



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:53 PM UTC

PDB ID : 3IE0 / pdb_00003ie0
Title : Crystal Structure of S378Y 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 : 2.73 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

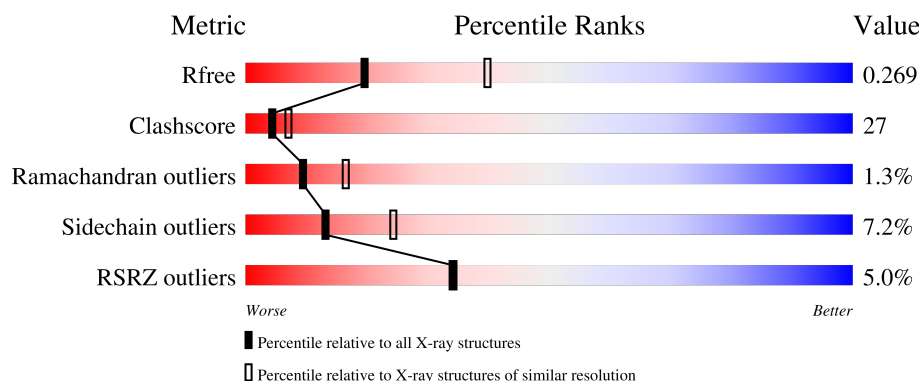
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.73 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	1819 (2.76-2.72)
Clashscore	190562	1866 (2.76-2.72)
Ramachandran outliers	187476	1830 (2.76-2.72)
Sidechain outliers	187428	1831 (2.76-2.72)
RSRZ outliers	180081	1819 (2.76-2.72)

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	63% 31% 5%
1	B	431	54% 39% 7%
1	C	431	6% 47% 48% 6%
1	D	431	13% 47% 49% .

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	B	433	-	-	X	-
2	SO4	B	446	-	-	X	-
2	SO4	B	448	-	-	X	-
2	SO4	D	433	-	-	X	-
3	FLC	B	451	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 13790 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.

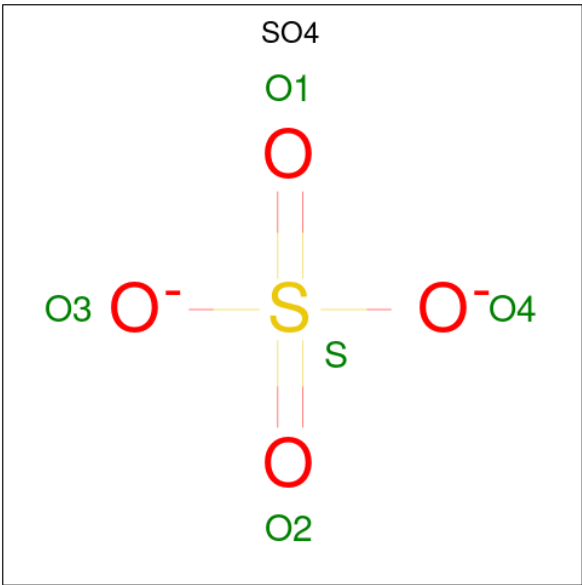
- Molecule 1 is a protein called Ribonuclease TTHA0252.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	431	Total	C	N	O	S	0	0	0
			3332	2133	597	594	8			
1	B	431	Total	C	N	O	S	0	0	0
			3332	2133	597	594	8			
1	C	431	Total	C	N	O	S	0	0	0
			3332	2133	597	594	8			
1	D	431	Total	C	N	O	S	0	0	0
			3332	2133	597	594	8			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	378	TYR	SER	engineered mutation	UNP Q5SLP1
B	378	TYR	SER	engineered mutation	UNP Q5SLP1
C	378	TYR	SER	engineered mutation	UNP Q5SLP1
D	378	TYR	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	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		
2	B	1	Total	O	S	0	0
			5	4	1		

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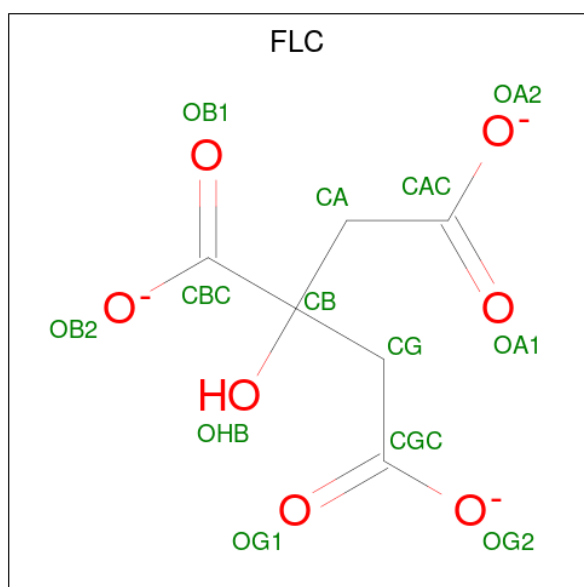
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total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

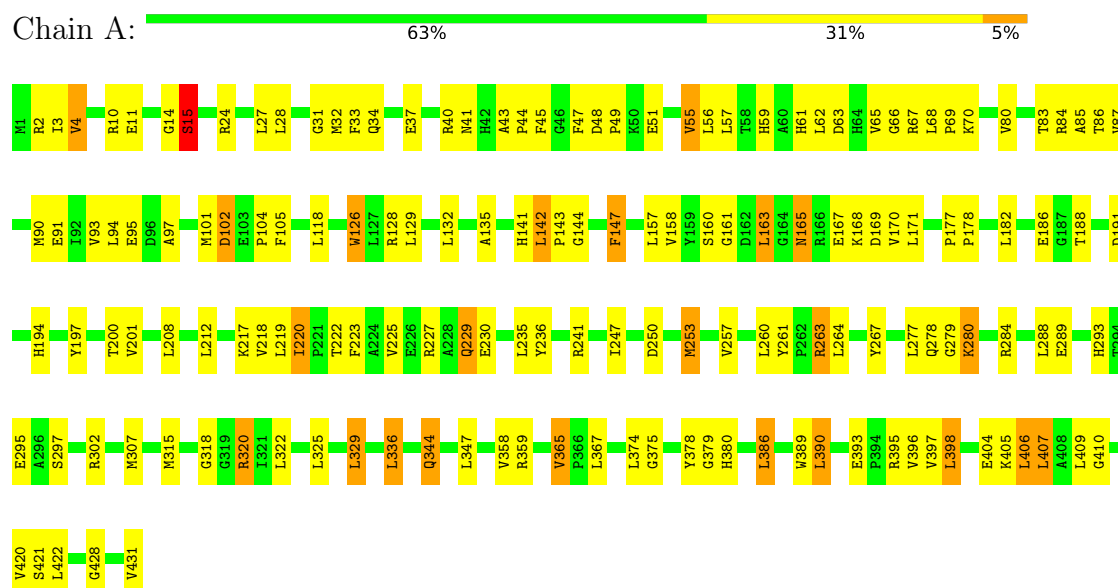
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	26	Total	O	0	0
			26	26		
5	B	33	Total	O	0	0
			33	33		
5	C	9	Total	O	0	0
			9	9		
5	D	12	Total	O	0	0
			12	12		

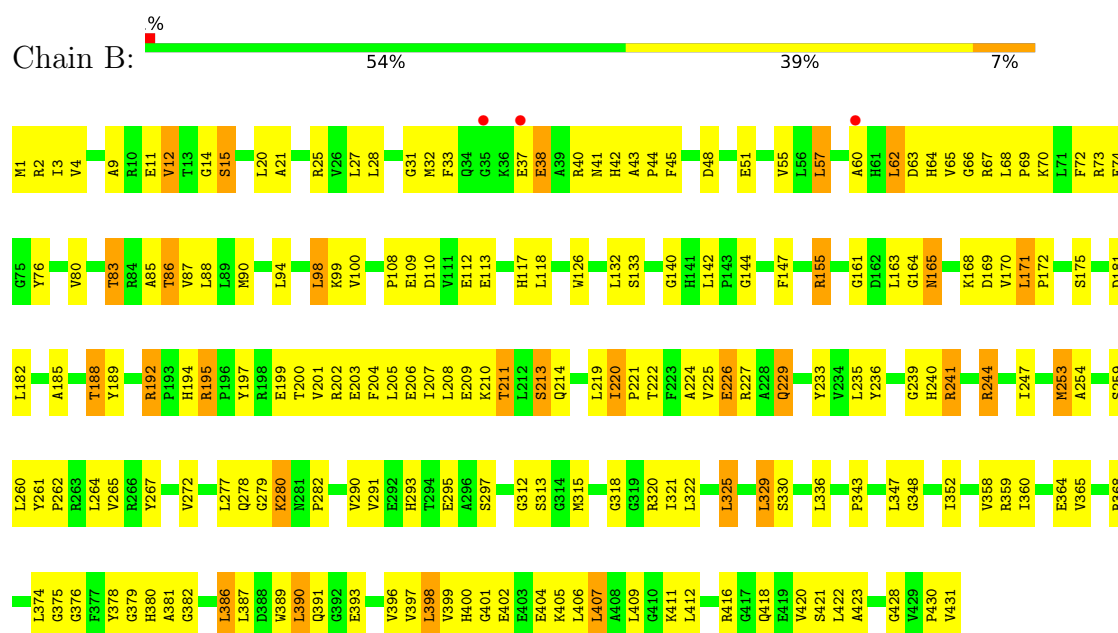
3 Residue-property plots

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.

