Full wwPDB X-ray Structure Validation Report ⓘ

Oct 24, 2023 – 11:30 AM EDT

PDB ID	:	3A4Y
Title	:	Crystal Structure of H61A 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:

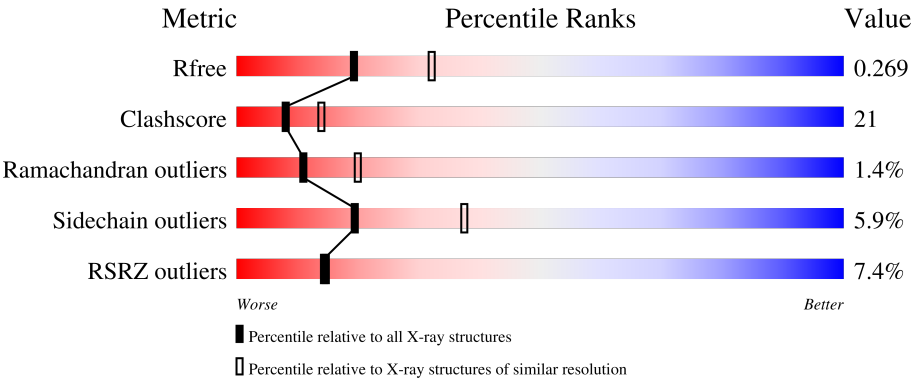
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (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 <=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	2% 68% 29% ·
1	B	431	2% 68% 28% ·
1	C	431	11% 54% 43% ·
1	D	431	15% 54% 44% ·

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	436	-	-	-	X
3	FLC	B	447	-	-	-	X

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 13743 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.

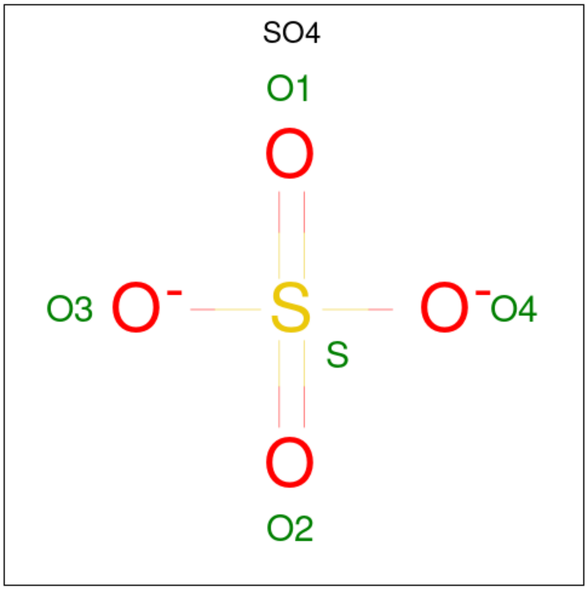
- Molecule 1 is a protein called Ribonuclease TTHA0252.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	431	Total	C	N	O	S	0	0	0
			3321	2124	595	594	8			
1	B	431	Total	C	N	O	S	0	0	0
			3321	2124	595	594	8			
1	C	431	Total	C	N	O	S	0	0	0
			3321	2124	595	594	8			
1	D	431	Total	C	N	O	S	0	0	0
			3321	2124	595	594	8			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	61	ALA	HIS	engineered mutation	UNP Q5SLP1
B	61	ALA	HIS	engineered mutation	UNP Q5SLP1
C	61	ALA	HIS	engineered mutation	UNP Q5SLP1
D	61	ALA	HIS	engineered mutation	UNP Q5SLP1

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

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

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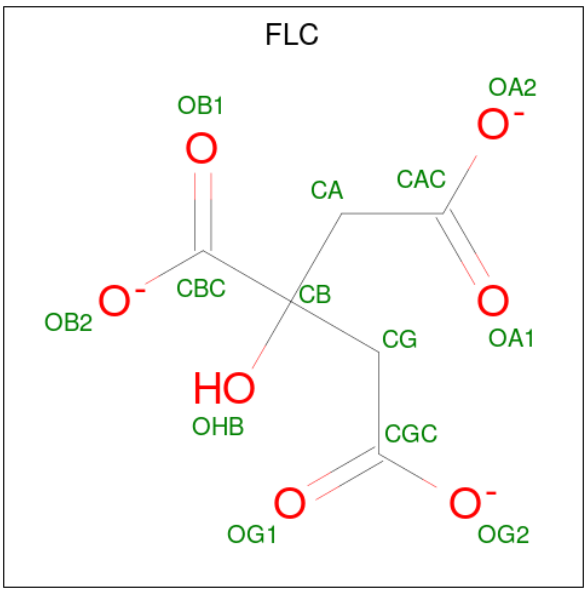
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0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

- Molecule 3 is CITRATE ANION (three-letter code: FLC) (formula: $C_6H_5O_7$).



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

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

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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	50	Total O 50 50	0	0
5	B	54	Total O 54 54	0	0

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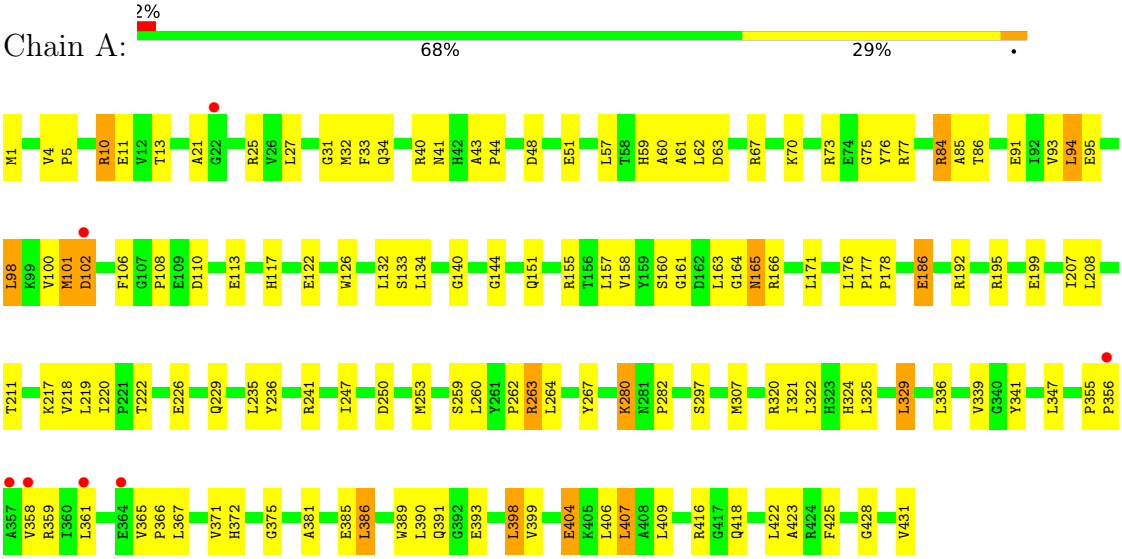
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	17	Total O 17 17	0	0
5	D	15	Total O 15 15	0	0

3 Residue-property plots (i)

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.

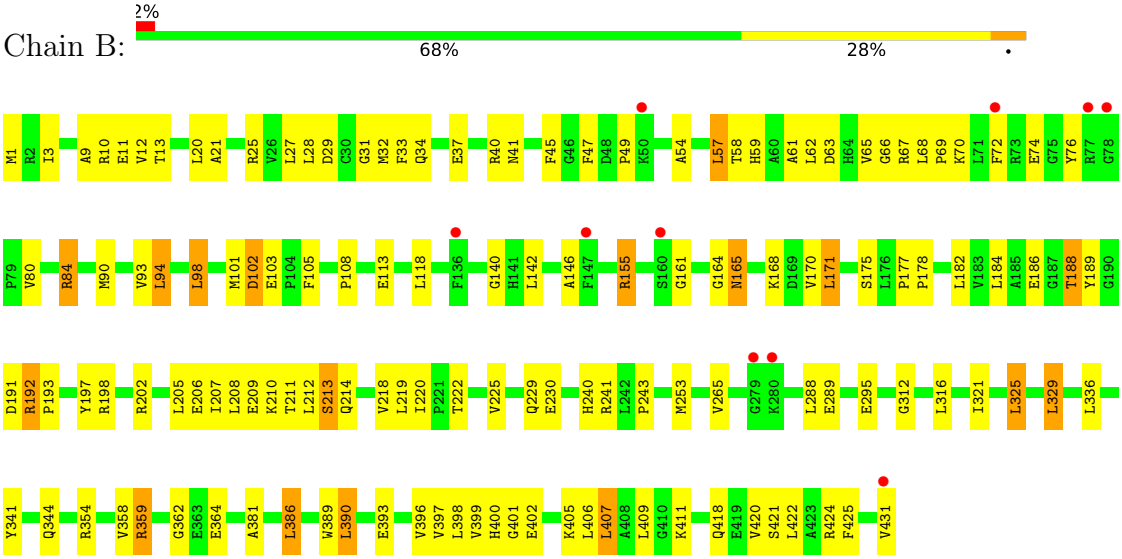
• Molecule 1: Ribonuclease TTHA0252

Chain A:



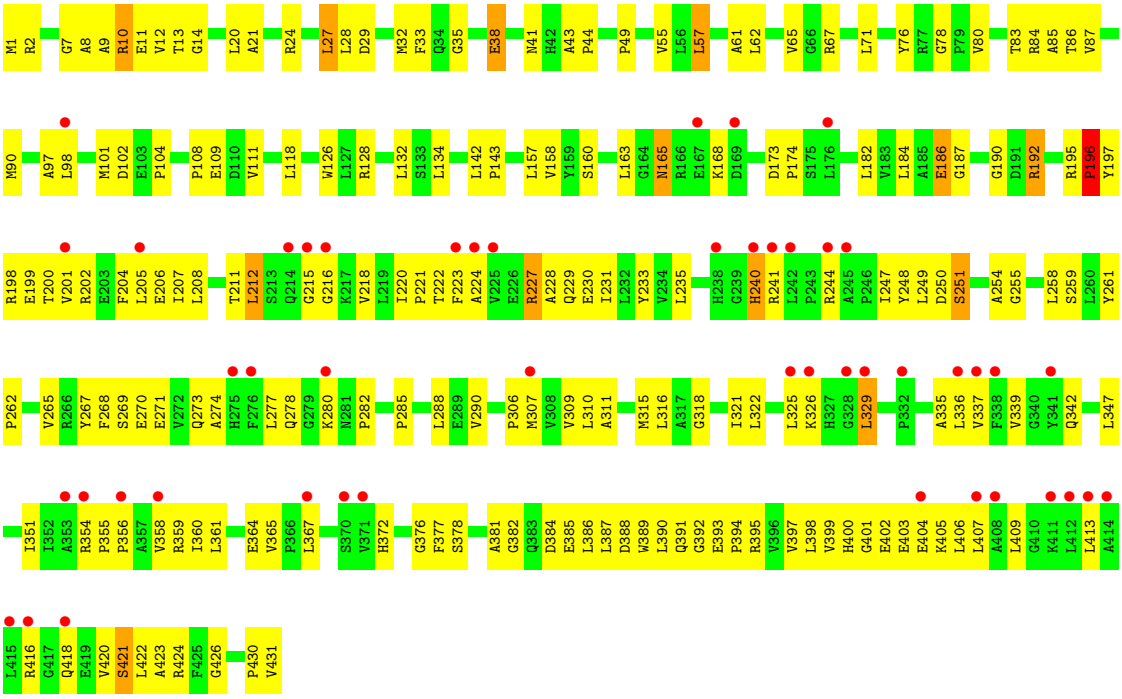
• Molecule 1: Ribonuclease TTHA0252

Chain B:



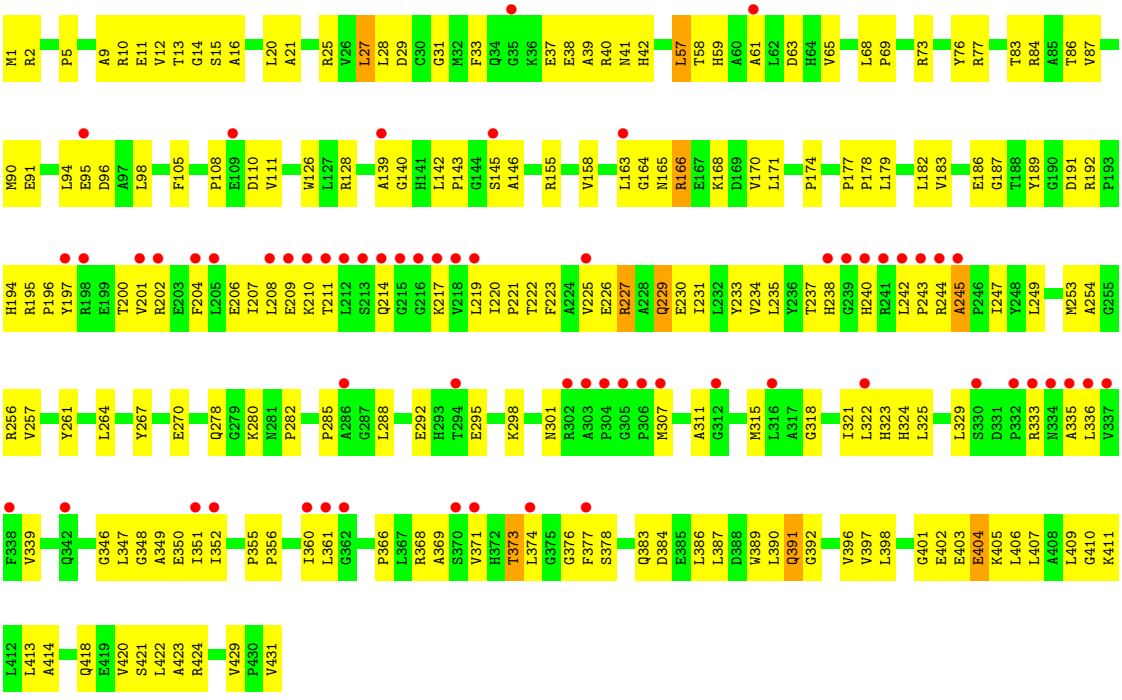
• Molecule 1: Ribonuclease TTHA0252

Chain C:



• Molecule 1: Ribonuclease TTHA0252

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	143.14Å 146.77Å 121.12Å 90.00° 109.24° 90.00°	Depositor
Resolution (Å)	50.00 – 2.50 39.18 – 2.50	Depositor EDS
% Data completeness (in resolution range)	96.4 (50.00-2.50) 96.3 (39.18-2.50)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.93 (at 2.51Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.239 , 0.282 0.227 , 0.269	Depositor DCC
R_{free} test set	8161 reflections (10.01%)	wwPDB-VP
Wilson B-factor (Å^2)	51.2	Xtriage
Anisotropy	0.105	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 45.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	13743	wwPDB-VP
Average B, all atoms (Å^2)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.79% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: ZN, SO4, 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	0.41	0/3401	0.67	1/4613 (0.0%)
1	B	0.39	0/3401	0.69	1/4613 (0.0%)
1	C	0.33	0/3401	0.59	0/4613
1	D	0.32	0/3401	0.58	0/4613
All	All	0.37	0/13604	0.64	2/18452 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	161	GLY	N-CA-C	-6.41	97.08	113.10
1	A	161	GLY	N-CA-C	-5.54	99.26	113.10

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	3321	0	3349	113	0
1	B	3321	0	3349	132	0
1	C	3321	0	3349	177	0
1	D	3321	0	3349	161	0
2	A	95	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	75	0	0	0	0
2	C	65	0	0	0	0
2	D	45	0	0	2	0
3	A	13	0	5	0	0
3	B	13	0	5	1	0
3	C	13	0	5	1	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	50	0	0	2	0
5	B	54	0	0	3	0
5	C	17	0	0	0	0
5	D	15	0	0	1	0
All	All	13743	0	13411	576	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 21.

