



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 04:50 PM UTC

PDB ID : 3A4Y / pdb_00003a4y
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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

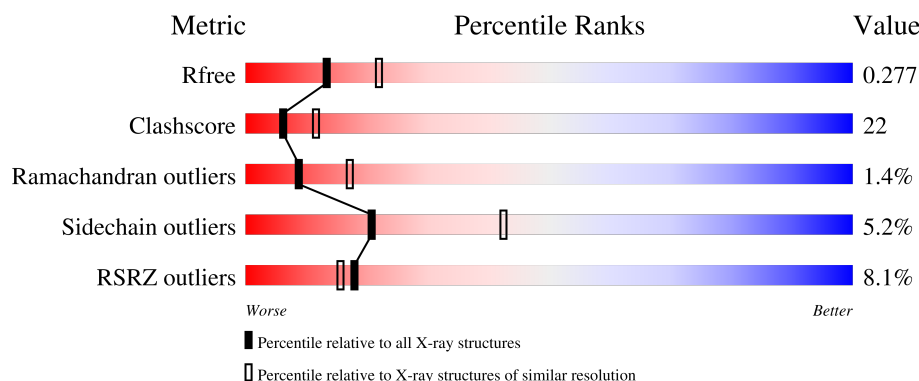
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	431	65% 31% 5%
1	B	431	2% 65% 32% .
1	C	431	13% 50% 47% .
1	D	431	16% 51% 46% .

2 Entry composition

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.

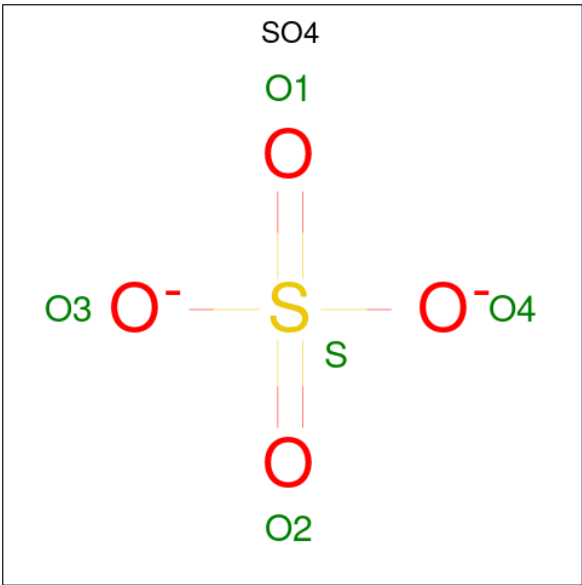
- Molecule 1 is a protein called Ribonuclease TTHA0252.

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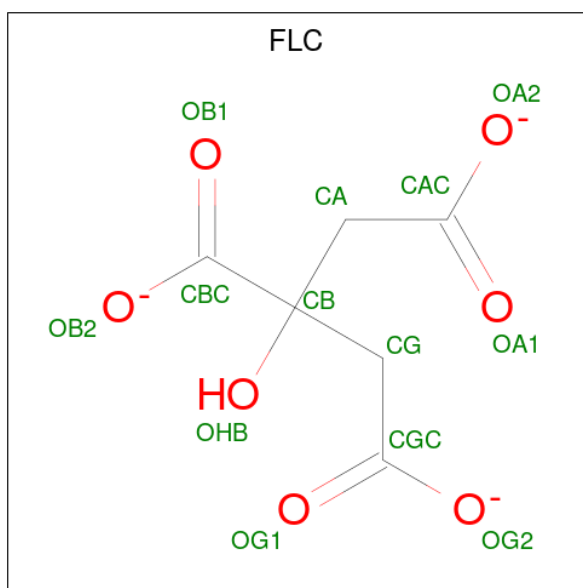
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	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	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	B	1	Total	C	O	0	0
			13	6	7		
3	C	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	1	Total	Zn	0	0
			1	1		
4	B	1	Total	Zn	0	0
			1	1		
4	C	1	Total	Zn	0	0
			1	1		
4	D	1	Total	Zn	0	0
			1	1		