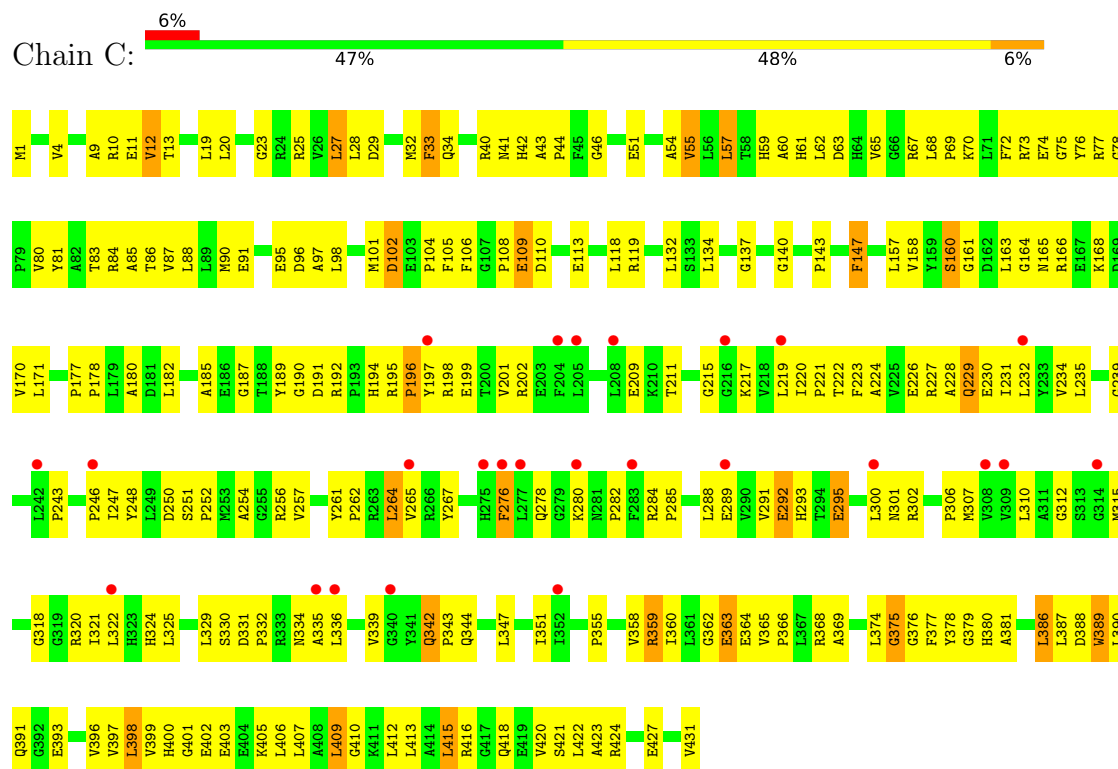
• Molecule 1: Ribonuclease TTHA0252



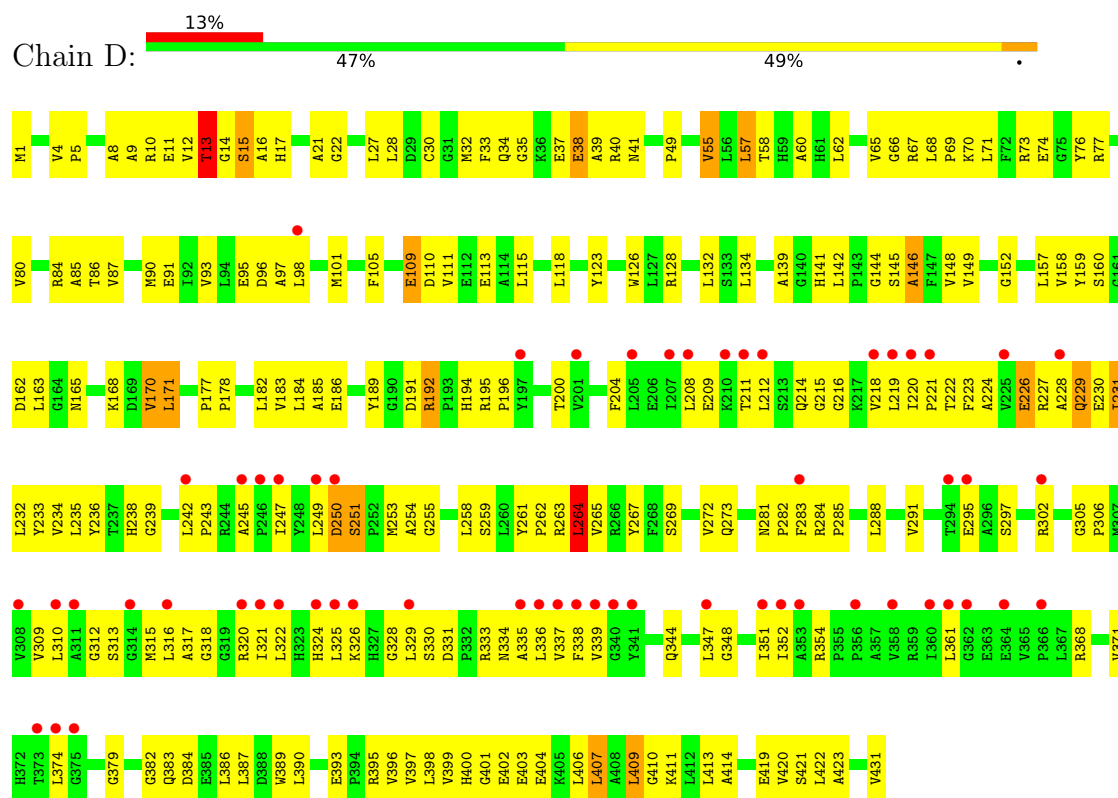
• Molecule 1: Ribonuclease TTHA0252



● 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	143.18Å 146.12Å 121.00Å 90.00° 109.51° 90.00°	Depositor
Resolution (Å)	50.00 – 2.73 50.00 – 2.73	Depositor EDS
% Data completeness (in resolution range)	96.1 (50.00-2.73) 96.1 (50.00-2.73)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.48 (at 2.73Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.218 , 0.272 0.216 , 0.269	Depositor DCC
R_{free} test set	6258 reflections (10.11%)	wwPDB-VP
Wilson B-factor (Å ²)	54.6	Xtriage
Anisotropy	0.067	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 53.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	13790	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.90% 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

5.1 Standard geometry

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	0.51	0/3414	1.03	14/4631 (0.3%)
1	B	0.49	0/3414	1.03	19/4631 (0.4%)
1	C	0.39	0/3414	0.91	12/4631 (0.3%)
1	D	0.38	0/3414	0.94	9/4631 (0.2%)
All	All	0.45	0/13656	0.98	54/18524 (0.3%)

There are no bond length outliers.

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	379	GLY	N-CA-C	14.27	131.03	112.77
1	B	225	VAL	N-CA-C	10.75	120.52	110.74
1	D	379	GLY	N-CA-C	10.16	124.93	112.64
1	A	170	VAL	N-CA-C	9.33	119.35	110.30
1	A	4	VAL	N-CA-C	7.92	116.07	107.60
1	A	225	VAL	N-CA-C	7.87	119.58	111.00
1	B	379	GLY	N-CA-C	7.35	128.19	115.62
1	D	60	ALA	N-CA-C	7.17	121.12	112.38
1	B	170	VAL	N-CA-C	7.10	117.23	110.42
1	C	265	VAL	N-CA-C	6.94	117.64	110.36
1	C	4	VAL	N-CA-C	6.83	114.90	107.60
1	B	265	VAL	N-CA-C	6.56	117.31	110.62
1	B	60	ALA	N-CA-C	6.51	121.07	113.20
1	D	4	VAL	N-CA-C	6.41	115.04	107.73
1	B	220	ILE	N-CA-C	6.30	114.38	108.15
1	C	160	SER	N-CA-C	6.26	118.91	111.71
1	D	170	VAL	N-CA-C	6.24	116.72	110.23
1	A	147	PHE	N-CA-C	-6.21	100.08	109.95
1	A	393	GLU	CA-C-N	6.11	125.59	119.24
1	A	393	GLU	C-N-CA	6.11	125.59	119.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	66	GLY	N-CA-C	6.09	121.37	113.27
1	A	220	ILE	N-CA-C	5.99	114.08	108.15
1	C	301	ASN	N-CA-C	-5.93	106.17	113.41
1	B	169	ASP	N-CA-C	5.86	120.56	113.41
1	D	146	ALA	N-CA-C	5.86	117.15	108.60
1	D	231	ILE	N-CA-C	-5.85	106.11	111.67
1	A	169	ASP	N-CA-C	5.75	120.42	113.41
1	B	161	GLY	N-CA-C	-5.74	101.36	111.80
1	C	170	VAL	N-CA-C	5.74	116.19	110.23
1	B	147	PHE	N-CA-C	-5.57	102.21	110.46
1	B	64	HIS	N-CA-C	-5.55	107.76	114.75
1	C	60	ALA	N-CA-C	5.53	119.65	113.01
1	C	147	PHE	N-CA-C	-5.51	101.60	110.14
1	D	393	GLU	CA-C-N	5.47	125.30	119.28
1	D	393	GLU	C-N-CA	5.47	125.30	119.28
1	C	12	VAL	N-CA-C	5.39	119.31	113.43
1	B	365	VAL	N-CA-C	5.39	113.36	107.60
1	C	161	GLY	N-CA-C	-5.37	100.98	110.86
1	A	293	HIS	N-CA-C	5.34	118.42	110.14
1	B	278	GLN	N-CA-C	-5.29	106.52	112.87
1	C	23	GLY	N-CA-C	-5.28	104.90	114.46
1	A	126	TRP	N-CA-C	5.25	118.17	109.46
1	A	161	GLY	N-CA-C	-5.19	99.86	112.01
1	B	181	ASP	N-CA-C	-5.17	105.72	112.23
1	C	33	PHE	N-CA-C	-5.16	102.84	110.48
1	A	365	VAL	N-CA-C	5.16	113.61	107.73
1	B	393	GLU	CA-C-N	5.14	124.76	119.05
1	B	393	GLU	C-N-CA	5.14	124.76	119.05
1	B	398	LEU	N-CA-C	5.03	117.60	110.50
1	B	280	LYS	N-CA-C	5.02	116.59	110.41
1	C	46	GLY	N-CA-C	-5.02	107.87	114.95
1	B	192	ARG	CA-C-N	5.02	126.13	120.66
1	B	192	ARG	C-N-CA	5.02	126.13	120.66
1	D	13	THR	N-CA-C	5.01	116.46	108.79

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	3332	0	3355	126	0
1	B	3332	0	3355	168	0
1	C	3332	0	3355	220	0
1	D	3332	0	3355	217	0
2	A	100	0	0	2	0
2	B	95	0	0	9	0
2	C	95	0	0	1	0
2	D	45	0	0	4	0
3	A	26	0	10	2	0
3	B	13	0	5	4	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	26	0	0	1	0
5	B	33	0	0	2	0
5	C	9	0	0	0	0
5	D	12	0	0	1	0
All	All	13790	0	13435	724	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 27.

