



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 03:07 PM GMT

PDB ID : 3IE1
Title : Crystal structure of H380A mutant TTHA0252 from *Thermus thermophilus* HB8 complexed with RNA
Authors : Ishikawa, H.; Nakagawa, N.; Kuramitsu, S.; Yokoyama, S.; Masui, R.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on : 2009-07-22
Resolution : 2.85 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

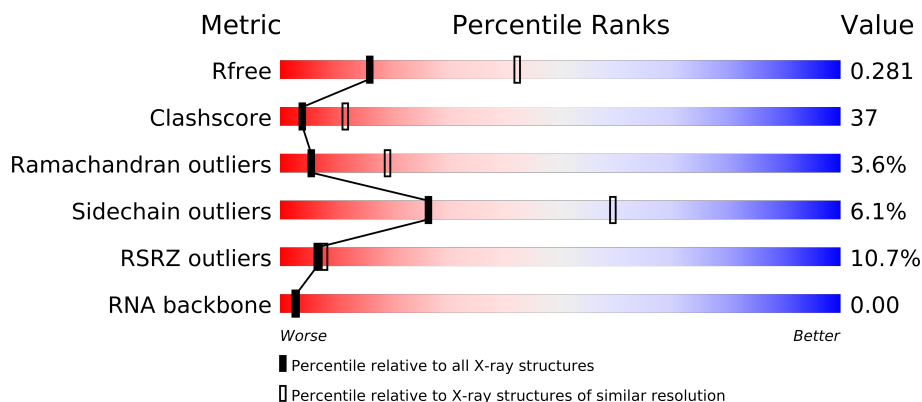
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.85 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}	66092	1524 (2.90-2.82)
Clashscore	79885	1879 (2.90-2.82)
Ramachandran outliers	78287	1824 (2.90-2.82)
Sidechain outliers	78261	1827 (2.90-2.82)
RSRZ outliers	66119	1526 (2.90-2.82)
RNA backbone	1838	1014 (3.32-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	431	
1	B	431	
1	C	431	
1	D	431	
2	E	4	
2	F	4	
2	G	4	
2	H	4	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	SO4	A	432	-	X
3	SO4	A	436	-	X
3	SO4	A	442	-	X
3	SO4	A	444	-	X
3	SO4	A	448	-	X
3	SO4	A	449	-	X
3	SO4	B	432	-	X
3	SO4	B	435	-	X
3	SO4	B	436	-	X
3	SO4	B	444	-	X
3	SO4	B	447	-	X
3	SO4	C	434	-	X
4	FLC	A	450	-	X
4	FLC	A	451	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 13910 atoms, of which 0 are hydrogen and 0 are deuterium.

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			

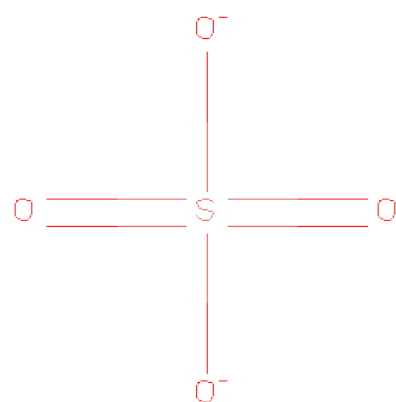
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	380	ALA	HIS	ENGINEERED	UNP Q5SLP1
B	380	ALA	HIS	ENGINEERED	UNP Q5SLP1
C	380	ALA	HIS	ENGINEERED	UNP Q5SLP1
D	380	ALA	HIS	ENGINEERED	UNP Q5SLP1

- Molecule 2 is a RNA chain called RNA (5'-R(P*UP*UP*UP*U)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	4	Total	C	N	O	P	0	0	0
			81	36	8	33	4			
2	F	4	Total	C	N	O	P	0	0	0
			81	36	8	33	4			
2	G	2	Total	C	N	O	P	0	0	0
			41	18	4	17	2			
2	H	4	Total	C	N	O	P	0	0	0
			81	36	8	33	4			

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

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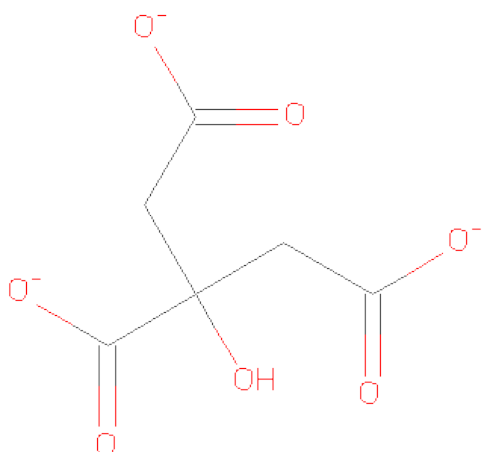
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total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

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

- Molecule 4 is CITRATE ANION (three-letter code: FLC) (formula: C₆H₅O₇).



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

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	14	Total	O	0	0
			14	14		
6	B	11	Total	O	0	0
			11	11		
6	C	4	Total	O	0	0
			4	4		

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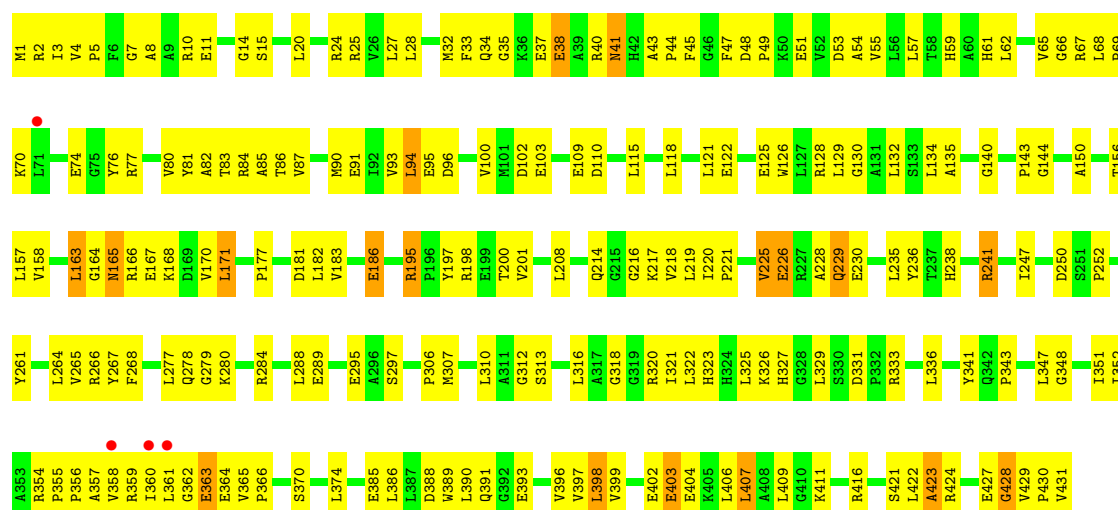
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	D	7	Total	O	0	0
			7	7		
6	E	1	Total	O	0	0
			1	1		
6	G	1	Total	O	0	0
			1	1		