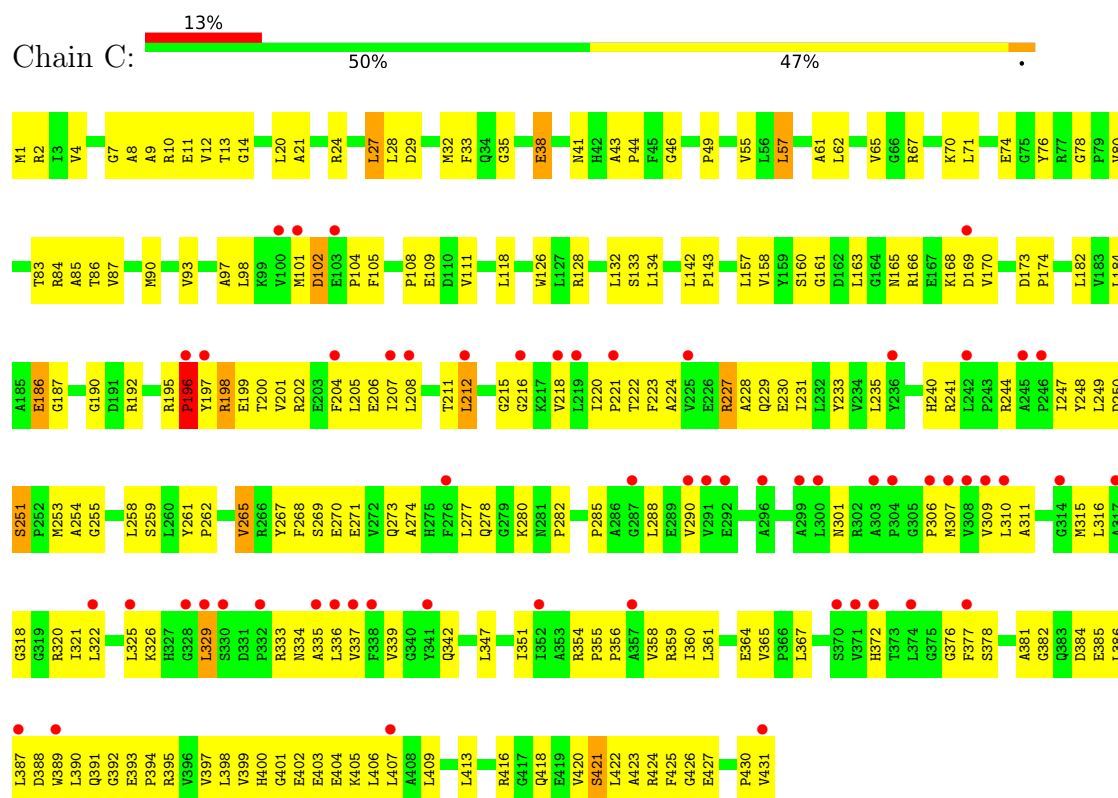
- Molecule 5 is water.

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

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



- 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	143.14Å 146.77Å 121.12Å 90.00° 109.24° 90.00°	Depositor
Resolution (Å)	50.00 – 2.50 50.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	96.4 (50.00-2.50) 96.4 (50.00-2.50)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.93 (at 2.51Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.239 , 0.282 0.235 , 0.277	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 , 46.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: FLC, SO4, ZN

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	0/3401	0.99	15/4613 (0.3%)
1	B	0.48	0/3401	1.00	14/4613 (0.3%)
1	C	0.40	0/3401	0.92	8/4613 (0.2%)
1	D	0.38	0/3401	0.93	10/4613 (0.2%)
All	All	0.44	0/13604	0.96	47/18452 (0.3%)

There are no bond length outliers.

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	170	VAL	N-CA-C	9.89	119.71	110.42
1	C	4	VAL	N-CA-C	8.66	116.12	107.55
1	B	60	ALA	N-CA-C	8.25	122.44	112.38
1	B	161	GLY	N-CA-C	-8.03	97.08	112.02
1	D	75	GLY	N-CA-C	7.82	124.00	114.69
1	A	192	ARG	N-CA-C	7.60	117.92	108.11
1	B	320	ARG	N-CA-C	7.51	120.42	111.33
1	A	305	GLY	N-CA-C	-7.44	103.07	112.00
1	B	169	ASP	N-CA-C	7.40	122.44	113.41
1	A	365	VAL	N-CA-C	7.38	115.94	107.89
1	B	147	PHE	N-CA-C	-7.25	99.48	110.14
1	D	60	ALA	N-CA-C	6.62	120.61	112.54
1	C	170	VAL	N-CA-C	6.57	116.70	110.53
1	A	169	ASP	N-CA-C	6.54	121.39	113.41
1	C	265	VAL	N-CA-C	6.36	117.87	110.62
1	A	41	ASN	N-CA-C	-6.16	105.76	113.28
1	A	60	ALA	N-CA-C	6.16	120.65	113.20
1	B	160	SER	N-CA-C	6.09	117.92	111.28
1	A	161	GLY	N-CA-C	-5.98	99.26	112.17
1	B	148	VAL	N-CA-C	5.96	117.06	108.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	126	TRP	N-CA-C	5.84	118.77	109.24
1	A	147	PHE	N-CA-C	-5.82	101.12	110.14
1	C	161	GLY	N-CA-C	-5.82	101.21	111.80
1	A	66	GLY	N-CA-C	5.79	119.90	112.83
1	A	33	PHE	N-CA-C	-5.77	101.15	110.32
1	C	46	GLY	N-CA-C	-5.75	106.85	114.95
1	D	176	LEU	N-CA-C	-5.63	102.02	110.24
1	D	225	VAL	N-CA-C	5.59	115.68	110.42
1	A	170	VAL	N-CA-C	5.51	115.65	110.30
1	B	192	ARG	CA-C-N	5.41	125.88	120.52
1	B	192	ARG	C-N-CA	5.41	125.88	120.52
1	D	161	GLY	N-CA-C	-5.30	101.16	111.02
1	C	166	ARG	N-CA-C	5.26	117.69	111.33
1	B	195	ARG	N-CA-C	-5.24	102.99	109.64
1	A	225	VAL	CA-C-N	-5.23	113.97	121.98
1	A	225	VAL	C-N-CA	-5.23	113.97	121.98
1	C	169	ASP	N-CA-C	5.19	120.26	113.88
1	B	166	ARG	N-CA-C	5.17	121.82	110.80
1	C	301	ASN	N-CA-C	-5.16	106.14	112.90
1	A	166	ARG	N-CA-C	5.14	119.03	112.34
1	D	64	HIS	N-CA-C	-5.09	107.00	114.39
1	B	231	ILE	N-CA-C	-5.09	105.58	110.72
1	D	66	GLY	N-CA-C	5.09	119.04	112.83
1	A	293	HIS	N-CA-C	5.07	117.37	109.52
1	B	365	VAL	N-CA-C	5.06	113.50	107.73
1	D	103	GLU	CA-C-N	5.00	125.23	119.83
1	D	103	GLU	C-N-CA	5.00	125.23	119.83