All (724) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:263:ARG:HH21	1:A:263:ARG:HB3	1.00	1.14
1:C:73:ARG:HH21	1:C:106:PHE:HA	1.23	1.03
1:C:235:LEU:HD13	1:C:247:ILE:HD13	1.40	1.02
1:D:13:THR:CG2	1:D:33:PHE:HA	1.91	1.00
1:B:430:PRO:HG3	2:B:446:SO4:O3	1.62	0.98
1:B:83:THR:HG22	1:B:86:THR:H	1.29	0.96
1:C:33:PHE:H	1:C:41:ASN:HD21	1.12	0.94
1:B:33:PHE:H	1:B:41:ASN:HD21	1.11	0.93
1:A:263:ARG:HB3	1:A:263:ARG:NH2	1.85	0.92
1:A:217:LYS:HE2	1:A:307:MET:HE3	1.49	0.91
1:D:235:LEU:HD13	1:D:247:ILE:HD13	1.50	0.91
1:A:263:ARG:HH21	1:A:263:ARG:CB	1.83	0.91
1:D:318:GLY:HA2	1:D:322:LEU:HD11	1.52	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:97:ALA:O	1:C:101:MET:HB2	1.75	0.86
1:C:342:GLN:HE21	1:C:342:GLN:HA	1.38	0.86
1:D:220:ILE:HG12	1:D:337:VAL:HB	1.59	0.85
1:B:37:GLU:HG3	1:B:40:ARG:HH11	1.40	0.85
1:B:48:ASP:OD2	1:B:51:GLU:HG2	1.78	0.84
1:B:57:LEU:HD23	1:B:90:MET:HE1	1.60	0.84
1:B:359:ARG:HD2	1:B:364:GLU:OE1	1.76	0.83
1:C:387:LEU:HB3	1:C:416:ARG:HH12	1.44	0.82
1:D:211:THR:HG21	1:D:335:ALA:HB2	1.62	0.82
1:B:411:LYS:HG3	3:B:451:FLC:HA1	1.61	0.81
1:C:315:MET:HE2	1:C:343:PRO:HD3	1.62	0.80
1:B:375:GLY:HA2	1:B:378:TYR:CE2	2.17	0.80
1:C:32:MET:HE2	1:C:105:PHE:HZ	1.47	0.80
1:D:86:THR:HG22	1:D:90:MET:HE2	1.63	0.79
1:C:101:MET:HE3	1:C:104:PRO:HA	1.64	0.79
1:D:157:LEU:HD12	1:D:158:VAL:H	1.47	0.79
1:C:87:VAL:HG13	1:C:118:LEU:HD13	1.65	0.78
1:D:182:LEU:HD23	1:D:431:VAL:HG22	1.65	0.78
1:D:291:VAL:HG13	2:D:433:SO4:O1	1.83	0.78
1:B:83:THR:HG21	1:B:144:GLY:CA	2.13	0.78
1:D:284:ARG:HD3	1:D:288:LEU:HD23	1.66	0.78
1:B:31:GLY:O	1:B:67:ARG:HG3	1.83	0.77
1:D:13:THR:HG21	1:D:34:GLN:H	1.49	0.77
1:D:33:PHE:H	1:D:41:ASN:HD21	1.31	0.77
1:C:209:GLU:OE2	1:C:243:PRO:HD3	1.85	0.77
1:A:91:GLU:O	1:A:95:GLU:HG2	1.86	0.76
1:C:342:GLN:HE21	1:C:343:PRO:HD2	1.51	0.76
1:B:12:VAL:HG12	1:B:401:GLY:HA2	1.68	0.76
1:A:10:ARG:HG2	1:A:10:ARG:HH11	1.51	0.76
1:C:222:THR:HG22	1:C:339:VAL:HG21	1.68	0.75
1:D:12:VAL:HG12	1:D:401:GLY:HA2	1.67	0.75
1:C:344:GLN:CD	1:C:344:GLN:H	1.95	0.75
1:B:33:PHE:N	1:B:41:ASN:HD21	1.85	0.74
1:A:182:LEU:HD11	1:A:397:VAL:HG23	1.71	0.73
1:C:403:GLU:O	1:C:407:LEU:HD23	1.88	0.73
1:D:229:GLN:HG3	1:D:261:TYR:CE1	2.23	0.73
1:C:227:ARG:NH1	1:C:378:TYR:HA	2.04	0.73
1:C:73:ARG:NH2	1:C:106:PHE:HA	2.01	0.72
1:C:25:ARG:HH11	1:C:51:GLU:HB3	1.53	0.72
1:C:160:SER:HB2	1:C:163:LEU:HD21	1.72	0.72
1:B:43:ALA:HB1	1:B:44:PRO:HD2	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:12:VAL:CG1	1:D:401:GLY:HA2	2.21	0.71
1:D:160:SER:HB2	1:D:163:LEU:HD21	1.72	0.71
1:B:83:THR:HG21	1:B:144:GLY:HA3	1.71	0.71
1:B:70:LYS:HE3	1:B:74:GLU:OE1	1.90	0.71
1:A:128:ARG:O	1:A:129:LEU:HD23	1.90	0.71
1:B:99:LYS:HE2	5:B:472:HOH:O	1.91	0.71
1:D:13:THR:HG23	1:D:33:PHE:HA	1.70	0.71
1:A:97:ALA:O	1:A:101:MET:HB2	1.91	0.70
1:B:37:GLU:HG3	1:B:40:ARG:NH1	2.07	0.70
1:B:236:TYR:OH	1:B:280:LYS:HD3	1.90	0.70
1:D:325:LEU:HG	1:D:329:LEU:HD11	1.72	0.70
1:C:198:ARG:HB3	1:C:198:ARG:NH2	2.06	0.69
1:B:1:MET:HG3	1:B:21:ALA:HB2	1.74	0.69
1:A:84:ARG:NH2	1:A:263:ARG:HH12	1.90	0.69
1:D:401:GLY:HA3	1:D:406:LEU:HD11	1.75	0.69
1:C:331:ASP:HB3	1:C:334:ASN:ND2	2.07	0.69
1:C:407:LEU:HD22	1:C:422:LEU:HD21	1.75	0.68
1:A:34:GLN:HE21	1:A:63:ASP:HB3	1.58	0.68
1:A:85:ALA:HB2	1:A:267:TYR:CD2	2.29	0.68
1:C:12:VAL:HG12	1:C:401:GLY:HA2	1.76	0.68
1:A:55:VAL:HG22	1:A:80:VAL:HG13	1.76	0.68
1:A:208:LEU:HD23	1:A:218:VAL:HG21	1.73	0.68
1:B:295:GLU:H	1:B:295:GLU:CD	2.01	0.67
1:C:342:GLN:NE2	1:C:343:PRO:HD2	2.09	0.67
1:C:409:LEU:HD22	1:C:413:LEU:HG	1.76	0.67
1:D:295:GLU:H	1:D:295:GLU:CD	2.01	0.67
1:B:57:LEU:HD23	1:B:90:MET:CE	2.25	0.67
1:A:83:THR:O	1:A:87:VAL:HG23	1.95	0.67
1:C:329:LEU:HD12	1:C:369:ALA:HB3	1.75	0.67
1:C:227:ARG:HH11	1:C:378:TYR:HA	1.60	0.66
1:D:258:LEU:HD11	1:D:283:PHE:HB3	1.75	0.66
1:A:165:ASN:C	1:A:165:ASN:HD22	2.03	0.66
1:A:302:ARG:HG2	1:A:302:ARG:HH21	1.59	0.66
1:D:326:LYS:HD2	1:D:361:LEU:HD12	1.76	0.66
1:C:229:GLN:HG3	1:C:261:TYR:CZ	2.29	0.66
1:A:85:ALA:HB2	1:A:267:TYR:CE2	2.32	0.65
1:B:401:GLY:C	1:B:406:LEU:HD11	2.21	0.65
1:C:27:LEU:HD13	1:C:29:ASP:O	1.96	0.65
1:C:160:SER:HB2	1:C:163:LEU:CD2	2.27	0.65
1:B:387:LEU:HB3	1:B:416:ARG:HH12	1.62	0.65
1:A:278:GLN:HB3	1:A:280:LYS:HE2	1.76	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:217:LYS:HE2	1:C:307:MET:HE3	1.79	0.64
1:A:344:GLN:H	1:A:344:GLN:CD	2.05	0.64
1:C:360:ILE:HD12	1:C:365:VAL:HG11	1.79	0.64
1:A:10:ARG:HG2	1:A:10:ARG:NH1	2.10	0.64
1:A:200:THR:CG2	1:A:374:LEU:HB3	2.27	0.64
1:A:404:GLU:CD	1:A:404:GLU:H	2.04	0.64
1:C:86:THR:O	1:C:90:MET:HB2	1.97	0.64
1:D:62:LEU:HD13	1:D:93:VAL:HG12	1.79	0.64
1:D:321:ILE:O	1:D:325:LEU:HD13	1.98	0.64
1:D:222:THR:HG22	1:D:339:VAL:HG21	1.78	0.64
1:D:168:LYS:HD3	1:D:230:GLU:OE1	1.98	0.64
1:D:171:LEU:H	1:D:171:LEU:HD22	1.62	0.64
1:C:84:ARG:HB3	1:C:267:TYR:OH	1.98	0.64
1:D:209:GLU:OE1	1:D:242:LEU:HA	1.97	0.64
1:C:57:LEU:HD23	1:C:90:MET:CE	2.27	0.63
1:C:189:TYR:CE1	1:C:380:HIS:HB2	2.33	0.63
1:D:228:ALA:HB3	1:D:229:GLN:NE2	2.13	0.63
1:D:302:ARG:HG2	1:D:302:ARG:HH21	1.63	0.63
1:B:325:LEU:O	1:B:329:LEU:HB2	1.99	0.63
1:C:221:PRO:HB3	1:C:321:ILE:HG12	1.81	0.63
1:D:227:ARG:HG2	1:D:227:ARG:HH21	1.63	0.63
1:A:32:MET:HE1	1:A:101:MET:HE1	1.81	0.63
1:A:288:LEU:HD12	1:A:289:GLU:H	1.62	0.63
1:C:420:VAL:HG22	1:C:421:SER:N	2.13	0.63
1:D:216:GLY:HA3	1:D:333:ARG:O	1.98	0.63
1:D:291:VAL:CG1	2:D:433:SO4:O1	2.46	0.63
1:B:430:PRO:CG	2:B:446:SO4:O3	2.43	0.63
1:C:424:ARG:HD2	1:C:427:GLU:OE2	1.99	0.62
1:A:347:LEU:HD11	1:A:358:VAL:HG11	1.81	0.62
1:B:98:LEU:HD11	1:B:108:PRO:HA	1.81	0.62
1:C:415:LEU:HD23	1:C:416:ARG:N	2.14	0.62
1:B:406:LEU:N	1:B:406:LEU:HD12	2.14	0.62
1:C:73:ARG:HH21	1:C:106:PHE:CA	2.07	0.62
1:B:65:VAL:HG11	1:B:90:MET:HG3	1.81	0.62
1:C:342:GLN:HE21	1:C:342:GLN:CA	2.07	0.62
1:D:5:PRO:HG2	1:D:423:ALA:HB1	1.82	0.62
1:C:410:GLY:HA2	1:C:420:VAL:HG21	1.81	0.62
1:D:32:MET:HE2	1:D:105:PHE:HZ	1.65	0.62
1:B:37:GLU:CG	1:B:40:ARG:HH11	2.10	0.62
1:A:220:ILE:HG22	1:A:222:THR:HG23	1.82	0.62
1:C:251:SER:HB3	1:C:254:ALA:HB3	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:342:GLN:HA	1:C:342:GLN:NE2	2.10	0.62
1:D:76:TYR:O	1:D:77:ARG:HD2	2.00	0.62
1:C:163:LEU:HD11	1:C:389:TRP:CE2	2.35	0.61
1:A:102:ASP:O	1:A:104:PRO:HD3	2.00	0.61
1:B:239:GLY:O	1:B:241:ARG:N	2.32	0.61
1:C:229:GLN:CD	1:C:229:GLN:H	2.08	0.61
1:C:302:ARG:HG2	1:C:302:ARG:HH21	1.65	0.61
1:D:32:MET:HG2	1:D:66:GLY:HA3	1.82	0.61
1:B:155:ARG:HD3	1:B:431:VAL:O	1.99	0.61
1:C:83:THR:O	1:C:87:VAL:HG23	1.99	0.61
1:B:407:LEU:HD13	1:B:422:LEU:HD21	1.81	0.61
1:D:128:ARG:HD2	5:D:454:HOH:O	1.99	0.61
1:D:33:PHE:N	1:D:41:ASN:HD21	1.98	0.61
1:D:284:ARG:HD3	1:D:288:LEU:CD2	2.31	0.61
1:B:98:LEU:HD11	1:B:108:PRO:CA	2.31	0.60
1:C:295:GLU:CD	1:C:295:GLU:H	2.07	0.60
1:B:229:GLN:HG3	1:B:261:TYR:CZ	2.36	0.60
1:C:57:LEU:HD23	1:C:90:MET:HE1	1.83	0.60
1:A:84:ARG:HH22	1:A:263:ARG:HH12	1.49	0.60
1:A:235:LEU:HD13	1:A:247:ILE:HD13	1.84	0.60
1:C:32:MET:HE2	1:C:105:PHE:CZ	2.33	0.60
1:C:318:GLY:HA2	1:C:322:LEU:CD1	2.30	0.60
1:D:347:LEU:O	1:D:351:ILE:HG13	2.01	0.60
1:B:200:THR:HG23	1:B:374:LEU:HB3	1.81	0.60
1:D:239:GLY:HA2	1:D:242:LEU:HG	1.84	0.60
1:B:165:ASN:HD22	1:B:165:ASN:C	2.10	0.60
1:C:291:VAL:HG12	1:C:292:GLU:N	2.16	0.60
1:D:259:SER:O	1:D:262:PRO:HD2	2.02	0.60
1:D:384:ASP:HA	1:D:387:LEU:HD12	1.82	0.60
1:A:229:GLN:H	1:A:229:GLN:CD	2.08	0.59
1:D:410:GLY:HA2	1:D:420:VAL:HG21	1.82	0.59
1:B:401:GLY:CA	1:B:406:LEU:HD11	2.32	0.59
1:C:215:GLY:HA2	1:C:306:PRO:HD3	1.84	0.59
1:C:12:VAL:HG23	1:C:13:THR:HG23	1.84	0.59
1:C:54:ALA:HA	1:C:76:TYR:OH	2.02	0.59
1:C:331:ASP:HB3	1:C:334:ASN:HD22	1.67	0.59
1:C:359:ARG:HG2	1:C:359:ARG:HH11	1.68	0.59
1:C:182:LEU:HD23	1:C:431:VAL:HG22	1.85	0.59
1:D:91:GLU:HG3	1:D:115:LEU:HD13	1.84	0.59
1:B:33:PHE:H	1:B:41:ASN:ND2	1.92	0.59
1:C:229:GLN:H	1:C:229:GLN:NE2	2.01	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:359:ARG:HH12	1:C:362:GLY:C	2.11	0.58
1:C:86:THR:HG22	1:C:90:MET:CE	2.33	0.58
