



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 03:12 AM UTC

PDB ID : 3IDZ / pdb_00003idz
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 : 2009-07-22
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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

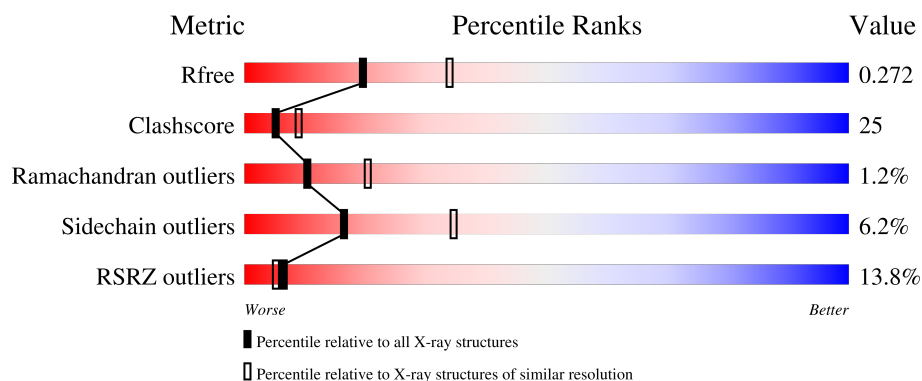
1 Overall quality at a glance

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}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	66% 29% 6%
1	B	431	3% 65% 31% .
1	C	431	22% 50% 44% 6%
1	D	431	29% 48% 48% .

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	443	-	-	X	-
2	SO4	B	441	-	-	X	-
2	SO4	D	432	-	-	X	-
3	FLC	A	454	-	-	X	-
3	FLC	B	456	-	-	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 mutation	UNP Q5SLP1
B	378	GLN	SER	engineered mutation	UNP Q5SLP1
C	378	GLN	SER	engineered mutation	UNP Q5SLP1
D	378	GLN	SER	engineered mutation	UNP Q5SLP1

- Molecule 2 is SULFATE ION (CCD ID: 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		
2	B	1	Total	O	S	0	0
			5	4	1		

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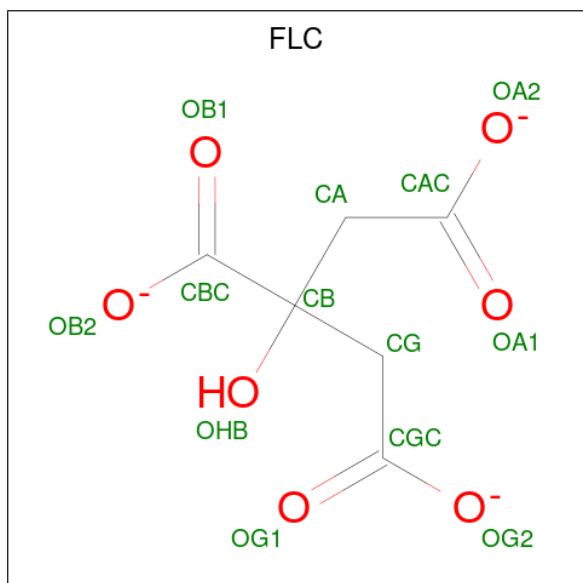
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	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 (CCD ID: FLC) (formula: $C_6H_5O_7^-$).



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 (CCD ID: ZN) (formula: Zn).

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

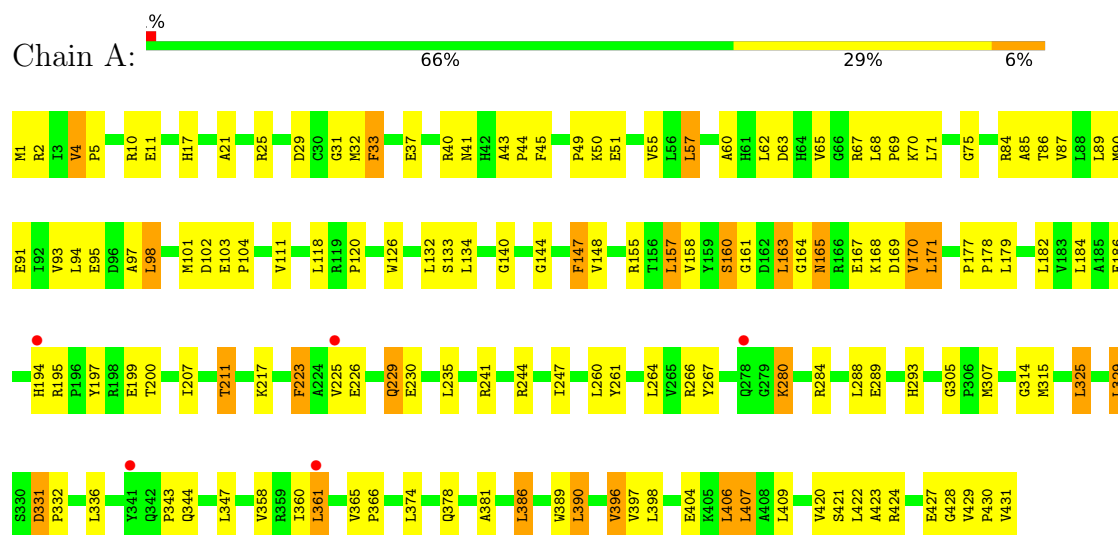
- Molecule 5 is water.

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		

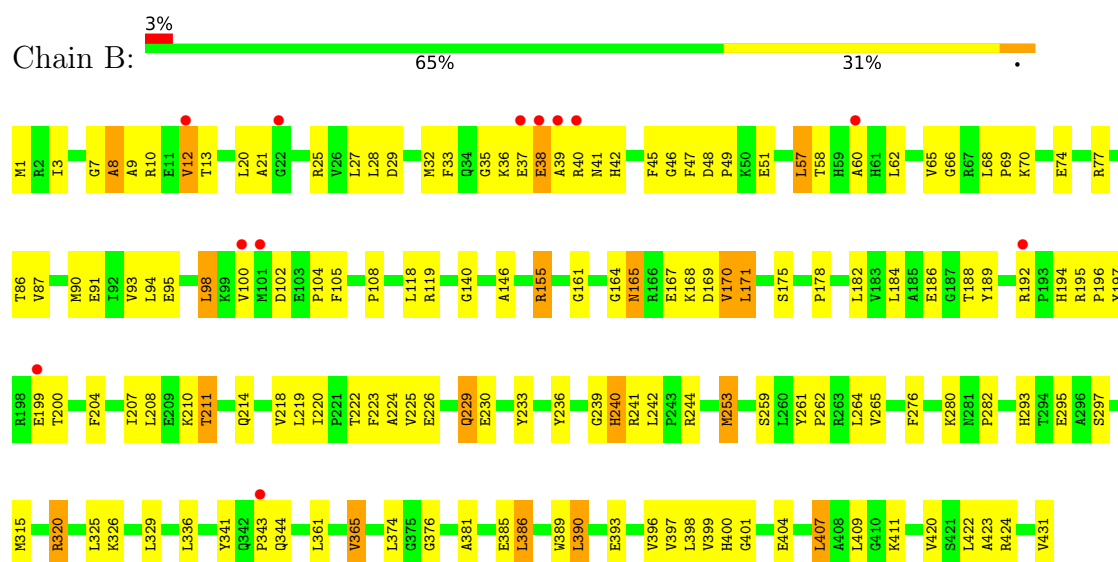
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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