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	121	0
1	B	3321	0	3349	134	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	3321	0	3349	186	0
1	D	3321	0	3349	171	0
2	A	95	0	0	1	0
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	605	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 22.

All (605) 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:C:101:MET:HE3	1:C:104:PRO:HA	1.44	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:32:MET:HE2	1:B:34:GLN:OE1	1.75	0.87
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
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:86:THR:HG22	1:D:90:MET:HE2	1.64	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:D:224:ALA:HB3	1:D:253:MET:HE2	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:381:ALA:HB1	1:C:385:GLU:HB2	1.71	0.70
1:B:421:SER:C	1:B:422:LEU:HD12	2.16	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
1:C:1:MET:HG3	1:C:21:ALA:HB2	1.75	0.69
1:B:90:MET:HE1	1:B:118:LEU:HD22	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:D:325:LEU:HA	1:D:329:LEU:HD13	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:A:133:SER:C	1:A:134:LEU:HD12	2.18	0.67
1:C:98:LEU:O	1:C:98:LEU:HD23	1.93	0.67
1:C:208:LEU:C	1:C:212:LEU:HD21	2.20	0.67
1:B:295:GLU:H	1:B:295:GLU:CD	2.01	0.67
1:B:57:LEU:HG	1:B:65:VAL:HG12	1.76	0.67
1:C:86:THR:HG22	1:C:90:MET:HE3	1.76	0.67
1:A:76:TYR:O	1:A:77:ARG:HD2	1.94	0.66
1:B:102:ASP:CG	1:B:103:GLU:H	2.01	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: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:B:401:GLY:C	1:B:406:LEU:HD11	2.22	0.63
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:7:GLY:HA3	1:C:14:GLY:O	1.98	0.63
1:A:404:GLU:CD	1:A:404:GLU:H	2.06	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:32:MET:HE3	1:A:62:LEU:HG	1.81	0.62
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:D:191:ASP:CG	1:D:405:LYS:HD2	2.25	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:32:MET:HE1	1:D:101:MET:HE1	1.83	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:D:404:GLU:H	1:D:404:GLU:CD	2.08	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:217:LYS:HE2	1:D:307:MET:HE3	1.84	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: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:B:86:THR:HG22	1:B:90:MET:HE2	1.84	0.58
1:D:295:GLU:H	1:D:295:GLU:CD	2.11	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:B:87:VAL:HA	1:B:90:MET:HE3	1.86	0.57
1:A:90:MET:HE1	1:A:118:LEU:HD22	1.87	0.57
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:217:LYS:HE2	1:A:307:MET:HE3	1.86	0.56
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:57:LEU:HD23	1:C:90:MET:HE1	1.88	0.56
1:C:160:SER:HB2	1:C:163:LEU:CD2	2.32	0.56
1:B:90:MET:HE1	1:B:118:LEU:CD2	2.35	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: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: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:347:LEU:C	1:C:347:LEU:HD23	2.32	0.55
1:C:93:VAL:HA	1:C:253:MET:HE1	1.89	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:31:GLY:HA3	1:D:63:ASP:C	2.32	0.54
1:D:209:GLU:HG2	1:D:243:PRO:HD2	1.88	0.54
1:C:32:MET:HE3	1:C:105:PHE:HZ	1.73	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:C:32:MET:HE3	1:C:105:PHE:CZ	2.43	0.52
1:A:229:GLN:H	1:A:229:GLN:CD	2.17	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: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: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:HD23	1:C:347:LEU:O	2.11	0.51
1:D:329:LEU:HA	1:D:369:ALA:HB3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:97:ALA:O	1:C:101:MET:HB2	2.11	0.51
1:C:195:ARG:O	1:C:196:PRO:C	2.54	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:C:409:LEU:HD23	1:C:409:LEU:C	2.35	0.51
1:D:229:GLN:H	1:D:229:GLN:NE2	2.09	0.51
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:157:LEU:HG	1:A:158:VAL:N	2.24	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
1:A:11:GLU:CD	1:A:40:ARG:HH12	2.18	0.50
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: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:B:101:MET:O	1:B:102:ASP:C	2.55	0.49
1:C:248:TYR:HB2	1:C:309:VAL:HG22	1.94	0.49
1:C:10:ARG:HG2	1:C:10:ARG:HH11	1.77	0.49
1:D:195:ARG:O	1:D:196:PRO:C	2.55	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:106:PHE:C	1:A:106:PHE:CD2	2.90	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:228:ALA:HB3	1:C:229:GLN:NE2	2.28	0.48
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:D:229:GLN:H	1:D:229:GLN:CD	2.20	0.48