All (576) 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:B:37:GLU:HG3	1:B:40:ARG:HH11	1.11	1.09
1:C:391:GLN:HA	1:C:416:ARG:HH12	1.22	1.04
1:D:211:THR:HG21	1:D:335:ALA:HB2	1.40	1.01
1:D:285:PRO:HD2	1:D:288:LEU:HD22	1.39	1.00
1:B:192:ARG:HG3	1:B:192:ARG:HH11	1.26	0.99
1:A:263:ARG:HH11	1:A:263:ARG:HB3	1.26	0.98
1:C:33:PHE:H	1:C:41:ASN:HD21	1.06	0.98
1:B:37:GLU:HG3	1:B:40:ARG:NH1	1.78	0.97
1:A:160:SER:HB2	1:A:163:LEU:HD21	1.44	0.95
1:C:160:SER:HB2	1:C:163:LEU:HD21	1.50	0.94
1:B:10:ARG:HH12	1:B:424:ARG:HG2	1.29	0.93
1:D:37:GLU:HB3	1:D:40:ARG:HH11	1.34	0.92
1:C:391:GLN:HA	1:C:416:ARG:NH1	1.85	0.90
1:D:91:GLU:O	1:D:95:GLU:HG2	1.71	0.90
1:D:33:PHE:H	1:D:41:ASN:HD21	1.18	0.90
1:C:98:LEU:HD11	1:C:108:PRO:HA	1.54	0.90
1:D:253:MET:HA	1:D:256:ARG:NH2	1.88	0.89
1:A:33:PHE:H	1:A:41:ASN:HD21	1.17	0.87
1:B:37:GLU:CG	1:B:40:ARG:HH11	1.87	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:98:LEU:HD11	1:B:108:PRO:HA	1.59	0.84
1:C:315:MET:HA	1:C:342:GLN:HE22	1.43	0.84
1:B:33:PHE:H	1:B:41:ASN:HD21	1.25	0.83
1:A:132:LEU:HG	1:A:134:LEU:HD11	1.60	0.83
1:D:10:ARG:NH2	1:D:424:ARG:HH11	1.76	0.82
1:D:12:VAL:HG12	1:D:401:GLY:HA2	1.61	0.82
1:A:235:LEU:HD13	1:A:247:ILE:HD13	1.62	0.80
1:A:34:GLN:HE21	1:A:63:ASP:HB3	1.46	0.80
1:D:360:ILE:HG22	1:D:361:LEU:HD13	1.65	0.79
1:D:398:LEU:HD21	1:D:409:LEU:HD12	1.64	0.79
1:A:25:ARG:HD2	1:A:51:GLU:O	1.82	0.78
1:A:34:GLN:NE2	1:A:63:ASP:HB3	1.99	0.78
1:B:9:ALA:O	1:B:11:GLU:HG2	1.84	0.77
1:B:10:ARG:NH1	1:B:424:ARG:HG2	1.99	0.77
1:C:205:LEU:HD13	1:C:241:ARG:HH21	1.50	0.77
1:C:98:LEU:HD12	1:C:111:VAL:HG21	1.66	0.77
1:B:10:ARG:HH12	1:B:424:ARG:CG	1.98	0.76
1:D:253:MET:HA	1:D:256:ARG:HH21	1.49	0.76
1:D:76:TYR:O	1:D:77:ARG:HD2	1.85	0.76
1:A:1:MET:HG2	1:A:431:VAL:HG21	1.67	0.76
1:A:263:ARG:HH11	1:A:263:ARG:CB	1.99	0.75
1:C:285:PRO:HD2	1:C:288:LEU:HD22	1.68	0.75
1:A:208:LEU:HD23	1:A:218:VAL:HG21	1.69	0.73
1:D:37:GLU:HB3	1:D:40:ARG:NH1	2.02	0.73
1:B:84:ARG:HG2	1:B:84:ARG:HH21	1.53	0.73
1:B:45:PHE:HB3	1:B:47:PHE:CE1	2.23	0.72
1:C:168:LYS:HE2	1:C:230:GLU:OE1	1.88	0.72
1:C:165:ASN:HB3	1:C:168:LYS:HD2	1.71	0.72
1:B:398:LEU:N	1:B:398:LEU:HD12	2.04	0.72
1:C:87:VAL:HG13	1:C:118:LEU:HD12	1.72	0.71
1:C:220:ILE:HB	1:C:310:LEU:HD23	1.70	0.71
1:B:168:LYS:HG2	1:B:197:TYR:CD2	2.26	0.71
1:C:212:LEU:HD23	1:C:212:LEU:H	1.54	0.71
1:A:84:ARG:HH11	1:A:84:ARG:HG3	1.55	0.70
1:C:381:ALA:HB1	1:C:385:GLU:HB2	1.71	0.70
1:B:192:ARG:HG3	1:B:192:ARG:NH1	1.98	0.70
1:C:201:VAL:O	1:C:205:LEU:HG	1.91	0.70
1:B:1:MET:HG3	1:B:21:ALA:HB2	1.72	0.70
1:D:37:GLU:CB	1:D:40:ARG:HH11	2.04	0.70
1:C:57:LEU:HD23	1:C:90:MET:CE	2.22	0.69
1:D:329:LEU:HD11	1:D:336:LEU:HD12	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1:MET:HG3	1:C:21:ALA:HB2	1.75	0.69
1:B:359:ARG:HH12	1:B:362:GLY:HA2	1.58	0.69
1:C:221:PRO:HB3	1:C:321:ILE:HG12	1.75	0.69
1:B:208:LEU:HD23	1:B:218:VAL:HG21	1.74	0.68
1:C:86:THR:HG22	1:C:90:MET:HE3	1.74	0.68
1:D:325:LEU:HA	1:D:329:LEU:HD13	1.76	0.68
1:C:57:LEU:HD23	1:C:90:MET:HE1	1.76	0.68
1:C:57:LEU:HG	1:C:65:VAL:HG12	1.76	0.68
1:C:222:THR:HG22	1:C:339:VAL:HG21	1.76	0.67
1:C:87:VAL:HG13	1:C:118:LEU:CD1	2.24	0.67
1:C:98:LEU:O	1:C:98:LEU:HD23	1.93	0.67
1:B:57:LEU:HG	1:B:65:VAL:HG12	1.76	0.67
1:A:76:TYR:O	1:A:77:ARG:HD2	1.94	0.66
1:A:166:ARG:HG2	1:A:385:GLU:OE2	1.96	0.66
1:B:182:LEU:HD11	1:B:397:VAL:HG23	1.77	0.66
1:C:220:ILE:HG22	1:C:222:THR:HG23	1.76	0.66
1:B:421:SER:C	1:B:422:LEU:HD12	2.16	0.66
1:B:381:ALA:HB3	1:B:386:LEU:HD13	1.78	0.65
1:B:295:GLU:OE2	1:B:295:GLU:N	2.27	0.65
1:C:33:PHE:H	1:C:41:ASN:ND2	1.87	0.65
1:C:231:ILE:O	1:C:235:LEU:HG	1.95	0.65
1:D:298:LYS:HA	1:D:301:ASN:ND2	2.12	0.65
1:B:37:GLU:HG3	1:B:40:ARG:CZ	2.25	0.65
1:A:132:LEU:HG	1:A:134:LEU:CD1	2.28	0.64
1:C:9:ALA:O	1:C:11:GLU:HG2	1.98	0.64
1:A:48:ASP:OD2	1:A:51:GLU:HG2	1.97	0.64
1:A:207:ILE:O	1:A:211:THR:HG23	1.97	0.64
1:D:200:THR:HG21	1:D:376:GLY:HA3	1.79	0.63
1:D:204:PHE:CE1	1:D:208:LEU:HD11	2.33	0.63
1:C:7:GLY:HA3	1:C:14:GLY:O	1.98	0.63
1:D:2:ARG:HG3	2:D:435:SO4:O3	1.98	0.63
1:B:37:GLU:HG3	1:B:40:ARG:HE	1.62	0.63
1:A:62:LEU:HD13	1:A:93:VAL:HG12	1.79	0.63
1:C:318:GLY:HA2	1:C:322:LEU:CD1	2.29	0.63
1:D:397:VAL:HG21	1:D:429:VAL:HG11	1.80	0.63
1:A:260:LEU:HD12	1:A:263:ARG:HD3	1.81	0.62
1:C:215:GLY:HA2	1:C:306:PRO:HD3	1.79	0.62
1:D:10:ARG:NH1	1:D:422:LEU:HB3	2.14	0.62
1:A:133:SER:C	1:A:134:LEU:HD12	2.18	0.62
1:C:208:LEU:C	1:C:212:LEU:HD21	2.20	0.62
1:B:295:GLU:H	1:B:295:GLU:CD	2.01	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:204:PHE:O	1:C:208:LEU:HD23	1.99	0.62
1:C:318:GLY:HA2	1:C:322:LEU:HD12	1.81	0.62
1:A:177:PRO:HD3	1:A:389:TRP:CE2	2.34	0.62
1:C:398:LEU:HD21	1:C:409:LEU:HD22	1.82	0.62
1:D:355:PRO:HB2	1:D:356:PRO:HD2	1.82	0.62
1:C:227:ARG:HH12	1:C:378:SER:HA	1.65	0.61
1:C:360:ILE:HG22	1:C:361:LEU:HD13	1.82	0.61
1:B:68:LEU:N	1:B:69:PRO:HD2	2.15	0.61
1:C:399:VAL:HG12	1:C:423:ALA:HB3	1.81	0.61
1:B:102:ASP:CG	1:B:103:GLU:H	2.01	0.61
1:C:316:LEU:HD13	1:C:347:LEU:HD22	1.82	0.61
1:B:208:LEU:HD21	1:B:218:VAL:HG11	1.82	0.61
1:D:168:LYS:HE2	1:D:230:GLU:OE1	2.00	0.61
1:B:59:HIS:HD2	1:B:142:LEU:HD22	1.66	0.61
1:B:401:GLY:CA	1:B:406:LEU:HD11	2.29	0.61
1:D:402:GLU:HB2	1:D:405:LYS:HG2	1.82	0.61
1:A:85:ALA:HB2	1:A:267:TYR:CD2	2.36	0.61
1:A:416:ARG:HD2	5:A:500:HOH:O	2.00	0.61
1:C:420:VAL:O	1:C:421:SER:HB3	2.01	0.61
1:A:100:VAL:O	1:A:101:MET:HB2	2.01	0.60
1:B:401:GLY:HA3	1:B:406:LEU:HD11	1.82	0.60
1:B:406:LEU:N	1:B:406:LEU:HD12	2.16	0.60
1:C:231:ILE:HG21	1:C:310:LEU:HD21	1.82	0.60
1:C:358:VAL:O	1:C:365:VAL:HG12	2.01	0.60
1:C:403:GLU:O	1:C:407:LEU:HD23	2.01	0.60
1:C:200:THR:HG21	1:C:376:GLY:HA3	1.83	0.60
1:D:128:ARG:HD2	5:D:445:HOH:O	2.00	0.60
1:D:249:LEU:HD11	1:D:254:ALA:HB3	1.82	0.60
1:A:91:GLU:O	1:A:95:GLU:HG2	2.02	0.60
1:B:62:LEU:HD13	1:B:93:VAL:HG12	1.83	0.60
1:D:182:LEU:HD23	1:D:431:VAL:HG22	1.83	0.60
1:B:37:GLU:HG3	1:B:40:ARG:NE	2.16	0.60
1:B:398:LEU:N	1:B:398:LEU:CD1	2.65	0.60
1:C:197:TYR:O	1:C:201:VAL:HG23	2.01	0.60
1:D:13:THR:HB	1:D:33:PHE:HA	1.83	0.60
1:D:155:ARG:HD3	1:D:431:VAL:O	2.01	0.60
1:C:321:ILE:O	1:C:325:LEU:HD13	2.01	0.60
1:D:386:LEU:O	1:D:390:LEU:HD23	2.02	0.60
1:A:1:MET:HG2	1:A:431:VAL:CG2	2.32	0.59
1:C:211:THR:HG21	1:C:335:ALA:HB2	1.83	0.59