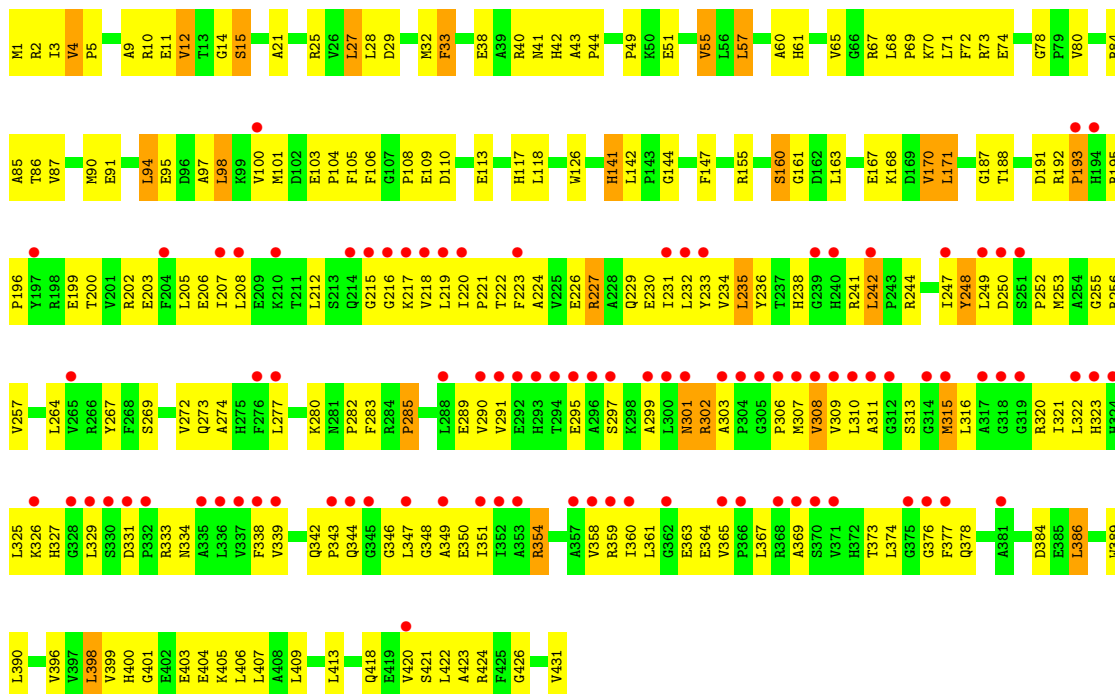


• Molecule 1: Ribonuclease TTHA0252

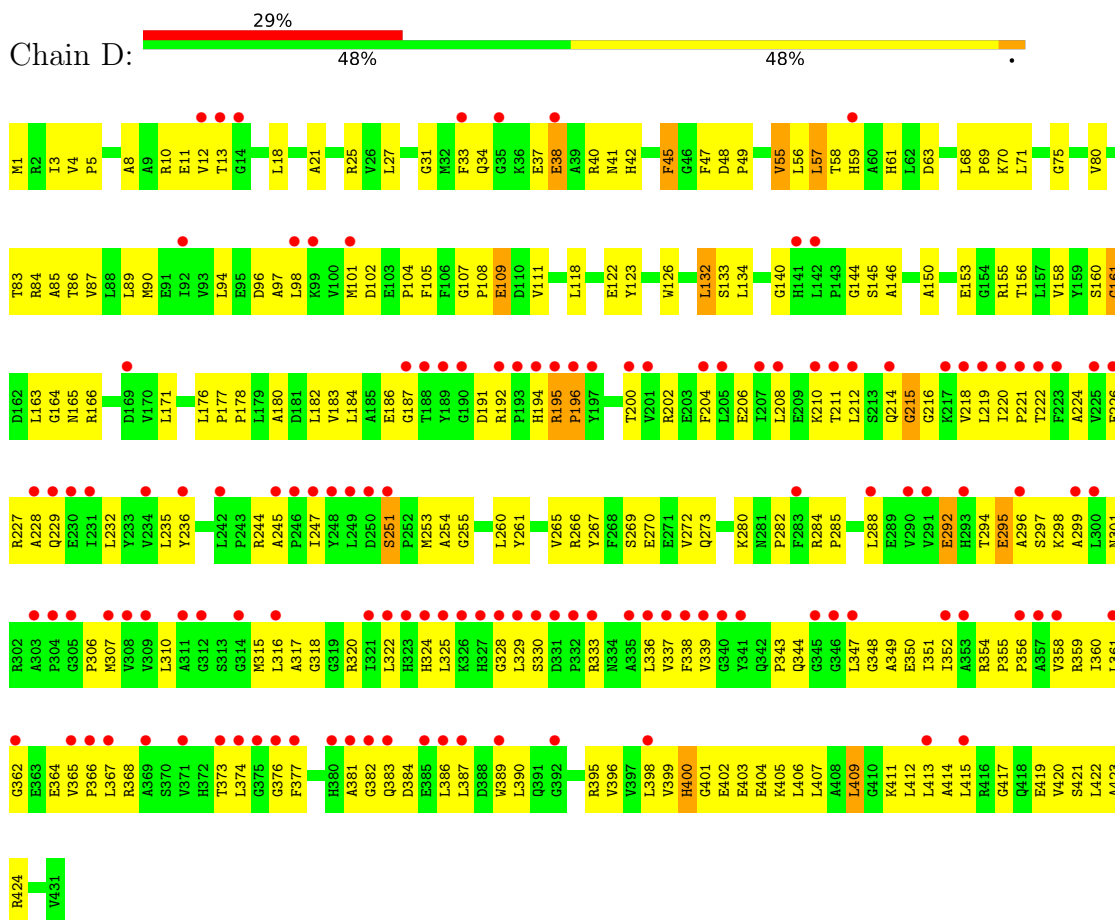


• Molecule 1: Ribonuclease TTHA0252





- 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 50.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.8 (50.00-2.50) 99.8 (50.00-2.50)	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 (10.03%)	wwPDB-VP
Wilson B-factor (Å ²)	54.9	Xtriage
Anisotropy	0.080	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 50.4	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	0.94	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: SO4, ZN, FLC

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	0.50	0/3410	0.99	18/4625 (0.4%)
1	B	0.48	1/3410 (0.0%)	1.03	13/4625 (0.3%)
1	C	0.39	0/3410	0.92	14/4625 (0.3%)
1	D	0.36	0/3410	0.88	6/4625 (0.1%)
All	All	0.44	1/13640 (0.0%)	0.96	51/18500 (0.3%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	365	VAL	CA-CB	6.25	1.59	1.54