1:A:168:LYS:HD3	1:A:230:GLU:OE1	2.03	0.58
1:D:13:THR:HG22	1:D:33:PHE:CD1	2.38	0.58
1:D:219:LEU:HD23	1:D:325:LEU:HD12	1.85	0.58
1:C:409:LEU:CD2	1:C:413:LEU:HG	2.34	0.58
1:B:401:GLY:HA3	1:B:406:LEU:HD11	1.85	0.58
1:D:396:VAL:HG12	1:D:398:LEU:HD12	1.84	0.58
1:C:232:LEU:HA	1:C:235:LEU:HD12	1.86	0.58
1:C:420:VAL:HG22	1:C:421:SER:H	1.67	0.58
1:B:142:LEU:CD2	1:B:226:GLU:HB3	2.33	0.58
1:D:222:THR:HG22	1:D:339:VAL:CG2	2.34	0.58
1:A:87:VAL:HG13	1:A:118:LEU:HD13	1.85	0.58
1:A:329:LEU:HD11	1:A:336:LEU:HD12	1.86	0.58
1:D:383:GLN:O	1:D:387:LEU:HG	2.04	0.58
1:C:219:LEU:N	1:C:219:LEU:HD12	2.19	0.57
1:D:13:THR:HG21	1:D:33:PHE:HA	1.80	0.57
1:D:157:LEU:HD12	1:D:158:VAL:N	2.16	0.57
1:C:55:VAL:HG22	1:C:80:VAL:HG13	1.86	0.57
1:C:374:LEU:C	1:C:376:GLY:H	2.13	0.57
1:B:411:LYS:HB2	3:B:451:FLC:OHB	2.04	0.57
1:C:220:ILE:HG22	1:C:222:THR:HG23	1.85	0.57
1:B:239:GLY:C	1:B:241:ARG:H	2.12	0.57
1:B:1:MET:HG3	1:B:21:ALA:CB	2.35	0.57
1:B:83:THR:HG21	1:B:144:GLY:HA2	1.86	0.57
1:D:229:GLN:HG3	1:D:261:TYR:CZ	2.39	0.57
1:C:197:TYR:O	1:C:201:VAL:HG23	2.04	0.57
1:A:34:GLN:NE2	1:A:63:ASP:HB3	2.19	0.57
1:C:252:PRO:HB2	2:C:434:SO4:O2	2.05	0.57
1:D:13:THR:HG22	1:D:33:PHE:HD1	1.68	0.57
1:D:330:SER:O	1:D:368:ARG:HB2	2.04	0.57
1:A:129:LEU:O	1:A:132:LEU:HB2	2.05	0.57
1:D:86:THR:O	1:D:90:MET:HB2	2.04	0.57
1:D:37:GLU:HB3	1:D:40:ARG:HE	1.70	0.56
1:A:45:PHE:HB3	1:A:47:PHE:CE1	2.40	0.56
1:D:32:MET:HE2	1:D:105:PHE:CZ	2.40	0.56
1:D:177:PRO:HD3	1:D:389:TRP:CE2	2.40	0.56
1:B:90:MET:O	1:B:94:LEU:HB2	2.04	0.56
1:D:11:GLU:C	1:D:401:GLY:H	2.13	0.56
1:A:398:LEU:HB3	1:A:406:LEU:HG	1.86	0.56
1:A:4:VAL:HG22	1:A:428:GLY:HA3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:395:ARG:HG3	1:D:419:GLU:HB3	1.88	0.56
1:C:388:ASP:O	1:C:391:GLN:HB3	2.05	0.56
1:D:325:LEU:HA	1:D:329:LEU:HD13	1.86	0.56
1:C:98:LEU:HD13	1:C:98:LEU:C	2.31	0.56
1:B:209:GLU:O	1:B:213:SER:HB2	2.05	0.56
1:D:297:SER:HB2	1:D:320:ARG:NH2	2.20	0.56
1:C:227:ARG:HG2	1:C:227:ARG:HH21	1.71	0.55
1:C:198:ARG:HB3	1:C:198:ARG:HH21	1.71	0.55
1:B:290:VAL:HB	2:B:437:SO4:O3	2.06	0.55
1:B:396:VAL:HG12	1:B:398:LEU:HD12	1.88	0.55
1:D:113:GLU:OE2	1:D:113:GLU:HA	2.05	0.55
1:D:354:ARG:NH1	1:D:371:VAL:HG23	2.22	0.55
1:C:393:GLU:O	1:C:418:GLN:HG2	2.06	0.55
1:D:177:PRO:HD3	1:D:389:TRP:NE1	2.21	0.55
1:D:221:PRO:HD2	1:D:337:VAL:O	2.06	0.55
1:B:411:LYS:CG	3:B:451:FLC:HA1	2.32	0.55
1:B:195:ARG:HD3	1:B:199:GLU:OE2	2.06	0.55
1:C:248:TYR:CE2	1:C:289:GLU:HG2	2.42	0.55
1:C:412:LEU:O	1:C:415:LEU:HD22	2.07	0.55
1:B:33:PHE:CE2	1:B:67:ARG:NH1	2.75	0.54
1:B:100:VAL:HG12	1:B:100:VAL:O	2.07	0.54
1:D:163:LEU:N	1:D:163:LEU:HD22	2.22	0.54
1:D:354:ARG:HH12	1:D:371:VAL:HG23	1.72	0.54
1:C:34:GLN:HE21	1:C:63:ASP:HB3	1.73	0.54
1:C:231:ILE:O	1:C:235:LEU:HG	2.07	0.54
1:A:165:ASN:ND2	1:A:167:GLU:H	2.06	0.54
1:C:318:GLY:HA2	1:C:322:LEU:HD11	1.89	0.54
1:D:49:PRO:HB3	1:D:71:LEU:HD12	1.89	0.54
1:B:20:LEU:HD21	1:B:25:ARG:HE	1.73	0.54
1:B:142:LEU:HD21	1:B:226:GLU:HB3	1.88	0.54
1:C:293:HIS:HB3	1:C:295:GLU:OE1	2.08	0.54
1:C:415:LEU:HD23	1:C:415:LEU:C	2.32	0.54
1:A:404:GLU:OE2	1:A:404:GLU:N	2.33	0.54
1:C:70:LYS:HE2	1:C:74:GLU:OE1	2.08	0.54
1:D:219:LEU:HD21	1:D:324:HIS:O	2.08	0.54
1:D:232:LEU:O	1:D:285:PRO:HD3	2.08	0.54
1:B:315:MET:SD	1:B:343:PRO:HD3	2.48	0.54
1:D:209:GLU:CD	1:D:243:PRO:HD3	2.32	0.54
1:B:229:GLN:CD	1:B:229:GLN:H	2.13	0.53
1:D:382:GLY:O	1:D:386:LEU:HD13	2.07	0.53
1:A:33:PHE:H	1:A:41:ASN:HD21	1.56	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:65:VAL:HG12	1:B:94:LEU:HD13	1.90	0.53
1:B:420:VAL:HG22	1:B:421:SER:N	2.23	0.53
1:D:37:GLU:HB3	1:D:40:ARG:HH11	1.73	0.53
1:D:231:ILE:C	1:D:233:TYR:H	2.16	0.53
1:A:41:ASN:O	1:A:70:LYS:HE3	2.08	0.53
1:A:86:THR:HG22	1:A:90:MET:HE2	1.91	0.53
1:A:250:ASP:OD2	1:A:297:SER:OG	2.26	0.53
1:D:182:LEU:HD11	1:D:397:VAL:HG23	1.90	0.53
1:D:204:PHE:CE1	1:D:208:LEU:HD11	2.43	0.53
1:A:396:VAL:HG12	1:A:398:LEU:HD13	1.91	0.53
1:C:109:GLU:CD	1:C:109:GLU:H	2.16	0.53
1:D:171:LEU:HD22	1:D:171:LEU:N	2.24	0.53
1:A:220:ILE:HG22	1:A:222:THR:CG2	2.39	0.53
1:D:13:THR:HG21	1:D:34:GLN:N	2.22	0.53
1:B:68:LEU:N	1:B:69:PRO:HD2	2.23	0.53
1:A:288:LEU:HD12	1:A:289:GLU:N	2.23	0.53
1:A:329:LEU:HG	1:A:367:LEU:HD13	1.89	0.53
1:C:113:GLU:HA	1:C:113:GLU:OE2	2.09	0.53
1:C:401:GLY:HA3	1:C:406:LEU:HD11	1.91	0.53
1:D:91:GLU:O	1:D:95:GLU:HG3	2.07	0.53
1:A:302:ARG:HG2	1:A:302:ARG:NH2	2.24	0.53
1:D:37:GLU:C	1:D:39:ALA:H	2.17	0.53
1:A:68:LEU:N	1:A:69:PRO:HD2	2.23	0.52
1:A:229:GLN:H	1:A:229:GLN:NE2	2.07	0.52
1:A:284:ARG:HD2	3:A:452:FLC:HA2	1.92	0.52
1:B:295:GLU:OE2	1:B:295:GLU:N	2.31	0.52
1:D:35:GLY:C	1:D:37:GLU:H	2.15	0.52
1:B:204:PHE:CZ	1:B:208:LEU:HD11	2.45	0.52
1:D:160:SER:HB3	1:D:185:ALA:HA	1.91	0.52
1:D:420:VAL:HG22	1:D:421:SER:N	2.24	0.52
1:A:142:LEU:HD22	1:A:143:PRO:HD2	1.92	0.52
1:B:389:TRP:HE3	1:B:390:LEU:HD13	1.75	0.52
1:A:320:ARG:HD3	3:A:453:FLC:OHB	2.10	0.52
1:A:395:ARG:NH2	1:A:431:VAL:OXT	2.40	0.52
1:C:227:ARG:HG2	1:C:227:ARG:NH2	2.24	0.52
1:A:253:MET:O	1:A:257:VAL:HG23	2.10	0.52
1:B:83:THR:HG22	1:B:86:THR:N	2.12	0.52
1:C:1:MET:HG2	1:C:431:VAL:HG21	1.91	0.52
1:C:407:LEU:CD2	1:C:422:LEU:HD21	2.38	0.52
1:D:316:LEU:C	1:D:318:GLY:H	2.18	0.52
1:D:325:LEU:HG	1:D:329:LEU:CD1	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:200:THR:HG23	1:A:374:LEU:HB3	1.93	0.51
1:C:209:GLU:CD	1:C:243:PRO:HD3	2.35	0.51
1:D:209:GLU:HG3	1:D:243:PRO:HD3	1.91	0.51
1:D:409:LEU:HD22	1:D:413:LEU:HG	1.91	0.51
1:A:375:GLY:HA2	1:A:378:TYR:CE2	2.45	0.51
1:B:382:GLY:O	1:B:386:LEU:HD22	2.10	0.51
1:B:411:LYS:HA	3:B:451:FLC:HG1	1.91	0.51
1:C:177:PRO:HD3	1:C:389:TRP:CE2	2.45	0.51
1:C:227:ARG:HH11	1:C:378:TYR:CA	2.23	0.51
1:D:312:GLY:HA2	1:D:313:SER:C	2.34	0.51
1:A:157:LEU:HG	1:A:158:VAL:N	2.22	0.51
1:A:165:ASN:C	1:A:165:ASN:ND2	2.68	0.51
1:C:42:HIS:CE1	1:C:105:PHE:HB3	2.44	0.51
1:D:57:LEU:HD21	1:D:68:LEU:HD22	1.90	0.51
1:B:200:THR:OG1	1:B:376:GLY:HA3	2.11	0.51
1:D:84:ARG:HB2	1:D:267:TYR:OH	2.10	0.51
1:D:85:ALA:HB2	1:D:267:TYR:CD2	2.45	0.51
1:B:70:LYS:O	1:B:74:GLU:HG3	2.11	0.51
1:C:85:ALA:HB2	1:C:267:TYR:CD2	2.45	0.51
1:D:141:HIS:O	1:D:142:LEU:HD23	2.10	0.51
1:A:11:GLU:CD	1:A:40:ARG:HH12	2.18	0.51
1:B:165:ASN:C	1:B:165:ASN:ND2	2.66	0.51
1:C:132:LEU:HD21	1:C:134:LEU:HD21	1.92	0.51
1:C:226:GLU:O	1:C:229:GLN:HG2	2.09	0.51
1:B:31:GLY:HA3	1:B:63:ASP:C	2.35	0.51
1:B:253:MET:O	1:B:254:ALA:C	2.53	0.51
1:B:416:ARG:CG	2:B:433:SO4:O3	2.59	0.51
1:D:33:PHE:H	1:D:41:ASN:ND2	2.03	0.51
1:A:37:GLU:OE2	1:A:37:GLU:HA	2.10	0.51
1:B:37:GLU:HA	1:B:37:GLU:OE2	2.10	0.51
1:C:68:LEU:HD11	1:C:72:PHE:HE1	1.75	0.51
1:D:10:ARG:HG2	1:D:10:ARG:HH11	1.76	0.51
1:C:231:ILE:HG21	1:C:310:LEU:HD21	1.93	0.51
1:C:315:MET:CE	1:C:343:PRO:HD3	2.37	0.51
1:A:86:THR:O	1:A:90:MET:HB2	2.11	0.51
1:C:28:LEU:O	1:C:29:ASP:HB2	2.11	0.51
1:B:140:GLY:O	1:B:164:GLY:HA3	2.11	0.50
1:C:12:VAL:HG12	1:C:401:GLY:CA	2.42	0.50
1:D:8:ALA:N	1:D:13:THR:O	2.37	0.50
1:B:199:GLU:HA	1:B:202:ARG:HH11	1.77	0.50
1:D:70:LYS:NZ	1:D:74:GLU:OE1	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:73:ARG:HD2	1:C:110:ASP:OD2	2.10	0.50
1:D:411:LYS:O	1:D:414:ALA:HB3	2.12	0.50
1:A:318:GLY:HA2	1:A:322:LEU:CD1	2.41	0.50
1:B:12:VAL:HG12	1:B:401:GLY:CA	2.38	0.50
1:B:293:HIS:HB3	2:B:441:SO4:O4	2.11	0.50
1:B:397:VAL:HG22	1:B:421:SER:OG	2.11	0.50
1:C:165:ASN:HB2	1:C:379:GLY:O	2.11	0.50
1:C:191:ASP:CG	1:C:192:ARG:HG3	2.37	0.50
1:D:62:LEU:HD13	1:D:93:VAL:CG1	2.42	0.50
1:B:73:ARG:HD2	1:B:110:ASP:OD2	2.12	0.50
1:C:228:ALA:HB3	1:C:229:GLN:NE2	2.27	0.50
1:D:211:THR:HG21	1:D:335:ALA:CB	2.38	0.50
1:A:191:ASP:CG	1:A:405:LYS:HD2	2.36	0.50
1:A:325:LEU:O	1:A:329:LEU:HB2	2.12	0.50
1:B:168:LYS:HG2	1:B:197:TYR:CE2	2.47	0.50
1:C:33:PHE:CD2	1:C:40:ARG:HB2	2.46	0.50
1:D:251:SER:HB3	1:D:254:ALA:HB3	1.94	0.50
1:D:264:LEU:HD13	1:D:264:LEU:N	2.27	0.50
1:C:95:GLU:O	1:C:98:LEU:HB3	2.11	0.50
1:D:1:MET:HG3	1:D:21:ALA:HB2	1.92	0.50
1:D:37:GLU:CB	1:D:40:ARG:HH11	2.25	0.50
1:D:139:ALA:HB2	1:D:146:ALA:HA	1.93	0.50