1:A:62:LEU:HD13	1:A:93:VAL:CG1	2.31	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:398:LEU:HB3	1:A:406:LEU:HG	1.84	0.59
1:C:165:ASN:HB3	1:C:168:LYS:CD	2.32	0.59
1:D:229:GLN:HG3	1:D:261:TYR:CZ	2.38	0.59
1:A:10:ARG:HG2	1:A:10:ARG:HH11	1.68	0.59
1:B:401:GLY:C	1:B:406:LEU:HD11	2.22	0.59
1:D:318:GLY:HA2	1:D:322:LEU:HD11	1.84	0.59
1:D:86:THR:O	1:D:90:MET:HB2	2.02	0.59
1:D:220:ILE:HG22	1:D:222:THR:HG23	1.84	0.59
1:D:285:PRO:HG2	1:D:288:LEU:HB2	1.84	0.59
1:C:33:PHE:N	1:C:41:ASN:HD21	1.89	0.58
1:A:259:SER:O	1:A:262:PRO:HD2	2.03	0.58
1:A:329:LEU:HG	1:A:367:LEU:HD13	1.85	0.58
1:A:4:VAL:HG22	1:A:428:GLY:HA3	1.86	0.58
1:B:207:ILE:O	1:B:211:THR:HG23	2.02	0.58
1:A:85:ALA:HB3	1:A:144:GLY:HA3	1.85	0.58
1:C:235:LEU:HD13	1:C:247:ILE:HD13	1.84	0.58
1:D:10:ARG:CZ	1:D:424:ARG:HG2	2.34	0.57
1:D:233:TYR:O	1:D:237:THR:HG23	2.04	0.57
1:D:403:GLU:O	1:D:407:LEU:HD13	2.03	0.57
1:D:12:VAL:HG12	1:D:401:GLY:CA	2.34	0.57
1:A:236:TYR:OH	1:A:280:LYS:HD3	2.04	0.57
1:A:329:LEU:HD11	1:A:336:LEU:HD12	1.87	0.57
1:C:83:THR:O	1:C:87:VAL:HG23	2.05	0.57
1:B:208:LEU:CD2	1:B:218:VAL:HG11	2.34	0.57
1:C:354:ARG:HA	1:C:367:LEU:HD21	1.87	0.57
1:A:85:ALA:HB2	1:A:267:TYR:CE2	2.40	0.57
1:D:197:TYR:O	1:D:201:VAL:HG23	2.05	0.57
1:D:98:LEU:HD11	1:D:108:PRO:HB3	1.86	0.57
1:D:191:ASP:CG	1:D:405:LYS:HD2	2.25	0.57
1:D:219:LEU:HD12	1:D:219:LEU:N	2.20	0.56
1:A:33:PHE:H	1:A:41:ASN:ND2	1.94	0.56
1:D:58:THR:O	1:D:145:SER:HA	2.05	0.56
1:C:160:SER:HB2	1:C:163:LEU:CD2	2.32	0.56
1:C:142:LEU:HG	1:C:143:PRO:HD2	1.88	0.56
1:D:163:LEU:HD11	1:D:389:TRP:CD2	2.41	0.56
1:D:221:PRO:HA	1:D:311:ALA:O	2.05	0.56
1:A:163:LEU:N	1:A:163:LEU:HD22	2.21	0.56
1:B:11:GLU:HB2	5:B:483:HOH:O	2.06	0.56
1:B:359:ARG:NH1	1:B:362:GLY:HA2	2.21	0.56
1:C:221:PRO:HA	1:C:311:ALA:O	2.05	0.55
1:D:404:GLU:H	1:D:404:GLU:CD	2.08	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:43:ALA:HB1	1:C:44:PRO:HD2	1.88	0.55
1:D:348:GLY:O	1:D:352:ILE:HG13	2.07	0.55
1:D:384:ASP:HA	1:D:387:LEU:HD12	1.87	0.55
1:B:90:MET:HE3	1:B:118:LEU:HD13	1.89	0.55
1:C:132:LEU:HG	1:C:134:LEU:HD11	1.89	0.55
1:D:219:LEU:HD21	1:D:324:HIS:O	2.06	0.55
1:B:70:LYS:NZ	1:B:74:GLU:OE1	2.34	0.55
1:B:168:LYS:HE2	1:B:230:GLU:OE1	2.06	0.55
1:C:1:MET:HG3	1:C:21:ALA:CB	2.37	0.55
1:D:83:THR:O	1:D:87:VAL:HG23	2.07	0.55
1:C:199:GLU:HA	1:C:202:ARG:HD3	1.89	0.55
1:C:101:MET:CE	1:C:104:PRO:HA	2.37	0.55
1:B:425:PHE:HZ	5:B:489:HOH:O	1.89	0.54
1:A:195:ARG:HE	1:A:199:GLU:HG3	1.72	0.54
1:B:98:LEU:HD11	1:B:108:PRO:CA	2.35	0.54
1:A:113:GLU:OE2	1:A:117:HIS:HE1	1.90	0.54
1:B:396:VAL:HG12	1:B:398:LEU:HD12	1.90	0.54
1:D:209:GLU:HG2	1:D:243:PRO:HD2	1.88	0.54
1:D:295:GLU:H	1:D:295:GLU:CD	2.11	0.54
1:A:4:VAL:HG22	1:A:428:GLY:CA	2.38	0.53
1:B:398:LEU:HD13	1:B:420:VAL:HG23	1.89	0.53
1:A:33:PHE:N	1:A:41:ASN:HD21	1.96	0.53
1:B:396:VAL:HG12	1:B:398:LEU:CD1	2.39	0.53
1:C:32:MET:SD	1:C:62:LEU:HG	2.48	0.53
1:C:347:LEU:HD21	1:C:351:ILE:HD11	1.90	0.53
1:C:61:ALA:O	1:C:65:VAL:HG22	2.09	0.53
1:B:28:LEU:O	1:B:29:ASP:HB2	2.08	0.53
1:B:61:ALA:O	1:B:65:VAL:HG22	2.08	0.53
1:B:398:LEU:CD1	1:B:420:VAL:HG23	2.39	0.53
1:B:407:LEU:HD13	1:B:422:LEU:HD21	1.90	0.53
1:B:47:PHE:O	1:B:49:PRO:HD3	2.09	0.53
1:C:84:ARG:HB3	1:C:267:TYR:OH	2.08	0.53
1:A:220:ILE:HG22	1:A:222:THR:HG23	1.91	0.53
1:B:32:MET:HE3	1:B:34:GLN:CG	2.38	0.53
1:B:32:MET:HE3	1:B:34:GLN:HG2	1.90	0.53
1:B:84:ARG:HG2	1:B:84:ARG:NH2	2.19	0.53
1:D:217:LYS:HG2	1:D:307:MET:HG2	1.91	0.53
1:A:41:ASN:O	1:A:70:LYS:HE3	2.08	0.53
1:B:420:VAL:HG22	1:B:421:SER:N	2.23	0.53
1:C:407:LEU:HD22	1:C:422:LEU:HD21	1.91	0.53
1:D:227:ARG:HH11	1:D:378:SER:HA	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:407:LEU:HD13	1:A:422:LEU:HD21	1.90	0.53
1:D:329:LEU:HA	1:D:369:ALA:CB	2.39	0.53
1:B:177:PRO:HD3	1:B:389:TRP:CE2	2.43	0.53
1:C:80:VAL:HB	1:C:118:LEU:HD23	1.91	0.53
1:B:31:GLY:HA3	1:B:63:ASP:O	2.08	0.52
1:A:241:ARG:HD3	2:A:449:SO4:O3	2.10	0.52
1:A:10:ARG:HG2	1:A:10:ARG:NH1	2.23	0.52
1:A:155:ARG:HD3	1:A:431:VAL:O	2.09	0.52
1:B:62:LEU:HD13	1:B:93:VAL:CG1	2.39	0.52
1:D:86:THR:HG22	1:D:90:MET:HE2	1.91	0.52
1:D:226:GLU:HG2	1:D:261:TYR:OH	2.10	0.52
1:D:222:THR:HG22	1:D:339:VAL:CG2	2.40	0.52
1:A:297:SER:OG	1:A:320:ARG:HD3	2.09	0.52
1:C:290:VAL:HG13	1:C:290:VAL:O	2.10	0.52
1:A:263:ARG:HB3	1:A:263:ARG:NH1	2.09	0.52
1:C:85:ALA:HB2	1:C:267:TYR:CD2	2.44	0.52
1:C:212:LEU:HD23	1:C:212:LEU:N	2.25	0.52
1:A:157:LEU:HG	1:A:158:VAL:N	2.24	0.52
1:D:86:THR:HG22	1:D:90:MET:CE	2.40	0.52
1:B:37:GLU:N	1:B:37:GLU:OE2	2.43	0.51
1:C:207:ILE:HD13	1:C:372:HIS:CG	2.45	0.51
1:D:187:GLY:HA2	1:D:386:LEU:HD21	1.90	0.51
1:B:168:LYS:HG2	1:B:197:TYR:CE2	2.45	0.51
1:C:347:LEU:O	1:C:347:LEU:HD23	2.11	0.51
1:D:329:LEU:HA	1:D:369:ALA:HB3	1.92	0.51
1:C:97:ALA:O	1:C:101:MET:HB2	2.11	0.51
1:C:249:LEU:HB3	1:C:290:VAL:HA	1.93	0.51
1:C:229:GLN:HG3	1:C:261:TYR:CZ	2.45	0.51
1:A:341:TYR:CE1	1:A:375:GLY:HA3	2.46	0.51
1:B:210:LYS:HD2	1:B:214:GLN:OE1	2.11	0.51
1:D:229:GLN:H	1:D:229:GLN:NE2	2.09	0.51
1:C:347:LEU:HD23	1:C:347:LEU:C	2.32	0.50
1:D:73:ARG:NH2	1:D:110:ASP:OD2	2.43	0.50
1:D:177:PRO:HD3	1:D:389:TRP:NE1	2.26	0.50
1:D:280:LYS:O	1:D:282:PRO:HD3	2.11	0.50
1:A:5:PRO:HG2	1:A:423:ALA:HB1	1.93	0.50
1:A:176:LEU:O	1:D:126:TRP:HB2	2.10	0.50
1:B:402:GLU:O	1:B:405:LYS:N	2.43	0.50
1:C:325:LEU:O	1:C:329:LEU:HB2	2.11	0.50
1:D:158:VAL:HB	1:D:183:VAL:HG22	1.93	0.50
1:D:351:ILE:HG22	1:D:371:VAL:HG21	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:32:MET:HA	1:C:67:ARG:HG3	1.93	0.50
1:D:420:VAL:HG22	1:D:421:SER:N	2.26	0.50
1:B:20:LEU:HD21	1:B:25:ARG:HE	1.77	0.50
1:B:37:GLU:CG	1:B:40:ARG:HE	2.24	0.50
1:C:35:GLY:O	1:C:38:GLU:HB2	2.11	0.50
1:C:384:ASP:HA	1:C:387:LEU:HD12	1.93	0.50
1:D:396:VAL:O	1:D:420:VAL:HG23	2.12	0.50
1:A:73:ARG:HB2	1:A:110:ASP:OD1	2.12	0.50
1:A:404:GLU:OE1	1:A:404:GLU:N	2.30	0.50
1:A:404:GLU:H	1:A:404:GLU:CD	2.06	0.50
1:C:182:LEU:HD11	1:C:397:VAL:HG23	1.94	0.50
1:D:58:THR:HB	1:D:146:ALA:O	2.12	0.50
1:D:244:ARG:O	1:D:245:ALA:HB2	2.12	0.50
1:C:98:LEU:HD11	1:C:108:PRO:CA	2.34	0.50
1:A:84:ARG:NH1	1:D:270:GLU:OE1	2.45	0.49
1:C:248:TYR:HB2	1:C:309:VAL:HG22	1.94	0.49
1:D:31:GLY:HA3	1:D:63:ASP:C	2.32	0.49
1:C:10:ARG:HG2	1:C:10:ARG:HH11	1.77	0.49
1:C:420:VAL:HG23	1:C:421:SER:N	2.26	0.49
1:C:347:LEU:HD11	1:C:360:ILE:HG12	1.94	0.49
1:A:263:ARG:HH11	1:A:263:ARG:CG	2.25	0.49
1:B:389:TRP:HE3	1:B:390:LEU:HD13	1.76	0.49
