



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 23, 2017 – 12:13 PM EDT

PDB ID : 3IDZ
Title : Crystal Structure of S378Q mutant TTHA0252 from *Thermus thermophilus* HB8
Authors : Ishikawa, H.; Nakagawa, N.; Kuramitsu, S.; Yokoyama, S.; Masui, R.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on : unknown
Resolution : 2.50 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	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20030345
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	rb-20030345

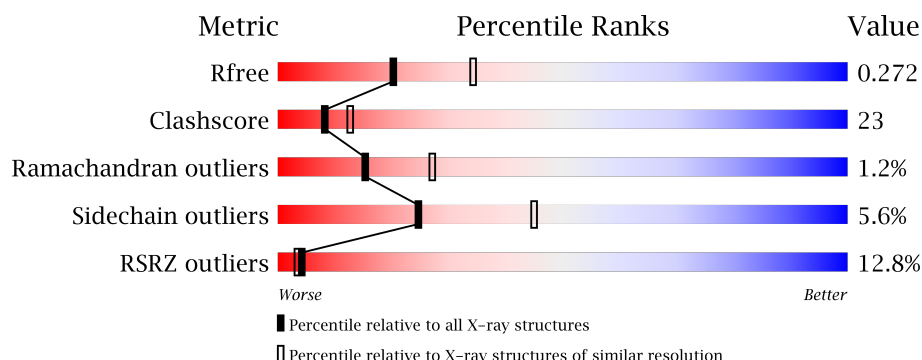
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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}	100719	3846 (2.50-2.50)
Clashscore	112137	4554 (2.50-2.50)
Ramachandran outliers	110173	4463 (2.50-2.50)
Sidechain outliers	110143	4465 (2.50-2.50)
RSRZ outliers	101464	3876 (2.50-2.50)

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	431	
1	B	431	
1	C	431	
1	D	431	

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	A	436	-	-	-	X
2	SO4	A	443	-	-	X	-
2	SO4	A	445	-	-	-	X
2	SO4	B	441	-	-	X	-
2	SO4	B	447	-	-	-	X
2	SO4	B	448	-	-	-	X
2	SO4	B	449	-	-	-	X
2	SO4	B	451	-	-	-	X
2	SO4	C	439	-	-	-	X
2	SO4	D	432	-	-	X	-
3	FLC	A	454	-	-	X	-
3	FLC	B	455	-	-	-	X
3	FLC	B	456	-	-	X	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 13823 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 Ribonuclease TTHA0252.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	431	Total	C	N	O	S	0	0	0
			3329	2129	598	594	8			
1	B	431	Total	C	N	O	S	0	0	0
			3329	2129	598	594	8			
1	C	431	Total	C	N	O	S	0	0	0
			3329	2129	598	594	8			
1	D	431	Total	C	N	O	S	0	0	0
			3329	2129	598	594	8			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	378	GLN	SER	ENGINEERED	UNP Q5SLP1
B	378	GLN	SER	ENGINEERED	UNP Q5SLP1
C	378	GLN	SER	ENGINEERED	UNP Q5SLP1
D	378	GLN	SER	ENGINEERED	UNP Q5SLP1

- 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	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		

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

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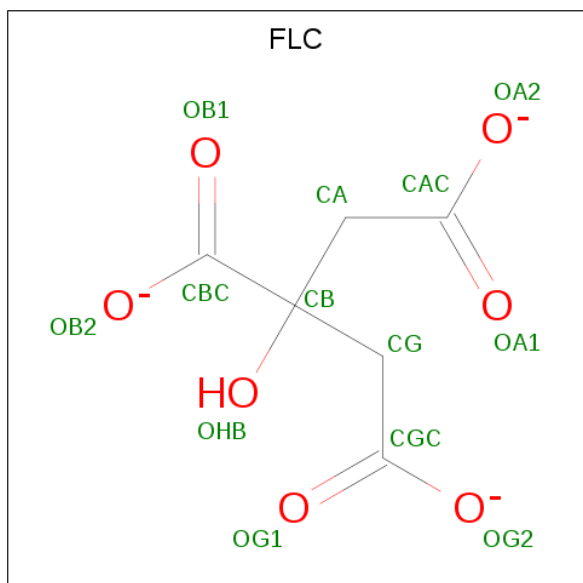
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total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

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

- Molecule 3 is CITRATE ANION (three-letter code: FLC) (formula: $\text{C}_6\text{H}_5\text{O}_7$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			13	6	7		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			13	6	7		
3	B	1	Total	C	O	0	0
			13	6	7		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	2	Total	Zn	0	0
			2	2		
4	A	2	Total	Zn	0	0
			2	2		
4	D	2	Total	Zn	0	0
			2	2		
4	C	2	Total	Zn	0	0
			2	2		

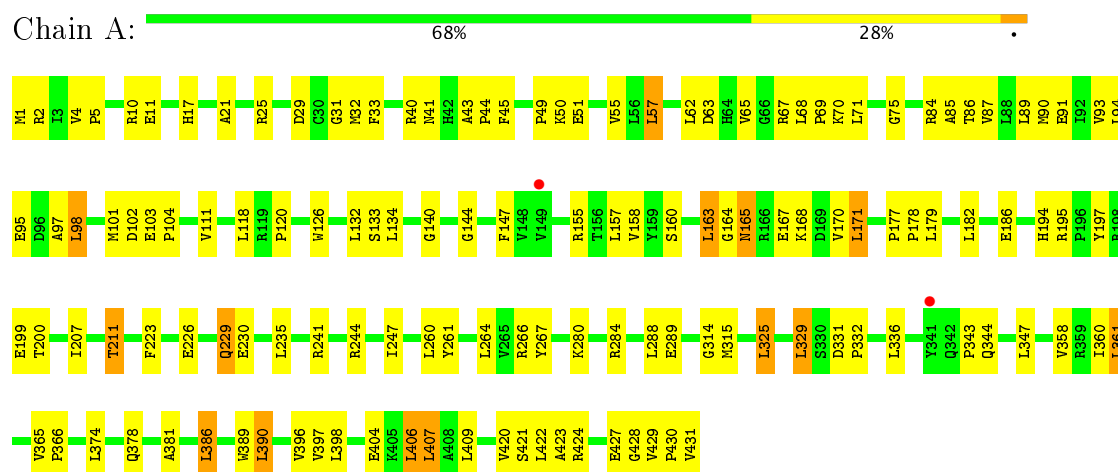
- Molecule 5 is water.

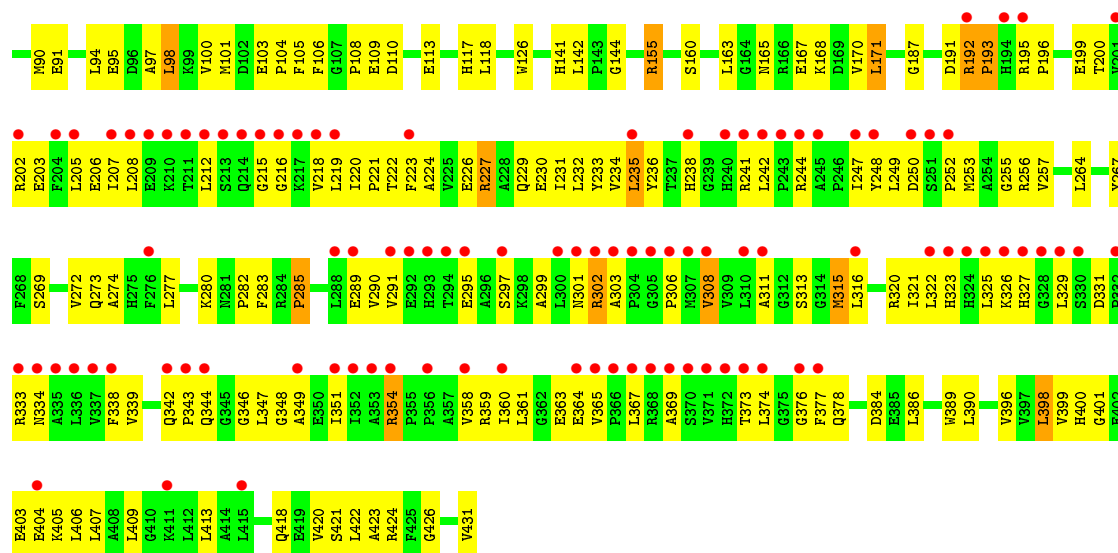
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	60	Total	O	0	0
			60	60		
5	B	41	Total	O	0	0
			41	41		
5	C	21	Total	O	0	0
			21	21		
5	D	8	Total	O	0	0
			8	8		

3 Residue-property plots

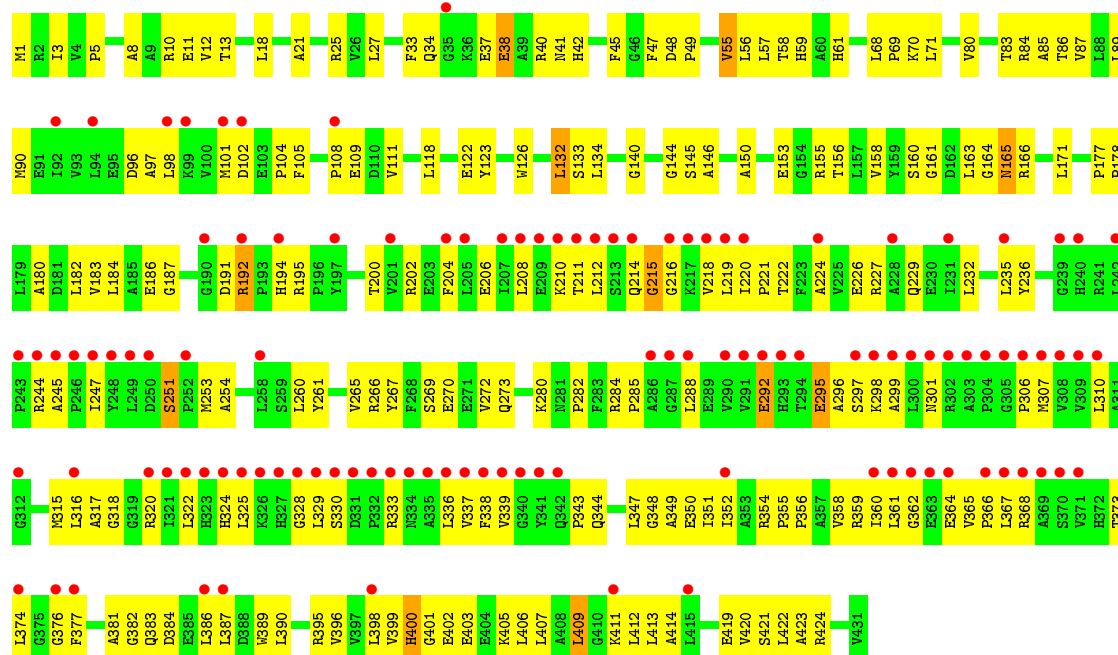
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: Ribonuclease TTHA0252





● Molecule 1: Ribonuclease TTHA0252



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	142.84Å 147.20Å 121.17Å 90.00° 109.52° 90.00°	Depositor
Resolution (Å)	50.00 – 2.50 49.67 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.8 (50.00-2.50) 99.8 (49.67-2.50)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.24 (at 2.51Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.240 , 0.278 0.235 , 0.272	Depositor DCC
R_{free} test set	8162 reflections (10.04%)	DCC
Wilson B-factor (Å ²)	54.9	Xtriage
Anisotropy	0.080	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 48.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	13823	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.63% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: FLC, ZN, 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	0.39	0/3410	0.67	0/4625
1	B	0.39	0/3410	0.69	0/4625
1	C	0.32	0/3410	0.58	0/4625
1	D	0.30	0/3410	0.57	0/4625
All	All	0.35	0/13640	0.63	0/18500

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	3329	0	3354	117	0
1	B	3329	0	3354	125	0
1	C	3329	0	3354	200	0
1	D	3329	0	3354	200	0
2	A	110	0	0	8	0
2	B	115	0	0	2	0
2	C	75	0	0	2	0
2	D	30	0	0	4	0
3	A	13	0	5	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	26	0	10	7	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
4	C	2	0	0	0	0
4	D	2	0	0	0	0
5	A	60	0	0	0	0
5	B	41	0	0	1	0
5	C	21	0	0	1	0
5	D	8	0	0	2	0
All	All	13823	0	13431	635	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 23.