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	170	VAL	N-CA-C	8.55	120.32	111.00
1	B	60	ALA	N-CA-C	7.99	122.59	113.01
1	A	170	VAL	N-CA-C	7.73	117.79	110.53
1	B	12	VAL	N-CA-C	7.28	120.19	111.09
1	C	170	VAL	N-CA-C	7.04	117.80	110.62
1	B	169	ASP	N-CA-C	6.71	121.55	113.23
1	B	46	GLY	N-CA-C	-6.63	105.36	114.64
1	A	60	ALA	N-CA-C	6.51	120.82	113.01
1	A	4	VAL	N-CA-C	6.43	114.48	107.60
1	A	33	PHE	N-CA-C	-6.35	101.12	110.52
1	B	93	VAL	N-CA-C	6.29	117.04	110.62
1	B	161	GLY	N-CA-C	-6.14	100.81	111.50
1	A	225	VAL	N-CA-C	6.12	117.67	111.00
1	B	225	VAL	N-CA-C	6.06	118.67	111.09
1	C	161	GLY	N-CA-C	-6.00	100.87	112.02
1	A	331	ASP	CA-C-N	5.99	125.67	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	331	ASP	C-N-CA	5.99	125.67	119.56
1	A	148	VAL	N-CA-C	5.96	116.88	108.36
1	C	4	VAL	N-CA-C	5.93	113.42	107.55
1	D	161	GLY	N-CA-C	-5.84	101.34	111.50
1	D	75	GLY	N-CA-C	5.80	122.75	115.21
1	B	365	VAL	N-CA-C	5.77	114.47	107.61
1	A	223	PHE	N-CA-C	-5.75	101.96	110.48
1	C	147	PHE	N-CA-C	-5.73	101.26	110.14
1	A	161	GLY	N-CA-C	-5.62	101.58	111.80
1	D	107	GLY	CA-C-N	5.51	125.03	119.19
1	D	107	GLY	C-N-CA	5.51	125.03	119.19
1	A	169	ASP	N-CA-C	5.50	120.27	113.50
1	C	60	ALA	N-CA-C	5.50	119.83	113.18
1	B	365	VAL	CA-C-N	5.49	125.41	119.76
1	B	365	VAL	C-N-CA	5.49	125.41	119.76
1	A	147	PHE	N-CA-C	-5.49	101.64	110.14
1	B	393	GLU	CA-C-N	5.46	125.11	119.05
1	B	393	GLU	C-N-CA	5.46	125.11	119.05
1	A	280	LYS	N-CA-C	5.45	117.78	108.90
1	A	305	GLY	N-CA-C	-5.40	105.52	112.00
1	D	4	VAL	N-CA-C	5.35	113.83	107.73
1	A	293	HIS	N-CA-C	5.32	118.25	109.85
1	C	141	HIS	N-CA-C	-5.24	108.65	114.62
1	A	160	SER	N-CA-C	5.22	117.87	111.82
1	A	184	LEU	N-CA-C	-5.19	99.33	108.20
1	A	396	VAL	N-CA-C	5.17	115.48	107.78
1	C	33	PHE	N-CA-C	-5.14	102.88	110.48
1	C	78	GLY	CA-C-N	5.13	125.03	119.85
1	C	78	GLY	C-N-CA	5.13	125.03	119.85
1	C	242	LEU	CA-C-N	5.12	125.04	119.76
1	C	242	LEU	C-N-CA	5.12	125.04	119.76
1	C	248	TYR	N-CA-C	5.11	117.56	109.24
1	D	45	PHE	N-CA-C	5.06	116.48	110.97
1	C	160	SER	N-CA-C	5.05	117.68	111.82
1	C	301	ASN	N-CA-C	-5.01	106.94	113.16

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	3329	0	3354	121	0
1	B	3329	0	3354	133	0
1	C	3329	0	3354	212	0
1	D	3329	0	3354	209	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
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	668	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 25.