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

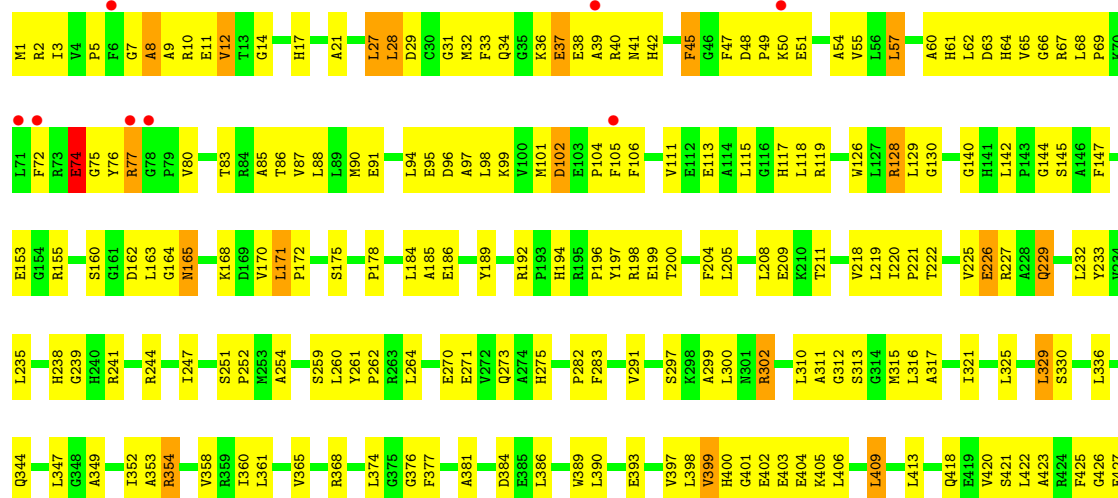
• Molecule 1: Ribonuclease TTHA0252

Chain A:



• Molecule 1: Ribonuclease TTHA0252

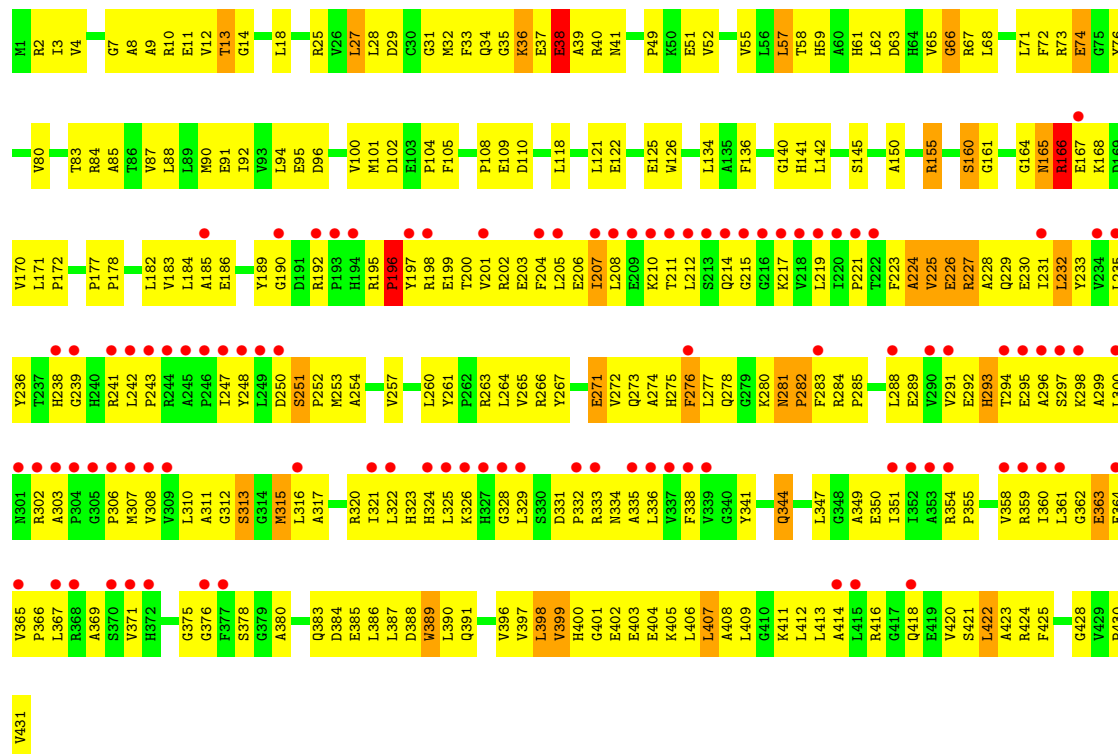
Chain B:



V431

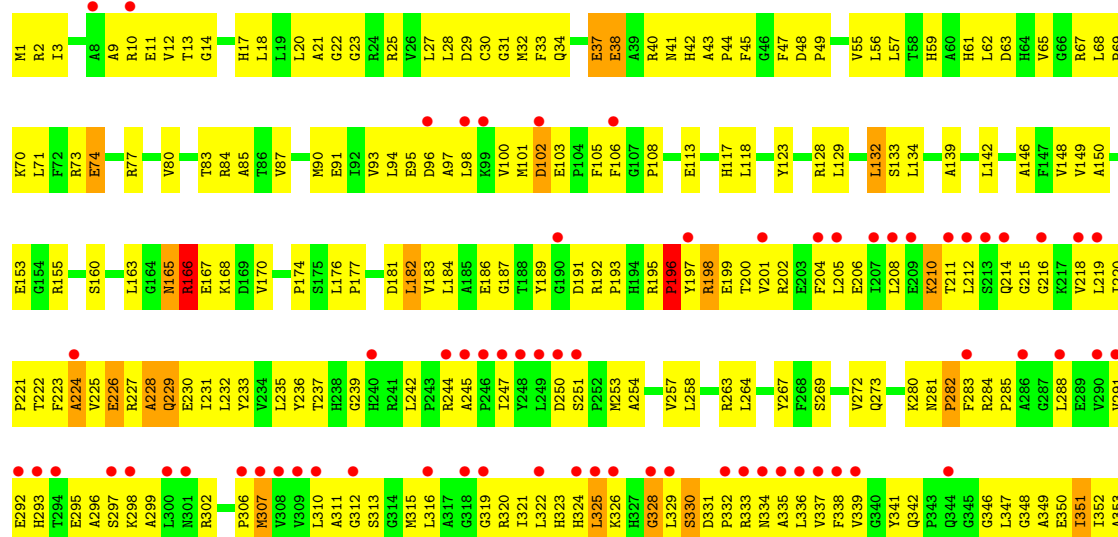
• Molecule 1: Ribonuclease TTHA0252

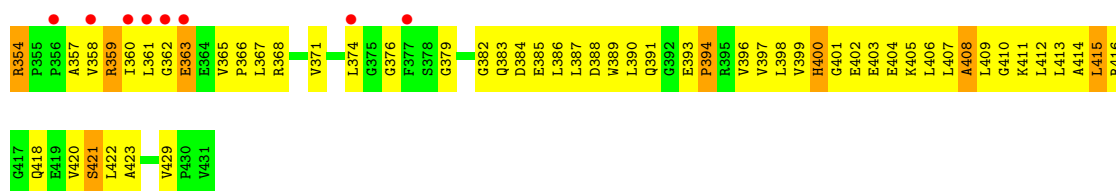
Chain C:



• Molecule 1: Ribonuclease TTHA0252

Chain D:





- Molecule 2: RNA (5'-R(P*UP*UP*UP*U)-3')

Chain E:



- Molecule 2: RNA (5'-R(P*UP*UP*UP*U)-3')

Chain F:



- Molecule 2: RNA (5'-R(P*UP*UP*UP*U)-3')

Chain G:



- Molecule 2: RNA (5'-R(P*UP*UP*UP*U)-3')

Chain H:



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	143.42Å 148.16Å 120.84Å 90.00° 109.61° 90.00°	Depositor
Resolution (Å)	50.00 – 2.85 49.92 – 2.85	Depositor EDS
% Data completeness (in resolution range)	97.2 (50.00-2.85) 97.5 (49.92-2.85)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.11 (at 2.86Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.231 , 0.291 0.223 , 0.281	Depositor DCC
R_{free} test set	5446 reflections (11.23%)	DCC
Wilson B-factor (Å ²)	65.4	Xtriage
Anisotropy	0.147	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 39.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 55129 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	13910	wwPDB-VP
Average B, all atoms (Å ²)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.35% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.44	0/3401	0.70	0/4613
1	B	0.44	0/3401	0.71	0/4613
1	C	0.33	0/3401	0.59	1/4613 (0.0%)
1	D	0.33	0/3401	0.58	0/4613
2	E	0.94	1/88 (1.1%)	0.85	0/132
2	F	1.03	1/88 (1.1%)	0.87	0/132
2	G	1.32	1/44 (2.3%)	0.82	0/64
2	H	0.97	1/88 (1.1%)	0.84	0/132
All	All	0.41	4/13912 (0.0%)	0.65	1/18912 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	E	0	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	1	U	OP3-P	-7.19	1.52	1.61
2	F	1	U	OP3-P	-7.16	1.52	1.61
2	G	1	U	OP3-P	-7.11	1.52	1.61
2	E	1	U	OP3-P	-6.32	1.53	1.61

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	161	GLY	N-CA-C	-5.33	99.79	113.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	E	1	U	Sidechain

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3321	0	3349	192	0
1	B	3321	0	3349	196	0
1	C	3321	0	3349	322	0
1	D	3321	0	3349	313	0
2	E	81	0	41	6	0
2	F	81	0	41	8	0
2	G	41	0	21	5	0
2	H	81	0	41	16	0
3	A	90	0	0	2	0
3	B	85	0	0	3	0
3	C	50	0	0	1	0
3	D	45	0	0	5	0
4	A	26	0	10	6	0
5	A	2	0	0	0	0
5	B	2	0	0	0	0
5	C	2	0	0	0	0
5	D	2	0	0	0	0
6	A	14	0	0	0	0
6	B	11	0	0	0	0
6	C	4	0	0	0	0
6	D	7	0	0	0	0
6	E	1	0	0	0	0
6	G	1	0	0	0	0
All	All	13910	0	13550	1026	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 37.

All (1026) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:363:GLU:HG2	1:C:364:GLU:H	1.26	0.99
1:D:37:GLU:HG3	1:D:40:ARG:HH11	1.26	0.99
1:C:359:ARG:HH12	1:C:362:GLY:HA2	1.25	0.99
1:D:1:MET:HG3	1:D:21:ALA:HB2	1.40	0.98
1:C:250:ASP:HB3	1:C:311:ALA:HB2	1.45	0.98
1:B:33:PHE:H	1:B:41:ASN:HD21	0.98	0.97
1:A:195:ARG:HB2	3:A:432:SO4:O3	1.64	0.96
1:A:220:ILE:HB	1:A:310:LEU:HD23	1.48	0.96
1:C:235:LEU:HD13	1:C:247:ILE:HD13	1.48	0.96
1:C:33:PHE:H	1:C:41:ASN:HD21	1.00	0.95
1:C:205:LEU:HA	1:C:208:LEU:HD12	1.49	0.92
1:D:33:PHE:H	1:D:41:ASN:HD21	1.11	0.92
1:D:359:ARG:HH12	1:D:362:GLY:HA2	1.37	0.90
1:A:228:ALA:HB3	1:A:229:GLN:NE2	1.86	0.90
1:C:403:GLU:O	1:C:407:LEU:HD13	1.71	0.90
1:B:238:HIS:O	1:B:241:ARG:HG2	1.75	0.86
1:B:360:ILE:HG22	1:B:361:LEU:HD13	1.55	0.86
1:C:359:ARG:HH12	1:C:362:GLY:CA	1.89	0.86
1:D:420:VAL:HG22	1:D:421:SER:H	1.42	0.85
1:D:57:LEU:HD21	1:D:80:VAL:CG1	2.07	0.85
1:C:62:LEU:HD22	2:G:2:U:H3'	1.59	0.85
1:C:420:VAL:HG22	1:C:421:SER:H	1.41	0.85
1:D:98:LEU:HD11	1:D:108:PRO:HA	1.58	0.84
1:C:250:ASP:HA	1:C:291:VAL:HB	1.57	0.84
1:A:10:ARG:HG3	1:A:10:ARG:HH11	1.42	0.84
1:D:258:LEU:HD11	1:D:283:PHE:HB3	1.58	0.84
1:B:401:GLY:HA3	1:B:406:LEU:HD11	1.60	0.84
1:D:191:ASP:OD2	1:D:192:ARG:HG2	1.77	0.83
1:B:349:ALA:HA	1:B:352:ILE:HD12	1.62	0.82
1:A:33:PHE:HB3	1:A:37:GLU:HB2	1.61	0.82
1:D:330:SER:O	1:D:368:ARG:HB2	1.80	0.82
1:A:235:LEU:HD13	1:A:247:ILE:HD13	1.61	0.82
1:B:33:PHE:N	1:B:41:ASN:HD21	1.77	0.81
1:A:20:LEU:HD22	1:A:25:ARG:HH11	1.43	0.81
1:D:168:LYS:HE2	1:D:230:GLU:OE2	1.79	0.81
1:C:221:PRO:HB3	1:C:321:ILE:HG12	1.62	0.81
1:D:165:ASN:HB3	1:D:168:LYS:HG3	1.62	0.81
1:A:411:LYS:HB2	4:A:451:FLC:OB2	1.80	0.81
1:C:88:LEU:HB3	1:C:260:LEU:HD21	1.61	0.81
1:D:45:PHE:HB3	1:D:47:PHE:CE1	2.14	0.81
1:C:420:VAL:HG22	1:C:421:SER:N	1.96	0.80
1:B:88:LEU:HD12	1:B:264:LEU:HD11	1.64	0.79