All (635) 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:C:247:ILE:HA	1:C:308:VAL:HG13	1.40	1.04
1:D:10:ARG:HH12	1:D:424:ARG:HG2	1.18	1.04
1:C:33:PHE:H	1:C:41:ASN:HD21	1.04	1.01
1:C:73:ARG:HH21	1:C:106:PHE:HA	1.26	0.98
1:B:33:PHE:H	1:B:41:ASN:HD21	0.96	0.94
1:D:10:ARG:NH1	1:D:424:ARG:HG2	1.82	0.94
1:A:280:LYS:HD3	3:A:454:FLC:OA2	1.68	0.92
1:D:235:LEU:HD13	1:D:247:ILE:HD13	1.51	0.91
1:C:212:LEU:HD22	1:C:306:PRO:HB2	1.53	0.90
1:B:33:PHE:N	1:B:41:ASN:HD21	1.70	0.90
1:C:160:SER:HB2	1:C:163:LEU:HD21	1.52	0.89
1:D:160:SER:HB2	1:D:163:LEU:HD21	1.53	0.87
1:A:2:ARG:HG3	2:A:443:SO4:O4	1.75	0.85
1:C:222:THR:HG22	1:C:339:VAL:HG21	1.58	0.85
1:B:33:PHE:H	1:B:41:ASN:ND2	1.76	0.84
1:D:222:THR:HG22	1:D:339:VAL:HG21	1.57	0.84
1:A:10:ARG:HG3	1:A:10:ARG:HH11	1.41	0.84
1:C:235:LEU:HD23	1:C:236:TYR:H	1.42	0.82
1:D:13:THR:HG21	1:D:34:GLN:HB2	1.61	0.82
1:B:37:GLU:HG3	1:B:40:ARG:HH11	1.44	0.82
1:B:320:ARG:HD3	3:B:455:FLC:HG2	1.61	0.81
1:A:33:PHE:H	1:A:41:ASN:HD21	1.26	0.81
1:A:2:ARG:CD	2:A:443:SO4:O4	2.29	0.80
1:C:326:LYS:HD2	1:C:361:LEU:HB2	1.62	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2:ARG:HD2	2:A:443:SO4:O4	1.81	0.80
1:C:221:PRO:HB3	1:C:321:ILE:HG12	1.62	0.80
1:C:360:ILE:HG22	1:C:361:LEU:HD22	1.61	0.80
1:A:50:LYS:HE2	1:A:75:GLY:HA3	1.64	0.78
1:A:2:ARG:CG	2:A:443:SO4:O4	2.32	0.78
1:D:215:GLY:HA2	1:D:306:PRO:HD3	1.65	0.77
1:B:168:LYS:HE2	1:B:230:GLU:OE1	1.86	0.76
1:D:329:LEU:HD11	1:D:336:LEU:HD12	1.66	0.76
1:D:33:PHE:H	1:D:41:ASN:HD21	1.32	0.76
1:B:10:ARG:NH1	1:B:424:ARG:HG2	2.00	0.76
1:A:25:ARG:HD3	1:A:51:GLU:O	1.86	0.76
1:B:196:PRO:HB2	1:B:199:GLU:HG2	1.68	0.76
1:A:62:LEU:HD13	1:A:93:VAL:HG12	1.67	0.75
1:C:351:ILE:HG12	1:C:358:VAL:HG21	1.67	0.75
1:A:1:MET:HG3	1:A:21:ALA:HB2	1.68	0.74
1:B:411:LYS:HA	3:B:456:FLC:HG1	1.70	0.74
1:D:359:ARG:HH12	1:D:362:GLY:HA2	1.51	0.74
1:B:226:GLU:HA	1:B:229:GLN:HE21	1.51	0.73
1:D:318:GLY:HA2	1:D:322:LEU:HD11	1.69	0.73
1:A:132:LEU:HG	1:A:134:LEU:HD11	1.69	0.73
1:D:59:HIS:CD2	1:D:61:HIS:HB2	2.23	0.73
1:A:366:PRO:HG2	2:A:449:SO4:O3	1.88	0.73
1:C:219:LEU:HD23	1:C:325:LEU:HD12	1.71	0.73
1:C:343:PRO:HG2	1:C:346:GLY:HA3	1.69	0.73
1:D:359:ARG:NH1	1:D:362:GLY:HA2	2.02	0.73
1:B:240:HIS:HE1	1:B:241:ARG:HH21	1.34	0.73
1:A:102:ASP:CG	1:A:103:GLU:H	1.93	0.72
1:B:320:ARG:HD3	3:B:455:FLC:CG	2.18	0.72
1:D:227:ARG:NH1	2:D:432:SO4:O4	2.21	0.72
1:D:37:GLU:HB3	1:D:40:ARG:HH11	1.54	0.72
1:D:184:LEU:HD11	1:D:399:VAL:HG21	1.71	0.72
1:A:360:ILE:HG22	1:A:361:LEU:HD22	1.72	0.71
1:B:182:LEU:HD11	1:B:397:VAL:HG23	1.71	0.71
1:A:244:ARG:HG2	1:A:244:ARG:HH11	1.55	0.71
1:C:220:ILE:HG22	1:C:222:THR:HG23	1.73	0.71
1:C:215:GLY:HA2	1:C:306:PRO:HD3	1.71	0.71
1:B:37:GLU:HB3	1:B:40:ARG:HE	1.56	0.70
1:B:229:GLN:HG3	1:B:261:TYR:CE1	2.27	0.70
1:D:227:ARG:NH1	2:D:432:SO4:O1	2.24	0.70
1:C:73:ARG:NH2	1:C:106:PHE:HA	2.03	0.70
1:D:399:VAL:HG12	1:D:400:HIS:N	2.06	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:235:LEU:HD23	1:C:236:TYR:N	2.05	0.70
1:A:200:THR:HG23	1:A:374:LEU:HB3	1.72	0.70
1:A:194:HIS:HB3	1:A:378:GLN:NE2	2.06	0.69
1:C:403:GLU:O	1:C:407:LEU:HD23	1.92	0.69
1:B:102:ASP:O	1:B:104:PRO:HD3	1.92	0.69
1:B:1:MET:HG3	1:B:21:ALA:HB2	1.74	0.69
1:C:12:VAL:HG12	1:C:401:GLY:HA2	1.74	0.69
1:C:232:LEU:HD11	1:C:249:LEU:HD13	1.74	0.69
1:A:10:ARG:HG3	1:A:10:ARG:NH1	2.05	0.68
1:B:398:LEU:N	1:B:398:LEU:HD12	2.08	0.68
1:D:245:ALA:HB1	1:D:307:MET:HA	1.75	0.68
1:C:302:ARG:C	1:C:302:ARG:HD2	2.15	0.67
1:C:91:GLU:O	1:C:95:GLU:HG2	1.94	0.67
1:B:25:ARG:HD3	1:B:51:GLU:O	1.95	0.67
1:C:250:ASP:HB3	1:C:311:ALA:HB2	1.77	0.67
1:D:360:ILE:HG22	1:D:361:LEU:HD23	1.77	0.67
1:A:223:PHE:HB2	2:A:436:SO4:O2	1.94	0.67
1:C:10:ARG:NH2	1:C:424:ARG:HH11	1.92	0.67
1:A:280:LYS:HZ3	3:A:454:FLC:HA2	1.60	0.67
1:C:315:MET:HA	1:C:342:GLN:HE22	1.60	0.66
1:C:235:LEU:HD11	1:C:285:PRO:HG3	1.76	0.66
1:D:218:VAL:HG23	1:D:307:MET:O	1.96	0.66
1:B:210:LYS:O	1:B:214:GLN:HG2	1.96	0.66
1:B:404:GLU:H	1:B:404:GLU:CD	1.98	0.66
1:A:280:LYS:NZ	3:A:454:FLC:HA2	2.10	0.65
1:C:170:VAL:HG12	1:C:171:LEU:HD13	1.77	0.65
1:C:325:LEU:O	1:C:329:LEU:HB2	1.96	0.65
1:C:70:LYS:HE2	1:C:74:GLU:OE1	1.96	0.65
1:B:398:LEU:HD13	1:B:420:VAL:HG23	1.78	0.65
1:D:325:LEU:O	1:D:329:LEU:HB2	1.95	0.65
1:A:89:LEU:HD23	1:A:260:LEU:HD23	1.79	0.65
1:B:170:VAL:HG12	1:B:171:LEU:HD13	1.79	0.65
1:D:386:LEU:O	1:D:390:LEU:HD23	1.97	0.65
1:C:420:VAL:HG22	1:C:421:SER:N	2.12	0.65
1:D:49:PRO:HB3	1:D:71:LEU:HD12	1.77	0.65
1:C:87:VAL:HG13	1:C:118:LEU:HD13	1.79	0.64
1:D:399:VAL:HG12	1:D:400:HIS:H	1.63	0.64
1:D:318:GLY:HA2	1:D:322:LEU:CD1	2.28	0.64
1:B:411:LYS:HG3	3:B:456:FLC:HA1	1.78	0.64
1:C:236:TYR:OH	1:C:280:LYS:HD3	1.97	0.64
1:A:97:ALA:O	1:A:101:MET:HB2	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:12:VAL:HG12	1:D:401:GLY:HA2	1.79	0.64
1:B:12:VAL:HG23	1:B:13:THR:HG23	1.79	0.64
1:B:226:GLU:CA	1:B:229:GLN:HE21	2.11	0.64
1:D:85:ALA:HB2	1:D:267:TYR:CE2	2.33	0.64
1:C:32:MET:HA	1:C:67:ARG:HG3	1.80	0.63
1:D:200:THR:HG21	1:D:376:GLY:HA3	1.79	0.63
1:C:97:ALA:O	1:C:101:MET:HB2	1.99	0.63
1:B:229:GLN:HG3	1:B:261:TYR:CZ	2.34	0.63
1:B:389:TRP:HE3	1:B:390:LEU:HD13	1.64	0.63
1:D:227:ARG:NH1	2:D:432:SO4:S	2.72	0.63
1:C:223:PHE:HD1	1:C:227:ARG:HG3	1.63	0.63
1:A:207:ILE:O	1:A:211:THR:HG23	1.99	0.63
1:A:229:GLN:NE2	1:A:229:GLN:H	1.97	0.63
1:B:297:SER:OG	1:B:320:ARG:HG2	1.98	0.63
1:C:321:ILE:O	1:C:325:LEU:HD13	1.99	0.62
1:D:399:VAL:HG22	1:D:423:ALA:HB3	1.81	0.62
1:C:420:VAL:HG22	1:C:421:SER:H	1.65	0.62
1:B:12:VAL:HG12	1:B:401:GLY:HA2	1.81	0.62
1:C:73:ARG:HD2	1:C:110:ASP:OD2	1.99	0.62
1:D:153:GLU:O	1:D:155:ARG:HG2	1.99	0.62
1:A:165:ASN:C	1:A:165:ASN:HD22	2.02	0.61
1:A:33:PHE:H	1:A:41:ASN:ND2	1.98	0.61
1:C:413:LEU:HD22	1:C:418:GLN:NE2	2.16	0.61
1:D:221:PRO:HD2	1:D:337:VAL:O	1.99	0.61
1:D:57:LEU:CD2	1:D:80:VAL:HG12	2.31	0.61
1:A:167:GLU:OE2	1:A:194:HIS:HE1	1.82	0.61
1:C:329:LEU:HG	1:C:367:LEU:HA	1.83	0.60
1:D:37:GLU:HB3	1:D:40:ARG:NH1	2.16	0.60
1:A:194:HIS:HB3	1:A:378:GLN:HE22	1.66	0.60
1:D:3:ILE:HD13	1:D:184:LEU:HD22	1.84	0.60
1:D:382:GLY:O	1:D:386:LEU:HD13	2.02	0.60
1:A:1:MET:N	2:A:443:SO4:O2	2.35	0.60
1:A:57:LEU:HG	1:A:65:VAL:HG12	1.84	0.60
1:B:398:LEU:N	1:B:398:LEU:CD1	2.65	0.60
1:D:57:LEU:HD21	1:D:80:VAL:CG1	2.31	0.60
1:C:27:LEU:HD13	1:C:29:ASP:O	2.01	0.60
1:C:359:ARG:HA	1:C:363:GLU:O	2.02	0.60
1:D:177:PRO:HD3	1:D:389:TRP:NE1	2.16	0.60
1:A:207:ILE:O	1:A:211:THR:CG2	2.50	0.59
1:B:35:GLY:O	1:B:38:GLU:HB2	2.02	0.59
1:B:240:HIS:CE1	1:B:241:ARG:HH21	2.19	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:132:LEU:HD22	1:D:134:LEU:HG	1.85	0.59
1:D:202:ARG:O	1:D:206:GLU:HG3	2.02	0.59
1:A:32:MET:HA	1:A:67:ARG:HG3	1.84	0.59
1:C:98:LEU:HD11	1:C:108:PRO:HA	1.85	0.59
1:C:218:VAL:HB	1:C:308:VAL:HA	1.83	0.59
1:D:98:LEU:HD11	1:D:108:PRO:HA	1.85	0.59
1:C:235:LEU:HD12	1:C:247:ILE:HD13	1.84	0.59
1:D:87:VAL:HG13	1:D:118:LEU:HD13	1.85	0.59
1:D:402:GLU:HB2	1:D:405:LYS:HG2	1.82	0.59
1:B:223:PHE:HB3	5:B:469:HOH:O	2.03	0.59
1:D:216:GLY:HA3	1:D:333:ARG:O	2.03	0.59
1:D:409:LEU:HD22	1:D:413:LEU:CD2	2.33	0.58
1:B:37:GLU:CG	1:B:40:ARG:HH11	2.14	0.58
1:D:298:LYS:HA	1:D:301:ASN:ND2	2.19	0.58
1:D:55:VAL:HG13	1:D:80:VAL:HA	1.84	0.58
1:D:386:LEU:HD23	1:D:409:LEU:HD11	1.86	0.58
1:C:360:ILE:HG22	1:C:361:LEU:CD2	2.31	0.58
1:D:220:ILE:HG12	1:D:337:VAL:HB	1.85	0.58
1:B:196:PRO:HD2	1:B:199:GLU:CD	2.24	0.57
1:D:11:GLU:O	1:D:401:GLY:N	2.29	0.57
1:A:86:THR:O	1:A:90:MET:HB2	2.04	0.57
1:C:386:LEU:O	1:C:390:LEU:HD23	2.04	0.57
1:C:216:GLY:O	1:C:306:PRO:HA	2.04	0.57
1:C:247:ILE:HA	1:C:308:VAL:CG1	2.25	0.57
1:C:316:LEU:HB3	1:C:347:LEU:HD23	1.87	0.57
1:C:98:LEU:HD11	1:C:108:PRO:CA	2.35	0.57
1:B:229:GLN:CD	1:B:229:GLN:H	2.08	0.57
1:C:269:SER:O	1:C:273:GLN:HG3	2.04	0.57
1:C:86:THR:HG22	1:C:90:MET:CE	2.35	0.57
1:A:91:GLU:O	1:A:95:GLU:HG2	2.04	0.57
1:D:208:LEU:HD23	1:D:218:VAL:HG11	1.85	0.57
1:D:210:LYS:O	1:D:214:GLN:HG2	2.04	0.57
1:D:229:GLN:H	1:D:229:GLN:NE2	2.03	0.57
1:D:383:GLN:O	1:D:387:LEU:HG	2.04	0.57
1:B:10:ARG:HH12	1:B:424:ARG:HG2	1.68	0.57
1:C:43:ALA:O	1:C:70:LYS:NZ	2.38	0.57
1:C:208:LEU:CD2	1:C:218:VAL:HG11	2.35	0.57
1:B:37:GLU:HG3	1:B:40:ARG:NH1	2.16	0.56
1:B:407:LEU:HD13	1:B:422:LEU:HD21	1.86	0.56
1:B:98:LEU:HD11	1:B:108:PRO:HB3	1.87	0.56
1:C:205:LEU:HD11	1:C:238:HIS:CG	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:224:ALA:CB	1:B:253:MET:HG2	2.36	0.56
1:C:403:GLU:HG2	1:C:407:LEU:HD23	1.86	0.56
1:D:202:ARG:CB	1:D:202:ARG:HH11	2.18	0.56
1:A:229:GLN:H	1:A:229:GLN:CD	2.09	0.56
1:C:167:GLU:OE1	1:C:196:PRO:HA	2.05	0.56
1:D:358:VAL:O	1:D:365:VAL:HG12	2.05	0.56
1:A:168:LYS:HE3	1:A:230:GLU:OE1	2.06	0.56
1:A:33:PHE:N	1:A:41:ASN:HD21	2.02	0.56
1:C:338:PHE:HD2	1:C:373:THR:HG22	1.70	0.56
1:D:166:ARG:HG3	1:D:166:ARG:O	2.05	0.56
1:C:160:SER:HB2	1:C:163:LEU:CD2	2.31	0.56
1:D:182:LEU:HD12	1:D:183:VAL:H	1.70	0.56
1:D:45:PHE:HB3	1:D:47:PHE:CE1	2.41	0.56
1:D:123:TYR:HE1	1:D:146:ALA:HB2	1.71	0.56
1:D:387:LEU:HD11	1:D:412:LEU:HD13	1.87	0.56
1:A:85:ALA:HB2	1:A:267:TYR:CD2	2.41	0.55
1:C:331:ASP:HB3	1:C:334:ASN:ND2	2.21	0.55
1:C:12:VAL:HG12	1:C:401:GLY:CA	2.35	0.55
1:C:57:LEU:HG	1:C:65:VAL:HG12	1.86	0.55
1:A:140:GLY:O	1:A:164:GLY:HA3	2.05	0.55
1:A:244:ARG:HG2	1:A:244:ARG:NH1	2.20	0.55
1:A:84:ARG:HD3	1:A:120:PRO:HB3	1.88	0.55
1:C:86:THR:HG22	1:C:90:MET:HE3	1.89	0.55
1:B:20:LEU:CD2	1:B:25:ARG:HE	2.20	0.55