1:D:331:ASP:HB3	1:D:334:ASN:ND2	2.27	0.50
1:C:199:GLU:HA	1:C:202:ARG:HE	1.77	0.49
1:D:401:GLY:CA	1:D:406:LEU:HD11	2.41	0.49
1:D:123:TYR:HE1	1:D:146:ALA:HB2	1.77	0.49
1:A:229:GLN:HG3	1:A:261:TYR:CZ	2.47	0.49
1:D:185:ALA:HB2	1:D:390:LEU:HD11	1.94	0.49
1:A:289:GLU:OE2	1:B:291:VAL:HA	2.12	0.49
1:C:13:THR:OG1	1:C:33:PHE:HA	2.12	0.49
1:D:208:LEU:O	1:D:212:LEU:HG	2.12	0.49
1:D:421:SER:C	1:D:422:LEU:HD12	2.37	0.49
1:A:344:GLN:H	1:A:344:GLN:NE2	2.09	0.49
1:B:85:ALA:HB2	1:B:267:TYR:CD2	2.47	0.49
1:A:217:LYS:HG2	1:A:307:MET:HG2	1.95	0.49
1:B:40:ARG:C	1:B:42:HIS:H	2.21	0.49
1:B:396:VAL:HG12	1:B:398:LEU:CD1	2.42	0.49
1:C:9:ALA:C	1:C:11:GLU:H	2.21	0.49
1:B:163:LEU:HD21	1:B:389:TRP:CD2	2.48	0.49
1:D:32:MET:HA	1:D:67:ARG:HG3	1.95	0.49
1:B:387:LEU:HB3	1:B:416:ARG:NH1	2.27	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:158:VAL:HG23	1:C:180:ALA:HB2	1.94	0.48
1:D:404:GLU:H	1:D:404:GLU:CD	2.21	0.48
1:B:236:TYR:C	1:B:236:TYR:CD2	2.90	0.48
1:C:101:MET:HE3	1:C:104:PRO:CA	2.38	0.48
1:C:358:VAL:O	1:C:365:VAL:HG12	2.13	0.48
1:B:348:GLY:O	1:B:352:ILE:HG13	2.13	0.48
1:A:295:GLU:CD	1:A:295:GLU:H	2.21	0.48
1:C:227:ARG:HH11	1:C:379:GLY:N	2.11	0.48
1:C:229:GLN:HG3	1:C:261:TYR:CE1	2.47	0.48
1:D:14:GLY:O	1:D:15:SER:C	2.55	0.48
1:D:250:ASP:O	1:D:251:SER:HB2	2.12	0.48
1:C:359:ARG:HG2	1:C:359:ARG:NH1	2.28	0.48
1:D:37:GLU:C	1:D:39:ALA:N	2.71	0.48
1:A:62:LEU:HD11	1:A:97:ALA:HB2	1.96	0.48
1:B:182:LEU:HD11	1:B:397:VAL:HG23	1.96	0.48
1:B:203:GLU:O	1:B:206:GLU:HB2	2.13	0.48
1:B:226:GLU:HG3	1:B:227:ARG:N	2.28	0.48
1:B:406:LEU:CD1	1:B:406:LEU:H	2.26	0.48
1:C:73:ARG:NH2	1:C:106:PHE:CA	2.72	0.48
1:D:97:ALA:O	1:D:101:MET:HB2	2.13	0.48
1:A:241:ARG:HD3	2:A:441:SO4:O3	2.13	0.48
1:B:14:GLY:O	1:B:15:SER:C	2.56	0.48
1:C:12:VAL:CG1	1:C:401:GLY:HA2	2.43	0.48
1:D:245:ALA:HB1	1:D:306:PRO:O	2.14	0.48
1:D:325:LEU:HB3	1:D:329:LEU:HD22	1.96	0.48
1:D:330:SER:O	1:D:368:ARG:HD2	2.14	0.48
1:D:420:VAL:HG22	1:D:421:SER:H	1.79	0.48
1:A:375:GLY:HA2	1:A:378:TYR:CZ	2.49	0.48
1:B:259:SER:O	1:B:262:PRO:HD2	2.14	0.48
1:D:16:ALA:C	1:D:17:HIS:CD2	2.91	0.48
1:A:43:ALA:HB1	1:A:44:PRO:HD2	1.95	0.48
1:C:381:ALA:HB3	1:C:386:LEU:CD1	2.44	0.48
1:D:195:ARG:O	1:D:196:PRO:C	2.57	0.48
1:A:3:ILE:HG23	1:A:3:ILE:O	2.12	0.47
1:C:347:LEU:O	1:C:351:ILE:HG13	2.14	0.47
1:D:38:GLU:O	1:D:38:GLU:HG2	2.12	0.47
1:B:224:ALA:HB1	1:B:253:MET:HG2	1.96	0.47
1:D:177:PRO:HD3	1:D:389:TRP:CD1	2.49	0.47
1:B:347:LEU:HD11	1:B:358:VAL:HG11	1.95	0.47
1:C:235:LEU:HD13	1:C:247:ILE:HG21	1.96	0.47
1:D:170:VAL:HG12	1:D:171:LEU:HD13	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:204:PHE:HB2	1:D:374:LEU:HD13	1.96	0.47
1:D:109:GLU:H	1:D:109:GLU:CD	2.22	0.47
1:C:217:LYS:HG2	1:C:307:MET:HG2	1.96	0.47
1:D:219:LEU:CD2	1:D:324:HIS:HB3	2.45	0.47
1:D:258:LEU:CD1	1:D:283:PHE:HB3	2.43	0.47
1:A:4:VAL:HG22	1:A:428:GLY:CA	2.43	0.47
1:B:188:THR:HG22	1:B:189:TYR:CD1	2.49	0.47
1:B:207:ILE:O	1:B:211:THR:HG22	2.14	0.47
1:B:416:ARG:HD2	1:B:418:GLN:OE1	2.15	0.47
1:C:331:ASP:OD2	1:C:332:PRO:HD2	2.15	0.47
1:D:231:ILE:C	1:D:233:TYR:N	2.72	0.47
1:B:37:GLU:O	1:B:38:GLU:C	2.57	0.47
1:B:406:LEU:N	1:B:406:LEU:CD1	2.76	0.47
1:C:25:ARG:NH1	1:C:51:GLU:HB3	2.26	0.47
1:D:12:VAL:HG23	1:D:12:VAL:O	2.14	0.47
1:D:398:LEU:O	1:D:399:VAL:HG13	2.15	0.47
1:D:37:GLU:O	1:D:39:ALA:N	2.48	0.47
1:A:318:GLY:HA2	1:A:322:LEU:HD12	1.97	0.47
1:D:65:VAL:HG11	1:D:90:MET:CG	2.45	0.47
1:A:59:HIS:CD2	1:A:61:HIS:HB2	2.50	0.47
1:B:277:LEU:C	1:B:279:GLY:N	2.72	0.47
1:B:297:SER:OG	1:B:320:ARG:HD3	2.15	0.47
1:D:13:THR:CG2	1:D:14:GLY:N	2.76	0.47
1:D:28:LEU:HB3	1:D:159:TYR:CD1	2.50	0.47
1:B:412:LEU:HD22	2:B:448:SO4:O3	2.15	0.46
1:B:404:GLU:HG3	1:B:405:LYS:N	2.30	0.46
1:D:148:VAL:HG12	1:D:149:VAL:N	2.30	0.46
1:D:336:LEU:C	1:D:336:LEU:HD23	2.41	0.46
1:D:348:GLY:O	1:D:352:ILE:HG13	2.14	0.46
1:A:2:ARG:HD3	5:A:461:HOH:O	2.15	0.46
1:B:233:TYR:CE1	1:B:272:VAL:HG22	2.50	0.46
1:C:91:GLU:O	1:C:95:GLU:HG2	2.14	0.46
1:D:168:LYS:CD	1:D:230:GLU:OE1	2.62	0.46
1:D:98:LEU:HD23	1:D:98:LEU:C	2.40	0.46
1:D:55:VAL:HG13	1:D:80:VAL:HG22	1.98	0.46
1:D:177:PRO:HB3	1:D:389:TRP:CZ2	2.50	0.46
1:B:229:GLN:HG3	1:B:261:TYR:CE1	2.51	0.46
1:C:9:ALA:O	1:C:11:GLU:HG2	2.15	0.46
1:C:88:LEU:HD12	1:C:264:LEU:HD11	1.98	0.46
1:D:226:GLU:O	1:D:229:GLN:HG2	2.16	0.46
1:C:43:ALA:O	1:C:70:LYS:NZ	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:32:MET:HE1	1:D:101:MET:CE	2.46	0.46
1:D:344:GLN:CD	1:D:344:GLN:H	2.24	0.46
1:A:420:VAL:HG22	1:A:421:SER:N	2.30	0.46
1:C:191:ASP:OD2	1:C:192:ARG:N	2.49	0.46
1:C:227:ARG:O	1:C:228:ALA:C	2.59	0.46
1:C:234:VAL:HG21	1:C:377:PHE:HE2	1.81	0.46
1:A:163:LEU:HD21	1:A:389:TRP:CD2	2.51	0.46
1:B:55:VAL:HG12	1:B:57:LEU:HD13	1.97	0.46
1:B:381:ALA:HB3	1:B:386:LEU:HD13	1.97	0.46
1:A:236:TYR:CD2	1:A:236:TYR:C	2.94	0.45
1:A:297:SER:OG	1:A:320:ARG:HG2	2.15	0.45
1:B:126:TRP:CE3	1:C:178:PRO:HB3	2.51	0.45
1:C:32:MET:HA	1:C:67:ARG:HG3	1.98	0.45
1:C:396:VAL:HG12	1:C:398:LEU:CD1	2.45	0.45
1:A:28:LEU:N	1:A:28:LEU:CD1	2.79	0.45
1:B:277:LEU:C	1:B:279:GLY:H	2.24	0.45
1:C:77:ARG:NE	1:C:113:GLU:OE1	2.49	0.45
1:A:24:ARG:HH11	1:A:24:ARG:HG2	1.82	0.45
1:B:3:ILE:HG23	1:B:3:ILE:O	2.16	0.45
1:B:43:ALA:HB1	1:B:44:PRO:CD	2.43	0.45
1:B:402:GLU:O	1:B:406:LEU:HD13	2.16	0.45
1:C:101:MET:O	1:C:102:ASP:C	2.59	0.45
1:C:198:ARG:HH21	1:C:198:ARG:CB	2.29	0.45
1:D:58:THR:O	1:D:145:SER:HA	2.16	0.45
1:D:211:THR:OG1	1:D:218:VAL:HG22	2.16	0.45
1:B:358:VAL:HG12	1:B:359:ARG:N	2.31	0.45
1:B:406:LEU:HD12	1:B:406:LEU:H	1.81	0.45
1:C:223:PHE:HZ	1:C:315:MET:HG3	1.81	0.45
1:C:375:GLY:HA2	1:C:378:TYR:CZ	2.51	0.45
1:D:55:VAL:CG1	1:D:80:VAL:HG22	2.47	0.45
1:D:402:GLU:O	1:D:403:GLU:C	2.60	0.45
1:C:220:ILE:HG22	1:C:222:THR:CG2	2.46	0.45
1:C:284:ARG:HH21	1:C:288:LEU:HD23	1.82	0.45
1:C:374:LEU:C	1:C:376:GLY:N	2.73	0.45
1:D:139:ALA:HB1	1:D:162:ASP:O	2.16	0.45
1:D:189:TYR:CE2	1:D:194:HIS:HE1	2.34	0.45
1:D:291:VAL:HA	2:D:433:SO4:O1	2.17	0.45
1:A:194:HIS:NE2	1:A:380:HIS:O	2.50	0.45
1:B:171:LEU:HB3	1:B:172:PRO:HD2	1.97	0.45
1:D:191:ASP:OD2	1:D:192:ARG:HG3	2.17	0.45
1:D:224:ALA:CB	1:D:254:ALA:HB2	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4:VAL:HA	1:A:428:GLY:HA2	1.99	0.45
1:A:407:LEU:HD13	1:A:422:LEU:HD21	1.99	0.45
1:B:73:ARG:HH21	1:B:73:ARG:HG3	1.81	0.45
1:B:113:GLU:OE2	1:B:113:GLU:HA	2.17	0.45
1:B:210:LYS:O	1:B:214:GLN:HG2	2.17	0.45
1:C:399:VAL:HG12	1:C:423:ALA:CB	2.46	0.45
1:D:232:LEU:HD11	1:D:249:LEU:HD13	1.97	0.45
1:D:269:SER:O	1:D:273:GLN:HG3	2.17	0.45
1:C:76:TYR:CZ	1:C:78:GLY:HA3	2.52	0.45
1:C:246:PRO:HG2	1:C:248:TYR:HE1	1.82	0.45
1:C:262:PRO:HA	1:C:276:PHE:CZ	2.52	0.45
1:C:420:VAL:CG2	1:C:421:SER:N	2.80	0.45
1:B:201:VAL:O	1:B:205:LEU:HG	2.17	0.45
1:C:43:ALA:HB1	1:C:44:PRO:HD2	1.99	0.45
1:D:10:ARG:HG2	1:D:10:ARG:NH1	2.32	0.45
1:D:85:ALA:HB2	1:D:267:TYR:CE2	2.52	0.45
1:D:215:GLY:O	1:D:305:GLY:HA3	2.16	0.45
1:A:14:GLY:O	1:A:15:SER:C	2.58	0.45
1:B:72:PHE:HE2	1:B:117:HIS:CG	2.34	0.45
1:C:344:GLN:CD	1:C:344:GLN:N	2.69	0.45
1:D:344:GLN:CD	1:D:344:GLN:N	2.75	0.45
1:B:244:ARG:H	1:B:244:ARG:NE	2.15	0.44
1:B:399:VAL:HG12	1:B:423:ALA:HB3	1.98	0.44
1:D:310:LEU:N	1:D:310:LEU:HD12	2.32	0.44
1:A:386:LEU:HD12	1:A:386:LEU:HA	1.88	0.44
1:B:375:GLY:HA2	1:B:378:TYR:CZ	2.51	0.44
1:C:235:LEU:O	1:C:239:GLY:N	2.50	0.44
1:C:291:VAL:CG1	1:C:292:GLU:N	2.80	0.44
1:D:68:LEU:N	1:D:69:PRO:HD2	2.31	0.44
1:D:223:PHE:CZ	1:D:315:MET:HG3	2.53	0.44
1:D:302:ARG:HG2	1:D:302:ARG:NH2	2.30	0.44
1:A:62:LEU:HD13	1:A:93:VAL:HG12	1.99	0.44
1:A:389:TRP:HE3	1:A:390:LEU:HD13	1.82	0.44
1:B:235:LEU:HD13	1:B:247:ILE:HD13	1.99	0.44
1:C:224:ALA:O	1:C:257:VAL:HG21	2.18	0.44
1:D:200:THR:CG2	1:D:374:LEU:HB3	2.48	0.44
1:B:40:ARG:C	1:B:42:HIS:N	2.73	0.44
1:C:168:LYS:HE3	1:C:378:TYR:O	2.17	0.44
1:C:421:SER:C	1:C:422:LEU:HD12	2.42	0.44
1:A:208:LEU:O	1:A:212:LEU:HG	2.18	0.44
1:A:223:PHE:CZ	1:A:315:MET:HE2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:330:SER:O	1:B:368:ARG:HD2	2.18	0.44