1:A:31:GLY:HA3	1:A:63:ASP:C	2.38	0.48
1:B:41:ASN:O	1:B:70:LYS:HE3	2.14	0.48
1:D:14:GLY:O	1:D:15:SER:C	2.57	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:425:PHE:C	1:A:425:PHE:CD2	2.91	0.47
1:B:58:THR:HB	1:B:146:ALA:O	2.14	0.47
1:D:376:GLY:C	1:D:378:SER:H	2.22	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:B:344:GLN:CD	1:B:344:GLN:H	2.22	0.47
1:C:98:LEU:HD12	1:C:111:VAL:CG2	2.42	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:86:THR:HG22	1:D:90:MET:CE	2.40	0.47
1:B:165:ASN:HD22	1:B:165:ASN:C	2.21	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:A:165:ASN:C	1:A:165:ASN:HD22	2.22	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:A:87:VAL:HA	1:A:90:MET:HE3	1.98	0.46
1:A:186:GLU:OE2	1:A:188:THR:OG1	2.33	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:165:ASN:C	1:B:165:ASN:ND2	2.74	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: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:C:404:GLU:H	1:C:404:GLU:CD	2.22	0.46
1:B:37:GLU:CD	1:B:40:ARG:HH11	2.24	0.45
1:B:178:PRO:HB3	1:C:126:TRP:CD2	2.51	0.45
1:D:32:MET:HE2	1:D:105:PHE:HZ	1.81	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:A:73:ARG:HB2	1:A:110:ASP:CG	2.42	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:A:371:VAL:C	1:A:372:HIS:CD2	2.95	0.45
1:C:401:GLY:HA3	1:C:406:LEU:HD11	1.99	0.45
1:D:238:HIS:C	1:D:240:HIS:H	2.24	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:B:31:GLY:HA3	1:B:63:ASP:C	2.42	0.45
1:A:4:VAL:HA	1:A:428:GLY:HA2	1.98	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
1:C:205:LEU:CD1	1:C:241:ARG:HH21	2.24	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: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:346:GLY:O	1:D:347:LEU:C	2.60	0.45
1:B:33:PHE:C	1:B:34:GLN:HG3	2.42	0.44
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:C:133:SER:C	1:C:134:LEU:HD12	2.42	0.44
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:C:197:TYR:O	1:C:198:ARG:C	2.60	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: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:B:68:LEU:N	1:B:69:PRO:CD	2.81	0.43
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
1:D:189:TYR:CD2	1:D:194:HIS:HE1	2.37	0.42
1:D:309:VAL:C	1:D:310:LEU:HD12	2.44	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: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:C:316:LEU:C	1:C:318:GLY:H	2.27	0.42
1:D:191:ASP:OD1	1:D:405:LYS:HD2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:101:MET:O	1:C:102:ASP:C	2.63	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:25:ARG:HD2	1:A:51:GLU:C	2.44	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:B:401:GLY:C	1:B:406:LEU:CD1	2.92	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
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:C:376:GLY:C	1:C:378:SER:H	2.27	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:C:70:LYS:NZ	1:C:74:GLU:OE1	2.50	0.41
1:D:366:PRO:HB2	1:D:368:ARG:NH1	2.36	0.41
1:A:90:MET:HE1	1:A:118:LEU:CD2	2.49	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:C:227:ARG:O	1:C:228:ALA:C	2.62	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:14:GLY:O	1:A:15:SER:C	2.63	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: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:B:274:ALA:O	1:B:275:HIS:C	2.63	0.41
1:D:231:ILE:O	1:D:235:LEU:HG	2.21	0.41
1:A:264:LEU:O	1:A:265:VAL:C	2.62	0.41
1:B:14:GLY:O	1:B:15:SER:C	2.62	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:1:MET:HE2	1:D:21:ALA:CB	2.50	0.41
1:D:35:GLY:C	1:D:37:GLU:H	2.27	0.41
1:D:87:VAL:HA	1:D:90:MET:HE3	2.03	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: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:C:425:PHE:C	1:C:427:GLU:H	2.28	0.41
1:D:211:THR:HA	1:D:214:GLN:HG2	2.02	0.41
1:A:75:GLY:O	1:A:77:ARG:HD3	2.21	0.40
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:170:VAL:HG12	1:B:171:LEU:HD13	2.03	0.40
1:B:187:GLY:O	1:B:188:THR:C	2.64	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:C:333:ARG:O	1:C:334:ASN:C	2.64	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: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
1:D:341:TYR:CD1	1:D:341:TYR:C	2.98	0.40
1:D:390:LEU:O	1:D:391:GLN:C	2.65	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	429/431 (100%)	402 (94%)	25 (6%)	2 (0%)	24	43
1	B	429/431 (100%)	393 (92%)	30 (7%)	6 (1%)	9	17
1	C	429/431 (100%)	376 (88%)	44 (10%)	9 (2%)	5	9
1	D	429/431 (100%)	384 (90%)	38 (9%)	7 (2%)	7	14
All	All	1716/1724 (100%)	1555 (91%)	137 (8%)	24 (1%)	9	17