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:37:GLU:HB2	1:D:40:ARG:HE	1.48	0.78
1:B:221:PRO:HB3	1:B:321:ILE:HG12	1.65	0.78
1:C:200:THR:HG21	1:C:376:GLY:HA3	1.65	0.78
1:C:192:ARG:HH12	1:C:405:LYS:NZ	1.82	0.77
1:B:27:LEU:HB3	1:B:55:VAL:HG12	1.67	0.77
1:D:211:THR:HG21	1:D:335:ALA:HB2	1.66	0.77
1:D:316:LEU:HB3	1:D:347:LEU:HD23	1.66	0.77
1:D:73:ARG:NH2	1:D:106:PHE:HA	1.98	0.77
1:D:57:LEU:HD21	1:D:80:VAL:HG12	1.67	0.77
1:D:284:ARG:HA	1:D:288:LEU:HD22	1.65	0.77
1:C:168:LYS:HE2	1:C:230:GLU:OE1	1.84	0.77
1:A:84:ARG:HG2	1:A:84:ARG:HH11	1.50	0.77
1:C:336:LEU:HB3	1:C:371:VAL:HG22	1.67	0.76
1:B:37:GLU:HG2	1:B:40:ARG:HH11	1.50	0.76
1:D:55:VAL:CG2	1:D:80:VAL:HG13	2.15	0.76
1:C:57:LEU:HD23	1:C:90:MET:HE2	1.66	0.76
1:C:197:TYR:O	1:C:201:VAL:HG23	1.85	0.76
1:A:348:GLY:O	1:A:352:ILE:HG13	1.86	0.76
1:B:33:PHE:H	1:B:41:ASN:ND2	1.81	0.75
1:D:399:VAL:HG12	1:D:400:HIS:H	1.51	0.75
1:D:215:GLY:HA2	1:D:306:PRO:HD3	1.67	0.75
1:D:200:THR:HG21	1:D:376:GLY:HA3	1.68	0.75
1:C:192:ARG:HH12	1:C:405:LYS:HZ1	1.34	0.75
1:C:211:THR:HG21	1:C:335:ALA:HB2	1.68	0.75
1:C:351:ILE:HG23	1:C:367:LEU:HD11	1.67	0.74
1:B:153:GLU:O	1:B:155:ARG:HG2	1.86	0.74
1:C:57:LEU:HD23	1:C:90:MET:CE	2.18	0.74
1:C:383:GLN:O	1:C:387:LEU:HG	1.86	0.74
1:A:228:ALA:HB3	1:A:229:GLN:HE22	1.50	0.74
1:C:227:ARG:HH21	1:C:378:SER:HA	1.51	0.74
1:C:232:LEU:HD21	1:C:288:LEU:HD13	1.70	0.73
1:D:222:THR:HG22	1:D:339:VAL:HG21	1.69	0.73
1:C:402:GLU:OE1	1:C:405:LYS:HE2	1.88	0.73
1:A:225:VAL:O	1:A:229:GLN:NE2	2.22	0.73
1:A:76:TYR:O	1:A:77:ARG:HD2	1.87	0.73
1:B:61:HIS:CD2	1:B:142:LEU:HD11	2.23	0.73
1:C:293:HIS:HB2	1:C:295:GLU:HG2	1.70	0.73
1:B:97:ALA:O	1:B:101:MET:HB2	1.89	0.73
1:A:347:LEU:HD11	1:A:358:VAL:HG11	1.70	0.73
1:D:84:ARG:HB3	1:D:267:TYR:OH	1.87	0.73
1:C:387:LEU:HB3	1:C:416:ARG:HH12	1.53	0.72
1:B:229:GLN:HA	1:B:232:LEU:HD12	1.72	0.72

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:91:GLU:O	1:A:95:GLU:HG2	1.90	0.72
1:C:215:GLY:HA2	1:C:306:PRO:HD3	1.72	0.72
1:A:10:ARG:HG3	1:A:10:ARG:NH1	2.04	0.72
1:B:196:PRO:HB2	1:B:199:GLU:HG2	1.72	0.72
1:D:170:VAL:HA	1:D:272:VAL:HG21	1.70	0.71
1:A:122:GLU:O	1:A:125:GLU:HB2	1.90	0.71
1:D:91:GLU:O	1:D:95:GLU:HG2	1.91	0.71
1:B:259:SER:O	1:B:262:PRO:HD2	1.91	0.71
1:D:403:GLU:O	1:D:407:LEU:HB2	1.91	0.71
1:D:128:ARG:O	1:D:129:LEU:HD23	1.91	0.71
1:A:208:LEU:HD23	1:A:218:VAL:HG21	1.72	0.71
1:C:49:PRO:HG3	1:C:74:GLU:HB3	1.73	0.70
1:A:183:VAL:HG21	1:A:393:GLU:HG3	1.72	0.70
1:D:102:ASP:CG	1:D:103:GLU:H	1.95	0.70
1:A:411:LYS:HD2	4:A:451:FLC:HG2	1.74	0.70
1:C:360:ILE:HG22	1:C:361:LEU:HD13	1.73	0.70
1:D:299:ALA:HA	1:D:302:ARG:HD3	1.74	0.70
1:A:200:THR:HG23	1:A:374:LEU:HB3	1.74	0.69
1:A:168:LYS:HE3	1:A:230:GLU:OE2	1.90	0.69
1:C:387:LEU:HB3	1:C:416:ARG:NH1	2.06	0.69
1:C:325:LEU:O	1:C:329:LEU:HD13	1.92	0.69
1:D:55:VAL:HG23	1:D:80:VAL:HG13	1.74	0.69
1:A:229:GLN:H	1:A:229:GLN:NE2	1.90	0.69
1:B:34:GLN:OE1	1:B:62:LEU:HD23	1.93	0.69
1:C:363:GLU:HG2	1:C:364:GLU:N	2.05	0.69
1:B:76:TYR:C	1:B:77:ARG:HD2	2.12	0.69
1:D:360:ILE:HG22	1:D:361:LEU:HD13	1.76	0.68
1:D:410:GLY:HA2	1:D:420:VAL:HG21	1.76	0.68
1:D:84:ARG:NH2	1:D:263:ARG:HH21	1.89	0.68
1:C:235:LEU:O	1:C:239:GLY:N	2.26	0.68
1:C:402:GLU:HB2	1:C:405:LYS:HG2	1.75	0.68
1:B:55:VAL:HG23	1:B:80:VAL:HG13	1.75	0.68
1:B:68:LEU:N	1:B:69:PRO:HD2	2.09	0.68
1:C:91:GLU:O	1:C:95:GLU:HG2	1.92	0.68
1:D:1:MET:HE2	1:D:21:ALA:HB1	1.75	0.68
1:C:13:THR:HG21	1:C:34:GLN:H	1.57	0.68
1:B:229:GLN:CD	1:B:229:GLN:H	1.97	0.68
1:A:166:ARG:HG2	1:A:385:GLU:OE2	1.94	0.68
1:B:192:ARG:HG2	1:B:192:ARG:HH11	1.57	0.68
1:A:407:LEU:HG	4:A:451:FLC:OB1	1.93	0.68
1:C:27:LEU:O	1:C:55:VAL:HG23	1.93	0.68
1:C:420:VAL:CG2	1:C:421:SER:H	2.07	0.68