1:C:65:VAL:HG11	1:C:90:MET:HG3	1.98	0.44
1:C:101:MET:CE	1:C:104:PRO:HA	2.43	0.44
1:C:191:ASP:OD2	1:C:192:ARG:HG3	2.18	0.44
1:C:302:ARG:HG2	1:C:302:ARG:NH2	2.32	0.44
1:C:359:ARG:NH1	1:C:363:GLU:N	2.65	0.44
1:D:215:GLY:HA2	1:D:306:PRO:HB3	2.00	0.44
1:B:396:VAL:O	1:B:420:VAL:HA	2.18	0.44
1:B:220:ILE:HG22	1:B:222:THR:HG23	1.98	0.44
1:B:221:PRO:HB3	1:B:321:ILE:HG12	2.00	0.44
1:B:325:LEU:HG	1:B:329:LEU:HD22	2.00	0.44
1:A:263:ARG:HH21	1:A:263:ARG:CG	2.31	0.44
1:C:98:LEU:HD13	1:C:98:LEU:O	2.17	0.44
1:C:409:LEU:HD22	1:C:413:LEU:CG	2.46	0.44
1:D:132:LEU:HG	1:D:134:LEU:HD11	1.99	0.44
1:B:207:ILE:O	1:B:211:THR:CG2	2.66	0.44
1:C:81:TYR:HA	1:C:119:ARG:O	2.18	0.44
1:C:226:GLU:HG3	1:C:227:ARG:N	2.31	0.44
1:C:410:GLY:CA	1:C:420:VAL:HG21	2.48	0.44
1:D:1:MET:HE1	1:D:152:GLY:N	2.33	0.44
1:D:182:LEU:HD12	1:D:183:VAL:H	1.82	0.44
1:B:416:ARG:O	1:B:416:ARG:HG2	2.17	0.43
1:C:20:LEU:HD23	1:C:25:ARG:HG2	2.00	0.43
1:B:233:TYR:CE1	1:B:282:PRO:HB2	2.53	0.43
1:C:359:ARG:HH12	1:C:363:GLU:N	2.16	0.43
1:D:87:VAL:HG13	1:D:118:LEU:HD13	1.99	0.43
1:D:221:PRO:HG3	1:D:338:PHE:CE1	2.54	0.43
1:D:236:TYR:N	1:D:285:PRO:HB3	2.34	0.43
1:B:195:ARG:HH11	1:B:195:ARG:HG2	1.83	0.43
1:B:325:LEU:HD12	1:B:325:LEU:HA	1.82	0.43
1:C:219:LEU:HD21	1:C:324:HIS:O	2.18	0.43
1:A:260:LEU:HD12	1:A:263:ARG:HD3	2.01	0.43
1:C:86:THR:HG22	1:C:90:MET:HE2	2.00	0.43
1:C:359:ARG:NH1	1:C:362:GLY:C	2.75	0.43
1:D:191:ASP:CG	1:D:192:ARG:HG3	2.43	0.43
1:C:20:LEU:CD2	1:C:25:ARG:HG2	2.48	0.43
1:D:9:ALA:O	1:D:11:GLU:HG2	2.19	0.43
1:D:85:ALA:HB3	1:D:144:GLY:HA3	2.01	0.43
1:B:98:LEU:HD11	1:B:108:PRO:HB3	2.00	0.43
1:C:235:LEU:CD1	1:C:247:ILE:HG21	2.48	0.43
1:C:284:ARG:HD3	1:C:288:LEU:HD23	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:420:VAL:CG2	1:C:421:SER:H	2.32	0.43
1:D:37:GLU:HA	1:D:37:GLU:OE2	2.19	0.43
1:D:223:PHE:HZ	1:D:315:MET:HG3	1.82	0.43
1:D:73:ARG:NH2	1:D:110:ASP:OD2	2.52	0.43
1:A:85:ALA:HB3	1:A:144:GLY:HA3	2.01	0.43
1:A:167:GLU:HB3	1:A:197:TYR:HB2	2.01	0.43
1:A:407:LEU:O	1:A:410:GLY:N	2.52	0.43
1:B:80:VAL:HB	1:B:118:LEU:HD23	2.00	0.43
1:A:347:LEU:CD1	1:A:358:VAL:HG11	2.49	0.43
1:B:126:TRP:CD2	1:C:178:PRO:HB3	2.53	0.43
1:B:188:THR:OG1	1:B:400:HIS:ND1	2.52	0.43
1:A:177:PRO:HD3	1:A:389:TRP:CE2	2.54	0.43
1:A:197:TYR:O	1:A:201:VAL:HG23	2.19	0.43
1:C:168:LYS:HD3	1:C:230:GLU:OE1	2.19	0.43
1:D:211:THR:O	1:D:214:GLN:HG2	2.18	0.43
1:D:234:VAL:HG13	1:D:238:HIS:HD2	1.83	0.43
1:B:239:GLY:C	1:B:241:ARG:N	2.76	0.42
1:B:318:GLY:HA2	1:B:322:LEU:HD11	1.99	0.42
1:C:374:LEU:O	1:C:376:GLY:N	2.52	0.42
1:D:17:HIS:ND1	1:D:184:LEU:HD21	2.34	0.42
1:C:34:GLN:NE2	1:C:63:ASP:HB3	2.32	0.42
1:C:355:PRO:HG2	1:C:358:VAL:HG22	2.00	0.42
1:D:111:VAL:O	1:D:115:LEU:HG	2.19	0.42
1:D:209:GLU:CG	1:D:243:PRO:HD3	2.49	0.42
1:D:253:MET:C	1:D:255:GLY:N	2.77	0.42
1:D:316:LEU:HB3	1:D:347:LEU:HD23	2.01	0.42
1:A:32:MET:HE2	1:A:105:PHE:HZ	1.84	0.42
1:A:126:TRP:CE3	1:A:135:ALA:HB2	2.55	0.42
1:A:329:LEU:HD12	1:A:329:LEU:HA	1.91	0.42
1:B:9:ALA:C	1:B:11:GLU:H	2.27	0.42
1:D:227:ARG:HH21	1:D:227:ARG:CG	2.32	0.42
1:C:194:HIS:CE1	1:C:378:TYR:HD1	2.37	0.42
1:D:110:ASP:O	1:D:113:GLU:N	2.52	0.42
1:A:31:GLY:HA3	1:A:63:ASP:C	2.44	0.42
1:B:57:LEU:HD22	1:B:80:VAL:CG1	2.50	0.42
1:C:168:LYS:NZ	1:C:377:PHE:O	2.52	0.42
1:C:312:GLY:O	1:C:321:ILE:HG22	2.19	0.42
1:D:49:PRO:HB3	1:D:71:LEU:CD1	2.49	0.42
1:D:182:LEU:HD12	1:D:183:VAL:N	2.34	0.42
1:B:32:MET:HE3	1:B:62:LEU:CD1	2.49	0.42
1:B:185:ALA:O	1:B:399:VAL:HG22	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:19:LEU:HD13	1:C:157:LEU:HD23	2.01	0.42
1:C:59:HIS:CD2	1:C:61:HIS:HB2	2.55	0.42
1:C:386:LEU:O	1:C:390:LEU:HD23	2.20	0.42
1:D:32:MET:HE1	1:D:101:MET:HE1	2.00	0.42
1:D:395:ARG:HD2	1:D:419:GLU:OE2	2.19	0.42
1:B:87:VAL:HG13	1:B:118:LEU:HD13	2.01	0.42
1:C:10:ARG:HG2	1:C:10:ARG:HH11	1.85	0.42
1:C:108:PRO:HD2	1:C:109:GLU:CD	2.45	0.42
1:D:91:GLU:HG3	1:D:115:LEU:CD1	2.49	0.42
1:D:170:VAL:HA	1:D:272:VAL:HG21	2.02	0.42
1:D:291:VAL:HG13	2:D:433:SO4:S	2.60	0.42
1:D:386:LEU:O	1:D:390:LEU:HD23	2.19	0.42
1:B:20:LEU:CD2	1:B:25:ARG:HE	2.32	0.42
1:B:68:LEU:HD11	1:B:72:PHE:HE1	1.85	0.42
1:B:391:GLN:NE2	2:B:433:SO4:O2	2.53	0.42
1:C:1:MET:HG2	1:C:431:VAL:CG2	2.50	0.42
1:C:330:SER:HA	1:C:366:PRO:O	2.20	0.42
1:D:87:VAL:HA	1:D:90:MET:HE3	2.02	0.42
1:D:220:ILE:HG23	1:D:337:VAL:O	2.20	0.42
1:B:194:HIS:NE2	1:B:380:HIS:O	2.52	0.42
1:B:387:LEU:HD13	2:B:448:SO4:O1	2.20	0.42
1:C:143:PRO:HG3	1:C:171:LEU:HD11	2.02	0.42
1:C:190:GLY:HA3	1:C:409:LEU:HB2	2.02	0.42
1:C:402:GLU:HB2	1:C:405:LYS:CG	2.49	0.42
1:C:65:VAL:HG11	1:C:90:MET:CG	2.50	0.42
1:C:330:SER:O	1:C:368:ARG:HD2	2.19	0.42
1:D:281:ASN:C	1:D:283:PHE:H	2.26	0.42
1:A:32:MET:HA	1:A:67:ARG:HG3	2.02	0.41
1:A:41:ASN:HD22	1:A:67:ARG:HD3	1.85	0.41
1:A:147:PHE:HB2	1:A:160:SER:HA	2.02	0.41
1:B:45:PHE:CZ	1:B:70:LYS:HG2	2.54	0.41
1:C:222:THR:HG22	1:C:339:VAL:CG2	2.44	0.41
1:B:359:ARG:HG2	1:B:359:ARG:HH11	1.86	0.41
1:C:32:MET:HG2	1:C:62:LEU:O	2.20	0.41
1:A:178:PRO:HB3	1:D:126:TRP:CE3	2.54	0.41
1:A:277:LEU:HD21	1:D:263:ARG:HG2	2.01	0.41
1:C:140:GLY:O	1:C:164:GLY:HA3	2.20	0.41
1:C:177:PRO:HD3	1:C:389:TRP:NE1	2.35	0.41
1:C:235:LEU:HB2	1:C:285:PRO:HB3	2.02	0.41
1:A:48:ASP:OD2	1:A:51:GLU:HG2	2.20	0.41
1:A:194:HIS:CE1	1:A:378:TYR:HB2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4:VAL:HA	1:B:428:GLY:HA2	2.02	0.41
1:B:88:LEU:HB3	1:B:260:LEU:HD21	2.01	0.41
1:B:236:TYR:HH	1:B:280:LYS:HD3	1.82	0.41
1:C:291:VAL:HG12	1:C:292:GLU:H	1.84	0.41
1:A:37:GLU:OE2	1:A:37:GLU:CA	2.69	0.41
1:A:48:ASP:HA	1:A:49:PRO:HD2	1.95	0.41
1:A:163:LEU:HD12	1:A:163:LEU:HA	1.83	0.41
1:B:312:GLY:HA2	1:B:313:SER:C	2.45	0.41
1:C:195:ARG:O	1:C:196:PRO:C	2.64	0.41
1:D:224:ALA:HB3	1:D:253:MET:HE2	2.02	0.41
1:D:409:LEU:HD22	1:D:413:LEU:CD1	2.50	0.41
1:B:325:LEU:HB3	1:B:360:ILE:HD13	2.02	0.41
1:C:137:GLY:HA3	1:C:147:PHE:CZ	2.56	0.41
1:C:75:GLY:O	1:C:76:TYR:C	2.61	0.41
1:C:77:ARG:HD3	1:C:77:ARG:HA	1.85	0.41
1:C:96:ASP:C	1:C:98:LEU:N	2.77	0.41
1:C:196:PRO:HB2	1:C:199:GLU:HG2	2.02	0.41
1:D:232:LEU:HD23	1:D:235:LEU:HD12	2.03	0.41
1:D:295:GLU:CD	1:D:295:GLU:N	2.73	0.41
1:D:409:LEU:HD22	1:D:413:LEU:CG	2.50	0.41
1:C:9:ALA:C	1:C:11:GLU:N	2.77	0.41
1:C:137:GLY:HA3	1:C:147:PHE:CE1	2.56	0.41
1:D:264:LEU:N	1:D:264:LEU:CD1	2.84	0.41
1:C:68:LEU:HB3	1:C:69:PRO:HD3	2.01	0.41
1:C:182:LEU:HD11	1:C:397:VAL:HG23	2.03	0.41
1:C:375:GLY:HA2	1:C:378:TYR:CE1	2.56	0.41
1:D:17:HIS:CD2	1:D:17:HIS:N	2.88	0.41
1:D:407:LEU:HD13	1:D:407:LEU:HA	1.88	0.41
1:A:277:LEU:C	1:A:279:GLY:H	2.29	0.41
1:B:402:GLU:OE1	1:B:405:LYS:HD2	2.21	0.41
1:B:416:ARG:HG3	2:B:433:SO4:O3	2.21	0.41
1:D:325:LEU:CA	1:D:329:LEU:HD13	2.51	0.41
1:A:126:TRP:CD2	1:D:178:PRO:HB3	2.56	0.40
1:B:2:ARG:CG	5:B:459:HOH:O	2.69	0.40
1:B:132:LEU:HD12	1:B:133:SER:H	1.85	0.40
1:A:229:GLN:CD	1:A:229:GLN:N	2.79	0.40
1:A:56:LEU:C	1:A:57:LEU:HD12	2.46	0.40
1:A:141:HIS:HA	2:A:448:SO4:O2	2.22	0.40
1:A:227:ARG:HH21	1:A:227:ARG:HG2	1.85	0.40
1:A:358:VAL:HG12	1:A:359:ARG:N	2.35	0.40
1:B:72:PHE:HA	1:B:76:TYR:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:244:ARG:H	1:B:244:ARG:CD	2.34	0.40
1:B:290:VAL:O	1:B:290:VAL:HG12	2.20	0.40
1:C:160:SER:OG	1:C:185:ALA:HA	2.21	0.40
1:C:192:ARG:HH11	1:C:192:ARG:HG2	1.87	0.40
1:C:250:ASP:HA	1:C:291:VAL:HB	2.03	0.40
1:C:280:LYS:O	1:C:282:PRO:HD3	2.20	0.40
1:C:402:GLU:O	1:C:406:LEU:HD13	2.21	0.40
1:D:309:VAL:C	1:D:310:LEU:HD12	2.46	0.40
1:A:178:PRO:HB3	1:D:126:TRP:CD2	2.56	0.40
1:C:248:TYR:CE2	1:C:300:LEU:HD21	2.56	0.40
1:B:110:ASP:C	1:B:112:GLU:N	2.79	0.40
1:C:211:THR:HG21	1:C:335:ALA:CB	2.52	0.40
1:C:227:ARG:HH11	1:C:378:TYR:C	2.29	0.40
1:D:11:GLU:O	1:D:400:HIS:HA	2.22	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%)	28 (6%)	1 (0%)	43	62
1	B	429/431 (100%)	387 (90%)	36 (8%)	6 (1%)	9	15
1	C	429/431 (100%)	370 (86%)	54 (13%)	5 (1%)	10	19
1	D	429/431 (100%)	376 (88%)	43 (10%)	10 (2%)	5	8
All	All	1716/1724 (100%)	1533 (89%)	161 (9%)	22 (1%)	9	16