1:D:101:MET:SD	1:D:104:PRO:HA	2.46	0.55
1:C:235:LEU:CD1	1:C:247:ILE:HD13	2.37	0.55
1:C:236:TYR:HD1	1:C:285:PRO:HA	1.72	0.55
1:A:85:ALA:HB2	1:A:267:TYR:CE2	2.42	0.55
1:C:205:LEU:HD13	1:C:241:ARG:HD2	1.89	0.55
1:C:359:ARG:HG3	1:C:364:GLU:OE2	2.06	0.55
1:B:140:GLY:O	1:B:164:GLY:HA3	2.07	0.55
1:B:239:GLY:C	1:B:241:ARG:H	2.10	0.55
1:C:233:TYR:CE1	1:C:282:PRO:HB2	2.42	0.55
1:D:8:ALA:O	1:D:399:VAL:HG13	2.07	0.55
1:D:220:ILE:HG22	1:D:222:THR:HG23	1.89	0.55
1:B:70:LYS:NZ	1:B:74:GLU:OE1	2.38	0.54
1:D:58:THR:O	1:D:145:SER:HA	2.06	0.54
1:B:241:ARG:HG3	1:B:242:LEU:N	2.23	0.54
1:B:396:VAL:HG12	1:B:398:LEU:HD12	1.90	0.54
1:C:227:ARG:HH22	1:C:377:PHE:C	2.11	0.54
1:B:10:ARG:HH12	1:B:424:ARG:CG	2.20	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:232:LEU:HD22	1:D:288:LEU:HD13	1.88	0.54
1:C:11:GLU:OE1	1:C:40:ARG:NH1	2.41	0.54
1:D:12:VAL:HG23	1:D:13:THR:HG23	1.89	0.54
1:D:177:PRO:HD3	1:D:389:TRP:CD1	2.42	0.54
1:D:37:GLU:CB	1:D:40:ARG:HH11	2.20	0.54
1:C:98:LEU:HD11	1:C:108:PRO:HB3	1.90	0.54
1:C:55:VAL:HG22	1:C:80:VAL:HG13	1.90	0.54
1:D:381:ALA:HB3	1:D:386:LEU:HD11	1.89	0.54
1:B:10:ARG:NH1	1:B:424:ARG:CG	2.69	0.54
1:C:170:VAL:HG12	1:C:171:LEU:CD1	2.38	0.54
1:B:200:THR:OG1	1:B:376:GLY:HA3	2.09	0.53
1:B:398:LEU:CD1	1:B:420:VAL:HG23	2.38	0.53
1:D:85:ALA:HB3	1:D:144:GLY:HA3	1.89	0.53
1:C:230:GLU:O	1:C:233:TYR:HB3	2.09	0.53
1:A:182:LEU:HD11	1:A:397:VAL:HG23	1.91	0.53
1:B:326:LYS:HD2	1:B:361:LEU:HB2	1.89	0.53
1:D:83:THR:O	1:D:87:VAL:HG23	2.07	0.53
1:C:155:ARG:HD3	1:C:431:VAL:O	2.08	0.53
1:C:215:GLY:HA2	1:C:306:PRO:CD	2.36	0.53
1:C:326:LYS:HD2	1:C:361:LEU:CB	2.38	0.53
1:C:200:THR:HG21	1:C:376:GLY:HA3	1.90	0.53
1:C:252:PRO:HB2	2:C:439:SO4:O2	2.09	0.53
1:D:354:ARG:HG3	1:D:354:ARG:HH11	1.74	0.53
1:A:266:ARG:NH2	1:D:273:GLN:HE22	2.07	0.53
1:A:229:GLN:HG3	1:A:261:TYR:CZ	2.44	0.53
1:D:161:GLY:O	1:D:186:GLU:HG2	2.08	0.53
1:D:177:PRO:HD3	1:D:389:TRP:CE2	2.44	0.53
1:A:84:ARG:NH2	1:D:270:GLU:OE1	2.42	0.53
1:D:349:ALA:HA	1:D:352:ILE:HD12	1.91	0.53
1:D:409:LEU:HD22	1:D:413:LEU:HD21	1.90	0.53
1:D:182:LEU:HD12	1:D:183:VAL:N	2.24	0.53
1:A:404:GLU:CD	1:A:404:GLU:H	2.12	0.52
1:D:211:THR:HG21	1:D:218:VAL:HG22	1.91	0.52
1:D:229:GLN:H	1:D:229:GLN:CD	2.11	0.52
1:D:5:PRO:HG2	1:D:423:ALA:HB1	1.92	0.52
1:B:200:THR:HG23	1:B:374:LEU:HB3	1.91	0.52
1:D:202:ARG:HB2	1:D:202:ARG:NH1	2.24	0.52
1:D:269:SER:OG	1:D:272:VAL:HG23	2.09	0.52
1:A:226:GLU:HA	1:A:229:GLN:HE21	1.74	0.52
1:B:47:PHE:O	1:B:49:PRO:HD3	2.09	0.52
1:C:168:LYS:HD2	1:C:378:GLN:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:284:ARG:HA	1:D:288:LEU:CD2	2.39	0.52
1:B:396:VAL:HG12	1:B:398:LEU:CD1	2.40	0.52
1:D:338:PHE:HB2	1:D:373:THR:HA	1.90	0.52
1:A:226:GLU:CA	1:A:229:GLN:HE21	2.23	0.52
1:C:84:ARG:HB3	1:C:267:TYR:OH	2.09	0.52
1:D:247:ILE:O	1:D:288:LEU:HA	2.09	0.52
1:C:233:TYR:HE1	1:C:282:PRO:HB2	1.74	0.52
1:D:163:LEU:N	1:D:163:LEU:HD22	2.25	0.52
1:C:248:TYR:HA	1:C:289:GLU:HB3	1.92	0.52
1:C:212:LEU:CD2	1:C:306:PRO:HB2	2.34	0.52
1:D:280:LYS:O	1:D:282:PRO:HD3	2.10	0.52
1:D:411:LYS:O	1:D:414:ALA:HB3	2.09	0.52
1:B:411:LYS:CG	3:B:456:FLC:HA1	2.40	0.51
1:D:403:GLU:O	1:D:407:LEU:HD23	2.10	0.51
1:A:102:ASP:CG	1:A:103:GLU:N	2.62	0.51
1:C:315:MET:HA	1:C:342:GLN:NE2	2.24	0.51
1:D:395:ARG:HG3	1:D:419:GLU:HB3	1.91	0.51
1:B:399:VAL:HG12	1:B:423:ALA:HB3	1.92	0.51
1:C:205:LEU:HD22	1:C:242:LEU:HD21	1.91	0.51
1:C:49:PRO:HB3	1:C:71:LEU:HD12	1.92	0.51
1:A:132:LEU:HG	1:A:134:LEU:CD1	2.39	0.51
1:C:57:LEU:HD23	1:C:90:MET:CE	2.39	0.51
1:A:347:LEU:HD11	1:A:358:VAL:HG11	1.92	0.51
1:A:424:ARG:HD3	1:A:427:GLU:OE1	2.10	0.51
1:C:208:LEU:O	1:C:212:LEU:HG	2.11	0.51
1:D:383:GLN:NE2	1:D:412:LEU:HD11	2.26	0.51
1:A:86:THR:HG22	1:A:90:MET:HE2	1.93	0.51
1:C:342:GLN:OE1	1:C:348:GLY:HA3	2.11	0.51
1:D:402:GLU:O	1:D:406:LEU:HD13	2.11	0.51
1:A:360:ILE:HG22	1:A:361:LEU:CD2	2.40	0.51
1:C:269:SER:OG	1:C:272:VAL:HG23	2.11	0.51
1:C:344:GLN:HA	1:C:344:GLN:HE21	1.76	0.51
1:D:316:LEU:C	1:D:318:GLY:H	2.14	0.51
1:B:220:ILE:HG22	1:B:222:THR:HG23	1.93	0.51
1:C:202:ARG:O	1:C:206:GLU:HG3	2.11	0.51
1:C:229:GLN:CD	1:C:229:GLN:H	2.13	0.51
1:C:274:ALA:O	1:C:277:LEU:HB3	2.11	0.51
1:C:10:ARG:HH21	1:C:424:ARG:HH11	1.59	0.51
1:A:84:ARG:NH1	1:A:120:PRO:HB2	2.27	0.51
1:B:45:PHE:HB3	1:B:47:PHE:CE1	2.45	0.51
1:C:10:ARG:HH21	1:C:424:ARG:HG2	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:299:ALA:O	1:C:303:ALA:HB2	2.10	0.51
1:C:233:TYR:HB2	1:C:283:PHE:CD1	2.45	0.50
1:D:420:VAL:HG22	1:D:421:SER:N	2.26	0.50
1:A:315:MET:SD	1:A:343:PRO:HD3	2.51	0.50
1:A:407:LEU:HD13	1:A:422:LEU:HD21	1.92	0.50
1:A:280:LYS:CD	3:A:454:FLC:OA2	2.51	0.50
1:C:68:LEU:HD11	1:C:72:PHE:HE1	1.77	0.50
1:B:224:ALA:HB1	1:B:253:MET:HG2	1.93	0.50
1:B:344:GLN:HA	1:B:344:GLN:OE1	2.10	0.50
1:D:219:LEU:HD21	1:D:324:HIS:O	2.11	0.50
1:B:389:TRP:CE3	1:B:390:LEU:HD13	2.46	0.50
1:B:155:ARG:CD	1:B:431:VAL:O	2.59	0.50
1:C:163:LEU:HD11	1:C:389:TRP:CE2	2.46	0.50
1:D:200:THR:CG2	1:D:376:GLY:HA3	2.42	0.50
1:C:68:LEU:HB3	1:C:69:PRO:HD3	1.92	0.50
1:B:168:LYS:HG2	1:B:197:TYR:CD2	2.46	0.50
1:B:57:LEU:HG	1:B:65:VAL:HG12	1.94	0.50
1:C:168:LYS:HE2	1:C:230:GLU:OE1	2.12	0.50
1:C:221:PRO:HA	1:C:311:ALA:O	2.11	0.50
1:C:227:ARG:NH2	1:C:377:PHE:HB3	2.27	0.50
1:A:389:TRP:HE3	1:A:390:LEU:HD13	1.76	0.50
1:C:203:GLU:O	1:C:207:ILE:HG13	2.12	0.49
1:C:396:VAL:HG12	1:C:398:LEU:HD13	1.93	0.49
1:D:13:THR:HB	1:D:33:PHE:HA	1.94	0.49
1:D:399:VAL:CG1	1:D:400:HIS:H	2.25	0.49
1:D:232:LEU:O	1:D:285:PRO:HD3	2.13	0.49
1:A:49:PRO:HB3	1:A:71:LEU:HD12	1.94	0.49
1:B:381:ALA:HB3	1:B:386:LEU:HD13	1.94	0.49
1:D:156:THR:O	1:D:180:ALA:HB1	2.11	0.49
1:D:57:LEU:CD2	1:D:80:VAL:CG1	2.89	0.49
1:C:208:LEU:HD21	1:C:218:VAL:HG11	1.93	0.49
1:D:355:PRO:HB2	1:D:356:PRO:HD2	1.95	0.49
1:A:165:ASN:ND2	1:A:167:GLU:H	2.09	0.49
1:B:7:GLY:O	1:B:9:ALA:N	2.46	0.49
1:D:399:VAL:CG1	1:D:400:HIS:N	2.74	0.49
1:A:10:ARG:NH1	1:A:423:ALA:O	2.43	0.49
1:B:184:LEU:HD11	1:B:399:VAL:HG11	1.95	0.49
1:D:140:GLY:O	1:D:164:GLY:HA3	2.13	0.49
1:D:224:ALA:HB3	1:D:253:MET:CE	2.43	0.49
1:D:55:VAL:CG1	1:D:80:VAL:HG22	2.43	0.49
1:A:160:SER:HB2	1:A:163:LEU:CD2	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:170:VAL:HG12	1:A:171:LEU:HD13	1.95	0.49
1:A:223:PHE:CE2	1:A:314:GLY:HA3	2.48	0.49
1:B:208:LEU:HD23	1:B:218:VAL:HG21	1.95	0.49
1:D:55:VAL:C	1:D:56:LEU:HD12	2.34	0.49
1:C:101:MET:CE	1:C:104:PRO:HA	2.43	0.48
1:D:158:VAL:HG23	1:D:180:ALA:HB2	1.94	0.48
1:D:396:VAL:HG12	1:D:398:LEU:HD12	1.94	0.48
1:C:221:PRO:HB3	1:C:321:ILE:CG1	2.37	0.48
1:D:59:HIS:HD2	1:D:61:HIS:HB2	1.77	0.48
1:D:55:VAL:HG13	1:D:80:VAL:HG13	1.94	0.48
1:A:11:GLU:CD	1:A:40:ARG:HH12	2.16	0.48
1:B:178:PRO:HB3	1:C:126:TRP:CD2	2.48	0.48
1:D:219:LEU:HD23	1:D:325:LEU:HG	1.94	0.48
1:A:85:ALA:HB3	1:A:144:GLY:HA3	1.94	0.48
1:A:2:ARG:NH1	2:A:448:SO4:O4	2.46	0.48
1:A:32:MET:HE3	1:A:62:LEU:HG	1.95	0.48
1:C:61:HIS:CD2	1:C:142:LEU:HD11	2.48	0.48
1:D:384:ASP:OD2	1:D:384:ASP:N	2.44	0.48
1:D:49:PRO:HB3	1:D:71:LEU:CD1	2.43	0.48
1:A:43:ALA:HB1	1:A:44:PRO:HD2	1.95	0.48
1:B:77:ARG:NE	2:B:441:SO4:O2	2.46	0.48
1:C:422:LEU:N	1:C:422:LEU:HD12	2.29	0.48
1:D:354:ARG:HG3	1:D:354:ARG:NH1	2.28	0.48
1:C:235:LEU:CD1	1:C:285:PRO:HG3	2.43	0.48
1:D:85:ALA:HB2	1:D:267:TYR:CD2	2.49	0.48
3:A:454:FLC:OG2	1:B:293:HIS:CE1	2.67	0.48
1:B:411:LYS:HB2	3:B:456:FLC:OHB	2.13	0.48
1:D:235:LEU:HB2	1:D:285:PRO:HG3	1.96	0.48
1:A:11:GLU:OE2	1:A:40:ARG:NH1	2.46	0.47
1:B:165:ASN:HD22	1:B:165:ASN:C	2.16	0.47
1:B:168:LYS:HG2	1:B:197:TYR:CE2	2.49	0.47
1:C:231:ILE:O	1:C:235:LEU:HD22	2.13	0.47
1:C:9:ALA:C	1:C:11:GLU:H	2.18	0.47
1:C:290:VAL:O	1:C:290:VAL:HG23	2.13	0.47
1:B:48:ASP:OD2	1:B:51:GLU:HG2	2.13	0.47
1:C:85:ALA:HB2	1:C:267:TYR:CD2	2.50	0.47
1:C:168:LYS:CE	1:C:230:GLU:OE1	2.63	0.47
1:C:25:ARG:NH1	1:C:51:GLU:HB3	2.29	0.47
1:C:27:LEU:CD1	1:C:29:ASP:O	2.62	0.47
1:A:147:PHE:HB2	1:A:160:SER:HA	1.96	0.47
1:B:182:LEU:HD11	1:B:397:VAL:CG2	2.41	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3:ILE:O	1:B:3:ILE:HG23	2.15	0.47
1:D:360:ILE:O	1:D:361:LEU:HB2	2.15	0.47
1:A:160:SER:HB2	1:A:163:LEU:HD21	1.95	0.47
1:A:223:PHE:CD2	1:A:314:GLY:HA3	2.50	0.47
1:A:29:ASP:HA	1:A:57:LEU:HD12	1.97	0.47
1:B:155:ARG:HD2	1:B:431:VAL:O	2.14	0.47
1:B:90:MET:HE3	1:B:118:LEU:HD13	1.97	0.47
1:C:1:MET:HG3	1:C:21:ALA:HB2	1.96	0.47
1:C:241:ARG:HG3	1:C:242:LEU:N	2.30	0.47
1:C:295:GLU:OE2	1:C:295:GLU:N	2.45	0.47
1:C:407:LEU:HD22	1:C:422:LEU:HD21	1.96	0.47
1:B:276:PHE:HA	1:B:280:LYS:O	2.14	0.47
1:B:68:LEU:N	1:B:69:PRO:HD2	2.30	0.47
1:D:211:THR:CG2	1:D:218:VAL:HG22	2.45	0.47
1:A:4:VAL:HG22	1:A:428:GLY:HA3	1.97	0.46
1:B:204:PHE:CZ	1:B:208:LEU:HD11	2.50	0.46
1:C:322:LEU:HD22	1:C:347:LEU:CD2	2.45	0.46
1:D:177:PRO:HB3	1:D:389:TRP:CZ2	2.50	0.46
1:A:177:PRO:HD3	1:A:389:TRP:CE2	2.51	0.46
1:A:5:PRO:HG2	1:A:423:ALA:HB1	1.97	0.46
1:B:91:GLU:O	1:B:95:GLU:HB2	2.15	0.46
1:D:298:LYS:HE3	5:D:445:HOH:O	2.15	0.46
1:D:322:LEU:CB	1:D:361:LEU:HD21	2.45	0.46
1:D:84:ARG:HG3	1:D:122:GLU:OE2	2.15	0.46
1:A:68:LEU:N	1:A:69:PRO:HD2	2.31	0.46
1:B:188:THR:HG22	1:B:189:TYR:CD1	2.50	0.46
1:B:241:ARG:CG	1:B:242:LEU:N	2.78	0.46
1:C:313:SER:HB2	1:C:315:MET:SD	2.56	0.46
1:D:347:LEU:O	1:D:350:GLU:HB3	2.16	0.46
1:B:262:PRO:O	1:B:265:VAL:HG23	2.16	0.46
1:C:85:ALA:HB2	1:C:267:TYR:CE2	2.51	0.46
1:A:168:LYS:HG2	1:A:197:TYR:CE2	2.50	0.46
1:C:229:GLN:CD	1:C:229:GLN:N	2.69	0.46
1:B:165:ASN:C	1:B:165:ASN:ND2	2.69	0.46