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 ⓘ

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%)	316 (93%)	25 (7%)	13	27
1	B	341/341 (100%)	317 (93%)	24 (7%)	14	29
1	C	341/341 (100%)	331 (97%)	10 (3%)	37	65
1	D	341/341 (100%)	329 (96%)	12 (4%)	32	58
All	All	1364/1364 (100%)	1293 (95%)	71 (5%)	21	42

All (71) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	LEU
1	A	57	LEU
1	A	94	LEU
1	A	98	LEU
1	A	102	ASP
1	A	142	LEU
1	A	165	ASN
1	A	171	LEU
1	A	186	GLU
1	A	192	ARG
1	A	219	LEU
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	406	LEU
1	A	407	LEU
1	A	409	LEU
1	A	416	ARG
1	B	27	LEU
1	B	57	LEU
1	B	84	ARG
1	B	94	LEU
1	B	98	LEU
1	B	142	LEU
1	B	157	LEU
1	B	165	ASN
1	B	171	LEU
1	B	175	SER
1	B	186	GLU
1	B	192	ARG
1	B	219	LEU
1	B	229	GLN
1	B	253	MET
1	B	265	VAL
1	B	325	LEU
1	B	329	LEU

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Mol	Chain	Res	Type
1	B	336	LEU
1	B	364	GLU
1	B	386	LEU
1	B	390	LEU
1	B	407	LEU
1	B	409	LEU
1	C	27	LEU
1	C	38	GLU
1	C	57	LEU
1	C	128	ARG
1	C	186	GLU
1	C	196	PRO
1	C	198	ARG
1	C	212	LEU
1	C	320	ARG
1	C	329	LEU
1	D	27	LEU
1	D	28	LEU
1	D	57	LEU
1	D	96	ASP
1	D	171	LEU
1	D	186	GLU
1	D	227	ARG
1	D	229	GLN
1	D	264	LEU
1	D	278	GLN
1	D	373	THR
1	D	391	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	GLN
1	A	41	ASN
1	A	117	HIS
1	A	165	ASN
1	A	275	HIS
1	A	383	GLN
1	A	391	GLN
1	B	41	ASN
1	B	59	HIS
1	B	165	ASN

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Mol	Chain	Res	Type
1	B	240	HIS
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	238	HIS
1	C	240	HIS
1	C	278	GLN
1	C	323	HIS
1	C	342	GLN
1	C	344	GLN
1	C	383	GLN
1	D	41	ASN
1	D	59	HIS
1	D	165	ASN
1	D	194	HIS
1	D	214	GLN
1	D	275	HIS
1	D	301	ASN
1	D	342	GLN