All (668) 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:D:224:ALA:HB3	1:D:253:MET:HE2	1.47	0.95
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:B:86:THR:HG22	1:B:90:MET:HE2	1.66	0.77
1:C:101:MET:HE3	1:C:104:PRO:HA	1.64	0.77
1:D:215:GLY:HA2	1:D:306:PRO:HD3	1.65	0.77
1:D:86:THR:HG22	1:D:90:MET:HE2	1.65	0.77
1:B:168:LYS:HE2	1:B:230:GLU:OE1	1.86	0.76
1:D:33:PHE:H	1:D:41:ASN:HD21	1.32	0.76
1:D:329:LEU:HD11	1:D:336:LEU:HD12	1.66	0.76
1:A:102:ASP:CG	1:A:103:GLU:H	1.93	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:C:217:LYS:HG2	1:C:307:MET:HE3	1.70	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:32:MET:HE3	1:A:62:LEU:HG	1.70	0.73
1:B:240:HIS:HE1	1:B:241:ARG:HH21	1.34	0.73
1:B:320:ARG:HD3	3:B:455:FLC:CG	2.18	0.72
1:C:302:ARG:HD2	1:C:302:ARG:C	2.15	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:HH11	1:A:244:ARG:HG2	1.55	0.71
1:A:280:LYS:HZ3	3:A:454:FLC:HA2	1.56	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:404:GLU:H	1:B:404:GLU:CD	1.98	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:315:MET:HA	1:C:342:GLN:HE22	1.60	0.66
1:A:165:ASN:C	1:A:165:ASN:HD22	2.02	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: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:70:LYS:HE2	1:C:74:GLU:OE1	1.96	0.65
1:C:325:LEU:O	1:C:329:LEU:HB2	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:B:87:VAL:HA	1:B:90:MET:HE3	1.80	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
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:A:217:LYS:HE2	1:A:307:MET:HE3	1.81	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:H	1:A:229:GLN:NE2	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:B:196:PRO:HD2	1:B:199:GLU:CD	2.24	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:229:GLN:CD	1:B:229:GLN:H	2.08	0.62
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:57:LEU:CD2	1:D:80:VAL:HG12	2.31	0.61
1:D:221:PRO:HD2	1:D:337:VAL:O	1.99	0.61
1:A:167:GLU:OE2	1:A:194:HIS:HE1	1.82	0.61
1:C:101:MET:HE3	1:C:104:PRO:CA	2.31	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:A:229:GLN:H	1:A:229:GLN:CD	2.09	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:239:GLY:C	1:B:241:ARG:H	2.10	0.59
1:D:87:VAL:HA	1:D:90:MET:HE3	1.84	0.59
1:B:240:HIS:CE1	1:B:241:ARG:HH21	2.19	0.59
1:C:227:ARG:HH22	1:C:377:PHE:C	2.11	0.59
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:55:VAL:HG13	1:D:80:VAL:HA	1.84	0.58
1:D:298:LYS:HA	1:D:301:ASN:ND2	2.19	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:D:229:GLN:H	1:D:229:GLN:CD	2.11	0.58
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:98:LEU:HD11	1:C:108:PRO:CA	2.35	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:86:THR:HG22	1:C:90:MET:CE	2.35	0.57
1:C:269:SER:O	1:C:273:GLN:HG3	2.04	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:A:404:GLU:CD	1:A:404:GLU:H	2.12	0.56
1:B:37:GLU:HG3	1:B:40:ARG:NH1	2.16	0.56
1:B:98:LEU:HD11	1:B:108:PRO:HB3	1.87	0.56
1:B:407:LEU:HD13	1:B:422:LEU:HD21	1.86	0.56
1:C:205:LEU:HD11	1:C:238:HIS:CG	2.40	0.56
1:B:224:ALA:CB	1:B:253:MET:HG2	2.36	0.56
1:C:167:GLU:OE1	1:C:196:PRO:HA	2.05	0.56
1:C:403:GLU:HG2	1:C:407:LEU:HD23	1.86	0.56
1:D:202:ARG:HH11	1:D:202:ARG:CB	2.18	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:O	1:D:166:ARG:HG3	2.05	0.56
1:C:229:GLN:CD	1:C:229:GLN:H	2.13	0.56
1:A:102:ASP:CG	1:A:103:GLU:N	2.62	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:C:331:ASP:HB3	1:C:334:ASN:ND2	2.21	0.55
1:D:316:LEU:C	1:D:318:GLY:H	2.14	0.55
1:A:84:ARG:HD3	1:A:120:PRO:HB3	1.88	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: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: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:B:10:ARG:HH12	1:B:424:ARG:CG	2.20	0.54
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:37:GLU:CB	1:D:40:ARG:HH11	2.20	0.54
1:D:177:PRO:HD3	1:D:389:TRP:CD1	2.42	0.54
1:C:55:VAL:HG22	1:C:80:VAL:HG13	1.90	0.54
1:C:98:LEU:HD11	1:C:108:PRO:HB3	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:32:MET:HE2	1:C:105:PHE:HZ	1.73	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:55:VAL:C	1:D:56:LEU:HD12	2.34	0.53
1:A:182:LEU:HD11	1:A:397:VAL:HG23	1.91	0.53
1:A:11:GLU:CD	1:A:40:ARG:HH12	2.16	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:84:ARG:NH2	1:D:270:GLU:OE1	2.42	0.53
1:A:165:ASN:C	1:A:165:ASN:ND2	2.67	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: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:D:211:THR:HG21	1:D:218:VAL:HG22	1.91	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:B:165:ASN:HD22	1:B:165:ASN:C	2.16	0.52
1:C:9:ALA:C	1:C:11:GLU:H	2.18	0.52
1:C:168:LYS:HD2	1:C:378:GLN:O	2.09	0.52
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:212:LEU:CD2	1:C:306:PRO:HB2	2.34	0.52
1:C:248:TYR:HA	1:C:289:GLU:HB3	1.92	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: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:49:PRO:HB3	1:C:71:LEU:HD12	1.92	0.51
1:C:205:LEU:HD22	1:C:242:LEU:HD21	1.91	0.51
1:A:132:LEU:HG	1:A:134:LEU:CD1	2.39	0.51
1:B:90:MET:HE1	1:B:118:LEU:HD22	1.93	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: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:HE21	1:C:344:GLN:HA	1.76	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: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:32:MET:HE2	1:B:105:PHE:HZ	1.76	0.51
1:B:45:PHE:HB3	1:B:47:PHE:CE1	2.45	0.51
1:B:165:ASN:C	1:B:165:ASN:ND2	2.69	0.51
1:C:10:ARG:HH21	1:C:424:ARG:HG2	1.76	0.51
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:280:LYS:CD	3:A:454:FLC:OA2	2.51	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: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:295:GLU:H	1:B:295:GLU:CD	2.15	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:344:GLN:OE1	1:B:344:GLN:HA	2.10	0.50
1:D:219:LEU:HD21	1:D:324:HIS:O	2.11	0.50
1:B:155:ARG:CD	1:B:431:VAL:O	2.59	0.50
1:B:389:TRP:CE3	1:B:390:LEU:HD13	2.46	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:57:LEU:HG	1:B:65:VAL:HG12	1.94	0.50
1:B:168:LYS:HG2	1:B:197:TYR:CD2	2.46	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:C:229:GLN:CD	1:C:229:GLN:N	2.69	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:A:31:GLY:HA3	1:A:63:ASP:C	2.37	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:57:LEU:CD2	1:D:80:VAL:CG1	2.89	0.49
1:D:156:THR:O	1:D:180:ALA:HB1	2.11	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:55:VAL:CG1	1:D:80:VAL:HG22	2.43	0.49
1:D:140:GLY:O	1:D:164:GLY:HA3	2.13	0.49
1:A:160:SER:HB2	1:A:163:LEU:CD2	2.42	0.49
1:C:253:MET:C	1:C:255:GLY:N	2.70	0.49
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:55:VAL:HG13	1:D:80:VAL:HG13	1.94	0.48
1:D:59:HIS:HD2	1:D:61:HIS:HB2	1.77	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:2:ARG:NH1	2:A:448:SO4:O4	2.46	0.48
1:A:85:ALA:HB3	1:A:144:GLY:HA3	1.94	0.48
1:C:109:GLU:CD	1:C:109:GLU:H	2.22	0.48
1:C:61:HIS:CD2	1:C:142:LEU:HD11	2.48	0.48
1:D:49:PRO:HB3	1:D:71:LEU:CD1	2.43	0.48
1:D:384:ASP:OD2	1:D:384:ASP:N	2.44	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:168:LYS:HG2	1:B:197:TYR:CE2	2.49	0.47
1:C:86:THR:HG22	1:C:90:MET:HE2	1.95	0.47
1:C:231:ILE:O	1:C:235:LEU:HD22	2.13	0.47
1:A:133:SER:C	1:A:134:LEU:HD12	2.40	0.47
1:C:290:VAL:HG23	1:C:290:VAL:O	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:25:ARG:NH1	1:C:51:GLU:HB3	2.29	0.47
1:C:168:LYS:CE	1:C:230:GLU:OE1	2.63	0.47
1:C:231:ILE:C	1:C:233:TYR:H	2.23	0.47
1:D:295:GLU:H	1:D:295:GLU:CD	2.22	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:3:ILE:HG23	1:B:3:ILE:O	2.15	0.47
1:B:182:LEU:HD11	1:B:397:VAL:CG2	2.41	0.47
1:C:374:LEU:C	1:C:376:GLY:H	2.23	0.47
1:D:360:ILE:O	1:D:361:LEU:HB2	2.15	0.47
1:A:29:ASP:HA	1:A:57:LEU:HD12	1.97	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:B:155:ARG:HD2	1:B:431:VAL:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1:MET:HG3	1:C:21:ALA:HB2	1.96	0.47
1:C:302:ARG:C	1:C:302:ARG:CD	2.88	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:68:LEU:N	1:B:69:PRO:HD2	2.30	0.47
1:B:276:PHE:HA	1:B:280:LYS:O	2.14	0.47
1:D:211:THR:CG2	1:D:218:VAL:HG22	2.45	0.47
1:D:226:GLU:C	1:D:229:GLN:HE21	2.23	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:5:PRO:HG2	1:A:423:ALA:HB1	1.97	0.46
1:A:177:PRO:HD3	1:A:389:TRP:CE2	2.51	0.46
1:B:91:GLU:O	1:B:95:GLU:HB2	2.15	0.46
1:D:84:ARG:HG3	1:D:122:GLU:OE2	2.15	0.46
1:D:229:GLN:CD	1:D:229:GLN:N	2.72	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: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: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: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: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:62:LEU:HD13	1:A:93:VAL:CG1	2.41	0.45
1:A:344:GLN:HE21	1:A:344:GLN:HA	1.80	0.45
1:C:14:GLY:O	1:C:15:SER:C	2.59	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:191:ASP:CG	1:D:405:LYS:HD2	2.41	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:OE2	1:D:295:GLU:N	2.49	0.45
1:D:68:LEU:N	1:D:69:PRO:HD2	2.30	0.45
1:D:132:LEU:HD23	1:D:133:SER:H	1.82	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:A:194:HIS:HB3	1:A:378:GLN:CD	2.41	0.45
1:B:192:ARG:HG2	1:B:192:ARG:HH11	1.81	0.45
1:B:199:GLU:HG3	1:B:200:THR:N	2.32	0.45
1:C:90:MET:O	1:C:94:LEU:HB2	2.15	0.45
1:C:235:LEU:HD21	1:C:285:PRO:HG3	1.98	0.45
1:D:186:GLU:HA	1:D:399:VAL:O	2.16	0.45
1:D:336:LEU:C	1:D:336:LEU:HD23	2.41	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:B:168:LYS:HE2	1:B:230:GLU:CD	2.41	0.45
1:C:354:ARG:NH1	1:C:354:ARG:HG3	2.30	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: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:C:191:ASP:OD1	1:C:405:LYS:HD3	2.17	0.45
1:C:248:TYR:CE2	1:C:289:GLU:HG2	2.52	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:HG3	1:C:244:ARG:HH11	1.81	0.44
1:B:184:LEU:HD11	1:B:399:VAL:CG1	2.48	0.44
2:B:441:SO4:O3	1:D:244:ARG:NH2	2.51	0.44
1:C:28:LEU:O	1:C:29:ASP:HB2	2.17	0.44
1:C:101:MET:CE	1:C:104:PRO:HA	2.43	0.44
1:C:142:LEU:CD2	1:C:226:GLU:HB2	2.47	0.44
1:C:323:HIS:O	1:C:327:HIS:HD2	2.00	0.44
1:B:77:ARG:HG2	1:B:77:ARG:HH11	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:400:HIS:O	1:B:400:HIS:ND1	2.50	0.44
1:C:163:LEU:N	1:C:163:LEU:HD22	2.32	0.44
1:D:215:GLY:HA2	1:D:306:PRO:CD	2.42	0.44
1:A:86:THR:HG22	1:A:90:MET:HE2	1.99	0.44
1:B:40:ARG:C	1:B:42:HIS:H	2.25	0.44
1:B:66:GLY:O	1:B:69:PRO:HD2	2.17	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:31:GLY:HA3	1:D:63:ASP:C	2.42	0.44
1:D:41:ASN:O	1:D:70:LYS:HE3	2.18	0.44
1:D:236:TYR:CA	1:D:285:PRO:HB3	2.48	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:97:ALA:O	1:D:101:MET:HB2	2.17	0.44
1:D:354:ARG:HG3	1:D:367:LEU:HD21	1.99	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:95:GLU:OE2	1:C:95:GLU:HA	2.17	0.44
1:C:205:LEU:HD11	1:C:238:HIS:ND1	2.33	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:7:GLY:C	1:B:9:ALA:N	2.76	0.43
1:C:113:GLU:OE2	1:C:117:HIS:HE1	2.00	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:12:VAL:HG23	1:D:13:THR:N	2.33	0.43
1:D:200:THR:OG1	1:D:376:GLY:HA3	2.17	0.43
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:B:404:GLU:CD	1:B:404:GLU:N	2.71	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:236:TYR:CD2	1:B:236:TYR:C	2.96	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: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:42:HIS:CE1	1:D:105:PHE:HB3	2.53	0.43
1:D:284:ARG:HA	1:D:288:LEU:HD23	2.01	0.43
1:D:294:THR:O	1:D:295:GLU:C	2.61	0.43
1:D:298:LYS:HA	1:D:301:ASN:HD22	1.82	0.43
1:A:126:TRP:CD2	1:D:178:PRO:HB3	2.53	0.43
1:A:284:ARG:HD2	3:A:454:FLC:OHB	2.19	0.43
1:C:367:LEU:O	1:C:367:LEU:HG	2.19	0.43
1:D:192:ARG:HD2	1:D:192:ARG:O	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:OD2	1:C:384:ASP:N	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:B:37:GLU:CB	1:B:40:ARG:HH11	2.32	0.43
1:C:43:ALA:HB1	1:C:44:PRO:HD2	2.01	0.43
1:C:208:LEU:HD23	1:C:218:VAL:HG11	2.01	0.43
1:D:195:ARG:O	1:D:196:PRO:C	2.62	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:229:GLN:CD	1:A:229:GLN:N	2.77	0.42
1:A:331:ASP:HA	1:A:332:PRO:HD2	1.84	0.42
1:B:58:THR:HB	1:B:146:ALA:O	2.19	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:C:227:ARG:HH12	1:C:378:GLN:HA	1.84	0.42
1:C:358:VAL:O	1:C:365:VAL:HG12	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:384:ASP:O	1:D:387:LEU:HB2	2.19	0.42
1:B:100:VAL:HG12	1:B:100:VAL:O	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:97:ALA:O	1:A:101:MET:HE3	2.19	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:10:ARG:NH2	1:C:424:ARG:NH1	2.63	0.42
1:D:320:ARG:O	1:D:320:ARG:HG2	2.19	0.42
1:A:155:ARG:HD3	1:A:431:VAL:O	2.19	0.42
1:C:309:VAL:C	1:C:310:LEU:HD12	2.45	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:A:420:VAL:HG22	1:A:421:SER:N	2.34	0.42
1:B:20:LEU:HD21	1:B:25:ARG:HE	1.84	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:40:ARG:C	1:B:42:HIS:N	2.77	0.42
1:B:178:PRO:HB3	1:C:126:TRP:CE3	2.54	0.42
1:B:259:SER:O	1:B:262:PRO:HD2	2.20	0.42
1:D:164:GLY:O	1:D:381:ALA:HB2	2.20	0.42
1:D:329:LEU:HD21	1:D:351:ILE:HD13	2.01	0.42
1:D:406:LEU:HD23	1:D:422:LEU:HG	2.02	0.42
1:C:344:GLN:HE21	1:C:344:GLN:CA	2.32	0.41
1:C:86:THR:HG22	1:C:90:MET:HE3	2.02	0.41
1:D:404:GLU:H	1:D:404:GLU:CD	2.28	0.41
1:C:42:HIS:CE1	1:C:105:PHE:HB3	2.56	0.41
1:C:187:GLY:O	1:C:188:THR:C	2.63	0.41
1:C:224:ALA:HB3	1:C:253:MET:HE2	2.01	0.41
1:D:202:ARG:HH11	1:D:202:ARG:HB2	1.84	0.41
1:D:229:GLN:HG3	1:D:261:TYR:CZ	2.55	0.41
1:D:310:LEU:N	1:D:310:LEU:HD12	2.34	0.41
1:B:10:ARG:HH11	1:B:424:ARG:HG2	1.82	0.41
1:B:28:LEU:O	1:B:29:ASP:HB2	2.20	0.41
1:C:101:MET:HE3	1:C:104:PRO:CB	2.51	0.41
1:C:233:TYR:HB2	1:C:283:PHE:HD1	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:109:GLU:CD	1:D:109:GLU:H	2.28	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
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:57:LEU:HD23	1:C:90:MET:HE1	2.01	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: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:B:239:GLY:C	1:B:241:ARG:N	2.74	0.41
1:C:3:ILE:HG23	1:C:3:ILE:O	2.21	0.41
1:C:33:PHE:CD2	1:C:40:ARG:HB2	2.55	0.41
1:C:224:ALA:O	1:C:257:VAL:HG21	2.21	0.41
1:C:386:LEU:HD23	1:C:409:LEU:CD1	2.51	0.41
1:D:89:LEU:HD23	1:D:260:LEU:HD23	2.03	0.41
1:D:98:LEU:HD12	1:D:111:VAL:HG21	2.03	0.41
1:D:269:SER:HB2	2:D:436:SO4:O2	2.21	0.41
1:D:381:ALA:HB3	1:D:386:LEU:CD1	2.50	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:B:7:GLY:O	1:B:8:ALA:C	2.64	0.40
1:D:227:ARG:O	1:D:228:ALA:C	2.65	0.40
1:D:415:LEU:C	1:D:417:GLY:H	2.28	0.40
1:A:422:LEU:O	1:A:423:ALA:C	2.65	0.40
1:B:194:HIS:HE2	1:B:385:GLU:CD	2.29	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:301:ASN:HB2	1:C:327:HIS:CG	2.57	0.40
1:C:348:GLY:C	1:C:350:GLU:N	2.76	0.40
1:D:253:MET:C	1:D:255:GLY:N	2.79	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	429/431 (100%)	400 (93%)	29 (7%)	0	100	100
1	B	429/431 (100%)	398 (93%)	27 (6%)	4 (1%)	14	27
1	C	429/431 (100%)	363 (85%)	59 (14%)	7 (2%)	7	14
1	D	429/431 (100%)	368 (86%)	51 (12%)	10 (2%)	5	8
All	All	1716/1724 (100%)	1529 (89%)	166 (10%)	21 (1%)	10	20