1:B:422:LEU:HD12	1:B:422:LEU:N	2.26	0.49
1:D:396:VAL:HG12	1:D:398:LEU:HD12	1.95	0.49
1:C:280:LYS:O	1:C:282:PRO:HD3	2.13	0.49
1:D:227:ARG:NH1	1:D:378:SER:HA	2.28	0.49
1:C:223:PHE:HB2	1:C:227:ARG:HB2	1.94	0.49
1:D:373:THR:O	1:D:373:THR:CG2	2.61	0.49
1:C:339:VAL:O	1:C:377:PHE:HB2	2.12	0.49
1:D:68:LEU:N	1:D:69:PRO:HD2	2.27	0.49
1:D:325:LEU:CA	1:D:329:LEU:HD13	2.43	0.49
1:A:43:ALA:HB1	1:A:44:PRO:HD2	1.95	0.48
1:D:20:LEU:HD23	1:D:25:ARG:HG2	1.95	0.48
1:D:143:PRO:HD3	1:D:226:GLU:HG3	1.95	0.48
1:D:166:ARG:O	1:D:166:ARG:HG2	2.13	0.48
1:B:192:ARG:NH1	1:B:192:ARG:CG	2.72	0.48
1:B:212:LEU:HB3	1:B:243:PRO:HG2	1.94	0.48
1:D:1:MET:HG3	1:D:21:ALA:HB2	1.95	0.48
1:B:84:ARG:HD2	5:B:452:HOH:O	2.12	0.48
1:C:101:MET:HE3	1:C:104:PRO:HA	1.95	0.48
1:C:228:ALA:HB3	1:C:229:GLN:NE2	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:10:ARG:NH2	1:D:424:ARG:NH1	2.54	0.48
1:D:98:LEU:HD12	1:D:111:VAL:HG21	1.94	0.48
1:B:90:MET:HE3	1:B:118:LEU:CD1	2.43	0.48
1:B:41:ASN:O	1:B:70:LYS:HE3	2.14	0.48
1:A:32:MET:HE3	1:A:62:LEU:HG	1.96	0.48
1:D:214:GLN:HE21	1:D:333:ARG:HA	1.79	0.48
1:A:98:LEU:HD11	1:A:108:PRO:HA	1.96	0.48
1:C:157:LEU:HG	1:C:158:VAL:N	2.28	0.48
1:C:385:GLU:O	1:C:388:ASP:HB2	2.13	0.48
1:D:223:PHE:HA	2:D:438:SO4:O3	2.13	0.47
1:A:229:GLN:H	1:A:229:GLN:CD	2.17	0.47
1:B:58:THR:HB	1:B:146:ALA:O	2.14	0.47
1:A:134:LEU:HD12	1:A:134:LEU:N	2.29	0.47
1:D:177:PRO:HD3	1:D:389:TRP:CE2	2.49	0.47
1:A:126:TRP:CD2	1:D:178:PRO:HB3	2.50	0.47
1:A:178:PRO:HB3	1:D:126:TRP:CE3	2.49	0.47
1:A:217:LYS:HG2	1:A:307:MET:HG2	1.96	0.47
1:D:238:HIS:O	1:D:242:LEU:HG	2.15	0.47
1:C:98:LEU:HD12	1:C:111:VAL:CG2	2.42	0.47
1:C:134:LEU:HD12	1:C:134:LEU:N	2.29	0.47
1:D:1:MET:HA	1:D:21:ALA:HB2	1.97	0.47
1:B:54:ALA:HA	1:B:76:TYR:OH	2.14	0.47
1:D:37:GLU:O	1:D:39:ALA:N	2.48	0.47
1:B:288:LEU:HD12	1:B:289:GLU:H	1.80	0.47
1:D:347:LEU:O	1:D:350:GLU:HB3	2.15	0.47
1:D:404:GLU:OE1	1:D:404:GLU:N	2.34	0.47
1:C:163:LEU:HD11	1:C:389:TRP:CE2	2.50	0.47
1:C:221:PRO:HD2	1:C:337:VAL:O	2.15	0.47
1:C:413:LEU:HD22	1:C:418:GLN:OE1	2.15	0.47
1:C:195:ARG:O	1:C:196:PRO:C	2.54	0.47
1:D:163:LEU:HD11	1:D:389:TRP:CE3	2.50	0.47
1:C:211:THR:HG21	1:C:335:ALA:CB	2.45	0.47
1:D:98:LEU:HD11	1:D:108:PRO:HA	1.97	0.47
1:B:402:GLU:O	1:B:405:LYS:HB2	2.15	0.46
1:C:399:VAL:HG12	1:C:423:ALA:CB	2.44	0.46
1:D:57:LEU:HD21	1:D:68:LEU:HD22	1.96	0.46
1:B:211:THR:O	1:B:214:GLN:HG2	2.15	0.46
1:C:224:ALA:HA	1:C:254:ALA:HB2	1.96	0.46
1:C:168:LYS:HD2	1:C:378:SER:O	2.15	0.46
1:C:192:ARG:HD2	1:C:192:ARG:O	2.15	0.46
1:D:230:GLU:O	1:D:234:VAL:HG23	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:86:THR:HG22	1:C:90:MET:CE	2.42	0.46
1:C:227:ARG:NH1	1:C:378:SER:HA	2.30	0.46
1:C:250:ASP:HB3	1:C:311:ALA:HB2	1.98	0.46
1:C:409:LEU:HD23	1:C:409:LEU:C	2.35	0.46
1:D:247:ILE:HB	1:D:288:LEU:HA	1.97	0.46
1:B:398:LEU:HD13	1:B:420:VAL:CG2	2.45	0.46
1:C:240:HIS:CD2	1:C:241:ARG:HG2	2.50	0.46
1:C:269:SER:O	1:C:273:GLN:HG3	2.14	0.46
1:C:277:LEU:HB3	1:C:278:GLN:HE21	1.80	0.46
1:D:11:GLU:O	1:D:401:GLY:N	2.31	0.46
1:D:189:TYR:CE2	1:D:194:HIS:HE1	2.33	0.46
1:C:2:ARG:NH2	1:C:430:PRO:HB3	2.31	0.46
1:D:411:LYS:O	1:D:414:ALA:HB3	2.15	0.46
1:A:25:ARG:NE	1:A:51:GLU:HB3	2.30	0.46
1:A:84:ARG:HG3	1:A:84:ARG:NH1	2.25	0.46
1:B:45:PHE:CD2	1:B:49:PRO:HG3	2.51	0.46
1:A:11:GLU:OE2	1:A:40:ARG:NH1	2.49	0.46
1:D:42:HIS:CE1	1:D:105:PHE:HB3	2.51	0.46
1:D:411:LYS:O	1:D:414:ALA:N	2.49	0.46
1:A:11:GLU:CD	1:A:40:ARG:HH12	2.18	0.46
1:B:406:LEU:N	1:B:406:LEU:CD1	2.77	0.46
1:C:274:ALA:O	1:C:277:LEU:HB3	2.16	0.46
1:B:178:PRO:HB3	1:C:126:TRP:CD2	2.51	0.45
1:A:393:GLU:OE1	1:A:393:GLU:HA	2.17	0.45
1:C:270:GLU:OE2	1:C:270:GLU:HA	2.15	0.45
1:C:306:PRO:O	1:C:307:MET:HB3	2.17	0.45
1:B:32:MET:CE	1:B:34:GLN:OE1	2.64	0.45
1:D:9:ALA:O	1:D:10:ARG:HB2	2.15	0.45
1:D:59:HIS:HD2	1:D:61:ALA:H	1.61	0.45
1:D:214:GLN:NE2	1:D:333:ARG:HA	2.32	0.45
1:C:401:GLY:HA3	1:C:406:LEU:HD11	1.99	0.45
1:A:280:LYS:O	1:A:282:PRO:HD3	2.17	0.45
1:B:140:GLY:O	1:B:164:GLY:HA3	2.17	0.45
1:A:25:ARG:HE	1:A:51:GLU:HB3	1.82	0.45
1:B:188:THR:HG22	1:B:189:TYR:CD1	2.51	0.45
1:C:413:LEU:HB2	1:C:420:VAL:HG11	1.99	0.45
1:A:59:HIS:HD2	1:A:61:ALA:H	1.64	0.45
1:A:4:VAL:HA	1:A:428:GLY:HA2	1.98	0.45
1:B:101:MET:O	1:B:102:ASP:C	2.55	0.45
1:C:14:GLY:HA3	1:C:33:PHE:CE1	2.52	0.45
1:C:76:TYR:CZ	1:C:78:GLY:HA3	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:205:LEU:CD1	1:C:241:ARG:HH21	2.24	0.45
1:D:195:ARG:O	1:D:196:PRO:C	2.55	0.45
1:B:407:LEU:HD13	1:B:422:LEU:CD2	2.47	0.45
1:C:359:ARG:NH1	1:C:364:GLU:OE2	2.50	0.45
1:B:102:ASP:CG	1:B:103:GLU:N	2.70	0.45
1:C:165:ASN:O	1:C:168:LYS:HG3	2.17	0.45
1:D:298:LYS:HA	1:D:301:ASN:HD21	1.80	0.45
1:D:168:LYS:CE	1:D:230:GLU:OE1	2.65	0.44
1:B:188:THR:HG22	1:B:189:TYR:CE1	2.52	0.44
1:B:406:LEU:CD1	1:B:406:LEU:H	2.30	0.44
1:D:98:LEU:HD11	1:D:108:PRO:CA	2.46	0.44
1:D:168:LYS:HD2	1:D:378:SER:O	2.17	0.44
1:B:70:LYS:O	1:B:74:GLU:HG3	2.16	0.44
1:B:202:ARG:O	1:B:206:GLU:HG3	2.17	0.44
1:A:106:PHE:C	1:A:106:PHE:CD2	2.90	0.44
1:C:381:ALA:HB1	1:C:385:GLU:CB	2.46	0.44
1:D:202:ARG:O	1:D:206:GLU:HG3	2.18	0.44
1:B:191:ASP:OD1	1:B:405:LYS:HE2	2.18	0.44
1:C:187:GLY:HA2	1:C:386:LEU:HD21	1.99	0.44
1:A:407:LEU:HD13	1:A:422:LEU:CD2	2.48	0.44
1:C:244:ARG:HG3	1:C:244:ARG:HH11	1.83	0.44
1:C:393:GLU:O	1:C:418:GLN:NE2	2.48	0.44
1:C:424:ARG:NH1	3:C:445:FLC:HG1	2.33	0.44
1:D:84:ARG:HB2	1:D:267:TYR:OH	2.17	0.44
1:B:192:ARG:HB2	1:B:193:PRO:HD2	2.00	0.44
1:D:229:GLN:H	1:D:229:GLN:CD	2.20	0.44
1:C:101:MET:HE2	1:C:104:PRO:HA	2.00	0.43
1:C:413:LEU:O	1:C:418:GLN:HB2	2.18	0.43
1:D:5:PRO:HG2	1:D:423:ALA:HB1	1.99	0.43
1:D:410:GLY:O	1:D:420:VAL:HG11	2.18	0.43
1:B:191:ASP:O	1:B:192:ARG:HB3	2.17	0.43
1:D:226:GLU:O	1:D:229:GLN:HG2	2.19	0.43
1:D:253:MET:HA	1:D:256:ARG:HH22	1.77	0.43
1:D:384:ASP:OD2	1:D:384:ASP:N	2.50	0.43
1:B:325:LEU:HG	1:B:329:LEU:HD21	2.01	0.43
1:D:376:GLY:C	1:D:378:SER:H	2.22	0.43
1:A:355:PRO:HB2	1:A:356:PRO:HD2	1.99	0.43
1:C:28:LEU:O	1:C:29:ASP:HB2	2.19	0.43
1:C:388:ASP:O	1:C:391:GLN:CB	2.66	0.43
1:A:31:GLY:HA3	1:A:63:ASP:C	2.38	0.43
1:B:68:LEU:N	1:B:69:PRO:CD	2.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:184:LEU:HD11	1:B:399:VAL:HG11	2.01	0.43
1:B:211:THR:OG1	1:B:218:VAL:HG23	2.17	0.43
1:B:393:GLU:O	1:B:418:GLN:HG2	2.19	0.43