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	240	HIS

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Mol	Chain	Res	Type
1	B	38	GLU
1	B	188	THR
1	B	241	ARG
1	C	375	GLY
1	C	400	HIS
1	D	38	GLU
1	D	226	GLU
1	D	317	ALA
1	D	328	GLY
1	A	15	SER
1	B	15	SER
1	C	102	ASP
1	D	22	GLY
1	D	30	CYS
1	D	282	PRO
1	D	15	SER
1	D	264	LEU
1	D	251	SER
1	B	66	GLY
1	C	196	PRO
1	C	187	GLY

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%)	313 (92%)	29 (8%)	10	18
1	B	342/342 (100%)	312 (91%)	30 (9%)	9	17
1	C	342/342 (100%)	318 (93%)	24 (7%)	14	26
1	D	342/342 (100%)	326 (95%)	16 (5%)	23	43
All	All	1368/1368 (100%)	1269 (93%)	99 (7%)	13	24

All (99) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	SER
1	A	27	LEU
1	A	55	VAL
1	A	65	VAL
1	A	94	LEU
1	A	102	ASP
1	A	142	LEU
1	A	163	LEU
1	A	165	ASN
1	A	171	LEU
1	A	186	GLU
1	A	188	THR
1	A	219	LEU
1	A	229	GLN
1	A	253	MET
1	A	263	ARG
1	A	264	LEU
1	A	280	LYS
1	A	320	ARG
1	A	329	LEU
1	A	336	LEU
1	A	344	GLN
1	A	365	VAL
1	A	386	LEU
1	A	390	LEU
1	A	398	LEU
1	A	406	LEU
1	A	407	LEU
1	A	409	LEU
1	B	12	VAL
1	B	27	LEU
1	B	28	LEU
1	B	57	LEU
1	B	62	LEU
1	B	83	THR
1	B	86	THR
1	B	98	LEU
1	B	109	GLU
1	B	155	ARG
1	B	165	ASN
1	B	171	LEU
1	B	175	SER
1	B	192	ARG

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Mol	Chain	Res	Type
1	B	195	ARG
1	B	211	THR
1	B	213	SER
1	B	219	LEU
1	B	226	GLU
1	B	229	GLN
1	B	244	ARG
1	B	253	MET
1	B	264	LEU
1	B	325	LEU
1	B	329	LEU
1	B	336	LEU
1	B	386	LEU
1	B	390	LEU
1	B	407	LEU
1	B	409	LEU
1	C	27	LEU
1	C	55	VAL
1	C	57	LEU
1	C	109	GLU
1	C	166	ARG
1	C	229	GLN
1	C	256	ARG
1	C	264	LEU
1	C	276	PHE
1	C	278	GLN
1	C	292	GLU
1	C	295	GLU
1	C	320	ARG
1	C	325	LEU
1	C	336	LEU
1	C	342	GLN
1	C	359	ARG
1	C	363	GLU
1	C	364	GLU
1	C	386	LEU
1	C	389	TRP
1	C	398	LEU
1	C	409	LEU
1	C	415	LEU
1	D	13	THR
1	D	27	LEU

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Mol	Chain	Res	Type
1	D	55	VAL
1	D	57	LEU
1	D	96	ASP
1	D	109	GLU
1	D	165	ASN
1	D	171	LEU
1	D	186	GLU
1	D	192	ARG
1	D	229	GLN
1	D	250	ASP
1	D	264	LEU
1	D	265	VAL
1	D	407	LEU
1	D	409	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	GLN
1	A	41	ASN
1	A	59	HIS
1	A	165	ASN
1	A	214	GLN
1	A	229	GLN
1	A	301	ASN
1	A	344	GLN
1	A	383	GLN
1	B	34	GLN
1	B	41	ASN
1	B	42	HIS
1	B	165	ASN
1	B	293	HIS
1	B	383	GLN
1	C	34	GLN
1	C	41	ASN
1	C	42	HIS
1	C	59	HIS
1	C	61	HIS
1	C	165	ASN
1	C	194	HIS
1	C	229	GLN
1	C	238	HIS

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Mol	Chain	Res	Type
1	C	275	HIS
1	C	323	HIS
1	C	342	GLN
1	D	34	GLN
1	D	41	ASN
1	D	59	HIS
1	D	165	ASN
1	D	194	HIS
1	D	214	GLN
1	D	229	GLN
1	D	238	HIS
1	D	301	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 78 ligands modelled in this entry, 8 are monoatomic - leaving 70 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	B	432	-	4,4,4	1.06	0	6,6,6	0.60	0
2	SO4	A	443	-	4,4,4	1.06	0	6,6,6	0.59	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SO4	A	436	-	4,4,4	1.07	0	6,6,6	0.57	0
2	SO4	B	433	-	4,4,4	1.06	0	6,6,6	0.58	0
3	FLC	B	451	-	12,12,12	2.28	5 (41%)	17,17,17	1.17	1 (5%)
2	SO4	B	446	-	4,4,4	1.09	0	6,6,6	0.57	0
2	SO4	D	436	-	4,4,4	1.07	0	6,6,6	0.57	0
2	SO4	A	440	-	4,4,4	1.06	0	6,6,6	0.56	0
2	SO4	C	446	-	4,4,4	1.08	0	6,6,6	0.57	0
2	SO4	A	432	-	4,4,4	1.09	0	6,6,6	0.57	0
2	SO4	C	443	-	4,4,4	1.09	0	6,6,6	0.55	0
2	SO4	A	446	-	4,4,4	1.07	0	6,6,6	0.57	0
2	SO4	D	438	-	4,4,4	1.04	0	6,6,6	0.60	0
2	SO4	A	434	-	4,4,4	1.06	0	6,6,6	0.57	0
2	SO4	C	439	-	4,4,4	1.08	0	6,6,6	0.57	0
2	SO4	A	444	-	4,4,4	1.07	0	6,6,6	0.57	0
2	SO4	C	436	-	4,4,4	1.07	0	6,6,6	0.57	0
2	SO4	C	437	-	4,4,4	1.10	0	6,6,6	0.57	0
2	SO4	D	439	-	4,4,4	1.09	0	6,6,6	0.60	0
2	SO4	A	450	-	4,4,4	1.05	0	6,6,6	0.59	0
2	SO4	B	435	-	4,4,4	1.06	0	6,6,6	0.60	0
2	SO4	A	447	-	4,4,4	1.08	0	6,6,6	0.57	0
2	SO4	A	445	-	4,4,4	1.05	0	6,6,6	0.57	0
2	SO4	A	438	-	4,4,4	1.08	0	6,6,6	0.56	0
2	SO4	B	448	-	4,4,4	1.06	0	6,6,6	0.58	0
2	SO4	A	435	-	4,4,4	1.06	0	6,6,6	0.56	0
2	SO4	B	449	-	4,4,4	1.09	0	6,6,6	0.57	0
2	SO4	D	433	-	4,4,4	1.09	0	6,6,6	0.62	0
2	SO4	C	433	-	4,4,4	1.09	0	6,6,6	0.56	0
3	FLC	A	452	-	12,12,12	1.64	4 (33%)	17,17,17	1.33	1 (5%)
2	SO4	B	439	-	4,4,4	0.99	0	6,6,6	0.63	0
2	SO4	A	448	-	4,4,4	1.07	0	6,6,6	0.59	0
2	SO4	C	448	-	4,4,4	1.10	0	6,6,6	0.57	0
2	SO4	B	441	-	4,4,4	1.07	0	6,6,6	0.58	0
2	SO4	C	450	-	4,4,4	1.07	0	6,6,6	0.58	0
2	SO4	A	449	-	4,4,4	1.10	0	6,6,6	0.53	0
2	SO4	C	444	-	4,4,4	1.09	0	6,6,6	0.57	0
2	SO4	B	442	-	4,4,4	1.07	0	6,6,6	0.56	0
2	SO4	C	447	-	4,4,4	1.06	0	6,6,6	0.58	0
2	SO4	C	434	-	4,4,4	1.07	0	6,6,6	0.57	0
2	SO4	D	435	-	4,4,4	1.07	0	6,6,6	0.57	0
2	SO4	A	439	-	4,4,4	1.06	0	6,6,6	0.56	0
2	SO4	A	441	-	4,4,4	1.04	0	6,6,6	0.61	0
2	SO4	B	444	-	4,4,4	1.08	0	6,6,6	0.57	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SO4	B	434	-	4,4,4	1.09	0	6,6,6	0.58	0
2	SO4	B	445	-	4,4,4	1.06	0	6,6,6	0.57	0
2	SO4	C	432	-	4,4,4	1.08	0	6,6,6	0.57	0
2	SO4	C	440	-	4,4,4	1.09	0	6,6,6	0.59	0
2	SO4	B	436	-	4,4,4	1.08	0	6,6,6	0.57	0
2	SO4	C	435	-	4,4,4	1.07	0	6,6,6	0.59	0
2	SO4	C	449	-	4,4,4	1.09	0	6,6,6	0.57	0
2	SO4	B	450	-	4,4,4	1.07	0	6,6,6	0.58	0
2	SO4	D	437	-	4,4,4	1.09	0	6,6,6	0.55	0
2	SO4	B	447	-	4,4,4	1.07	0	6,6,6	0.57	0
2	SO4	B	440	-	4,4,4	1.10	0	6,6,6	0.54	0
2	SO4	B	443	-	4,4,4	1.09	0	6,6,6	0.60	0
2	SO4	C	442	-	4,4,4	1.07	0	6,6,6	0.57	0
2	SO4	B	437	-	4,4,4	1.06	0	6,6,6	0.59	0
2	SO4	C	441	-	4,4,4	1.07	0	6,6,6	0.59	0
2	SO4	C	445	-	4,4,4	1.07	0	6,6,6	0.56	0
2	SO4	C	438	-	4,4,4	1.10	0	6,6,6	0.57	0
2	SO4	D	434	-	4,4,4	1.10	0	6,6,6	0.57	0
2	SO4	A	451	-	4,4,4	1.09	0	6,6,6	0.62	0
2	SO4	D	432	-	4,4,4	1.07	0	6,6,6	0.59	0
3	FLC	A	453	-	12,12,12	1.69	5 (41%)	17,17,17	1.32	1 (5%)
2	SO4	B	438	-	4,4,4	1.09	0	6,6,6	0.57	0
2	SO4	D	440	-	4,4,4	1.10	0	6,6,6	0.56	0
2	SO4	A	433	-	4,4,4	1.08	0	6,6,6	0.56	0
2	SO4	A	442	-	4,4,4	1.10	0	6,6,6	0.56	0
2	SO4	A	437	-	4,4,4	1.10	0	6,6,6	0.56	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	451	-	-	0/16/16/16	-
3	FLC	A	452	-	-	0/16/16/16	-
3	FLC	A	453	-	-	0/16/16/16	-