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

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Mol	Chain	Res	Type
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%)	316 (92%)	26 (8%)	12	26
1	B	342/342 (100%)	315 (92%)	27 (8%)	11	24
1	C	342/342 (100%)	325 (95%)	17 (5%)	22	44
1	D	342/342 (100%)	327 (96%)	15 (4%)	25	50
All	All	1368/1368 (100%)	1283 (94%)	85 (6%)	16	34

All (85) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	GLU
1	A	55	VAL
1	A	57	LEU
1	A	94	LEU
1	A	98	LEU
1	A	157	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

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Mol	Chain	Res	Type
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
1	B	27	LEU
1	B	57	LEU
1	B	62	LEU
1	B	94	LEU
1	B	98	LEU
1	B	119	ARG
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	320	ARG
1	B	325	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	12	VAL

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Mol	Chain	Res	Type
1	C	27	LEU
1	C	55	VAL
1	C	57	LEU
1	C	94	LEU
1	C	98	LEU
1	C	103	GLU
1	C	171	LEU
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	386	LEU
1	C	398	LEU
1	D	27	LEU
1	D	38	GLU
1	D	55	VAL
1	D	57	LEU
1	D	94	LEU
1	D	96	ASP
1	D	109	GLU
1	D	132	LEU
1	D	171	LEU
1	D	176	LEU
1	D	195	ARG
1	D	196	PRO
1	D	265	VAL
1	D	292	GLU
1	D	409	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	ASN
1	A	165	ASN
1	A	229	GLN
1	A	273	GLN
1	A	344	GLN
1	A	378	GLN
1	B	41	ASN