1:C:187:GLY:HA2	1:C:386:LEU:HD21	1.97	0.46
1:D:1:MET:HG3	1:D:21:ALA:HB2	1.97	0.46
1:A:165:ASN:C	1:A:165:ASN:ND2	2.67	0.46
1:B:315:MET:SD	1:B:343:PRO:HD3	2.56	0.46
1:C:253:MET:HB2	1:C:256:ARG:NH1	2.30	0.46
1:C:280:LYS:O	1:C:282:PRO:HD3	2.16	0.46
1:B:295:GLU:H	1:B:295:GLU:CD	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:90:MET:HE3	1:B:118:LEU:CD1	2.46	0.46
1:C:344:GLN:HA	1:C:344:GLN:NE2	2.30	0.46
1:C:399:VAL:HG12	1:C:423:ALA:HB3	1.98	0.46
1:D:285:PRO:HD2	1:D:288:LEU:HD22	1.98	0.46
1:D:322:LEU:HB3	1:D:361:LEU:HD21	1.98	0.46
1:D:389:TRP:HE3	1:D:390:LEU:HD22	1.81	0.46
1:A:344:GLN:HA	1:A:344:GLN:HE21	1.80	0.45
1:A:62:LEU:HD13	1:A:93:VAL:CG1	2.41	0.45
1:A:178:PRO:HB3	1:D:126:TRP:CD2	2.52	0.45
1:C:141:HIS:O	1:C:142:LEU:HD23	2.17	0.45
1:C:250:ASP:HA	1:C:291:VAL:HB	1.99	0.45
1:C:398:LEU:HB3	1:C:406:LEU:HG	1.98	0.45
1:D:86:THR:HG22	1:D:90:MET:HE2	1.98	0.45
1:B:178:PRO:HD3	1:C:126:TRP:CD1	2.51	0.45
1:B:396:VAL:O	1:B:420:VAL:HA	2.15	0.45
1:D:295:GLU:N	1:D:295:GLU:OE2	2.49	0.45
1:D:132:LEU:HD23	1:D:133:SER:H	1.82	0.45
1:D:68:LEU:N	1:D:69:PRO:HD2	2.30	0.45
1:C:100:VAL:HG12	1:C:100:VAL:O	2.16	0.45
1:A:155:ARG:NH1	1:A:431:VAL:OXT	2.49	0.45
1:B:192:ARG:HH11	1:B:192:ARG:HG2	1.81	0.45
1:B:199:GLU:HG3	1:B:200:THR:N	2.32	0.45
1:C:235:LEU:HD21	1:C:285:PRO:HG3	1.98	0.45
1:C:90:MET:O	1:C:94:LEU:HB2	2.15	0.45
1:D:186:GLU:HA	1:D:399:VAL:O	2.16	0.45
1:D:165:ASN:ND2	1:D:194:HIS:NE2	2.65	0.45
1:D:251:SER:OG	1:D:254:ALA:HB3	2.17	0.45
1:C:354:ARG:NH1	1:C:354:ARG:HG3	2.30	0.45
1:A:31:GLY:HA3	1:A:63:ASP:C	2.37	0.45
1:B:167:GLU:OE2	1:B:194:HIS:HE1	1.99	0.45
1:C:420:VAL:CG2	1:C:421:SER:N	2.80	0.45
1:D:204:PHE:CZ	1:D:208:LEU:HD11	2.52	0.45
1:D:232:LEU:HA	1:D:235:LEU:HD12	1.98	0.45
1:C:248:TYR:CE2	1:C:289:GLU:HG2	2.52	0.45
1:C:191:ASP:OD1	1:C:405:LYS:HD3	2.17	0.45
1:C:4:VAL:HA	1:C:5:PRO:HD3	1.82	0.45
1:C:98:LEU:HD11	1:C:108:PRO:CB	2.46	0.45
1:A:358:VAL:O	1:A:365:VAL:HG12	2.18	0.44
1:C:235:LEU:CG	1:C:285:PRO:HG3	2.47	0.44
1:C:244:ARG:HH11	1:C:244:ARG:HG3	1.81	0.44
1:B:184:LEU:HD11	1:B:399:VAL:CG1	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:441:SO4:O3	1:D:244:ARG:NH2	2.51	0.44
1:C:142:LEU:CD2	1:C:226:GLU:HB2	2.47	0.44
1:C:28:LEU:O	1:C:29:ASP:HB2	2.17	0.44
1:C:323:HIS:O	1:C:327:HIS:HD2	2.00	0.44
1:B:400:HIS:O	1:B:400:HIS:ND1	2.50	0.44
1:B:77:ARG:HG2	1:B:77:ARG:HH11	1.83	0.44
1:C:163:LEU:HD22	1:C:163:LEU:N	2.32	0.44
1:D:215:GLY:HA2	1:D:306:PRO:CD	2.42	0.44
1:B:66:GLY:O	1:B:69:PRO:HD2	2.17	0.44
1:C:253:MET:C	1:C:255:GLY:N	2.70	0.44
1:D:315:MET:SD	1:D:343:PRO:HD3	2.57	0.44
1:D:344:GLN:HA	1:D:344:GLN:NE2	2.33	0.44
1:D:236:TYR:CA	1:D:285:PRO:HB3	2.48	0.44
1:D:41:ASN:O	1:D:70:LYS:HE3	2.18	0.44
1:A:98:LEU:HD12	1:A:111:VAL:HG21	2.00	0.44
1:C:1:MET:HG2	1:C:431:VAL:HG21	2.00	0.44
1:C:2:ARG:HG3	2:C:445:SO4:O1	2.18	0.44
1:C:333:ARG:HH21	1:C:333:ARG:HG3	1.83	0.44
1:D:204:PHE:CD1	1:D:377:PHE:HZ	2.35	0.44
1:A:325:LEU:O	1:A:329:LEU:HB2	2.17	0.44
1:D:354:ARG:HG3	1:D:367:LEU:HD21	1.99	0.44
1:D:97:ALA:O	1:D:101:MET:HB2	2.17	0.44
1:A:165:ASN:HD21	1:A:167:GLU:HB2	1.83	0.44
1:A:429:VAL:HG13	1:A:430:PRO:HD2	1.99	0.44
1:C:205:LEU:HD11	1:C:238:HIS:ND1	2.33	0.44
1:C:95:GLU:HA	1:C:95:GLU:OE2	2.17	0.44
1:D:18:LEU:HD11	1:D:25:ARG:HB3	2.00	0.44
1:D:409:LEU:HD22	1:D:413:LEU:HD23	2.00	0.44
1:C:329:LEU:HD12	1:C:369:ALA:HB3	2.00	0.44
1:D:322:LEU:HB3	1:D:361:LEU:CD2	2.48	0.44
1:A:45:PHE:CZ	1:A:70:LYS:HD3	2.53	0.43
1:B:86:THR:HG22	1:B:90:MET:HE2	1.99	0.43
1:C:109:GLU:CD	1:C:109:GLU:H	2.22	0.43
1:C:113:GLU:OE2	1:C:117:HIS:HE1	2.00	0.43
1:D:12:VAL:HG23	1:D:13:THR:N	2.33	0.43
1:D:266:ARG:HB3	5:D:442:HOH:O	2.18	0.43
1:C:32:MET:HB2	1:C:41:ASN:OD1	2.17	0.43
1:C:403:GLU:HG2	1:C:407:LEU:CD2	2.47	0.43
1:A:1:MET:HG3	1:A:21:ALA:CB	2.45	0.43
1:A:57:LEU:HD23	1:A:90:MET:CE	2.48	0.43
1:D:200:THR:OG1	1:D:376:GLY:HA3	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:397:VAL:HG12	1:A:423:ALA:HB2	2.01	0.43
1:C:329:LEU:HD11	1:C:367:LEU:CD1	2.48	0.43
1:B:239:GLY:O	1:B:241:ARG:N	2.51	0.43
1:C:57:LEU:HD22	1:C:80:VAL:CG1	2.48	0.43
1:D:208:LEU:O	1:D:212:LEU:HG	2.18	0.43
1:D:330:SER:O	1:D:368:ARG:HB2	2.18	0.43
1:D:395:ARG:CG	1:D:419:GLU:HB3	2.48	0.43
1:B:220:ILE:HG22	1:B:222:THR:CG2	2.49	0.43
1:C:227:ARG:NH2	1:C:377:PHE:O	2.51	0.43
1:D:202:ARG:CB	1:D:202:ARG:NH1	2.81	0.43
1:D:232:LEU:HD23	1:D:235:LEU:HD12	2.00	0.43
1:D:295:GLU:CD	1:D:295:GLU:H	2.22	0.43
1:D:384:ASP:HA	1:D:387:LEU:HD12	2.00	0.43
1:A:102:ASP:O	1:A:104:PRO:HD3	2.19	0.43
1:D:284:ARG:HA	1:D:288:LEU:HD23	2.01	0.43
1:D:298:LYS:HA	1:D:301:ASN:HD22	1.82	0.43
1:D:42:HIS:CE1	1:D:105:PHE:HB3	2.53	0.43
1:A:284:ARG:HD2	3:A:454:FLC:OHB	2.19	0.43
1:C:367:LEU:HG	1:C:367:LEU:O	2.19	0.43
1:A:126:TRP:CD2	1:D:178:PRO:HB3	2.53	0.43
1:D:192:ARG:O	1:D:192:ARG:HD2	2.19	0.43
1:D:329:LEU:CD1	1:D:336:LEU:HD12	2.44	0.43
1:A:396:VAL:O	1:A:420:VAL:HG23	2.19	0.43
1:B:207:ILE:O	1:B:211:THR:HG23	2.19	0.43
1:C:384:ASP:N	1:C:384:ASP:OD2	2.51	0.43
1:D:132:LEU:HD23	1:D:133:SER:N	2.34	0.43
1:D:229:GLN:HG3	1:D:261:TYR:CE1	2.54	0.43
1:A:133:SER:C	1:A:134:LEU:HD12	2.40	0.43
1:B:37:GLU:CB	1:B:40:ARG:HH11	2.32	0.43
1:C:208:LEU:HD23	1:C:218:VAL:HG11	2.01	0.43
1:C:43:ALA:HB1	1:C:44:PRO:HD2	2.01	0.43
1:D:344:GLN:HA	1:D:344:GLN:HE21	1.84	0.43
1:A:398:LEU:HB3	1:A:406:LEU:HG	2.01	0.42
1:B:398:LEU:HD13	1:B:420:VAL:CG2	2.48	0.42
1:D:232:LEU:HD13	1:D:288:LEU:HD21	2.00	0.42
1:A:84:ARG:NH1	1:A:120:PRO:CB	2.82	0.42
1:A:331:ASP:HA	1:A:332:PRO:HD2	1.84	0.42
1:B:155:ARG:HD3	1:B:431:VAL:O	2.19	0.42
1:B:207:ILE:O	1:B:211:THR:CG2	2.67	0.42
1:B:58:THR:HB	1:B:146:ALA:O	2.19	0.42
1:C:231:ILE:C	1:C:233:TYR:H	2.23	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:358:VAL:O	1:C:365:VAL:HG12	2.19	0.42
1:C:227:ARG:HH12	1:C:378:GLN:HA	1.84	0.42
1:D:384:ASP:O	1:D:387:LEU:HB2	2.19	0.42
1:B:100:VAL:O	1:B:100:VAL:HG12	2.19	0.42
1:C:85:ALA:HB3	1:C:144:GLY:HA3	2.02	0.42
1:D:85:ALA:HB2	1:D:267:TYR:CZ	2.54	0.42
1:A:360:ILE:CG2	1:A:361:LEU:HD22	2.47	0.42
1:C:33:PHE:H	1:C:41:ASN:ND2	1.89	0.42
1:C:80:VAL:HB	1:C:118:LEU:HD23	2.00	0.42
1:C:315:MET:O	1:C:316:LEU:HB2	2.19	0.42
1:C:374:LEU:C	1:C:376:GLY:H	2.23	0.42
1:A:420:VAL:HG22	1:A:421:SER:N	2.34	0.42
1:C:10:ARG:NH2	1:C:424:ARG:NH1	2.63	0.42
1:D:229:GLN:CD	1:D:229:GLN:N	2.72	0.42
1:D:320:ARG:HG2	1:D:320:ARG:O	2.19	0.42
1:A:155:ARG:HD3	1:A:431:VAL:O	2.19	0.42
1:C:420:VAL:CG2	1:C:421:SER:H	2.31	0.42
1:D:134:LEU:HD23	1:D:150:ALA:HB2	2.01	0.42
1:D:359:ARG:HA	1:D:364:GLU:HA	2.02	0.42
1:A:87:VAL:HG13	1:A:118:LEU:HD13	2.00	0.42
1:B:20:LEU:HD21	1:B:25:ARG:HE	1.84	0.42
1:D:226:GLU:C	1:D:229:GLN:HE21	2.23	0.42
1:B:37:GLU:O	1:B:39:ALA:N	2.53	0.42
1:D:296:ALA:O	1:D:299:ALA:HB3	2.20	0.42
1:A:381:ALA:HB3	1:A:386:LEU:HD13	2.02	0.42
1:B:259:SER:O	1:B:262:PRO:HD2	2.20	0.42
1:B:178:PRO:HB3	1:C:126:TRP:CE3	2.54	0.42
1:D:329:LEU:HD21	1:D:351:ILE:HD13	2.01	0.42
1:D:164:GLY:O	1:D:381:ALA:HB2	2.20	0.42
1:D:406:LEU:HD23	1:D:422:LEU:HG	2.02	0.42
1:C:344:GLN:CA	1:C:344:GLN:HE21	2.32	0.41
1:C:42:HIS:CE1	1:C:105:PHE:HB3	2.56	0.41
1:D:202:ARG:HB2	1:D:202:ARG:HH11	1.84	0.41
1:D:229:GLN:HG3	1:D:261:TYR:CZ	2.55	0.41
1:D:310:LEU:HD12	1:D:310:LEU:N	2.34	0.41
1:B:28:LEU:O	1:B:29:ASP:HB2	2.20	0.41
1:B:10:ARG:HH11	1:B:424:ARG:HG2	1.82	0.41
1:C:233:TYR:HB2	1:C:283:PHE:HD1	1.84	0.41
1:D:204:PHE:HB2	1:D:374:LEU:HD13	2.01	0.41
1:A:200:THR:CG2	1:A:374:LEU:HB3	2.46	0.41
1:B:244:ARG:HG2	1:B:244:ARG:HH11	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:320:ARG:HD3	3:B:455:FLC:HG1	2.01	0.41
1:C:241:ARG:HG3	1:C:242:LEU:H	1.86	0.41
1:C:404:GLU:HG3	5:C:465:HOH:O	2.19	0.41
1:D:297:SER:OG	1:D:320:ARG:HD3	2.20	0.41
1:D:348:GLY:O	1:D:352:ILE:HG13	2.19	0.41
3:A:454:FLC:OG2	1:B:293:HIS:NE2	2.53	0.41
1:C:192:ARG:HA	1:C:193:PRO:HD3	1.92	0.41
1:C:234:VAL:O	1:C:238:HIS:HB2	2.20	0.41
1:B:29:ASP:HA	1:B:57:LEU:HD12	2.03	0.41
1:C:297:SER:OG	1:C:320:ARG:HD3	2.21	0.41
1:D:48:ASP:HA	1:D:49:PRO:HD2	1.81	0.41
1:A:5:PRO:HA	1:A:17:HIS:ND1	2.36	0.41
1:B:404:GLU:CD	1:B:404:GLU:N	2.71	0.41
1:D:365:VAL:HA	1:D:366:PRO:HD3	1.92	0.41
1:B:204:PHE:HB2	1:B:374:LEU:HD13	2.03	0.41
1:C:14:GLY:O	1:C:15:SER:C	2.59	0.41
1:C:3:ILE:HG23	1:C:3:ILE:O	2.21	0.41
1:D:269:SER:HB2	2:D:436:SO4:O2	2.21	0.41
1:C:224:ALA:O	1:C:257:VAL:HG21	2.21	0.41
1:C:33:PHE:CD2	1:C:40:ARG:HB2	2.55	0.41
1:C:386:LEU:HD23	1:C:409:LEU:CD1	2.51	0.41
1:D:98:LEU:HD12	1:D:111:VAL:HG21	2.03	0.41
1:D:381:ALA:HB3	1:D:386:LEU:CD1	2.50	0.41
1:D:89:LEU:HD23	1:D:260:LEU:HD23	2.03	0.41
1:D:191:ASP:CG	1:D:405:LYS:HD2	2.41	0.41
1:A:157:LEU:HG	1:A:158:VAL:N	2.32	0.40
1:C:200:THR:HG21	1:C:376:GLY:CA	2.51	0.40
1:D:165:ASN:HD21	1:D:194:HIS:CE1	2.39	0.40
1:A:235:LEU:HD13	1:A:247:ILE:HD13	2.04	0.40
1:A:194:HIS:HB3	1:A:378:GLN:CD	2.41	0.40
1:B:40:ARG:C	1:B:42:HIS:H	2.25	0.40
1:C:196:PRO:HB2	1:C:199:GLU:HG2	2.03	0.40
1:C:343:PRO:O	1:C:349:ALA:HB2	2.22	0.40
1:D:336:LEU:HD23	1:D:336:LEU:C	2.41	0.40
1:A:288:LEU:HD12	1:A:289:GLU:H	1.87	0.40
1:B:233:TYR:CE1	1:B:282:PRO:HB2	2.56	0.40
1:C:301:ASN:HB2	1:C:327:HIS:CG	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	429/431 (100%)	400 (93%)	29 (7%)	0	100	100
1	B	429/431 (100%)	398 (93%)	27 (6%)	4 (1%)	20	36
1	C	429/431 (100%)	363 (85%)	59 (14%)	7 (2%)	11	19
1	D	429/431 (100%)	368 (86%)	51 (12%)	10 (2%)	7	11
All	All	1716/1724 (100%)	1529 (89%)	166 (10%)	21 (1%)	15	27