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 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	432	-	4,4,4	1.09	0	6,6,6	0.57	0
2	SO4	A	434	-	4,4,4	1.06	0	6,6,6	0.58	0
2	SO4	C	443	-	4,4,4	1.07	0	6,6,6	0.57	0
2	SO4	D	439	-	4,4,4	1.08	0	6,6,6	0.57	0
2	SO4	B	444	-	4,4,4	1.07	0	6,6,6	0.55	0
2	SO4	D	435	-	4,4,4	1.08	0	6,6,6	0.57	0
2	SO4	B	440	-	4,4,4	1.07	0	6,6,6	0.57	0
2	SO4	A	441	-	4,4,4	1.07	0	6,6,6	0.56	0
2	SO4	D	436	-	4,4,4	1.08	0	6,6,6	0.56	0
2	SO4	A	448	-	4,4,4	1.11	0	6,6,6	0.57	0
2	SO4	B	435	-	4,4,4	1.09	0	6,6,6	0.58	0
2	SO4	B	442	-	4,4,4	1.09	0	6,6,6	0.58	0
2	SO4	B	446	-	4,4,4	1.09	0	6,6,6	0.57	0
2	SO4	A	443	-	4,4,4	1.04	0	6,6,6	0.64	0
2	SO4	B	438	-	4,4,4	1.06	0	6,6,6	0.59	0
2	SO4	B	439	-	4,4,4	1.04	0	6,6,6	0.57	0
2	SO4	B	433	-	4,4,4	1.07	0	6,6,6	0.56	0
2	SO4	B	436	-	4,4,4	1.09	0	6,6,6	0.58	0
2	SO4	A	442	-	4,4,4	1.07	0	6,6,6	0.56	0
2	SO4	A	447	-	4,4,4	1.08	0	6,6,6	0.55	0
2	SO4	C	444	-	4,4,4	1.05	0	6,6,6	0.59	0
2	SO4	A	449	-	4,4,4	1.08	0	6,6,6	0.60	0
2	SO4	C	435	-	4,4,4	1.04	0	6,6,6	0.61	0
2	SO4	B	434	-	4,4,4	1.06	0	6,6,6	0.57	0
3	FLC	C	445	-	12,12,12	1.63	5 (41%)	17,17,17	1.28	1 (5%)
2	SO4	A	445	-	4,4,4	1.07	0	6,6,6	0.57	0
2	SO4	D	440	-	4,4,4	1.08	0	6,6,6	0.54	0
2	SO4	B	445	-	4,4,4	1.07	0	6,6,6	0.60	0
2	SO4	A	450	-	4,4,4	1.09	0	6,6,6	0.56	0
2	SO4	D	438	-	4,4,4	1.09	0	6,6,6	0.56	0
2	SO4	D	433	-	4,4,4	1.09	0	6,6,6	0.56	0
2	SO4	A	435	-	4,4,4	1.07	0	6,6,6	0.62	0
2	SO4	B	443	-	4,4,4	1.03	0	6,6,6	0.60	0
3	FLC	B	447	-	12,12,12	1.67	5 (41%)	17,17,17	1.31	1 (5%)
3	FLC	A	451	-	12,12,12	1.59	3 (25%)	17,17,17	1.31	1 (5%)
2	SO4	A	439	-	4,4,4	1.08	0	6,6,6	0.56	0
2	SO4	B	432	-	4,4,4	1.06	0	6,6,6	0.58	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SO4	A	444	-	4,4,4	1.06	0	6,6,6	0.58	0
2	SO4	A	440	-	4,4,4	1.10	0	6,6,6	0.55	0
2	SO4	B	441	-	4,4,4	1.06	0	6,6,6	0.57	0
2	SO4	C	434	-	4,4,4	1.05	0	6,6,6	0.57	0
2	SO4	D	434	-	4,4,4	1.07	0	6,6,6	0.58	0
2	SO4	A	433	-	4,4,4	1.09	0	6,6,6	0.61	0
2	SO4	C	437	-	4,4,4	1.08	0	6,6,6	0.56	0
2	SO4	A	436	-	4,4,4	1.09	0	6,6,6	0.57	0
2	SO4	A	438	-	4,4,4	1.05	0	6,6,6	0.58	0
2	SO4	B	437	-	4,4,4	1.08	0	6,6,6	0.57	0
2	SO4	D	437	-	4,4,4	1.08	0	6,6,6	0.58	0
2	SO4	C	432	-	4,4,4	1.09	0	6,6,6	0.56	0
2	SO4	A	446	-	4,4,4	1.08	0	6,6,6	0.57	0
2	SO4	C	439	-	4,4,4	1.05	0	6,6,6	0.58	0
2	SO4	C	433	-	4,4,4	1.06	0	6,6,6	0.58	0
2	SO4	A	432	-	4,4,4	1.08	0	6,6,6	0.57	0
2	SO4	C	438	-	4,4,4	1.08	0	6,6,6	0.59	0
2	SO4	C	440	-	4,4,4	1.08	0	6,6,6	0.56	0
2	SO4	C	436	-	4,4,4	1.05	0	6,6,6	0.58	0
2	SO4	A	437	-	4,4,4	1.06	0	6,6,6	0.58	0
2	SO4	C	442	-	4,4,4	1.07	0	6,6,6	0.57	0
2	SO4	C	441	-	4,4,4	1.04	0	6,6,6	0.58	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	FLC	B	447	-	-	0/16/16/16	-
3	FLC	A	451	-	-	0/16/16/16	-
3	FLC	C	445	-	-	0/16/16/16	-

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	451	FLC	OG2-CGC	-2.77	1.21	1.30
3	B	447	FLC	CG-CB	2.70	1.57	1.54
3	A	451	FLC	OA2-CAC	-2.65	1.22	1.30
3	C	445	FLC	OA2-CAC	-2.61	1.22	1.30
3	B	447	FLC	OA2-CAC	-2.55	1.22	1.30
3	B	447	FLC	CA-CB	2.50	1.57	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	447	FLC	OG2-CGC	-2.45	1.22	1.30
3	C	445	FLC	OG2-CGC	-2.44	1.22	1.30
3	C	445	FLC	CA-CB	2.42	1.57	1.54
3	C	445	FLC	CG-CB	2.14	1.56	1.54
3	C	445	FLC	OB1-CBC	2.11	1.28	1.22
3	B	447	FLC	OB1-CBC	2.04	1.28	1.22
3	A	451	FLC	OB1-CBC	2.04	1.28	1.22

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	451	FLC	OB2-CBC-CB	3.74	120.32	113.14
3	B	447	FLC	OB2-CBC-CB	3.67	120.19	113.14
3	C	445	FLC	OB2-CBC-CB	3.64	120.13	113.14

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	435	SO4	1	0
2	A	449	SO4	1	0
3	C	445	FLC	1	0
2	D	438	SO4	1	0
3	B	447	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, 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%)	-0.11	1 (0%) 91 89	22, 41, 63, 86	0
1	B	431/431 (100%)	0.14	9 (2%) 63 59	24, 43, 68, 87	0
1	C	431/431 (100%)	0.83	58 (13%) 7 5	28, 71, 111, 122	0
1	D	431/431 (100%)	0.91	71 (16%) 4 3	33, 67, 126, 131	0
All	All	1724/1724 (100%)	0.44	139 (8%) 18 15	22, 51, 115, 131	0