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Mol	Chain	Res	Type
1	B	61	HIS
1	B	151	GLN
1	B	165	ASN
1	B	229	GLN
1	B	238	HIS
1	B	240	HIS
1	B	275	HIS
1	B	278	GLN
1	B	301	ASN
1	B	383	GLN
1	B	391	GLN
1	C	41	ASN
1	C	141	HIS
1	C	151	GLN
1	C	165	ASN
1	C	278	GLN
1	C	327	HIS
1	C	342	GLN
1	C	344	GLN
1	C	372	HIS
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	273	GLN
1	D	293	HIS
1	D	327	HIS
1	D	344	GLN
1	D	372	HIS
1	D	380	HIS
1	D	383	GLN

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 [i](#)

There are no oligosaccharides 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	435	-	4,4,4	1.04	0	6,6,6	0.59	0
2	SO4	A	446	-	4,4,4	1.09	0	6,6,6	0.57	0
2	SO4	B	452	-	4,4,4	1.06	0	6,6,6	0.60	0
2	SO4	C	438	-	4,4,4	1.09	0	6,6,6	0.57	0
2	SO4	D	434	-	4,4,4	1.07	0	6,6,6	0.58	0
2	SO4	B	448	-	4,4,4	1.11	0	6,6,6	0.55	0
2	SO4	C	437	-	4,4,4	1.07	0	6,6,6	0.58	0
2	SO4	A	432	-	4,4,4	1.08	0	6,6,6	0.57	0
2	SO4	C	444	-	4,4,4	1.09	0	6,6,6	0.57	0
2	SO4	B	453	-	4,4,4	1.02	0	6,6,6	0.60	0
3	FLC	A	454	-	12,12,12	2.11	5 (41%)	17,17,17	1.22	1 (5%)
2	SO4	A	445	-	4,4,4	1.08	0	6,6,6	0.58	0
2	SO4	A	452	-	4,4,4	1.07	0	6,6,6	0.59	0
2	SO4	C	439	-	4,4,4	1.07	0	6,6,6	0.56	0
2	SO4	C	433	-	4,4,4	1.08	0	6,6,6	0.59	0
2	SO4	D	437	-	4,4,4	1.06	0	6,6,6	0.58	0
2	SO4	A	433	-	4,4,4	1.11	0	6,6,6	0.61	0
2	SO4	A	437	-	4,4,4	1.07	0	6,6,6	0.58	0
2	SO4	B	435	-	4,4,4	1.08	0	6,6,6	0.56	0
2	SO4	B	439	-	4,4,4	1.11	0	6,6,6	0.55	0
2	SO4	C	436	-	4,4,4	1.10	0	6,6,6	0.56	0
2	SO4	B	432	-	4,4,4	1.07	0	6,6,6	0.58	0
2	SO4	A	444	-	4,4,4	1.06	0	6,6,6	0.59	0
2	SO4	C	440	-	4,4,4	1.07	0	6,6,6	0.58	0
2	SO4	A	442	-	4,4,4	1.07	0	6,6,6	0.56	0
2	SO4	A	453	-	4,4,4	1.07	0	6,6,6	0.58	0
2	SO4	C	435	-	4,4,4	1.08	0	6,6,6	0.56	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SO4	B	433	-	4,4,4	1.07	0	6,6,6	0.56	0
2	SO4	B	451	-	4,4,4	1.07	0	6,6,6	0.57	0
2	SO4	B	438	-	4,4,4	1.07	0	6,6,6	0.58	0
2	SO4	A	443	-	4,4,4	1.07	0	6,6,6	0.56	0
2	SO4	C	432	-	4,4,4	1.09	0	6,6,6	0.56	0
2	SO4	B	434	-	4,4,4	1.05	0	6,6,6	0.60	0
2	SO4	C	441	-	4,4,4	1.05	0	6,6,6	0.58	0
3	FLC	B	456	-	12,12,12	2.13	5 (41%)	17,17,17	1.21	1 (5%)
2	SO4	B	454	-	4,4,4	1.04	0	6,6,6	0.60	0
2	SO4	D	435	-	4,4,4	1.09	0	6,6,6	0.57	0
2	SO4	C	445	-	4,4,4	1.10	0	6,6,6	0.56	0
2	SO4	B	436	-	4,4,4	1.07	0	6,6,6	0.57	0
2	SO4	B	449	-	4,4,4	1.08	0	6,6,6	0.56	0
2	SO4	A	439	-	4,4,4	1.06	0	6,6,6	0.58	0
2	SO4	B	450	-	4,4,4	1.04	0	6,6,6	0.59	0
2	SO4	B	446	-	4,4,4	1.07	0	6,6,6	0.58	0
2	SO4	A	438	-	4,4,4	1.05	0	6,6,6	0.58	0
2	SO4	B	440	-	4,4,4	1.08	0	6,6,6	0.57	0
2	SO4	B	443	-	4,4,4	1.06	0	6,6,6	0.57	0
2	SO4	B	447	-	4,4,4	1.07	0	6,6,6	0.57	0
2	SO4	A	434	-	4,4,4	1.08	0	6,6,6	0.59	0
2	SO4	C	434	-	4,4,4	1.05	0	6,6,6	0.58	0
2	SO4	A	449	-	4,4,4	1.06	0	6,6,6	0.59	0
2	SO4	C	442	-	4,4,4	1.08	0	6,6,6	0.56	0
2	SO4	D	433	-	4,4,4	1.09	0	6,6,6	0.56	0
2	SO4	B	442	-	4,4,4	1.08	0	6,6,6	0.57	0
2	SO4	A	448	-	4,4,4	1.09	0	6,6,6	0.57	0
2	SO4	A	436	-	4,4,4	1.05	0	6,6,6	0.58	0
2	SO4	A	441	-	4,4,4	1.06	0	6,6,6	0.58	0
2	SO4	D	436	-	4,4,4	1.04	0	6,6,6	0.60	0
3	FLC	B	455	-	12,12,12	1.57	3 (25%)	17,17,17	1.36	1 (5%)
2	SO4	B	441	-	4,4,4	1.07	0	6,6,6	0.56	0
2	SO4	A	447	-	4,4,4	1.08	0	6,6,6	0.56	0
2	SO4	C	443	-	4,4,4	1.07	0	6,6,6	0.58	0
2	SO4	A	450	-	4,4,4	1.09	0	6,6,6	0.59	0
2	SO4	A	451	-	4,4,4	1.08	0	6,6,6	0.57	0
2	SO4	B	445	-	4,4,4	1.02	0	6,6,6	0.60	0
2	SO4	C	446	-	4,4,4	1.07	0	6,6,6	0.58	0
2	SO4	D	432	-	4,4,4	1.08	0	6,6,6	0.57	0
2	SO4	B	444	-	4,4,4	1.08	0	6,6,6	0.55	0
2	SO4	B	437	-	4,4,4	1.03	0	6,6,6	0.53	0
2	SO4	A	440	-	4,4,4	1.06	0	6,6,6	0.58	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
3	FLC	B	456	-	-	0/16/16/16	-
3	FLC	B	455	-	-	0/16/16/16	-
3	FLC	A	454	-	-	0/16/16/16	-

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	456	FLC	CB-CBC	-4.82	1.48	1.53
3	A	454	FLC	CB-CBC	-4.73	1.48	1.53
3	B	455	FLC	OA2-CAC	-2.92	1.21	1.30
3	B	456	FLC	OG2-CGC	-2.70	1.21	1.30
3	A	454	FLC	OG2-CGC	-2.69	1.21	1.30
3	B	455	FLC	OG2-CGC	-2.47	1.22	1.30
3	A	454	FLC	OA2-CAC	-2.45	1.22	1.30
3	B	456	FLC	OA2-CAC	-2.43	1.22	1.30
3	B	456	FLC	CA-CB	2.36	1.56	1.54
3	A	454	FLC	CA-CB	2.26	1.56	1.54
3	A	454	FLC	CG-CB	2.19	1.56	1.54
3	B	456	FLC	CG-CB	2.13	1.56	1.54
3	B	455	FLC	OB1-CBC	2.06	1.28	1.22