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:95:GLU:O	1:B:98:LEU:HB2	1.94	0.68
1:D:62:LEU:HD13	1:D:93:VAL:HG12	1.75	0.68
1:A:134:LEU:HD23	1:A:150:ALA:HA	1.75	0.68
1:A:37:GLU:HB3	1:A:40:ARG:HD3	1.76	0.67
1:D:321:ILE:HG13	1:D:325:LEU:HD13	1.75	0.67
1:D:37:GLU:CG	1:D:40:ARG:HH11	2.05	0.67
1:C:49:PRO:HB3	1:C:71:LEU:HD12	1.77	0.67
1:D:14:GLY:HA2	1:D:31:GLY:O	1.95	0.66
1:A:220:ILE:HB	1:A:310:LEU:CD2	2.24	0.66
1:D:199:GLU:HA	1:D:202:ARG:HE	1.60	0.66
1:A:45:PHE:HB3	1:A:47:PHE:CE1	2.31	0.66
1:D:206:GLU:O	1:D:210:LYS:HD3	1.94	0.66
1:D:139:ALA:O	1:D:174:PRO:HG3	1.95	0.66
1:A:128:ARG:O	1:A:129:LEU:HD23	1.95	0.66
1:C:87:VAL:HG13	1:C:118:LEU:CD1	2.25	0.66
1:B:163:LEU:HD21	1:B:389:TRP:CD2	2.31	0.66
1:C:182:LEU:HD23	1:C:431:VAL:HG22	1.76	0.66
1:C:208:LEU:HD13	1:C:242:LEU:HD13	1.76	0.66
1:D:331:ASP:HB2	1:D:334:ASN:ND2	2.11	0.66
1:D:166:ARG:HG3	1:D:166:ARG:O	1.95	0.66
1:D:359:ARG:HH12	1:D:362:GLY:CA	2.09	0.66
1:D:229:GLN:NE2	1:D:229:GLN:H	1.93	0.65
1:B:313:SER:HB3	2:F:3:U:C6	2.30	0.65
1:D:177:PRO:HD3	1:D:389:TRP:NE1	2.10	0.65
1:C:233:TYR:CE1	1:C:282:PRO:HB2	2.32	0.65
1:D:383:GLN:O	1:D:387:LEU:HG	1.96	0.65
1:A:217:LYS:HE2	1:A:307:MET:HE2	1.78	0.65
1:D:336:LEU:HD13	1:D:371:VAL:HG22	1.79	0.65
1:A:96:ASP:O	1:A:100:VAL:HG23	1.97	0.65
1:B:48:ASP:OD2	1:B:51:GLU:HG2	1.97	0.65
1:D:90:MET:HE3	1:D:118:LEU:HD13	1.78	0.64
1:B:225:VAL:O	1:B:229:GLN:NE2	2.30	0.64
1:D:2:ARG:NH1	3:D:437:SO4:S	2.70	0.64
1:C:87:VAL:HG13	1:C:118:LEU:HD13	1.78	0.64
1:B:7:GLY:HA3	1:B:14:GLY:O	1.97	0.64
1:D:224:ALA:HB3	1:D:253:MET:CE	2.27	0.64
1:D:224:ALA:HB3	1:D:253:MET:HE2	1.80	0.64
1:D:212:LEU:HD22	1:D:306:PRO:HB2	1.80	0.64
1:D:37:GLU:HG3	1:D:40:ARG:NH1	2.07	0.64
1:D:73:ARG:HH21	1:D:106:PHE:HA	1.61	0.64
1:D:9:ALA:O	1:D:11:GLU:HG2	1.98	0.64
1:C:280:LYS:O	1:C:282:PRO:HD3	1.98	0.63

