	SER	4.8
1	B	314	GLU	4.8
1	A	424	THR	4.7
1	C	81	ASN	4.7
1	C	119	VAL	4.7
1	C	143	ILE	4.6
1	C	138	GLU	4.6
1	B	107	ALA	4.6
1	D	106	VAL	4.5
1	C	79	GLY	4.5
1	C	108	VAL	4.5
1	C	90	THR	4.4
1	B	457	VAL	4.4
1	C	105	MET	4.4
1	C	141	LYS	4.2
1	B	37	HIS	4.2
1	A	313	GLY	4.2
1	D	77	LEU	4.2
1	C	144	CYS	4.2
1	C	115	THR	4.1
1	C	438	LEU	4.1
1	C	35	PHE	4.1
1	A	119	VAL	4.1
1	D	249	VAL	4.1
1	B	459	SER	4.0
1	C	107	ALA	4.0
1	D	79	GLY	4.0
1	C	135	THR	4.0
1	A	115	THR	3.9
1	A	314	GLU	3.9
1	D	83	VAL	3.8
1	A	137	ILE	3.8
1	B	460	GLY	3.8
1	B	458	PRO	3.7
1	C	162	GLY	3.7

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Mol	Chain	Res	Type	RSRZ
1	C	75	MET	3.7
1	C	142	VAL	3.7
1	C	120	GLY	3.6
1	A	428	ASP	3.6
1	C	1	MET	3.6
1	A	143	ILE	3.6
1	C	127	ASP	3.6
1	B	291	THR	3.6
1	D	55	SER	3.5
1	D	312	SER	3.5
1	C	111	GLU	3.5
1	C	154	GLU	3.5
1	B	57	THR	3.5
1	C	92	THR	3.5
1	C	312	SER	3.5
1	C	101	GLY	3.5
1	C	74	THR	3.5
1	D	443	ALA	3.5
1	C	40	TYR	3.5
1	B	134	VAL	3.5
1	D	105	MET	3.4
1	C	327	ILE	3.4
1	D	233	ILE	3.4
1	D	38	GLY	3.4
1	C	109	THR	3.4
1	C	289	ARG	3.4
1	A	423	ILE	3.4
1	D	461	THR	3.4
1	C	106	VAL	3.4
1	C	104	GLU	3.3
1	C	95	THR	3.3
1	D	147	LEU	3.3
1	D	325	VAL	3.3
1	A	454	GLY	3.3
1	D	85	LEU	3.3
1	D	107	ALA	3.3
1	A	249	VAL	3.3
1	C	82	ASP	3.3
1	B	456	LEU	3.2
1	C	83	VAL	3.2
1	B	139	GLY	3.2
1	D	80	GLY	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	118	SER	3.2
1	A	462	THR	3.2
1	C	133	GLU	3.2
1	C	171	ALA	3.2
1	B	106	VAL	3.2
1	A	1	MET	3.2
1	B	58	GLY	3.1
1	C	323	GLU	3.1
1	A	37	HIS	3.1
1	B	142	VAL	3.1
1	C	94	THR	3.1
1	A	379	GLN	3.1
1	C	41	ALA	3.1
1	B	98	SER	3.1
1	D	207	LEU	3.1
1	D	139	GLY	3.1
1	C	78	GLU	3.1
1	C	151	ASP	3.1
1	C	469	VAL	3.1
1	B	100	ILE	3.0
1	A	420	VAL	3.0
1	D	457	VAL	3.0
1	A	122	THR	3.0
1	C	76	LYS	3.0
1	D	76	LYS	3.0
1	C	170	LEU	3.0
1	C	93	PHE	3.0
1	A	279	MET	3.0
1	C	57	THR	3.0
1	A	107	ALA	3.0
1	C	174	ASP	3.0
1	A	139	GLY	3.0
1	A	77	LEU	3.0
1	B	401	THR	2.9
1	A	457	VAL	2.9
1	B	113	PHE	2.9
1	B	120	GLY	2.9
1	A	419	LEU	2.9
1	A	422	GLU	2.9
1	C	156	LYS	2.9
1	D	449	VAL	2.9
1	C	128	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	106	VAL	2.9
1	B	461	THR	2.9
1	A	456	LEU	2.9
1	B	470	LEU	2.9
1	A	41	ALA	2.9
1	A	135	THR	2.9
1	A	85	LEU	2.9
1	B	303	LEU	2.9
1	C	38	GLY	2.8
1	C	39	ASP	2.8
1	C	470	LEU	2.8
1	A	40	TYR	2.8
1	C	91	PHE	2.8
1	D	81	ASN	2.8
1	B	127	ASP	2.8
1	B	103	SER	2.8
1	D	455	ALA	2.7
1	C	147	LEU	2.7
1	B	96	ASP	2.7
1	A	201	ILE	2.7
1	D	448	VAL	2.7
1	D	290	PRO	2.7
1	B	147	LEU	2.7
1	B	379	GLN	2.7
1	A	58	GLY	2.7
1	C	458	PRO	2.7
1	A	95	THR	2.6
1	A	114	THR	2.6
1	B	146	VAL	2.6
1	B	189	VAL	2.6
1	C	423	ILE	2.6
1	D	460	GLY	2.6
1	D	439	GLN	2.6
1	C	117	LEU	2.6
1	A	90	THR	2.6
1	B	104	GLU	2.6
1	B	93	PHE	2.6
1	D	438	LEU	2.6
1	B	39	ASP	2.6
1	B	143	ILE	2.6
1	C	461	THR	2.6
1	B	20	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	73	ARG	2.6
1	D	82	ASP	2.6
1	D	155	ASN	2.5
1	A	443	ALA	2.5
1	B	193	PHE	2.5
1	D	209	ALA	2.5
1	D	269	ARG	2.5
1	B	312	SER	2.5