1:C:326:LYS:HD2	1:C:361:LEU:HD22	1.99	0.43
1:D:14:GLY:O	1:D:15:SER:C	2.57	0.43
1:D:98:LEU:HD11	1:D:108:PRO:CB	2.48	0.43
1:A:177:PRO:HD3	1:A:389:TRP:NE1	2.34	0.43
1:A:347:LEU:HD11	1:A:358:VAL:HG11	2.01	0.43
1:B:188:THR:OG1	1:B:400:HIS:CE1	2.71	0.43
1:C:402:GLU:HB2	1:C:405:LYS:HG2	2.00	0.43
1:D:170:VAL:HG21	1:D:230:GLU:HG3	2.01	0.43
1:D:225:VAL:O	1:D:257:VAL:HG11	2.18	0.43
1:B:45:PHE:HE1	1:B:67:ARG:HD2	1.84	0.43
1:B:155:ARG:HD2	1:B:431:VAL:O	2.18	0.43
1:C:86:THR:O	1:C:90:MET:HB2	2.19	0.43
1:C:216:GLY:O	1:C:306:PRO:HA	2.19	0.43
1:D:219:LEU:N	1:D:219:LEU:CD1	2.80	0.43
1:D:295:GLU:OE2	1:D:295:GLU:N	2.28	0.43
1:B:10:ARG:NH1	1:B:424:ARG:CG	2.72	0.43
1:C:24:ARG:HH21	1:C:24:ARG:HG2	1.83	0.43
1:C:382:GLY:O	1:C:386:LEU:HD13	2.19	0.43
1:D:323:HIS:ND1	1:D:361:LEU:HD21	2.34	0.43
1:A:407:LEU:HD12	1:A:407:LEU:HA	1.91	0.43
1:A:425:PHE:C	1:A:425:PHE:CD2	2.91	0.43
1:B:33:PHE:H	1:B:41:ASN:ND2	2.05	0.43
1:C:184:LEU:HD12	1:C:397:VAL:HB	2.01	0.43
1:A:132:LEU:HD12	1:A:151:GLN:O	2.18	0.43
1:C:12:VAL:HG23	1:C:13:THR:HG23	2.01	0.43
1:C:186:GLU:HA	1:C:399:VAL:O	2.19	0.43
1:C:398:LEU:HD12	1:C:398:LEU:N	2.34	0.43
1:D:383:GLN:O	1:D:387:LEU:HG	2.19	0.43
1:B:211:THR:OG1	1:B:218:VAL:CG2	2.67	0.42
1:C:20:LEU:O	1:C:21:ALA:HB2	2.19	0.42
1:C:49:PRO:HB3	1:C:71:LEU:HD12	2.00	0.42
1:C:173:ASP:HA	1:C:174:PRO:HD3	1.87	0.42
1:D:29:ASP:HA	1:D:57:LEU:HD12	2.00	0.42
1:D:223:PHE:CZ	1:D:315:MET:HG3	2.54	0.42
1:C:27:LEU:HD13	1:C:29:ASP:O	2.19	0.42
1:C:251:SER:OG	1:C:254:ALA:HB3	2.19	0.42
1:D:140:GLY:O	1:D:164:GLY:HA3	2.19	0.42
1:D:177:PRO:HB3	1:D:389:TRP:CZ2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:189:TYR:CD2	1:D:194:HIS:HE1	2.37	0.42
1:A:13:THR:OG1	1:A:33:PHE:HA	2.20	0.42
1:A:372:HIS:CD2	1:A:372:HIS:N	2.88	0.42
1:B:165:ASN:HD22	1:B:165:ASN:C	2.21	0.42
1:B:344:GLN:CD	1:B:344:GLN:H	2.22	0.42
1:C:358:VAL:HG12	1:C:359:ARG:N	2.33	0.42
1:A:84:ARG:HG3	1:A:122:GLU:OE2	2.18	0.42
1:A:186:GLU:HA	1:A:399:VAL:O	2.18	0.42
1:B:411:LYS:HB2	3:B:447:FLC:OHB	2.20	0.42
1:C:259:SER:O	1:C:262:PRO:HD2	2.19	0.42
1:A:32:MET:HB2	1:A:41:ASN:OD1	2.20	0.42
1:C:258:LEU:O	1:C:261:TYR:HB2	2.19	0.42
1:A:84:ARG:NH1	1:A:84:ARG:CG	2.82	0.42
1:A:226:GLU:HA	1:A:229:GLN:OE1	2.19	0.42
1:A:321:ILE:HG23	1:A:322:LEU:N	2.34	0.42
1:D:191:ASP:OD1	1:D:405:LYS:HD2	2.20	0.42
1:D:221:PRO:HB3	1:D:321:ILE:HG12	2.00	0.42
1:B:325:LEU:O	1:B:329:LEU:HD22	2.20	0.42
1:C:55:VAL:HG12	1:C:57:LEU:HD13	2.02	0.42
1:C:386:LEU:N	1:C:386:LEU:HD12	2.34	0.42
1:C:395:ARG:NH1	1:C:431:VAL:HA	2.35	0.42
1:B:80:VAL:HB	1:B:118:LEU:HD23	2.02	0.42
1:C:336:LEU:HD23	1:C:337:VAL:N	2.35	0.42
1:D:207:ILE:O	1:D:210:LYS:HB3	2.19	0.42
1:D:346:GLY:O	1:D:349:ALA:N	2.52	0.42
1:A:32:MET:HA	1:A:67:ARG:HG3	2.00	0.42
1:A:381:ALA:HB3	1:A:386:LEU:HD13	2.02	0.42
1:C:87:VAL:HG13	1:C:118:LEU:HD13	1.99	0.42
1:C:316:LEU:HD13	1:C:347:LEU:CD2	2.49	0.42
1:D:223:PHE:HZ	1:D:315:MET:HG3	1.85	0.42
1:D:227:ARG:NH1	1:D:377:PHE:O	2.42	0.42
1:A:1:MET:HA	1:A:21:ALA:HB2	2.01	0.42
1:A:140:GLY:O	1:A:164:GLY:HA3	2.19	0.42
1:C:108:PRO:HD2	1:C:109:GLU:OE2	2.19	0.42
1:D:28:LEU:O	1:D:29:ASP:HB2	2.20	0.42
1:A:25:ARG:HG2	1:A:25:ARG:HH21	1.85	0.41
1:A:365:VAL:HG12	1:A:366:PRO:O	2.20	0.41
1:B:184:LEU:HD11	1:B:399:VAL:CG1	2.49	0.41
1:C:222:THR:HG22	1:C:339:VAL:CG2	2.47	0.41
1:C:233:TYR:OH	1:C:271:GLU:HG2	2.19	0.41
1:C:244:ARG:HG3	1:C:244:ARG:NH1	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:94:LEU:HD12	1:A:94:LEU:HA	1.77	0.41
1:A:178:PRO:HB3	1:D:126:TRP:CD2	2.55	0.41
1:B:354:ARG:HG3	1:B:354:ARG:O	2.20	0.41
1:A:393:GLU:O	1:A:418:GLN:NE2	2.40	0.41
5:A:477:HOH:O	1:D:179:LEU:HB3	2.21	0.41
1:B:209:GLU:O	1:B:213:SER:HB2	2.19	0.41
1:D:366:PRO:HB2	1:D:368:ARG:NH1	2.36	0.41
1:A:60:ALA:N	1:A:86:THR:HG23	2.35	0.41
1:B:220:ILE:HG22	1:B:222:THR:HG23	2.01	0.41
1:B:165:ASN:C	1:B:165:ASN:ND2	2.74	0.41
1:B:189:TYR:HE2	1:B:341:TYR:CD2	2.38	0.41
1:B:358:VAL:HG12	1:B:359:ARG:N	2.36	0.41
1:D:200:THR:HG22	1:D:377:PHE:CE1	2.56	0.41
1:D:360:ILE:O	1:D:361:LEU:HB2	2.21	0.41
1:C:32:MET:HB2	1:C:32:MET:HE3	1.89	0.41
1:C:85:ALA:HB2	1:C:267:TYR:CE2	2.56	0.41
1:C:202:ARG:O	1:C:206:GLU:HG3	2.20	0.41
1:D:65:VAL:CG1	1:D:94:LEU:HD11	2.51	0.41
1:D:204:PHE:HD2	1:D:374:LEU:HD12	1.85	0.41
1:D:373:THR:O	1:D:373:THR:HG22	2.21	0.41
1:A:76:TYR:O	1:A:77:ARG:CD	2.67	0.41
1:A:165:ASN:C	1:A:165:ASN:HD22	2.22	0.41
1:C:404:GLU:H	1:C:404:GLU:CD	2.22	0.41
1:D:231:ILE:O	1:D:235:LEU:HG	2.21	0.41
1:B:3:ILE:HG23	1:B:3:ILE:O	2.21	0.41
1:B:37:GLU:CD	1:B:40:ARG:HH11	2.24	0.41
1:B:72:PHE:CD2	1:B:113:GLU:HG3	2.56	0.41
1:B:312:GLY:O	1:B:321:ILE:HG22	2.21	0.41
1:C:10:ARG:NH2	1:C:422:LEU:HB2	2.36	0.41
1:C:187:GLY:HA2	1:C:386:LEU:CD2	2.51	0.41
1:C:277:LEU:HB3	1:C:278:GLN:NE2	2.36	0.41
1:D:142:LEU:HD21	1:D:225:VAL:HG11	2.02	0.41
1:D:413:LEU:O	1:D:418:GLN:HB2	2.20	0.41
1:A:73:ARG:HB2	1:A:110:ASP:CG	2.42	0.41
1:A:250:ASP:OD2	1:A:324:HIS:NE2	2.52	0.41
1:C:224:ALA:O	1:C:254:ALA:HA	2.21	0.41
1:C:265:VAL:HA	1:C:268:PHE:HD2	1.86	0.41
1:C:392:GLY:H	1:C:416:ARG:NH1	2.19	0.41
1:D:211:THR:HA	1:D:214:GLN:HG2	2.02	0.41
1:D:238:HIS:C	1:D:240:HIS:H	2.24	0.41
1:A:75:GLY:O	1:A:77:ARG:HD3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:222:THR:HG22	1:A:339:VAL:HG21	2.04	0.40
1:B:45:PHE:HB3	1:B:47:PHE:CD1	2.55	0.40
1:B:189:TYR:CE2	1:B:341:TYR:CD2	3.08	0.40
1:C:200:THR:CG2	1:C:376:GLY:HA3	2.50	0.40
1:B:12:VAL:HG23	1:B:13:THR:HG23	2.03	0.40
1:B:406:LEU:HD12	1:B:406:LEU:H	1.85	0.40
1:C:355:PRO:HB2	1:C:356:PRO:HD2	2.03	0.40
1:C:395:ARG:HH21	1:C:395:ARG:HG3	1.86	0.40
1:B:90:MET:O	1:B:94:LEU:HB2	2.22	0.40
1:C:386:LEU:O	1:C:390:LEU:HD23	2.21	0.40
1:D:139:ALA:O	1:D:174:PRO:HG3	2.21	0.40
1:A:98:LEU:HD11	1:A:108:PRO:CA	2.52	0.40
1:A:359:ARG:HG3	1:A:359:ARG:NH2	2.37	0.40
1:B:31:GLY:HA3	1:B:63:ASP:C	2.42	0.40
1:B:170:VAL:HG12	1:B:171:LEU:HD13	2.03	0.40
1:B:205:LEU:HD13	1:B:241:ARG:HD2	2.03	0.40
1:C:190:GLY:HA3	1:C:409:LEU:HB2	2.03	0.40
1:C:255:GLY:O	1:C:258:LEU:HB3	2.22	0.40
1:D:401:GLY:HA3	1:D:406:LEU:HD11	2.04	0.40
1:A:126:TRP:CD1	1:D:178:PRO:HD3	2.57	0.40
1:A:371:VAL:C	1:A:372:HIS:CD2	2.95	0.40
1:B:33:PHE:C	1:B:34:GLN:HG3	2.42	0.40
1:C:212:LEU:HD22	1:C:218:VAL:HG21	2.03	0.40
1:D:27:LEU:HD23	1:D:27:LEU:HA	1.88	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%)	402 (94%)	25 (6%)	2 (0%)	29 48