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	36	LYS
1	B	8	ALA
1	B	38	GLU
1	B	240	HIS
1	C	193	PRO
1	D	292	GLU
1	D	295	GLU
1	D	400	HIS
1	C	15	SER
1	D	102	ASP
1	D	187	GLY
1	D	328	GLY
1	C	227	ARG
1	C	38	GLU
1	C	285	PRO
1	D	317	ALA
1	C	400	HIS
1	D	38	GLU
1	D	215	GLY
1	C	426	GLY
1	D	251	SER

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	342/342 (100%)	318 (93%)	24 (7%)	18	33
1	B	342/342 (100%)	318 (93%)	24 (7%)	18	33
1	C	342/342 (100%)	326 (95%)	16 (5%)	30	54
1	D	342/342 (100%)	329 (96%)	13 (4%)	38	64
All	All	1368/1368 (100%)	1291 (94%)	77 (6%)	25	45

All (77) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	55	VAL
1	A	57	LEU
1	A	94	LEU
1	A	98	LEU
1	A	163	LEU
1	A	165	ASN
1	A	171	LEU
1	A	179	LEU
1	A	186	GLU
1	A	195	ARG
1	A	199	GLU
1	A	211	THR
1	A	229	GLN
1	A	241	ARG
1	A	264	LEU
1	A	325	LEU
1	A	329	LEU
1	A	336	LEU
1	A	361	LEU
1	A	386	LEU
1	A	390	LEU
1	A	406	LEU
1	A	407	LEU
1	A	409	LEU