1	D	95	THR	2.5
1	D	401	THR	2.5
1	D	458	PRO	2.5
1	D	267	CYS	2.5
1	A	146	VAL	2.5
1	C	45	GLN	2.5
1	A	182	CYS	2.5
1	B	178	LEU	2.5
1	A	133	GLU	2.5
1	D	279	MET	2.5
1	C	136	ALA	2.5
1	A	311	LEU	2.5
1	C	460	GLY	2.5
1	C	88	GLY	2.5
1	B	129	LEU	2.5
1	C	424	THR	2.5
1	B	91	PHE	2.4
1	A	138	GLU	2.4
1	D	143	ILE	2.4
1	A	136	ALA	2.4
1	A	441	GLY	2.4
1	C	14	THR	2.4
1	C	67	THR	2.4
1	C	121	ASN	2.4
1	B	152	LEU	2.4
1	A	312	SER	2.4
1	B	119	VAL	2.4
1	C	201	ILE	2.4
1	C	110	TYR	2.4
1	C	85	LEU	2.4
1	D	178	LEU	2.4
1	B	293	ALA	2.4
1	D	354	ILE	2.4
1	C	129	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	456	LEU	2.4
1	D	117	LEU	2.4
1	B	153	GLY	2.4
1	A	142	VAL	2.4
1	A	439	GLN	2.4
1	B	26	ALA	2.4
1	D	41	ALA	2.4
1	B	444	HIS	2.4
1	B	137	ILE	2.4
1	B	50	LEU	2.4
1	A	461	THR	2.4
1	B	233	ILE	2.3
1	A	33	LEU	2.3
1	B	117	LEU	2.3
1	B	209	ALA	2.3
1	C	293	ALA	2.3
1	A	253	VAL	2.3
1	D	108	VAL	2.3
1	A	35	PHE	2.3
1	D	141	LYS	2.3
1	B	430	TYR	2.3
1	A	214	ASN	2.3
1	B	55	SER	2.3
1	D	324	ALA	2.3
1	B	221	ILE	2.3
1	A	164	SER	2.3
1	B	368	LYS	2.3
1	A	144	CYS	2.3
1	B	370	ASP	2.3
1	D	470	LEU	2.3
1	A	163	VAL	2.3
1	C	459	SER	2.3
1	A	39	ASP	2.3
1	B	85	LEU	2.3
1	D	33	LEU	2.3
1	D	132	MET	2.3
1	C	97	LYS	2.3
1	A	36	SER	2.3
1	A	162	GLY	2.3
1	A	446	GLY	2.3
1	C	165	ILE	2.3
1	C	445	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	431	ARG	2.2
1	D	152	LEU	2.2
1	A	125	VAL	2.2
1	A	120	GLY	2.2
1	B	439	GLN	2.2
1	B	149	ASN	2.2
1	D	138	GLU	2.2
1	B	279	MET	2.2
1	A	118	SER	2.2
1	C	167	LEU	2.2
1	C	58	GLY	2.2
1	D	88	GLY	2.2
1	B	462	THR	2.2
1	D	11	GLY	2.2
1	C	321	PRO	2.2
1	A	96	ASP	2.2
1	A	170	LEU	2.2
1	C	370	ASP	2.2
1	C	457	VAL	2.2
1	A	431	ARG	2.2
1	B	121	ASN	2.2
1	A	10	ILE	2.2
1	B	125	VAL	2.2
1	C	55	SER	2.2
1	B	18	GLU	2.1
1	B	81	ASN	2.1
1	B	331	ILE	2.1
1	D	90	THR	2.1
1	D	98	SER	2.1
1	C	140	ASN	2.1
1	B	53	VAL	2.1
1	A	18	GLU	2.1
1	B	92	THR	2.1
1	C	221	ILE	2.1
1	D	100	ILE	2.1
1	D	140	ASN	2.1
1	B	19	MET	2.1
1	A	79	GLY	2.1
1	B	101	GLY	2.1
1	D	70	PRO	2.1
1	C	163	VAL	2.1
1	A	149	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	224	GLN	2.1
1	D	198	SER	2.1
1	A	155	ASN	2.1
1	A	78	GLU	2.1
1	B	289	ARG	2.1
1	D	67	THR	2.1
1	A	105	MET	2.1
1	A	113	PHE	2.1
1	B	40	TYR	2.1
1	A	340	ASN	2.1
1	C	12	PRO	2.1
1	B	327	ILE	2.0
1	B	77	LEU	2.0
1	B	9	THR	2.0
1	C	446	GLY	2.0
1	D	309	VAL	2.0
1	B	210	HIS	2.0
1	D	321	PRO	2.0
1	A	121	ASN	2.0
1	A	331	ILE	2.0
1	C	354	ILE	2.0
1	B	138	GLU	2.0
1	B	234	LEU	2.0
1	B	247	LEU	2.0
1	C	42	GLU	2.0
1	C	178	LEU	2.0
1	C	206	HIS	2.0
1	B	428	ASP	2.0
1	C	449	VAL	2.0
1	D	142	VAL	2.0
1	D	270	ALA	2.0
1	A	157	GLY	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 [i](#)

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(\AA^2)	Q<0.9
2	SO4	C	703	5/5	0.93	0.25	1.57	18,19,20,22	0
2	SO4	B	702	5/5	0.85	0.31	1.36	18,19,20,22	0
2	SO4	D	704	5/5	0.92	0.25	1.24	18,19,20,22	0
2	SO4	A	701	5/5	0.92	0.23	0.68	18,19,20,22	0

6.5 Other polymers [i](#)

There are no such residues in this entry.