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:H:3:U:H2'	2:H:4:U:C5'	2.27	0.63
1:C:211:THR:HG21	1:C:335:ALA:CB	2.28	0.63
1:B:330:SER:O	1:B:368:ARG:HB2	1.98	0.63
1:C:3:ILE:HD12	1:C:18:LEU:O	1.99	0.63
1:B:12:VAL:HG12	1:B:401:GLY:CA	2.28	0.63
1:A:1:MET:HG2	1:A:431:VAL:HG21	1.79	0.63
1:C:416:ARG:HD2	1:C:418:GLN:OE1	1.98	0.63
1:C:316:LEU:HD11	1:C:338:PHE:CE1	2.34	0.63
1:C:207:ILE:O	1:C:207:ILE:HG22	1.99	0.63
1:D:87:VAL:HG13	1:D:118:LEU:HD13	1.80	0.63
1:C:232:LEU:O	1:C:283:PHE:HA	1.99	0.63
1:C:224:ALA:HA	1:C:254:ALA:HB2	1.80	0.63
1:D:396:VAL:HG12	1:D:398:LEU:HD12	1.81	0.63
1:D:236:TYR:CA	1:D:285:PRO:HB3	2.27	0.62
1:D:420:VAL:HG22	1:D:421:SER:N	2.13	0.62
1:D:10:ARG:HG3	1:D:10:ARG:HH11	1.64	0.62
1:C:359:ARG:NH1	1:C:362:GLY:HA2	2.07	0.62
1:C:351:ILE:HG22	1:C:371:VAL:HG21	1.81	0.62
1:D:57:LEU:CD2	1:D:80:VAL:HG12	2.29	0.62
1:D:10:ARG:NH1	1:D:422:LEU:HB3	2.15	0.62
1:C:236:TYR:N	1:C:285:PRO:HB3	2.14	0.62
1:A:358:VAL:HG12	1:A:359:ARG:N	2.15	0.62
1:D:177:PRO:HD3	1:D:389:TRP:CE2	2.33	0.62
1:B:3:ILE:HD11	1:B:17:HIS:HB3	1.82	0.62
1:A:85:ALA:HB2	1:A:267:TYR:CE2	2.34	0.62
1:C:384:ASP:HA	1:C:387:LEU:HD12	1.82	0.62
1:B:37:GLU:CG	1:B:40:ARG:HE	2.13	0.61
1:B:347:LEU:HD11	1:B:358:VAL:HG11	1.82	0.61
1:C:92:ILE:HD11	1:C:260:LEU:HD22	1.82	0.61
1:D:236:TYR:HA	1:D:285:PRO:HB3	1.83	0.61
1:D:18:LEU:HD11	1:D:25:ARG:HB3	1.83	0.61
1:A:59:HIS:CD2	1:A:61:HIS:HB2	2.36	0.61
1:B:111:VAL:O	1:B:115:LEU:HG	2.01	0.61
1:B:72:PHE:HE2	1:B:117:HIS:ND1	1.99	0.61
1:C:233:TYR:HE1	1:C:282:PRO:HB2	1.63	0.61
1:B:401:GLY:HA3	1:B:406:LEU:CD1	2.30	0.61
1:D:319:GLY:HA2	2:H:3:U:H1'	1.81	0.61
1:D:2:ARG:NH1	3:D:437:SO4:O4	2.33	0.61
1:B:7:GLY:O	1:B:9:ALA:N	2.34	0.61
1:A:33:PHE:H	1:A:41:ASN:HD21	1.47	0.60
1:B:204:PHE:HB2	1:B:374:LEU:HD13	1.83	0.60
1:D:325:LEU:O	1:D:329:LEU:HD13	2.01	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:31:GLY:HA3	1:B:63:ASP:C	2.21	0.60
1:C:32:MET:HA	1:C:67:ARG:HG3	1.83	0.60
1:D:1:MET:HG3	1:D:21:ALA:CB	2.25	0.60
1:C:12:VAL:HG12	1:C:400:HIS:C	2.22	0.60
1:B:208:LEU:CD2	1:B:218:VAL:HG11	2.32	0.60
2:H:3:U:H2'	2:H:4:U:H5''	1.83	0.60
1:D:232:LEU:HD22	1:D:288:LEU:HD13	1.83	0.60
1:D:382:GLY:O	1:D:386:LEU:HD13	2.02	0.60
1:B:299:ALA:O	1:B:302:ARG:HD2	2.01	0.60
1:A:325:LEU:O	1:A:329:LEU:HB2	2.01	0.60
1:C:83:THR:O	1:C:87:VAL:HG23	2.01	0.60
1:C:278:GLN:O	1:C:280:LYS:HG3	2.02	0.60
2:G:1:U:O2'	2:G:2:U:H5''	2.01	0.60
1:D:100:VAL:HG13	2:H:3:U:C4	2.37	0.60
1:D:399:VAL:HG12	1:D:400:HIS:N	2.15	0.60
1:A:24:ARG:HA	1:A:53:ASP:OD2	2.02	0.60
1:B:192:ARG:HG2	1:B:192:ARG:NH1	2.16	0.60
1:D:325:LEU:O	1:D:329:LEU:HB2	2.02	0.60
1:A:221:PRO:HB3	1:A:321:ILE:HG12	1.82	0.60
1:A:411:LYS:HA	4:A:451:FLC:HA2	1.81	0.59
2:G:2:U:O2	2:G:2:U:H2'	2.01	0.59
1:A:20:LEU:HD22	1:A:25:ARG:NH1	2.15	0.59
1:A:200:THR:CG2	1:A:374:LEU:HB3	2.31	0.59
1:B:91:GLU:O	1:B:95:GLU:HG2	2.01	0.59
1:B:353:ALA:O	1:B:354:ARG:CB	2.51	0.59
1:D:250:ASP:HB3	1:D:311:ALA:HB2	1.84	0.59
1:D:399:VAL:HG22	1:D:423:ALA:CB	2.33	0.59
1:D:322:LEU:HD13	1:D:361:LEU:HD11	1.84	0.59
1:C:14:GLY:HA2	1:C:31:GLY:C	2.23	0.59
1:C:336:LEU:CB	1:C:371:VAL:HG22	2.32	0.59
1:A:198:ARG:NH2	1:A:198:ARG:HG3	2.16	0.59
1:D:299:ALA:HA	1:D:302:ARG:CD	2.32	0.59
1:C:217:LYS:HG2	1:C:307:MET:HG2	1.85	0.58
1:A:68:LEU:N	1:A:69:PRO:HD2	2.18	0.58
1:B:381:ALA:HB3	1:B:386:LEU:HD13	1.85	0.58
1:C:90:MET:SD	1:C:118:LEU:HD11	2.42	0.58
1:D:163:LEU:N	1:D:163:LEU:HD12	2.18	0.58
1:B:200:THR:OG1	1:B:376:GLY:HA3	2.03	0.58
1:B:252:PRO:HD2	2:F:4:U:OP1	2.03	0.58
1:C:252:PRO:HD2	3:C:436:SO4:S	2.43	0.58
1:A:157:LEU:HG	1:A:158:VAL:N	2.15	0.58
1:C:413:LEU:HD22	1:C:418:GLN:NE2	2.19	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:H:1:U:O2'	2:H:2:U:H4'	2.03	0.58
1:D:61:HIS:HA	2:H:2:U:OP2	2.03	0.58
1:C:33:PHE:CD2	1:C:40:ARG:HB2	2.38	0.58
1:D:13:THR:HG21	1:D:34:GLN:HB2	1.84	0.58
1:D:208:LEU:HD23	1:D:218:VAL:HG11	1.85	0.58