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Mol	Chain	Res	Type
1	B	27	LEU
1	B	57	LEU
1	B	62	LEU
1	B	94	LEU
1	B	98	LEU
1	B	155	ARG
1	B	165	ASN
1	B	171	LEU
1	B	175	SER
1	B	186	GLU
1	B	195	ARG
1	B	211	THR
1	B	219	LEU
1	B	229	GLN
1	B	253	MET
1	B	264	LEU
1	B	329	LEU
1	B	336	LEU
1	B	341	TYR
1	B	365	VAL
1	B	386	LEU
1	B	390	LEU
1	B	407	LEU
1	B	409	LEU
1	C	55	VAL
1	C	57	LEU
1	C	98	LEU
1	C	103	GLU
1	C	155	ARG
1	C	165	ASN
1	C	171	LEU
1	C	192	ARG
1	C	195	ARG
1	C	235	LEU
1	C	264	LEU
1	C	302	ARG
1	C	308	VAL
1	C	315	MET
1	C	354	ARG
1	C	398	LEU
1	D	27	LEU
1	D	38	GLU

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Mol	Chain	Res	Type
1	D	55	VAL
1	D	96	ASP
1	D	109	GLU
1	D	132	LEU
1	D	165	ASN
1	D	171	LEU
1	D	192	ARG
1	D	195	ARG
1	D	265	VAL
1	D	292	GLU
1	D	409	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	ASN
1	A	59	HIS
1	A	165	ASN
1	A	229	GLN
1	A	344	GLN
1	A	378	GLN
1	B	41	ASN
1	B	61	HIS
1	B	165	ASN
1	B	229	GLN
1	B	238	HIS
1	B	240	HIS
1	B	380	HIS
1	B	383	GLN
1	C	41	ASN
1	C	117	HIS
1	C	165	ASN
1	C	323	HIS
1	C	342	GLN
1	C	344	GLN
1	D	41	ASN
1	D	151	GLN
1	D	165	ASN
1	D	229	GLN
1	D	238	HIS
1	D	240	HIS
1	D	293	HIS