All (139) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	339	VAL	4.2
1	D	322	LEU	4.2
1	D	367	LEU	4.1
1	D	338	PHE	4.1
1	C	329	LEU	4.0
1	C	308	VAL	3.9
1	D	330	SER	3.8
1	B	431	VAL	3.7
1	D	361	LEU	3.6
1	D	335	ALA	3.5
1	D	201	VAL	3.5
1	C	212	LEU	3.5
1	D	340	GLY	3.4
1	C	336	LEU	3.4
1	D	316	LEU	3.4
1	D	312	GLY	3.4
1	C	236	TYR	3.3
1	C	341	TYR	3.3
1	C	242	LEU	3.3
1	D	337	VAL	3.3
1	C	216	GLY	3.3

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Mol	Chain	Res	Type	RSRZ
1	D	311	ALA	3.3
1	D	305	GLY	3.2
1	D	245	ALA	3.2
1	C	225	VAL	3.2
1	D	225	VAL	3.1
1	C	317	ALA	3.1
1	D	300	LEU	3.0
1	C	207	ILE	3.0
1	C	292	GLU	3.0
1	C	337	VAL	3.0
1	B	341	TYR	3.0
1	C	300	LEU	3.0
1	C	291	VAL	2.9
1	C	322	LEU	2.9
1	D	212	LEU	2.9
1	C	310	LEU	2.9
1	C	407	LEU	2.9
1	D	219	LEU	2.9
1	B	72	PHE	2.9
1	D	358	VAL	2.8
1	C	290	VAL	2.8
1	B	35	GLY	2.8
1	D	356	PRO	2.8
1	C	296	ALA	2.8
1	C	169	ASP	2.7
1	D	197	TYR	2.7
1	D	324	HIS	2.7
1	D	204	PHE	2.7
1	D	290	VAL	2.7
1	C	197	TYR	2.7
1	D	326	LYS	2.6
1	D	366	PRO	2.6
1	D	362	GLY	2.6
1	C	304	PRO	2.6
1	C	307	MET	2.6
1	D	207	ILE	2.6
1	D	208	LEU	2.6
1	D	357	ALA	2.6
1	D	238	HIS	2.6
1	D	351	ILE	2.5
1	D	352	ILE	2.5
1	D	293	HIS	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	335	ALA	2.5
1	D	306	PRO	2.5
1	D	360	ILE	2.5
1	C	219	LEU	2.5
1	D	327	HIS	2.5
1	D	365	VAL	2.5
1	D	328	GLY	2.4
1	D	347	LEU	2.4
1	C	338	PHE	2.4
1	D	211	THR	2.4
1	C	374	LEU	2.4
1	D	415	LEU	2.4
1	D	218	VAL	2.4
1	C	330	SER	2.4
1	B	428	GLY	2.4
1	C	309	VAL	2.4
1	C	371	VAL	2.4
1	C	245	ALA	2.4
1	D	376	GLY	2.3
1	C	332	PRO	2.3
1	C	208	LEU	2.3
1	D	321	ILE	2.3
1	C	218	VAL	2.3
1	D	221	PRO	2.3
1	D	299	ALA	2.3
1	D	332	PRO	2.3
1	C	314	GLY	2.3
1	D	240	HIS	2.3
1	D	98	LEU	2.3
1	D	220	ILE	2.3
1	B	39	ALA	2.2
1	C	303	ALA	2.2
1	D	228	ALA	2.2
1	D	294	THR	2.2
1	D	217	LYS	2.2
1	C	221	PRO	2.2
1	C	299	ALA	2.2
1	C	372	HIS	2.2
1	B	280	LYS	2.2
1	D	345	GLY	2.2
1	D	302	ARG	2.2
1	C	204	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	246	PRO	2.2
1	D	334	ASN	2.2
1	D	373	THR	2.2
1	C	325	LEU	2.2
1	C	377	PHE	2.2
1	B	52	VAL	2.2
1	D	224	ALA	2.2
1	C	287	GLY	2.2
1	D	249	LEU	2.2
1	C	357	ALA	2.1
1	D	286	ALA	2.1
1	D	369	ALA	2.1
1	D	329	LEU	2.1
1	D	336	LEU	2.1
1	C	196	PRO	2.1
1	A	225	VAL	2.1
1	D	35	GLY	2.1
1	C	276	PHE	2.1
1	D	341	TYR	2.1
1	C	370	SER	2.1
1	D	348	GLY	2.1
1	C	101	MET	2.1
1	D	342	GLN	2.0
1	C	100	VAL	2.0
1	D	205	LEU	2.0
1	D	325	LEU	2.0
1	C	103	GLU	2.0
1	C	352	ILE	2.0
1	C	306	PRO	2.0
1	B	45	PHE	2.0
1	C	431	VAL	2.0
1	C	387	LEU	2.0
1	C	328	GLY	2.0
1	C	389	TRP	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	SO4	D	438	5/5	0.41	0.15	137,137,137,137	0
3	FLC	C	445	13/13	0.43	0.14	117,119,121,121	0
2	SO4	C	433	5/5	0.54	0.11	140,141,141,141	0
2	SO4	A	441	5/5	0.54	0.10	143,143,143,143	0
2	SO4	A	448	5/5	0.54	0.15	150,150,150,150	0
2	SO4	B	438	5/5	0.56	0.15	136,136,137,137	0
2	SO4	C	441	5/5	0.58	0.12	151,151,151,152	0
2	SO4	C	444	5/5	0.60	0.14	129,130,130,131	0
2	SO4	B	446	5/5	0.63	0.18	118,119,119,120	0
2	SO4	A	438	5/5	0.64	0.11	122,123,123,123	0
2	SO4	C	437	5/5	0.64	0.13	115,115,116,116	0
2	SO4	A	440	5/5	0.65	0.12	136,136,137,137	0
2	SO4	C	440	5/5	0.65	0.09	140,140,140,141	0
3	FLC	A	451	13/13	0.65	0.19	108,109,111,112	0
2	SO4	A	436	5/5	0.65	0.22	155,155,155,156	0
2	SO4	B	432	5/5	0.67	0.09	120,120,120,120	0
2	SO4	B	434	5/5	0.67	0.09	129,129,129,129	0
2	SO4	A	439	5/5	0.68	0.15	133,134,134,134	0
2	SO4	A	445	5/5	0.68	0.10	114,114,114,114	0
2	SO4	A	432	5/5	0.68	0.21	135,136,136,136	0
2	SO4	A	450	5/5	0.69	0.10	127,127,128,128	0
2	SO4	C	432	5/5	0.70	0.12	104,105,106,106	0
2	SO4	A	437	5/5	0.70	0.10	125,125,125,126	0
2	SO4	A	447	5/5	0.70	0.15	134,134,134,134	0
3	FLC	B	447	13/13	0.71	0.24	104,111,113,113	0
2	SO4	C	436	5/5	0.73	0.10	114,114,115,115	0
2	SO4	D	435	5/5	0.73	0.10	133,133,133,133	0
2	SO4	D	432	5/5	0.74	0.10	140,140,140,141	0
2	SO4	D	439	5/5	0.75	0.09	137,137,137,137	0
2	SO4	B	442	5/5	0.75	0.11	100,101,101,102	0
2	SO4	B	437	5/5	0.76	0.11	121,121,122,122	0
2	SO4	D	433	5/5	0.76	0.08	123,123,123,123	0