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	429/431 (100%)	393 (92%)	30 (7%)	6 (1%)	11 20
1	C	429/431 (100%)	376 (88%)	44 (10%)	9 (2%)	7 11
1	D	429/431 (100%)	384 (90%)	38 (9%)	7 (2%)	9 17
All	All	1716/1724 (100%)	1555 (91%)	137 (8%)	24 (1%)	11 20

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	102	ASP
1	C	102	ASP
1	C	394	PRO
1	A	101	MET
1	B	225	VAL
1	B	240	HIS
1	B	316	LEU
1	C	421	SER
1	D	38	GLU
1	D	166	ARG
1	C	8	ALA
1	C	196	PRO
1	D	391	GLN
1	A	102	ASP
1	B	188	THR
1	D	245	ALA
1	B	66	GLY
1	C	227	ARG
1	C	400	HIS
1	D	16	ALA
1	D	292	GLU
1	C	426	GLY
1	D	392	GLY
1	C	251	SER

5.3.2 Protein sidechains (i)

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	341/341 (100%)	315 (92%)	26 (8%)	13 25
1	B	341/341 (100%)	314 (92%)	27 (8%)	12 24
1	C	341/341 (100%)	328 (96%)	13 (4%)	33 58
1	D	341/341 (100%)	327 (96%)	14 (4%)	30 55
All	All	1364/1364 (100%)	1284 (94%)	80 (6%)	19 37

All (80) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	ARG
1	A	27	LEU
1	A	57	LEU
1	A	84	ARG
1	A	94	LEU
1	A	98	LEU
1	A	102	ASP
1	A	165	ASN
1	A	171	LEU
1	A	186	GLU
1	A	192	ARG
1	A	219	LEU
1	A	253	MET
1	A	263	ARG
1	A	264	LEU
1	A	280	LYS
1	A	325	LEU
1	A	329	LEU
1	A	361	LEU
1	A	386	LEU
1	A	390	LEU
1	A	391	GLN
1	A	398	LEU
1	A	404	GLU
1	A	407	LEU
1	A	409	LEU
1	B	27	LEU
1	B	57	LEU
1	B	84	ARG
1	B	94	LEU
1	B	98	LEU
1	B	105	PHE
1	B	155	ARG

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Mol	Chain	Res	Type
1	B	165	ASN
1	B	171	LEU
1	B	175	SER
1	B	186	GLU
1	B	192	ARG
1	B	198	ARG
1	B	213	SER
1	B	219	LEU
1	B	229	GLN
1	B	253	MET
1	B	265	VAL
1	B	325	LEU
1	B	329	LEU
1	B	336	LEU
1	B	359	ARG
1	B	364	GLU
1	B	386	LEU
1	B	390	LEU
1	B	407	LEU
1	B	409	LEU
1	C	10	ARG
1	C	27	LEU
1	C	38	GLU
1	C	57	LEU
1	C	128	ARG
1	C	165	ASN
1	C	186	GLU
1	C	192	ARG
1	C	196	PRO
1	C	198	ARG
1	C	212	LEU
1	C	240	HIS
1	C	329	LEU
1	D	27	LEU
1	D	57	LEU
1	D	96	ASP
1	D	165	ASN
1	D	171	LEU
1	D	186	GLU
1	D	192	ARG
1	D	227	ARG
1	D	229	GLN

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Mol	Chain	Res	Type
1	D	264	LEU
1	D	278	GLN
1	D	373	THR
1	D	391	GLN
1	D	404	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	GLN
1	A	41	ASN
1	A	59	HIS
1	A	117	HIS
1	A	165	ASN
1	A	275	HIS
1	A	383	GLN
1	B	41	ASN
1	B	59	HIS
1	B	165	ASN
1	B	383	GLN
1	C	41	ASN
1	C	42	HIS
1	C	59	HIS
1	C	165	ASN
1	C	229	GLN
1	C	240	HIS
1	C	275	HIS
1	C	278	GLN
1	C	323	HIS
1	C	344	GLN
1	C	380	HIS
1	D	41	ASN
1	D	59	HIS
1	D	165	ASN
1	D	194	HIS
1	D	214	GLN
1	D	301	ASN

5.3.3 RNA

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 63 ligands modelled in this entry, 4 are monoatomic - leaving 59 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	D	438	-	4,4,4	1.03	0	6,6,6	0.64	0
2	SO4	A	446	-	4,4,4	1.02	0	6,6,6	0.65	0
2	SO4	A	444	-	4,4,4	1.00	0	6,6,6	0.66	0
2	SO4	A	449	-	4,4,4	1.03	0	6,6,6	0.69	0
2	SO4	B	440	-	4,4,4	1.01	0	6,6,6	0.65	0
2	SO4	C	436	-	4,4,4	0.99	0	6,6,6	0.67	0
2	SO4	D	433	-	4,4,4	1.03	0	6,6,6	0.65	0
2	SO4	A	436	-	4,4,4	1.03	0	6,6,6	0.66	0
2	SO4	C	441	-	4,4,4	0.98	0	6,6,6	0.66	0
2	SO4	B	441	-	4,4,4	1.01	0	6,6,6	0.65	0
2	SO4	C	432	-	4,4,4	1.03	0	6,6,6	0.64	0
2	SO4	A	450	-	4,4,4	1.03	0	6,6,6	0.64	0
2	SO4	B	436	-	4,4,4	1.03	0	6,6,6	0.67	0
2	SO4	C	433	-	4,4,4	1.01	0	6,6,6	0.66	0
2	SO4	A	434	-	4,4,4	1.00	0	6,6,6	0.67	0
2	SO4	A	447	-	4,4,4	1.02	0	6,6,6	0.63	0
2	SO4	D	432	-	4,4,4	1.03	0	6,6,6	0.66	0
2	SO4	C	440	-	4,4,4	1.03	0	6,6,6	0.65	0
2	SO4	C	434	-	4,4,4	0.99	0	6,6,6	0.65	0
2	SO4	A	438	-	4,4,4	0.99	0	6,6,6	0.66	0
2	SO4	D	435	-	4,4,4	1.02	0	6,6,6	0.66	0
2	SO4	B	439	-	4,4,4	0.98	0	6,6,6	0.66	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	SO4	A	448	-	4,4,4	1.06	0	6,6,6	0.65	0
2	SO4	C	439	-	4,4,4	1.00	0	6,6,6	0.66	0
3	FLC	B	447	-	12,12,12	1.66	4 (33%)	17,17,17	1.42	1 (5%)
2	SO4	A	433	-	4,4,4	1.04	0	6,6,6	0.70	0
2	SO4	A	435	-	4,4,4	1.01	0	6,6,6	0.70	0
2	SO4	A	439	-	4,4,4	1.03	0	6,6,6	0.64	0
2	SO4	C	444	-	4,4,4	0.99	0	6,6,6	0.67	0
2	SO4	D	440	-	4,4,4	1.03	0	6,6,6	0.61	0
2	SO4	B	438	-	4,4,4	1.00	0	6,6,6	0.67	0
2	SO4	A	441	-	4,4,4	1.01	0	6,6,6	0.64	0
2	SO4	A	445	-	4,4,4	1.01	0	6,6,6	0.65	0
2	SO4	B	434	-	4,4,4	1.00	0	6,6,6	0.65	0
2	SO4	B	435	-	4,4,4	1.03	0	6,6,6	0.66	0
2	SO4	B	446	-	4,4,4	1.03	0	6,6,6	0.66	0
2	SO4	D	436	-	4,4,4	1.02	0	6,6,6	0.64	0
2	SO4	B	444	-	4,4,4	1.02	0	6,6,6	0.61	0
2	SO4	B	445	-	4,4,4	1.01	0	6,6,6	0.68	0
2	SO4	B	433	-	4,4,4	1.01	0	6,6,6	0.64	0
2	SO4	A	432	-	4,4,4	1.02	0	6,6,6	0.65	0
2	SO4	D	439	-	4,4,4	1.02	0	6,6,6	0.65	0
2	SO4	C	437	-	4,4,4	1.03	0	6,6,6	0.65	0
2	SO4	C	443	-	4,4,4	1.02	0	6,6,6	0.66	0
2	SO4	C	442	-	4,4,4	1.01	0	6,6,6	0.64	0
3	FLC	A	451	-	12,12,12	1.58	2 (16%)	17,17,17	1.42	1 (5%)
3	FLC	C	445	-	12,12,12	1.62	5 (41%)	17,17,17	1.39	1 (5%)
2	SO4	A	442	-	4,4,4	1.02	0	6,6,6	0.64	0
2	SO4	A	443	-	4,4,4	0.98	0	6,6,6	0.74	0
2	SO4	B	432	-	4,4,4	1.00	0	6,6,6	0.67	0
2	SO4	C	438	-	4,4,4	1.03	0	6,6,6	0.67	0
2	SO4	A	437	-	4,4,4	1.01	0	6,6,6	0.67	0
2	SO4	D	434	-	4,4,4	1.02	0	6,6,6	0.67	0
2	SO4	C	435	-	4,4,4	0.98	0	6,6,6	0.70	0
2	SO4	D	437	-	4,4,4	1.03	0	6,6,6	0.67	0
2	SO4	B	442	-	4,4,4	1.03	0	6,6,6	0.67	0
2	SO4	B	443	-	4,4,4	0.97	0	6,6,6	0.70	0
2	SO4	A	440	-	4,4,4	1.04	0	6,6,6	0.63	0
2	SO4	B	437	-	4,4,4	1.02	0	6,6,6	0.65	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	447	-	-	0/16/16/16	-
3	FLC	A	451	-	-	0/16/16/16	-
3	FLC	C	445	-	-	0/16/16/16	-

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	447	FLC	CG-CB	2.79	1.57	1.53
3	A	451	FLC	OG2-CGC	-2.70	1.21	1.30
3	B	447	FLC	CA-CB	2.59	1.57	1.53
3	A	451	FLC	OA2-CAC	-2.59	1.22	1.30
3	C	445	FLC	OA2-CAC	-2.54	1.22	1.30
3	C	445	FLC	CA-CB	2.51	1.57	1.53
3	B	447	FLC	OA2-CAC	-2.48	1.22	1.30
3	B	447	FLC	OG2-CGC	-2.38	1.22	1.30
3	C	445	FLC	OG2-CGC	-2.38	1.22	1.30
3	C	445	FLC	CG-CB	2.24	1.56	1.53
3	C	445	FLC	OB1-CBC	2.04	1.28	1.22