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Mol	Chain	Res	Type
1	D	301	ASN
1	D	327	HIS
1	D	344	GLN
1	D	372	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 77 ligands modelled in this entry, 8 are monoatomic - leaving 69 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	$\# Z > 2$
2	SO4	A	432	-	4,4,4	1.05	0	6,6,6	0.65	0
2	SO4	A	433	-	4,4,4	1.08	0	6,6,6	0.70	0
2	SO4	A	434	-	4,4,4	1.04	0	6,6,6	0.67	0
2	SO4	A	435	-	4,4,4	1.00	0	6,6,6	0.67	0
2	SO4	A	436	-	4,4,4	1.02	0	6,6,6	0.66	0
2	SO4	A	437	-	4,4,4	1.03	0	6,6,6	0.65	0
2	SO4	A	438	-	4,4,4	1.01	0	6,6,6	0.66	0
2	SO4	A	439	-	4,4,4	1.03	0	6,6,6	0.66	0
2	SO4	A	440	-	4,4,4	1.02	0	6,6,6	0.66	0
2	SO4	A	441	-	4,4,4	1.03	0	6,6,6	0.66	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SO4	A	442	-	4,4,4	1.04	0	6,6,6	0.63	0
2	SO4	A	443	-	4,4,4	1.03	0	6,6,6	0.64	0
2	SO4	A	444	-	4,4,4	1.03	0	6,6,6	0.67	0
2	SO4	A	445	-	4,4,4	1.06	0	6,6,6	0.66	0
2	SO4	A	446	-	4,4,4	1.06	0	6,6,6	0.65	0
2	SO4	A	447	-	4,4,4	1.05	0	6,6,6	0.64	0
2	SO4	A	448	-	4,4,4	1.06	0	6,6,6	0.65	0
2	SO4	A	449	-	4,4,4	1.03	0	6,6,6	0.67	0
2	SO4	A	450	-	4,4,4	1.06	0	6,6,6	0.67	0
2	SO4	A	451	-	4,4,4	1.05	0	6,6,6	0.65	0
2	SO4	A	452	-	4,4,4	1.04	0	6,6,6	0.67	0
2	SO4	A	453	-	4,4,4	1.04	0	6,6,6	0.65	0
3	FLC	A	454	-	3,12,12	1.11	0	3,17,17	0.20	0
2	SO4	B	432	-	4,4,4	1.03	0	6,6,6	0.65	0
2	SO4	B	433	-	4,4,4	1.04	0	6,6,6	0.64	0
2	SO4	B	434	-	4,4,4	1.02	0	6,6,6	0.68	0
2	SO4	B	435	-	4,4,4	1.05	0	6,6,6	0.64	0
2	SO4	B	436	-	4,4,4	1.04	0	6,6,6	0.65	0
2	SO4	B	437	-	4,4,4	0.99	0	6,6,6	0.60	0
2	SO4	B	438	-	4,4,4	1.03	0	6,6,6	0.65	0
2	SO4	B	439	-	4,4,4	1.08	0	6,6,6	0.63	0
2	SO4	B	440	-	4,4,4	1.05	0	6,6,6	0.65	0
2	SO4	B	441	-	4,4,4	1.04	0	6,6,6	0.64	0
2	SO4	B	442	-	4,4,4	1.05	0	6,6,6	0.65	0
2	SO4	B	443	-	4,4,4	1.03	0	6,6,6	0.65	0
2	SO4	B	444	-	4,4,4	1.05	0	6,6,6	0.62	0
2	SO4	B	445	-	4,4,4	0.98	0	6,6,6	0.68	0
2	SO4	B	446	-	4,4,4	1.04	0	6,6,6	0.66	0
2	SO4	B	447	-	4,4,4	1.04	0	6,6,6	0.65	0
2	SO4	B	448	-	4,4,4	1.08	0	6,6,6	0.63	0
2	SO4	B	449	-	4,4,4	1.05	0	6,6,6	0.63	0
2	SO4	B	450	-	4,4,4	1.01	0	6,6,6	0.67	0
2	SO4	B	451	-	4,4,4	1.04	0	6,6,6	0.65	0
2	SO4	B	452	-	4,4,4	1.03	0	6,6,6	0.68	0
2	SO4	B	453	-	4,4,4	0.98	0	6,6,6	0.68	0
2	SO4	B	454	-	4,4,4	1.01	0	6,6,6	0.68	0
3	FLC	B	455	-	3,12,12	0.87	0	3,17,17	1.06	0
3	FLC	B	456	-	3,12,12	1.13	0	3,17,17	0.20	0
2	SO4	C	432	-	4,4,4	1.06	0	6,6,6	0.64	0
2	SO4	C	433	-	4,4,4	1.05	0	6,6,6	0.67	0
2	SO4	C	434	-	4,4,4	1.02	0	6,6,6	0.66	0
2	SO4	C	435	-	4,4,4	1.05	0	6,6,6	0.64	0
2	SO4	C	436	-	4,4,4	1.07	0	6,6,6	0.63	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SO4	C	437	-	4,4,4	1.04	0	6,6,6	0.65	0
2	SO4	C	438	-	4,4,4	1.06	0	6,6,6	0.65	0
2	SO4	C	439	-	4,4,4	1.04	0	6,6,6	0.63	0
2	SO4	C	440	-	4,4,4	1.04	0	6,6,6	0.66	0
2	SO4	C	441	-	4,4,4	1.02	0	6,6,6	0.66	0
2	SO4	C	442	-	4,4,4	1.05	0	6,6,6	0.63	0
2	SO4	C	443	-	4,4,4	1.04	0	6,6,6	0.65	0
2	SO4	C	444	-	4,4,4	1.06	0	6,6,6	0.65	0
2	SO4	C	445	-	4,4,4	1.07	0	6,6,6	0.63	0
2	SO4	C	446	-	4,4,4	1.04	0	6,6,6	0.65	0
2	SO4	D	432	-	4,4,4	1.05	0	6,6,6	0.65	0
2	SO4	D	433	-	4,4,4	1.06	0	6,6,6	0.64	0
2	SO4	D	434	-	4,4,4	1.04	0	6,6,6	0.66	0
2	SO4	D	435	-	4,4,4	1.06	0	6,6,6	0.65	0
2	SO4	D	436	-	4,4,4	1.00	0	6,6,6	0.68	0
2	SO4	D	437	-	4,4,4	1.03	0	6,6,6	0.66	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
2	SO4	A	432	-	-	0/0/0/0	0/0/0/0
2	SO4	A	433	-	-	0/0/0/0	0/0/0/0
2	SO4	A	434	-	-	0/0/0/0	0/0/0/0
2	SO4	A	435	-	-	0/0/0/0	0/0/0/0
2	SO4	A	436	-	-	0/0/0/0	0/0/0/0
2	SO4	A	437	-	-	0/0/0/0	0/0/0/0
2	SO4	A	438	-	-	0/0/0/0	0/0/0/0
2	SO4	A	439	-	-	0/0/0/0	0/0/0/0
2	SO4	A	440	-	-	0/0/0/0	0/0/0/0
2	SO4	A	441	-	-	0/0/0/0	0/0/0/0
2	SO4	A	442	-	-	0/0/0/0	0/0/0/0
2	SO4	A	443	-	-	0/0/0/0	0/0/0/0
2	SO4	A	444	-	-	0/0/0/0	0/0/0/0
2	SO4	A	445	-	-	0/0/0/0	0/0/0/0
2	SO4	A	446	-	-	0/0/0/0	0/0/0/0
2	SO4	A	447	-	-	0/0/0/0	0/0/0/0
2	SO4	A	448	-	-	0/0/0/0	0/0/0/0
2	SO4	A	449	-	-	0/0/0/0	0/0/0/0
2	SO4	A	450	-	-	0/0/0/0	0/0/0/0
2	SO4	A	451	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SO4	A	452	-	-	0/0/0/0	0/0/0/0
2	SO4	A	453	-	-	0/0/0/0	0/0/0/0
3	FLC	A	454	-	-	0/6/16/16	0/0/0/0
2	SO4	B	432	-	-	0/0/0/0	0/0/0/0
2	SO4	B	433	-	-	0/0/0/0	0/0/0/0
2	SO4	B	434	-	-	0/0/0/0	0/0/0/0
2	SO4	B	435	-	-	0/0/0/0	0/0/0/0
2	SO4	B	436	-	-	0/0/0/0	0/0/0/0
2	SO4	B	437	-	-	0/0/0/0	0/0/0/0
2	SO4	B	438	-	-	0/0/0/0	0/0/0/0
2	SO4	B	439	-	-	0/0/0/0	0/0/0/0
2	SO4	B	440	-	-	0/0/0/0	0/0/0/0
2	SO4	B	441	-	-	0/0/0/0	0/0/0/0
2	SO4	B	442	-	-	0/0/0/0	0/0/0/0
2	SO4	B	443	-	-	0/0/0/0	0/0/0/0
2	SO4	B	444	-	-	0/0/0/0	0/0/0/0
2	SO4	B	445	-	-	0/0/0/0	0/0/0/0
2	SO4	B	446	-	-	0/0/0/0	0/0/0/0
2	SO4	B	447	-	-	0/0/0/0	0/0/0/0
2	SO4	B	448	-	-	0/0/0/0	0/0/0/0
2	SO4	B	449	-	-	0/0/0/0	0/0/0/0
2	SO4	B	450	-	-	0/0/0/0	0/0/0/0
2	SO4	B	451	-	-	0/0/0/0	0/0/0/0
2	SO4	B	452	-	-	0/0/0/0	0/0/0/0
2	SO4	B	453	-	-	0/0/0/0	0/0/0/0
2	SO4	B	454	-	-	0/0/0/0	0/0/0/0
3	FLC	B	455	-	-	0/6/16/16	0/0/0/0
3	FLC	B	456	-	-	0/6/16/16	0/0/0/0
2	SO4	C	432	-	-	0/0/0/0	0/0/0/0
2	SO4	C	433	-	-	0/0/0/0	0/0/0/0
2	SO4	C	434	-	-	0/0/0/0	0/0/0/0
2	SO4	C	435	-	-	0/0/0/0	0/0/0/0
2	SO4	C	436	-	-	0/0/0/0	0/0/0/0
2	SO4	C	437	-	-	0/0/0/0	0/0/0/0
2	SO4	C	438	-	-	0/0/0/0	0/0/0/0
2	SO4	C	439	-	-	0/0/0/0	0/0/0/0
2	SO4	C	440	-	-	0/0/0/0	0/0/0/0
2	SO4	C	441	-	-	0/0/0/0	0/0/0/0
2	SO4	C	442	-	-	0/0/0/0	0/0/0/0
2	SO4	C	443	-	-	0/0/0/0	0/0/0/0
2	SO4	C	444	-	-	0/0/0/0	0/0/0/0
2	SO4	C	445	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SO4	C	446	-	-	0/0/0/0	0/0/0/0
2	SO4	D	432	-	-	0/0/0/0	0/0/0/0
2	SO4	D	433	-	-	0/0/0/0	0/0/0/0
2	SO4	D	434	-	-	0/0/0/0	0/0/0/0
2	SO4	D	435	-	-	0/0/0/0	0/0/0/0
2	SO4	D	436	-	-	0/0/0/0	0/0/0/0
2	SO4	D	437	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

12 monomers are involved in 30 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	436	SO4	1	0
2	A	443	SO4	5	0
2	A	448	SO4	1	0
2	A	449	SO4	1	0
3	A	454	FLC	7	0
2	B	441	SO4	2	0
3	B	455	FLC	3	0
3	B	456	FLC	4	0
2	C	439	SO4	1	0
2	C	445	SO4	1	0
2	D	432	SO4	3	0
2	D	436	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	431/431 (100%)	0.09	2 (0%) 90 91	24, 43, 67, 82	0
1	B	431/431 (100%)	0.12	8 (1%) 67 69	24, 43, 68, 88	0
1	C	431/431 (100%)	1.16	98 (22%) 1 1	28, 75, 133, 137	0
1	D	431/431 (100%)	1.52	112 (25%) 1 0	36, 80, 142, 146	0
All	All	1724/1724 (100%)	0.72	220 (12%) 4 3	24, 53, 132, 146	0

All (220) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	374	LEU	9.9
1	D	326	LYS	9.8
1	C	219	LEU	9.3
1	D	219	LEU	9.2
1	D	322	LEU	9.2
1	C	326	LYS	8.5
1	D	212	LEU	8.2
1	D	208	LEU	8.2
1	C	329	LEU	8.1
1	C	216	GLY	8.0
1	C	336	LEU	8.0
1	D	300	LEU	7.9
1	C	337	VAL	7.8
1	D	242	LEU	7.8
1	D	338	PHE	7.8
1	D	329	LEU	7.5
1	D	245	ALA	7.1
1	C	242	LEU	7.0
1	D	218	VAL	6.9
1	D	330	SER	6.8
1	C	335	ALA	6.7

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Mol	Chain	Res	Type	RSRZ
1	D	307	MET	6.6
1	C	306	PRO	6.5
1	D	244	ARG	6.5
1	C	371	VAL	6.4
1	C	218	VAL	6.3
1	C	214	GLN	6.3
1	C	305	GLY	6.2
1	C	303	ALA	6.0
1	C	338	PHE	6.0
1	D	332	PRO	5.9
1	C	217	LYS	5.8
1	D	361	LEU	5.7
1	D	249	LEU	5.6
1	D	339	VAL	5.6
1	D	306	PRO	5.5
1	C	241	ARG	5.5
1	D	368	ARG	5.5
1	D	360	ILE	5.5
1	D	309	VAL	5.4
1	D	239	GLY	5.4
1	D	211	THR	5.3
1	C	333	ARG	5.3
1	D	288	LEU	5.3
1	D	328	GLY	5.3
1	D	228	ALA	5.3
1	D	325	LEU	5.3
1	D	250	ASP	5.2
1	D	302	ARG	5.2
1	C	245	ALA	5.1
1	D	371	VAL	5.0
1	D	220	ILE	5.0
1	C	304	PRO	4.9
1	D	377	PHE	4.9
1	D	213	SER	4.8
1	D	369	ALA	4.7
1	C	354	ARG	4.7
1	D	335	ALA	4.6
1	C	213	SER	4.6
1	D	192	ARG	4.6
1	D	201	VAL	4.6
1	D	324	HIS	4.6
1	D	316	LEU	4.6