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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	0.77	0.13	131,131,131,132	0
2	SO4	B	435	5/5	0.79	0.11	114,114,114,114	0
2	SO4	B	436	5/5	0.80	0.12	116,116,116,117	0
2	SO4	B	440	5/5	0.80	0.16	89,90,91,92	0
2	SO4	C	439	5/5	0.82	0.10	121,121,121,122	0
2	SO4	A	442	5/5	0.82	0.12	97,98,99,99	0
2	SO4	A	446	5/5	0.83	0.09	110,111,111,111	0
2	SO4	C	438	5/5	0.83	0.13	105,105,105,105	0
2	SO4	B	441	5/5	0.84	0.09	90,91,91,91	0
2	SO4	D	434	5/5	0.84	0.11	116,116,116,116	0
2	SO4	A	434	5/5	0.85	0.09	119,120,120,120	0
2	SO4	B	445	5/5	0.86	0.09	81,82,83,83	0
2	SO4	C	435	5/5	0.87	0.11	87,88,89,89	0
2	SO4	C	443	5/5	0.87	0.08	102,102,102,103	0
2	SO4	B	433	5/5	0.87	0.11	97,97,98,99	0
4	ZN	B	448	1/1	0.89	0.09	84,84,84,84	0
2	SO4	A	443	5/5	0.90	0.11	76,77,77,79	0
2	SO4	B	439	5/5	0.91	0.10	72,74,74,74	0
2	SO4	D	440	5/5	0.93	0.08	81,82,83,83	0
2	SO4	B	444	5/5	0.93	0.09	45,49,50,51	0
2	SO4	D	437	5/5	0.93	0.11	88,88,89,90	0
2	SO4	A	444	5/5	0.93	0.08	82,82,82,83	0
2	SO4	B	443	5/5	0.93	0.09	60,61,62,63	0
4	ZN	C	446	1/1	0.93	0.09	100,100,100,100	0
4	ZN	D	441	1/1	0.93	0.11	92,92,92,92	0
2	SO4	C	442	5/5	0.94	0.07	64,64,66,66	0
2	SO4	D	436	5/5	0.94	0.07	67,67,68,69	0
2	SO4	A	433	5/5	0.94	0.14	59,61,62,64	0
2	SO4	A	449	5/5	0.94	0.08	40,44,46,47	0
4	ZN	A	452	1/1	0.97	0.06	80,80,80,80	0
2	SO4	A	435	5/5	0.97	0.08	43,44,46,50	0

6.5 Other polymers [i](#)

There are no such residues in this entry.