1:D:332:PRO:HA	1:D:368:ARG:O	2.03	0.58
1:A:186:GLU:HA	1:A:399:VAL:O	2.03	0.58
1:A:3:ILE:O	1:A:428:GLY:HA2	2.03	0.58
1:B:33:PHE:HB3	1:B:37:GLU:HB2	1.85	0.58
1:C:232:LEU:HD13	1:C:288:LEU:HD22	1.86	0.58
1:D:350:GLU:HG3	1:D:351:ILE:N	2.19	0.58
1:D:297:SER:HB2	1:D:320:ARG:HH11	1.69	0.58
1:D:239:GLY:HA2	1:D:242:LEU:HD12	1.86	0.58
1:D:229:GLN:CD	1:D:229:GLN:H	2.08	0.58
1:A:217:LYS:HE2	1:A:307:MET:CE	2.34	0.58
1:A:404:GLU:CD	1:A:404:GLU:H	2.06	0.58
1:C:61:HIS:CD2	1:C:142:LEU:HD11	2.38	0.57
1:C:182:LEU:HD12	1:C:183:VAL:N	2.19	0.57
1:C:299:ALA:O	1:C:303:ALA:HB2	2.04	0.57
1:D:13:THR:HB	1:D:33:PHE:HA	1.86	0.57
1:D:225:VAL:O	1:D:229:GLN:NE2	2.37	0.57
1:B:185:ALA:O	1:B:399:VAL:HG22	2.03	0.57
1:C:277:LEU:HB3	1:C:278:GLN:NE2	2.19	0.57
1:A:266:ARG:NH2	1:D:273:GLN:HE22	2.03	0.57
1:B:220:ILE:HB	1:B:310:LEU:HD23	1.86	0.57
1:C:208:LEU:HD13	1:C:242:LEU:CD1	2.33	0.57
1:D:32:MET:HE1	1:D:105:PHE:CZ	2.39	0.57
1:A:85:ALA:HB2	1:A:267:TYR:CD2	2.39	0.57
1:B:178:PRO:HB3	1:C:126:TRP:CE3	2.40	0.57
1:B:86:THR:HG22	1:B:90:MET:CE	2.35	0.57
1:B:221:PRO:HA	1:B:311:ALA:O	2.04	0.57
1:C:336:LEU:O	1:C:371:VAL:HA	2.04	0.57
1:D:269:SER:OG	1:D:272:VAL:HG23	2.04	0.57
1:D:68:LEU:N	1:D:69:PRO:HD2	2.19	0.57
1:B:168:LYS:HG2	1:B:197:TYR:CD2	2.39	0.57
1:C:388:ASP:O	1:C:391:GLN:HB2	2.04	0.57
1:C:55:VAL:HG13	1:C:80:VAL:HG13	1.87	0.57
1:D:321:ILE:O	1:D:325:LEU:HB2	2.04	0.57
1:D:83:THR:O	1:D:87:VAL:HG23	2.04	0.57
1:A:170:VAL:HG21	1:A:230:GLU:HG3	1.86	0.57
1:D:186:GLU:HA	1:D:399:VAL:O	2.04	0.57
2:F:1:U:H2'	2:F:2:U:O5'	2.04	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:34:GLN:NE2	1:C:62:LEU:HD23	2.18	0.57
1:A:32:MET:HE3	1:A:66:GLY:HA3	1.87	0.57
1:C:170:VAL:HG12	1:C:171:LEU:HD12	1.87	0.57
1:C:204:PHE:CE1	1:C:208:LEU:HD11	2.39	0.57
1:D:31:GLY:O	1:D:67:ARG:HD3	2.04	0.57
1:B:10:ARG:HD3	1:B:403:GLU:OE2	2.04	0.57
1:B:252:PRO:HD2	2:F:4:U:P	2.45	0.57
1:D:235:LEU:HD13	1:D:247:ILE:HD13	1.87	0.57
1:A:360:ILE:HG22	1:A:361:LEU:HD13	1.87	0.57
1:A:65:VAL:HG12	1:A:94:LEU:HD11	1.87	0.56
1:D:399:VAL:HG22	1:D:423:ALA:HB2	1.87	0.56
1:B:220:ILE:HG22	1:B:222:THR:HG23	1.88	0.56
1:C:228:ALA:HB3	1:C:229:GLN:HE21	1.69	0.56
1:B:172:PRO:HA	3:B:440:SO4:O1	2.05	0.56
1:C:250:ASP:OD1	1:C:320:ARG:HD2	2.05	0.56
1:C:236:TYR:OH	1:C:280:LYS:HE2	2.05	0.56
1:B:349:ALA:CA	1:B:352:ILE:HD12	2.35	0.56
1:D:251:SER:HB3	1:D:254:ALA:HB3	1.86	0.56
1:C:312:GLY:HA2	1:C:313:SER:O	2.05	0.56
1:D:204:PHE:CE1	1:D:208:LEU:HD11	2.41	0.56
1:B:65:VAL:HG11	1:B:90:MET:SD	2.45	0.56
1:C:59:HIS:HB3	1:C:145:SER:HA	1.87	0.56
1:C:10:ARG:HH21	1:C:424:ARG:HG2	1.70	0.56
1:C:224:ALA:HB3	1:C:253:MET:CE	2.36	0.56
1:D:224:ALA:O	1:D:257:VAL:HG21	2.05	0.56
1:D:337:VAL:CG1	1:D:374:LEU:HD12	2.36	0.56
1:B:32:MET:SD	1:B:62:LEU:HD21	2.46	0.56
1:C:142:LEU:CD2	1:C:226:GLU:HB2	2.36	0.56
1:D:315:MET:HA	1:D:342:GLN:HE22	1.69	0.56
1:B:142:LEU:CD2	1:B:226:GLU:HB2	2.35	0.56
1:C:250:ASP:OD2	1:C:291:VAL:HG11	2.06	0.56
1:B:315:MET:O	1:B:317:ALA:N	2.39	0.56
1:A:360:ILE:CG2	1:A:361:LEU:HD13	2.35	0.56
1:C:294:THR:HG22	1:C:298:LYS:HG2	1.87	0.55
1:A:235:LEU:CD1	1:A:247:ILE:HD13	2.35	0.55
1:C:121:LEU:HD23	1:C:136:PHE:CE2	2.41	0.55
1:D:123:TYR:HE1	1:D:146:ALA:HB2	1.70	0.55
1:C:336:LEU:HD13	1:C:351:ILE:HG21	1.89	0.55
1:D:224:ALA:HB1	1:D:254:ALA:CA	2.36	0.55
1:D:353:ALA:O	1:D:354:ARG:HB2	2.05	0.55
1:D:307:MET:HG3	1:D:307:MET:O	2.04	0.55
1:B:128:ARG:HD3	1:C:177:PRO:O	2.06	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:316:LEU:HD11	1:C:338:PHE:CZ	2.42	0.55
1:B:90:MET:O	1:B:94:LEU:HB2	2.07	0.55
1:C:65:VAL:HG12	1:C:94:LEU:HD11	1.89	0.55
1:C:171:LEU:HB3	1:C:172:PRO:HD2	1.87	0.55
1:B:88:LEU:HD13	1:B:260:LEU:HD11	1.87	0.55
1:D:59:HIS:CD2	1:D:61:HIS:H	2.25	0.55
1:C:221:PRO:HA	1:C:311:ALA:O	2.07	0.55
1:D:224:ALA:HB1	1:D:254:ALA:HA	1.87	0.55
1:C:277:LEU:HB3	1:C:278:GLN:HE21	1.71	0.55