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Mol	Chain	Res	Type	RSRZ
1	D	231	ILE	4.5
1	D	367	LEU	4.5
1	C	366	PRO	4.5
1	C	250	ASP	4.4
1	D	304	PRO	4.4
1	C	353	ALA	4.4
1	D	333	ARG	4.3
1	D	362	GLY	4.3
1	C	301	ASN	4.3
1	C	238	HIS	4.3
1	C	209	GLU	4.3
1	C	302	ARG	4.3
1	D	287	GLY	4.2
1	D	214	GLN	4.2
1	D	305	GLY	4.2
1	C	368	ARG	4.2
1	C	247	ILE	4.1
1	D	308	VAL	4.1
1	D	323	HIS	4.1
1	D	312	GLY	4.1
1	D	286	ALA	4.1
1	D	246	PRO	4.0
1	C	294	THR	4.0
1	D	337	VAL	4.0
1	C	367	LEU	4.0
1	D	194	HIS	4.0
1	D	217	LYS	4.0
1	C	300	LEU	3.9
1	C	291	VAL	3.9
1	D	209	GLU	3.9
1	C	244	ARG	3.9
1	D	248	TYR	3.9
1	C	343	PRO	3.8
1	C	307	MET	3.8
1	C	377	PHE	3.8
1	D	207	ILE	3.8
1	C	358	VAL	3.7
1	C	240	HIS	3.7
1	C	322	LEU	3.7
1	C	370	SER	3.7
1	C	369	ALA	3.7
1	C	210	LYS	3.7

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Mol	Chain	Res	Type	RSRZ
1	D	334	ASN	3.7
1	C	293	HIS	3.7
1	D	303	ALA	3.7
1	D	204	PHE	3.6
1	C	208	LEU	3.6
1	D	331	ASP	3.6
1	D	336	LEU	3.6
1	D	235	LEU	3.6
1	C	205	LEU	3.6
1	D	99	LYS	3.5
1	D	216	GLY	3.5
1	D	342	GLN	3.5
1	D	340	GLY	3.5
1	C	311	ALA	3.5
1	C	372	HIS	3.4
1	C	316	LEU	3.4
1	B	78	GLY	3.4
1	C	373	THR	3.3
1	D	297	SER	3.3
1	C	332	PRO	3.3
1	D	205	LEU	3.3
1	C	376	GLY	3.3
1	A	341	TYR	3.3
1	D	294	THR	3.2
1	C	325	LEU	3.2
1	D	341	TYR	3.2
1	C	415	LEU	3.2
1	C	334	ASN	3.2
1	D	92	ILE	3.1
1	C	248	TYR	3.1
1	C	252	PRO	3.1
1	C	342	GLN	3.1
1	D	101	MET	3.1
1	C	374	LEU	3.1
1	D	102	ASP	3.1
1	C	360	ILE	3.0
1	D	98	LEU	3.0
1	C	295	GLU	3.0
1	D	240	HIS	3.0
1	D	224	ALA	3.0
1	D	298	LYS	3.0
1	D	299	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	310	LEU	3.0
1	C	243	PRO	3.0
1	C	207	ILE	2.9
1	D	293	HIS	2.9
1	C	364	GLU	2.9
1	C	330	SER	2.9
1	D	301	ASN	2.9
1	C	195	ARG	2.9
1	B	240	HIS	2.9
1	C	251	SER	2.8
1	D	370	SER	2.8
1	C	194	HIS	2.8
1	C	323	HIS	2.8
1	C	328	GLY	2.7
1	D	291	VAL	2.7
1	D	197	TYR	2.7
1	D	321	ILE	2.7
1	C	215	GLY	2.7
1	C	212	LEU	2.6
1	C	352	ILE	2.6
1	D	247	ILE	2.6
1	C	288	LEU	2.6
1	C	310	LEU	2.6
1	C	202	ARG	2.6
1	D	210	LYS	2.6
1	D	352	ILE	2.6
1	D	366	PRO	2.6
1	D	387	LEU	2.6
1	D	363	GLU	2.6
1	C	344	GLN	2.6
1	D	411	LYS	2.5
1	D	252	PRO	2.5
1	D	327	HIS	2.5
1	C	289	GLU	2.5
1	C	356	PRO	2.5
1	C	324	HIS	2.4
1	D	35	GLY	2.4
1	D	94	LEU	2.4
1	C	404	GLU	2.4
1	D	108	PRO	2.4
1	D	320	ARG	2.3
1	B	72	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	201	VAL	2.3
1	D	243	PRO	2.3
1	C	351	ILE	2.3
1	C	327	HIS	2.3
1	C	308	VAL	2.2
1	C	276	PHE	2.2
1	C	411	LYS	2.2
1	B	192	ARG	2.2
1	C	223	PHE	2.2
1	C	349	ALA	2.2
1	C	292	GLU	2.2
1	D	290	VAL	2.2
1	D	376	GLY	2.2
1	B	77	ARG	2.2
1	B	225	VAL	2.2
1	B	280	LYS	2.2
1	D	415	LEU	2.2
1	C	297	SER	2.2
1	C	365	VAL	2.1
1	C	192	ARG	2.1
1	C	235	LEU	2.1
1	C	204	PHE	2.1
1	D	258	LEU	2.1
1	D	190	GLY	2.1
1	D	292	GLU	2.1
1	A	149	VAL	2.1
1	D	364	GLU	2.0
1	D	386	LEU	2.0
1	C	211	THR	2.0
1	D	398	LEU	2.0
1	B	51	GLU	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	SO4	A	445	5/5	0.73	0.69	19.76	137,138,138,139	0
2	SO4	B	447	5/5	0.70	0.36	11.21	143,143,143,143	0
3	FLC	B	456	13/13	0.71	0.46	8.07	98,104,109,109	0
3	FLC	B	455	13/13	0.60	0.40	6.81	110,110,111,112	0
2	SO4	B	449	5/5	0.86	0.36	6.67	144,144,144,145	0
2	SO4	A	436	5/5	0.87	0.40	4.51	156,156,156,156	0
2	SO4	C	439	5/5	0.65	0.41	3.06	149,149,149,149	0
2	SO4	B	448	5/5	0.85	0.34	2.98	145,145,145,145	0
2	SO4	B	451	5/5	0.72	0.37	2.14	140,140,140,140	0
2	SO4	A	452	5/5	0.82	0.27	1.65	128,128,128,129	0
2	SO4	A	434	5/5	0.98	0.17	1.16	41,42,44,45	0
2	SO4	B	440	5/5	0.87	0.23	1.16	110,110,110,111	0
2	SO4	A	447	5/5	0.80	0.20	0.87	128,128,128,129	0
2	SO4	C	446	5/5	0.94	0.20	0.53	101,101,101,102	0
2	SO4	D	437	5/5	0.90	0.22	0.26	126,127,127,127	0
2	SO4	B	453	5/5	0.96	0.13	0.17	54,55,57,57	0
2	SO4	C	435	5/5	0.72	0.22	0.11	155,155,155,155	0
2	SO4	D	436	5/5	0.94	0.18	0.10	90,90,91,91	0
2	SO4	A	435	5/5	0.97	0.16	-0.15	52,53,55,58	0
2	SO4	A	443	5/5	0.78	0.18	-0.47	135,136,136,136	0
2	SO4	C	440	5/5	0.79	0.33	-0.48	148,148,148,148	0
2	SO4	A	450	5/5	0.91	0.14	-0.57	98,98,99,100	0
4	ZN	D	438	1/1	0.93	0.15	-0.59	101,101,101,101	0
2	SO4	B	438	5/5	0.97	0.15	-0.99	64,65,66,67	0
2	SO4	B	437	5/5	0.98	0.13	-1.05	47,47,51,52	0
2	SO4	A	433	5/5	0.97	0.16	-1.24	52,56,58,59	0
2	SO4	D	432	5/5	0.86	0.15	-1.40	117,117,117,117	0
4	ZN	C	447	1/1	0.82	0.11	-1.41	117,117,117,117	0
2	SO4	C	444	5/5	0.89	0.12	-1.65	113,113,113,113	0
2	SO4	A	437	5/5	0.96	0.10	-1.80	77,77,78,78	0
4	ZN	C	448	1/1	0.85	0.11	-1.85	115,115,115,115	0
4	ZN	D	439	1/1	0.97	0.06	-3.08	94,94,94,94	0
4	ZN	A	456	1/1	0.97	0.07	-3.32	72,72,72,72	0
2	SO4	C	443	5/5	0.95	0.11	-3.91	102,103,103,103	0
4	ZN	B	457	1/1	0.94	0.05	-4.25	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	ZN	A	455	1/1	0.99	0.04	-5.57	67,67,67,67	0
4	ZN	B	458	1/1	0.93	0.06	-11.60	79,79,79,79	0
2	SO4	B	443	5/5	0.91	0.19	-	118,119,119,119	0
2	SO4	B	436	5/5	0.87	0.16	-	120,121,121,121	0
3	FLC	A	454	13/13	0.67	0.38	-	103,106,110,110	0
2	SO4	C	434	5/5	0.95	0.09	-	111,111,111,111	0
2	SO4	C	437	5/5	0.84	0.24	-	144,144,144,145	0
2	SO4	A	451	5/5	0.82	0.29	-	137,137,138,138	0
2	SO4	B	439	5/5	0.81	0.35	-	135,135,135,136	0
2	SO4	B	442	5/5	0.92	0.19	-	119,119,119,119	0
2	SO4	A	439	5/5	0.91	0.13	-	136,136,136,136	0
2	SO4	C	436	5/5	0.86	0.27	-	138,138,139,139	0
2	SO4	B	445	5/5	0.83	0.30	-	142,142,142,142	0
2	SO4	A	440	5/5	0.79	0.17	-	122,123,123,123	0
2	SO4	A	448	5/5	0.90	0.18	-	98,98,99,99	0
2	SO4	B	454	5/5	0.80	0.17	-	123,124,124,124	0
2	SO4	C	442	5/5	0.85	0.15	-	111,111,111,112	0
2	SO4	C	438	5/5	0.69	0.40	-	143,143,144,144	0
2	SO4	A	453	5/5	0.84	0.18	-	122,122,122,123	0
2	SO4	A	441	5/5	0.88	0.13	-	136,137,137,137	0
2	SO4	B	435	5/5	0.92	0.12	-	98,99,100,100	0
2	SO4	A	442	5/5	0.92	0.18	-	96,96,96,98	0
2	SO4	B	452	5/5	0.89	0.28	-	98,98,99,99	0
2	SO4	B	432	5/5	0.96	0.15	-	110,110,110,110	0
2	SO4	C	441	5/5	0.98	0.13	-	71,71,72,73	0
2	SO4	C	433	5/5	0.83	0.24	-	121,121,121,122	0
2	SO4	C	445	5/5	0.86	0.15	-	128,128,128,128	0
2	SO4	B	441	5/5	0.84	0.33	-	159,159,160,160	0
2	SO4	D	433	5/5	0.89	0.12	-	123,124,124,124	0
2	SO4	C	432	5/5	0.92	0.18	-	90,91,92,92	0
2	SO4	B	433	5/5	0.96	0.12	-	91,91,92,92	0
2	SO4	B	446	5/5	0.94	0.10	-	84,84,85,85	0
2	SO4	D	434	5/5	0.96	0.12	-	81,82,82,83	0
2	SO4	A	449	5/5	0.67	0.24	-	135,135,135,136	0
2	SO4	B	450	5/5	0.96	0.10	-	79,79,80,81	0
2	SO4	B	444	5/5	0.89	0.23	-	116,116,117,117	0
2	SO4	B	434	5/5	0.79	0.45	-	148,148,148,149	0
2	SO4	A	446	5/5	0.85	0.30	-	131,131,132,132	0
2	SO4	D	435	5/5	0.86	0.17	-	132,132,132,132	0
2	SO4	A	438	5/5	0.90	0.21	-	116,116,116,116	0
2	SO4	A	432	5/5	0.75	0.16	-	138,138,138,139	0
2	SO4	A	444	5/5	0.90	0.14	-	109,109,110,110	0

6.5 Other polymers [i](#)

There are no such residues in this entry.