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	451	FLC	OB2-CBC-CB	4.19	120.32	113.05
3	B	447	FLC	OB2-CBC-CB	4.11	120.19	113.05
3	C	445	FLC	OB2-CBC-CB	4.07	120.13	113.05

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	438	SO4	1	0
2	A	449	SO4	1	0
2	D	435	SO4	1	0
3	B	447	FLC	1	0
3	C	445	FLC	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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%)	0.00	7 (1%) 72 74	22, 41, 63, 86	0
1	B	431/431 (100%)	0.09	10 (2%) 60 63	24, 43, 68, 87	0
1	C	431/431 (100%)	0.63	48 (11%) 5 5	28, 71, 111, 122	0
1	D	431/431 (100%)	0.84	63 (14%) 2 2	33, 67, 126, 131	0
All	All	1724/1724 (100%)	0.39	128 (7%) 14 15	22, 51, 115, 131	0

All (128) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	201	VAL	6.6
1	D	219	LEU	6.0
1	D	212	LEU	6.0
1	C	341	TYR	5.4
1	D	208	LEU	5.4
1	C	415	LEU	5.2
1	D	306	PRO	5.0
1	D	218	VAL	4.9
1	D	338	PHE	4.7
1	D	211	THR	4.6
1	C	244	ARG	4.5
1	D	316	LEU	4.5
1	D	302	ARG	4.5
1	D	242	LEU	4.4
1	D	362	GLY	4.3
1	D	333	ARG	4.3
1	C	216	GLY	4.1
1	D	238	HIS	4.1
1	D	336	LEU	4.0
1	D	245	ALA	4.0
1	D	294	THR	3.9

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Mol	Chain	Res	Type	RSRZ
1	D	198	ARG	3.9
1	D	240	HIS	3.8
1	D	244	ARG	3.7
1	C	407	LEU	3.7
1	D	213	SER	3.6
1	D	351	ILE	3.6
1	C	354	ARG	3.6
1	D	239	GLY	3.6
1	D	330	SER	3.6
1	C	358	VAL	3.5
1	C	370	SER	3.5
1	C	329	LEU	3.4
1	D	241	ARG	3.4
1	D	335	ALA	3.4
1	D	205	LEU	3.4
1	C	225	VAL	3.4
1	C	240	HIS	3.4
1	D	139	ALA	3.3
1	C	241	ARG	3.3
1	D	214	GLN	3.2
1	D	304	PRO	3.2
1	B	280	LYS	3.1
1	C	326	LYS	3.1
1	D	371	VAL	3.1
1	D	332	PRO	3.0
1	C	280	LYS	3.0
1	B	72	PHE	3.0
1	D	352	ILE	3.0
1	A	357	ALA	3.0
1	B	77	ARG	3.0
1	D	361	LEU	3.0
1	D	209	GLU	2.9
1	C	411	LYS	2.9
1	A	358	VAL	2.9
1	D	377	PHE	2.9
1	C	337	VAL	2.8
1	D	225	VAL	2.8
1	C	412	LEU	2.8
1	D	210	LYS	2.8
1	D	35	GLY	2.8
1	C	367	LEU	2.8
1	D	322	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	374	LEU	2.7
1	D	334	ASN	2.7
1	C	224	ALA	2.7
1	C	214	GLN	2.7
1	D	337	VAL	2.7
1	C	242	LEU	2.7
1	C	338	PHE	2.7
1	C	238	HIS	2.6
1	C	169	ASP	2.6
1	D	243	PRO	2.6
1	C	418	GLN	2.6
1	D	202	ARG	2.6
1	A	361	LEU	2.6
1	C	408	ALA	2.6
1	C	353	ALA	2.5
1	A	356	PRO	2.5
1	C	276	PHE	2.5
1	C	404	GLU	2.5
1	D	216	GLY	2.5
1	B	136	PHE	2.5
1	C	328	GLY	2.5
1	C	414	ALA	2.5
1	D	312	GLY	2.5
1	D	95	GLU	2.4
1	C	356	PRO	2.4
1	C	371	VAL	2.4
1	D	360	ILE	2.4
1	B	279	GLY	2.4
1	D	370	SER	2.4
1	C	336	LEU	2.3
1	A	364	GLU	2.3
1	C	223	PHE	2.3
1	C	167	GLU	2.3
1	D	342	GLN	2.3
1	C	98	LEU	2.2
1	D	286	ALA	2.2
1	D	109	GLU	2.2
1	C	201	VAL	2.2
1	B	78	GLY	2.2
1	D	305	GLY	2.2
1	C	245	ALA	2.2
1	B	50	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	197	TYR	2.1
1	B	147	PHE	2.1
1	C	176	LEU	2.1
1	C	307	MET	2.1
1	C	332	PRO	2.1
1	D	145	SER	2.1
1	A	102	ASP	2.1
1	C	205	LEU	2.1
1	C	215	GLY	2.1
1	B	431	VAL	2.1
1	D	61	ALA	2.1
1	C	275	HIS	2.1
1	C	325	LEU	2.1
1	C	413	LEU	2.1
1	D	307	MET	2.0
1	D	303	ALA	2.0
1	B	160	SER	2.0
1	A	22	GLY	2.0
1	C	416	ARG	2.0
1	D	215	GLY	2.0
1	D	163	LEU	2.0
1	D	204	PHE	2.0
1	D	217	LYS	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 monosaccharides 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, 95^{th} 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(Å^2)	Q<0.9
3	FLC	B	447	13/13	0.56	0.50	104,111,113,113	0
3	FLC	C	445	13/13	0.62	0.30	117,119,121,121	0
3	FLC	A	451	13/13	0.70	0.35	108,109,111,112	0
2	SO4	C	441	5/5	0.73	0.25	151,151,151,152	0
2	SO4	D	439	5/5	0.75	0.34	137,137,137,137	0
2	SO4	A	447	5/5	0.75	0.23	134,134,134,134	0
2	SO4	A	436	5/5	0.76	0.58	155,155,155,156	0
2	SO4	B	438	5/5	0.77	0.22	136,136,137,137	0
2	SO4	C	444	5/5	0.78	0.18	129,130,130,131	0
2	SO4	A	439	5/5	0.80	0.29	133,134,134,134	0
2	SO4	A	448	5/5	0.81	0.32	150,150,150,150	0
2	SO4	A	440	5/5	0.81	0.16	136,136,137,137	0
2	SO4	A	441	5/5	0.82	0.27	143,143,143,143	0
2	SO4	D	435	5/5	0.82	0.14	133,133,133,133	0
2	SO4	D	438	5/5	0.83	0.26	137,137,137,137	0
4	ZN	C	446	1/1	0.83	0.10	100,100,100,100	0
2	SO4	A	445	5/5	0.84	0.33	114,114,114,114	0
2	SO4	A	438	5/5	0.84	0.29	122,123,123,123	0
2	SO4	B	446	5/5	0.84	0.30	118,119,119,120	0
2	SO4	C	439	5/5	0.85	0.15	121,121,121,122	0
2	SO4	A	437	5/5	0.86	0.30	125,125,125,126	0
2	SO4	C	433	5/5	0.86	0.18	140,141,141,141	0
2	SO4	D	433	5/5	0.87	0.19	123,123,123,123	0
2	SO4	B	442	5/5	0.87	0.14	100,101,101,102	0
2	SO4	B	437	5/5	0.87	0.15	121,121,122,122	0
2	SO4	B	440	5/5	0.87	0.24	89,90,91,92	0
2	SO4	C	436	5/5	0.88	0.27	114,114,115,115	0
2	SO4	B	433	5/5	0.88	0.18	97,97,98,99	0
2	SO4	B	435	5/5	0.88	0.23	114,114,114,114	0
2	SO4	B	436	5/5	0.88	0.20	116,116,116,117	0
2	SO4	B	434	5/5	0.89	0.25	129,129,129,129	0
2	SO4	C	434	5/5	0.89	0.36	131,131,131,132	0
2	SO4	A	450	5/5	0.89	0.20	127,127,128,128	0
2	SO4	C	438	5/5	0.89	0.15	105,105,105,105	0
2	SO4	C	432	5/5	0.89	0.12	104,105,106,106	0
2	SO4	C	440	5/5	0.90	0.27	140,140,140,141	0
2	SO4	A	442	5/5	0.90	0.14	97,98,99,99	0
2	SO4	A	432	5/5	0.90	0.26	135,136,136,136	0
2	SO4	D	432	5/5	0.90	0.21	140,140,140,141	0
4	ZN	B	448	1/1	0.91	0.06	84,84,84,84	0
2	SO4	C	437	5/5	0.91	0.20	115,115,116,116	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	SO4	B	432	5/5	0.92	0.23	120,120,120,120	0
2	SO4	A	434	5/5	0.93	0.16	119,120,120,120	0
2	SO4	D	434	5/5	0.93	0.12	116,116,116,116	0
2	SO4	B	445	5/5	0.95	0.10	81,82,83,83	0
2	SO4	D	437	5/5	0.95	0.15	88,88,89,90	0
2	SO4	A	446	5/5	0.95	0.22	110,111,111,111	0
2	SO4	B	439	5/5	0.95	0.14	72,74,74,74	0
2	SO4	D	440	5/5	0.95	0.17	81,82,83,83	0
2	SO4	C	443	5/5	0.96	0.06	102,102,102,103	0
2	SO4	B	443	5/5	0.96	0.14	60,61,62,63	0
2	SO4	B	441	5/5	0.96	0.09	90,91,91,91	0
4	ZN	A	452	1/1	0.97	0.08	80,80,80,80	0
2	SO4	A	443	5/5	0.97	0.23	76,77,77,79	0
2	SO4	B	444	5/5	0.97	0.20	45,49,50,51	0
4	ZN	D	441	1/1	0.97	0.15	92,92,92,92	0
2	SO4	A	449	5/5	0.98	0.10	40,44,46,47	0
2	SO4	C	442	5/5	0.98	0.09	64,64,66,66	0
2	SO4	D	436	5/5	0.98	0.07	67,67,68,69	0
2	SO4	A	435	5/5	0.98	0.14	43,44,46,50	0
2	SO4	A	444	5/5	0.98	0.09	82,82,82,83	0
2	SO4	A	433	5/5	0.98	0.10	59,61,62,64	0
2	SO4	C	435	5/5	0.98	0.19	87,88,89,89	0

6.5 Other polymers (i)

There are no such residues in this entry.