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	455	FLC	OB2-CBC-CB	3.76	120.36	113.14
3	A	454	FLC	OB2-CBC-CB	3.09	119.06	113.14
3	B	456	FLC	OB2-CBC-CB	3.05	118.99	113.14

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
3	A	454	FLC	7	0
2	C	439	SO4	1	0
2	A	443	SO4	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	456	FLC	4	0
2	C	445	SO4	1	0
2	A	449	SO4	1	0
2	A	448	SO4	1	0
2	A	436	SO4	1	0
2	D	436	SO4	1	0
3	B	455	FLC	3	0
2	B	441	SO4	2	0
2	D	432	SO4	3	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	431/431 (100%)	0.03	5 (1%) 76 73	24, 43, 67, 82	0
1	B	431/431 (100%)	0.18	12 (2%) 55 50	24, 43, 68, 88	0
1	C	431/431 (100%)	1.15	94 (21%) 2 2	28, 75, 133, 137	0
1	D	431/431 (100%)	1.43	127 (29%) 1 1	36, 80, 142, 146	0
All	All	1724/1724 (100%)	0.70	238 (13%) 6 5	24, 53, 132, 146	0

All (238) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	290	VAL	5.9
1	D	228	ALA	5.5
1	C	219	LEU	4.8
1	D	322	LEU	4.8
1	D	362	GLY	4.8
1	D	328	GLY	4.7
1	C	296	ALA	4.6
1	C	305	GLY	4.6
1	D	377	PHE	4.5
1	D	329	LEU	4.4
1	D	338	PHE	4.4
1	C	326	LYS	4.3
1	C	338	PHE	4.3
1	D	361	LEU	4.3
1	C	328	GLY	4.2
1	C	365	VAL	4.2
1	D	223	PHE	4.2
1	C	301	ASN	4.2
1	C	217	LYS	4.1
1	C	218	VAL	4.1
1	D	219	LEU	4.1