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	451	FLC	CB-CBC	-5.62	1.47	1.53
3	A	452	FLC	OA2-CAC	-2.66	1.22	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	451	FLC	OG2-CGC	-2.62	1.22	1.30
3	A	452	FLC	CA-CB	2.52	1.57	1.54
3	A	452	FLC	OG2-CGC	-2.49	1.22	1.30
3	A	453	FLC	OA2-CAC	-2.47	1.22	1.30
3	A	453	FLC	CB-CBC	2.43	1.56	1.53
3	B	451	FLC	CA-CB	2.40	1.56	1.54
3	A	453	FLC	OG2-CGC	-2.40	1.22	1.30
3	A	453	FLC	CA-CB	2.35	1.56	1.54
3	B	451	FLC	OA2-CAC	-2.29	1.23	1.30
3	A	453	FLC	OB1-CBC	2.16	1.28	1.22
3	A	452	FLC	CG-CB	2.03	1.56	1.54
3	B	451	FLC	OB1-CBC	2.01	1.28	1.22

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	452	FLC	OB2-CBC-CB	3.87	120.56	113.14
3	A	453	FLC	OB2-CBC-CB	3.77	120.38	113.14
3	B	451	FLC	OB2-CBC-CB	2.62	118.16	113.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

12 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	433	SO4	3	0
3	B	451	FLC	4	0
2	B	446	SO4	2	0
2	B	448	SO4	2	0
2	D	433	SO4	4	0
3	A	452	FLC	1	0
2	A	448	SO4	1	0
2	B	441	SO4	1	0
2	C	434	SO4	1	0
2	A	441	SO4	1	0
2	B	437	SO4	1	0
3	A	453	FLC	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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%)	-0.29	0 100 100	22, 40, 63, 89	0
1	B	431/431 (100%)	-0.10	3 (0%) 84 84	22, 43, 74, 93	0
1	C	431/431 (100%)	0.51	25 (5%) 29 28	26, 72, 125, 136	0
1	D	431/431 (100%)	0.82	58 (13%) 7 6	34, 75, 147, 153	0
All	All	1724/1724 (100%)	0.23	86 (4%) 34 34	22, 51, 129, 153	0

All (86) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	311	ALA	4.0
1	C	352	ILE	4.0
1	D	362	GLY	3.9
1	D	316	LEU	3.7
1	D	208	LEU	3.7
1	D	336	LEU	3.7
1	D	339	VAL	3.7
1	D	374	LEU	3.4
1	D	338	PHE	3.4
1	D	322	LEU	3.4
1	D	249	LEU	3.3
1	D	310	LEU	3.2
1	D	340	GLY	3.2
1	D	361	LEU	3.2
1	D	245	ALA	3.1
1	D	225	VAL	3.1
1	D	375	GLY	3.1
1	D	360	ILE	3.1
1	D	212	LEU	3.0
1	D	211	THR	3.0
1	D	221	PRO	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	314	GLY	2.9
1	D	326	LYS	2.9
1	D	329	LEU	2.9
1	D	353	ALA	2.8
1	D	308	VAL	2.8
1	D	324	HIS	2.8
1	C	289	GLU	2.8
1	B	35	GLY	2.8
1	C	208	LEU	2.7
1	C	335	ALA	2.7
1	D	218	VAL	2.7
1	D	250	ASP	2.6
1	D	219	LEU	2.6
1	C	283	PHE	2.6
1	C	205	LEU	2.5
1	C	232	LEU	2.5
1	D	364	GLU	2.5
1	D	358	VAL	2.5
1	C	242	LEU	2.5
1	D	320	ARG	2.5
1	C	340	GLY	2.5
1	D	341	TYR	2.5
1	D	242	LEU	2.4
1	C	265	VAL	2.4
1	C	322	LEU	2.4
1	D	98	LEU	2.4
1	D	205	LEU	2.4
1	D	325	LEU	2.4
1	D	207	ILE	2.4
1	C	300	LEU	2.3
1	C	314	GLY	2.3
1	C	275	HIS	2.3
1	D	294	THR	2.3
1	C	216	GLY	2.3
1	D	351	ILE	2.2
1	D	210	LYS	2.2
1	C	197	TYR	2.2
1	C	309	VAL	2.2
1	B	37	GLU	2.2
1	C	219	LEU	2.2
1	C	308	VAL	2.2
1	D	373	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	356	PRO	2.2
1	D	347	LEU	2.2
1	D	352	ILE	2.2
1	B	60	ALA	2.2
1	D	335	ALA	2.2
1	D	197	TYR	2.2
1	C	280	LYS	2.2
1	D	321	ILE	2.1
1	D	220	ILE	2.1
1	D	337	VAL	2.1
1	C	204	PHE	2.1
1	D	228	ALA	2.1
1	D	246	PRO	2.1
1	D	366	PRO	2.1
1	C	276	PHE	2.1
1	D	295	GLU	2.1
1	D	283	PHE	2.1
1	D	302	ARG	2.0
1	C	246	PRO	2.0
1	C	277	LEU	2.0
1	C	336	LEU	2.0
1	D	247	ILE	2.0
1	D	201	VAL	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.

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SO4	C	434	5/5	0.36	0.14	146,146,147,147	0
2	SO4	D	434	5/5	0.40	0.17	163,163,164,164	0
2	SO4	B	433	5/5	0.53	0.17	171,171,171,171	0
2	SO4	D	436	5/5	0.53	0.13	170,170,170,170	0
2	SO4	C	447	5/5	0.55	0.10	153,154,154,154	0
2	SO4	C	433	5/5	0.55	0.10	141,141,141,141	0
2	SO4	B	448	5/5	0.55	0.20	178,178,178,178	0
2	SO4	C	442	5/5	0.56	0.12	139,140,140,140	0
2	SO4	B	436	5/5	0.59	0.15	148,148,149,149	0
2	SO4	C	438	5/5	0.59	0.13	138,138,139,139	0
2	SO4	A	437	5/5	0.61	0.12	148,148,149,149	0
2	SO4	A	435	5/5	0.61	0.11	142,142,143,143	0
2	SO4	C	445	5/5	0.61	0.12	162,162,163,163	0
2	SO4	C	444	5/5	0.64	0.13	118,118,118,118	0
3	FLC	A	452	13/13	0.66	0.19	108,111,112,112	0
2	SO4	B	450	5/5	0.67	0.15	137,137,138,138	0
2	SO4	D	435	5/5	0.67	0.12	126,127,127,127	0
2	SO4	B	434	5/5	0.67	0.12	136,136,136,137	0
2	SO4	D	433	5/5	0.67	0.10	156,157,158,158	0
2	SO4	A	433	5/5	0.68	0.11	121,121,122,122	0
2	SO4	A	442	5/5	0.69	0.20	141,141,141,142	0
2	SO4	B	444	5/5	0.69	0.10	124,124,124,124	0
2	SO4	C	432	5/5	0.69	0.11	131,131,132,132	0
2	SO4	A	446	5/5	0.70	0.17	113,114,114,114	0
2	SO4	A	436	5/5	0.70	0.09	131,131,131,131	0
2	SO4	C	441	5/5	0.72	0.16	147,147,147,147	0
2	SO4	C	436	5/5	0.72	0.11	139,139,139,139	0
2	SO4	A	450	5/5	0.73	0.13	145,145,145,145	0
2	SO4	C	446	5/5	0.73	0.12	119,120,120,120	0
2	SO4	C	437	5/5	0.73	0.12	133,134,134,134	0
2	SO4	A	447	5/5	0.73	0.11	125,126,126,126	0
2	SO4	A	434	5/5	0.74	0.08	117,117,117,118	0
2	SO4	B	437	5/5	0.75	0.23	169,169,170,170	0
2	SO4	B	446	5/5	0.75	0.12	154,154,155,155	0
2	SO4	B	438	5/5	0.75	0.12	110,110,111,111	0
2	SO4	A	438	5/5	0.76	0.17	130,130,131,131	0
3	FLC	A	453	13/13	0.76	0.17	122,123,124,124	0
2	SO4	D	437	5/5	0.77	0.12	109,110,110,110	0
2	SO4	D	438	5/5	0.77	0.13	110,110,111,111	0
2	SO4	B	445	5/5	0.77	0.08	114,115,115,115	0
2	SO4	C	449	5/5	0.77	0.12	114,114,114,115	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SO4	B	441	5/5	0.78	0.11	117,118,119,119	0
2	SO4	B	435	5/5	0.79	0.14	101,101,102,103	0
2	SO4	A	439	5/5	0.81	0.14	91,92,92,93	0
2	SO4	C	450	5/5	0.81	0.09	116,116,116,116	0
2	SO4	A	443	5/5	0.82	0.12	123,124,124,124	0
2	SO4	B	442	5/5	0.83	0.13	121,122,123,123	0
2	SO4	C	443	5/5	0.83	0.08	102,102,103,103	0
4	ZN	A	455	1/1	0.83	0.13	88,88,88,88	0
2	SO4	A	432	5/5	0.84	0.13	103,103,104,104	0
2	SO4	A	448	5/5	0.85	0.22	135,135,136,136	0
2	SO4	B	449	5/5	0.86	0.13	98,98,99,99	0
2	SO4	A	445	5/5	0.86	0.10	101,102,103,103	0
2	SO4	C	448	5/5	0.87	0.09	97,97,98,98	0
2	SO4	A	444	5/5	0.87	0.12	111,111,111,111	0
2	SO4	B	447	5/5	0.87	0.12	121,121,121,121	0
2	SO4	B	432	5/5	0.88	0.10	76,77,79,79	0
4	ZN	C	452	1/1	0.88	0.12	125,125,125,125	0
2	SO4	B	440	5/5	0.90	0.11	81,81,82,83	0
2	SO4	C	439	5/5	0.90	0.09	105,105,105,105	0
4	ZN	B	453	1/1	0.91	0.10	88,88,88,88	0
4	ZN	B	452	1/1	0.91	0.12	74,74,74,74	0
4	ZN	D	442	1/1	0.91	0.11	121,121,121,121	0
3	FLC	B	451	13/13	0.92	0.13	68,70,79,80	0
2	SO4	D	432	5/5	0.92	0.09	80,80,81,82	0
2	SO4	D	439	5/5	0.92	0.08	67,67,68,69	0
2	SO4	A	440	5/5	0.93	0.07	81,81,82,82	0
2	SO4	C	440	5/5	0.93	0.11	87,87,88,88	0
2	SO4	B	443	5/5	0.93	0.09	57,59,60,61	0
2	SO4	C	435	5/5	0.93	0.10	71,72,73,73	0
2	SO4	D	440	5/5	0.94	0.06	85,85,85,86	0
2	SO4	A	449	5/5	0.95	0.10	48,49,52,53	0
4	ZN	C	451	1/1	0.95	0.08	82,82,82,82	0
2	SO4	A	451	5/5	0.96	0.08	56,58,60,62	0
4	ZN	A	454	1/1	0.96	0.07	72,72,72,72	0
2	SO4	B	439	5/5	0.97	0.07	45,45,49,49	0
4	ZN	D	441	1/1	0.97	0.11	98,98,98,98	0
2	SO4	A	441	5/5	0.97	0.06	43,45,48,49	0

6.5 Other polymers ⓘ

There are no such residues in this entry.