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Mol	Chain	Res	Type	RSRZ
1	C	366	PRO	4.0
1	D	311	ALA	3.9
1	D	353	ALA	3.9
1	D	208	LEU	3.9
1	D	375	GLY	3.8
1	D	326	LYS	3.8
1	C	329	LEU	3.8
1	C	336	LEU	3.8
1	D	339	VAL	3.8
1	D	204	PHE	3.8
1	D	220	ILE	3.8
1	C	300	LEU	3.7
1	D	330	SER	3.7
1	C	319	GLY	3.7
1	D	249	LEU	3.7
1	C	308	VAL	3.6
1	D	242	LEU	3.6
1	C	318	GLY	3.6
1	D	305	GLY	3.6
1	D	382	GLY	3.6
1	D	201	VAL	3.5
1	D	205	LEU	3.5
1	D	197	TYR	3.5
1	D	373	THR	3.4
1	C	197	TYR	3.4
1	D	325	LEU	3.4
1	C	368	ARG	3.4
1	C	288	LEU	3.4
1	D	299	ALA	3.4
1	D	308	VAL	3.3
1	C	194	HIS	3.3
1	D	327	HIS	3.3
1	D	303	ALA	3.3
1	D	236	TYR	3.3
1	D	374	LEU	3.3
1	C	376	GLY	3.3
1	D	218	VAL	3.3
1	D	376	GLY	3.2
1	C	311	ALA	3.2
1	C	352	ILE	3.2
1	D	92	ILE	3.2
1	D	245	ALA	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	343	PRO	3.2
1	D	358	VAL	3.2
1	D	365	VAL	3.2
1	D	207	ILE	3.2
1	C	291	VAL	3.1
1	C	375	GLY	3.1
1	D	296	ALA	3.1
1	C	250	ASP	3.1
1	C	277	LEU	3.1
1	C	310	LEU	3.1
1	D	225	VAL	3.1
1	D	312	GLY	3.1
1	C	353	ALA	3.1
1	C	208	LEU	3.1
1	D	194	HIS	3.1
1	C	371	VAL	3.1
1	C	292	GLU	3.0
1	C	315	MET	3.0
1	D	212	LEU	3.0
1	D	221	PRO	3.0
1	C	216	GLY	3.0
1	C	309	VAL	3.0
1	C	299	ALA	3.0
1	C	335	ALA	3.0
1	D	210	LYS	3.0
1	D	251	SER	3.0
1	C	193	PRO	2.9
1	D	291	VAL	2.9
1	C	204	PHE	2.9
1	D	331	ASP	2.9
1	D	307	MET	2.9
1	C	247	ILE	2.9
1	D	321	ILE	2.9
1	C	323	HIS	2.9
1	D	229	GLN	2.9
1	C	297	SER	2.9
1	C	220	ILE	2.9
1	C	337	VAL	2.9
1	D	323	HIS	2.8
1	C	307	MET	2.8
1	A	341	TYR	2.8
1	C	207	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	371	VAL	2.8
1	C	322	LEU	2.8
1	B	192	ARG	2.8
1	C	304	PRO	2.8
1	D	337	VAL	2.8
1	C	249	LEU	2.8
1	C	303	ALA	2.8
1	D	347	LEU	2.8
1	B	199	GLU	2.8
1	D	385	GLU	2.8
1	D	193	PRO	2.8
1	D	356	PRO	2.8
1	D	381	ALA	2.8
1	C	377	PHE	2.8
1	C	358	VAL	2.7
1	C	242	LEU	2.7
1	D	188	THR	2.7
1	D	14	GLY	2.7
1	C	369	ALA	2.7
1	C	231	ILE	2.7
1	B	38	GLU	2.7
1	D	293	HIS	2.7
1	D	35	GLY	2.7
1	D	231	ILE	2.7
1	B	100	VAL	2.7
1	D	192	ARG	2.7
1	D	387	LEU	2.7
1	D	345	GLY	2.6
1	D	386	LEU	2.6
1	D	288	LEU	2.6
1	D	290	VAL	2.6
1	D	369	ALA	2.6
1	D	169	ASP	2.6
1	D	246	PRO	2.6
1	C	223	PHE	2.6
1	D	234	VAL	2.6
1	C	306	PRO	2.6
1	A	194	HIS	2.6
1	D	367	LEU	2.5
1	B	37	GLU	2.5
1	D	33	PHE	2.5
1	D	141	HIS	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	211	THR	2.5
1	C	360	ILE	2.5
1	D	352	ILE	2.5
1	C	100	VAL	2.5
1	D	324	HIS	2.5
1	D	247	ILE	2.5
1	D	98	LEU	2.5
1	D	415	LEU	2.5
1	C	362	GLY	2.4
1	D	190	GLY	2.4
1	D	230	GLU	2.4
1	C	232	LEU	2.4
1	C	294	THR	2.4
1	D	336	LEU	2.4
1	C	240	HIS	2.4
1	C	339	VAL	2.4
1	D	12	VAL	2.4
1	C	370	SER	2.4
1	D	366	PRO	2.4
1	C	312	GLY	2.4
1	C	344	GLN	2.4
1	D	195	ARG	2.4
1	C	276	PHE	2.4
1	C	420	VAL	2.4
1	D	196	PRO	2.4
1	C	251	SER	2.4
1	C	215	GLY	2.4
1	D	101	MET	2.4
1	C	330	SER	2.3
1	D	333	ARG	2.3
1	D	283	PHE	2.3
1	D	217	LYS	2.3
1	C	317	ALA	2.3
1	C	314	GLY	2.3
1	D	187	GLY	2.3
1	D	248	TYR	2.3
1	D	309	VAL	2.3
1	D	222	THR	2.3
1	C	347	LEU	2.3
1	D	250	ASP	2.3
1	D	38	GLU	2.3
1	D	341	TYR	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	239	GLY	2.3
1	D	304	PRO	2.3
1	D	214	GLN	2.2
1	D	142	LEU	2.2
1	B	343	PRO	2.2
1	C	381	ALA	2.2
1	C	345	GLY	2.2
1	D	316	LEU	2.2
1	C	351	ILE	2.2
1	C	359	ARG	2.2
1	B	60	ALA	2.2
1	D	383	GLN	2.2
1	D	346	GLY	2.2
1	C	265	VAL	2.2
1	D	99	LYS	2.2
1	D	380	HIS	2.2
1	D	300	LEU	2.2
1	B	40	ARG	2.2
1	A	225	VAL	2.1
1	C	293	HIS	2.1
1	B	22	GLY	2.1
1	D	332	PRO	2.1
1	D	335	ALA	2.1
1	D	357	ALA	2.1
1	D	340	GLY	2.1
1	C	332	PRO	2.1
1	D	59	HIS	2.1
1	A	278	GLN	2.1
1	C	349	ALA	2.1
1	A	361	LEU	2.1
1	D	13	THR	2.1
1	C	295	GLU	2.1
1	C	233	TYR	2.1
1	C	210	LYS	2.1
1	B	12	VAL	2.1
1	B	39	ALA	2.1
1	C	357	ALA	2.1
1	D	389	TRP	2.1
1	D	413	LEU	2.0
1	D	226	GLU	2.0
1	D	189	TYR	2.0
1	C	324	HIS	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	214	GLN	2.0
1	D	398	LEU	2.0
1	D	314	GLY	2.0
1	D	392	GLY	2.0
1	D	200	THR	2.0
1	B	101	MET	2.0
1	C	331	ASP	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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. 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	B-factors(Å ²)	Q<0.9
2	SO4	C	439	5/5	0.36	0.16	149,149,149,149	0
2	SO4	B	445	5/5	0.41	0.12	142,142,142,142	0
2	SO4	A	432	5/5	0.41	0.13	138,138,138,139	0
2	SO4	A	446	5/5	0.42	0.17	131,131,132,132	0
2	SO4	C	437	5/5	0.47	0.10	144,144,144,145	0
2	SO4	C	436	5/5	0.55	0.15	138,138,139,139	0
2	SO4	C	435	5/5	0.62	0.15	155,155,155,155	0
2	SO4	B	454	5/5	0.62	0.13	123,124,124,124	0
2	SO4	C	438	5/5	0.64	0.12	143,143,144,144	0
2	SO4	A	438	5/5	0.65	0.12	116,116,116,116	0
2	SO4	A	440	5/5	0.65	0.11	122,123,123,123	0
2	SO4	A	443	5/5	0.66	0.12	135,136,136,136	0
2	SO4	A	451	5/5	0.66	0.17	137,137,138,138	0
2	SO4	C	433	5/5	0.66	0.15	121,121,121,122	0
2	SO4	B	439	5/5	0.66	0.17	135,135,135,136	0
2	SO4	D	433	5/5	0.66	0.12	123,124,124,124	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SO4	C	440	5/5	0.67	0.13	148,148,148,148	0
2	SO4	B	441	5/5	0.67	0.09	159,159,160,160	0
2	SO4	B	451	5/5	0.68	0.13	140,140,140,140	0
2	SO4	B	447	5/5	0.68	0.21	143,143,143,143	0
2	SO4	A	449	5/5	0.69	0.13	135,135,135,136	0
2	SO4	A	452	5/5	0.69	0.13	128,128,128,129	0
2	SO4	A	453	5/5	0.70	0.14	122,122,122,123	0
2	SO4	C	445	5/5	0.70	0.11	128,128,128,128	0
2	SO4	B	436	5/5	0.70	0.13	120,121,121,121	0
3	FLC	A	454	13/13	0.70	0.22	103,106,110,110	0
3	FLC	B	455	13/13	0.73	0.22	110,110,111,112	0
2	SO4	A	445	5/5	0.74	0.27	137,138,138,139	0
2	SO4	A	439	5/5	0.74	0.10	136,136,136,136	0
2	SO4	A	441	5/5	0.75	0.09	136,137,137,137	0
2	SO4	B	448	5/5	0.76	0.15	145,145,145,145	0
2	SO4	B	444	5/5	0.76	0.15	116,116,117,117	0
2	SO4	A	447	5/5	0.76	0.16	128,128,128,129	0
2	SO4	C	432	5/5	0.76	0.11	90,91,92,92	0
2	SO4	A	442	5/5	0.76	0.12	96,96,96,98	0
2	SO4	D	437	5/5	0.77	0.13	126,127,127,127	0
2	SO4	B	434	5/5	0.77	0.12	148,148,148,149	0
2	SO4	B	449	5/5	0.77	0.13	144,144,144,145	0
2	SO4	D	435	5/5	0.78	0.11	132,132,132,132	0
2	SO4	B	443	5/5	0.78	0.12	118,119,119,119	0
2	SO4	C	434	5/5	0.79	0.07	111,111,111,111	0
2	SO4	C	442	5/5	0.79	0.11	111,111,111,112	0
2	SO4	D	432	5/5	0.81	0.11	117,117,117,117	0
2	SO4	A	436	5/5	0.81	0.19	156,156,156,156	0
2	SO4	B	442	5/5	0.82	0.09	119,119,119,119	0
2	SO4	A	448	5/5	0.83	0.12	98,98,99,99	0
2	SO4	A	450	5/5	0.83	0.16	98,98,99,100	0
2	SO4	D	436	5/5	0.83	0.14	90,90,91,91	0
2	SO4	B	435	5/5	0.84	0.10	98,99,100,100	0
2	SO4	C	446	5/5	0.84	0.11	101,101,101,102	0
2	SO4	B	440	5/5	0.84	0.15	110,110,110,111	0
2	SO4	B	452	5/5	0.85	0.13	98,98,99,99	0
2	SO4	B	432	5/5	0.85	0.07	110,110,110,110	0
2	SO4	C	443	5/5	0.85	0.09	102,103,103,103	0
3	FLC	B	456	13/13	0.85	0.26	98,104,109,109	0
2	SO4	A	444	5/5	0.86	0.09	109,109,110,110	0
2	SO4	C	444	5/5	0.86	0.11	113,113,113,113	0
2	SO4	B	433	5/5	0.87	0.10	91,91,92,92	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	ZN	C	447	1/1	0.87	0.13	117,117,117,117	0
2	SO4	B	450	5/5	0.90	0.08	79,79,80,81	0
4	ZN	C	448	1/1	0.91	0.10	115,115,115,115	0
4	ZN	D	438	1/1	0.91	0.14	101,101,101,101	0
2	SO4	C	441	5/5	0.92	0.08	71,71,72,73	0
4	ZN	A	456	1/1	0.93	0.10	72,72,72,72	0
2	SO4	A	437	5/5	0.93	0.08	77,77,78,78	0
2	SO4	B	446	5/5	0.93	0.09	84,84,85,85	0
2	SO4	D	434	5/5	0.93	0.08	81,82,82,83	0
4	ZN	B	457	1/1	0.94	0.07	72,72,72,72	0
2	SO4	B	453	5/5	0.94	0.09	54,55,57,57	0
2	SO4	A	435	5/5	0.94	0.11	52,53,55,58	0
2	SO4	A	433	5/5	0.94	0.12	52,56,58,59	0
4	ZN	B	458	1/1	0.95	0.08	79,79,79,79	0
2	SO4	B	438	5/5	0.95	0.09	64,65,66,67	0
2	SO4	A	434	5/5	0.96	0.07	41,42,44,45	0
2	SO4	B	437	5/5	0.97	0.07	47,47,51,52	0
4	ZN	D	439	1/1	0.97	0.06	94,94,94,94	0
4	ZN	A	455	1/1	0.99	0.04	67,67,67,67	0

6.5 Other polymers [i](#)

There are no such residues in this entry.