1:B:330:SER:O	1:B:368:ARG:HD2	2.07	0.55
1:A:165:ASN:HD21	1:A:167:GLU:HB2	1.71	0.55
1:C:350:GLU:CD	1:C:358:VAL:HG13	2.27	0.55
1:C:214:GLN:HE21	1:C:333:ARG:HB3	1.70	0.55
1:A:163:LEU:HD21	1:A:389:TRP:CD2	2.41	0.55
1:C:404:GLU:CD	1:C:404:GLU:H	2.10	0.55
1:C:274:ALA:O	1:C:278:GLN:HG2	2.06	0.54
1:D:31:GLY:HA3	1:D:63:ASP:C	2.27	0.54
1:D:390:LEU:HD12	1:D:390:LEU:N	2.23	0.54
1:B:251:SER:HB3	1:B:254:ALA:HB3	1.89	0.54
1:B:404:GLU:H	1:B:404:GLU:CD	2.11	0.54
1:C:12:VAL:HG12	1:C:401:GLY:N	2.22	0.54
1:D:221:PRO:HD2	1:D:337:VAL:O	2.06	0.54
1:A:128:ARG:C	1:A:129:LEU:HD23	2.28	0.54
1:D:65:VAL:CG1	1:D:94:LEU:HD11	2.38	0.54
1:A:126:TRP:HB2	1:D:176:LEU:O	2.08	0.54
1:D:402:GLU:O	1:D:406:LEU:HD13	2.07	0.54
1:B:401:GLY:CA	1:B:406:LEU:HD11	2.36	0.54
1:A:182:LEU:HD11	1:A:397:VAL:HG23	1.90	0.54
1:D:331:ASP:HB2	1:D:334:ASN:HD22	1.72	0.54
1:D:59:HIS:NE2	1:D:61:HIS:HB2	2.23	0.54
1:B:8:ALA:HB1	1:B:400:HIS:HA	1.90	0.54
1:A:24:ARG:HE	1:A:130:GLY:HA3	1.73	0.54
1:C:55:VAL:HG22	1:C:57:LEU:CD1	2.37	0.54
1:A:177:PRO:HD3	1:A:389:TRP:CE2	2.43	0.54
1:D:182:LEU:HD12	1:D:183:VAL:N	2.23	0.54
1:C:362:GLY:O	1:C:363:GLU:HB2	2.07	0.54
1:A:197:TYR:O	1:A:201:VAL:HG23	2.07	0.53
1:B:3:ILE:HG12	1:B:184:LEU:HD22	1.90	0.53
1:B:204:PHE:HB2	1:B:374:LEU:CD1	2.39	0.53
1:A:347:LEU:CD1	1:A:358:VAL:HG11	2.37	0.53
2:H:1:U:O4'	2:H:1:U:O2	2.27	0.53
1:C:224:ALA:O	1:C:257:VAL:HG21	2.08	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:12:VAL:HG12	1:B:401:GLY:HA2	1.88	0.53
1:B:422:LEU:HD12	1:B:422:LEU:N	2.23	0.53
1:C:232:LEU:HD22	1:C:285:PRO:HD2	1.89	0.53
1:D:332:PRO:HB3	1:D:368:ARG:HB3	1.90	0.53
1:C:102:ASP:O	1:C:104:PRO:HD3	2.08	0.53
1:C:231:ILE:C	1:C:233:TYR:H	2.12	0.53
1:C:202:ARG:HG3	1:C:203:GLU:N	2.23	0.53
1:B:55:VAL:CG2	1:B:80:VAL:HG13	2.39	0.53
1:C:351:ILE:CG2	1:C:371:VAL:HG21	2.39	0.53
1:D:338:PHE:O	1:D:374:LEU:HB2	2.09	0.53
1:D:411:LYS:O	1:D:415:LEU:HB2	2.07	0.53
1:C:420:VAL:CG2	1:C:421:SER:N	2.64	0.53
1:C:360:ILE:CG2	1:C:361:LEU:HD13	2.39	0.53
1:B:402:GLU:O	1:B:405:LYS:N	2.40	0.53
1:D:291:VAL:CG1	1:D:296:ALA:HB3	2.39	0.53
1:B:37:GLU:HG3	1:B:40:ARG:NE	2.23	0.53
1:B:32:MET:HE3	1:B:62:LEU:HD11	1.90	0.53
1:A:397:VAL:HG12	1:A:423:ALA:HB2	1.90	0.53
1:C:398:LEU:CD1	1:C:398:LEU:H	2.21	0.53
1:C:406:LEU:HB3	1:C:422:LEU:CD2	2.38	0.53
1:C:406:LEU:HD23	1:C:422:LEU:HD23	1.90	0.53
1:D:231:ILE:HG21	1:D:310:LEU:HD21	1.91	0.53
1:B:54:ALA:HA	1:B:76:TYR:OH	2.08	0.53
1:C:398:LEU:HD13	1:C:398:LEU:H	1.74	0.53
1:A:357:ALA:HB2	1:A:366:PRO:HA	1.91	0.53
1:C:250:ASP:HB3	1:C:311:ALA:CB	2.31	0.52
1:D:13:THR:HG21	1:D:34:GLN:H	1.74	0.52
1:D:168:LYS:HA	1:D:197:TYR:CD1	2.44	0.52
1:C:409:LEU:HD23	1:C:413:LEU:HG	1.90	0.52
1:A:32:MET:HA	1:A:67:ARG:HG3	1.91	0.52
1:C:224:ALA:HB3	1:C:253:MET:HE3	1.91	0.52
1:C:235:LEU:HD12	1:C:285:PRO:HG3	1.91	0.52
1:D:57:LEU:N	1:D:57:LEU:HD22	2.25	0.52
1:D:85:ALA:HB2	1:D:267:TYR:CD2	2.44	0.52
1:C:238:HIS:O	1:C:241:ARG:HG2	2.08	0.52
1:D:32:MET:HA	1:D:67:ARG:HD2	1.91	0.52
1:D:299:ALA:O	1:D:302:ARG:HG2	2.08	0.52
1:A:216:GLY:O	1:A:306:PRO:HA	2.08	0.52
1:A:14:GLY:HA3	1:A:33:PHE:CE1	2.44	0.52
1:A:2:ARG:NH1	3:A:446:SO4:O3	2.43	0.52
1:A:102:ASP:CG	1:A:103:GLU:H	2.13	0.52
1:D:367:LEU:HG	1:D:367:LEU:O	2.10	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:37:GLU:CG	1:B:40:ARG:NE	2.73	0.52
2:F:1:U:C2'	2:F:2:U:O5'	2.57	0.52
1:C:266:ARG:HA	1:C:273:GLN:NE2	2.24	0.52
1:D:228:ALA:HB3	1:D:229:GLN:NE2	2.25	0.52
1:A:411:LYS:CD	4:A:451:FLC:HG2	2.38	0.52
1:C:182:LEU:HD12	1:C:183:VAL:H	1.75	0.52
1:D:291:VAL:HG13	1:D:296:ALA:HB3	1.92	0.52
1:A:355:PRO:HB2	1:A:356:PRO:HD2	1.91	0.52
1:D:90:MET:HE3	1:D:118:LEU:CD1	2.39	0.52
1:B:325:LEU:O	1:B:329:LEU:HD22	2.10	0.52
1:B:37:GLU:O	1:B:39:ALA:N	2.42	0.52
1:A:115:LEU:HD23	1:A:118:LEU:HD11	1.92	0.52
1:D:227:ARG:NH1	1:D:379:GLY:H	2.08	0.52
1:B:27:LEU:CB	1:B:55:VAL:HG12	2.39	0.52
1:D:214:GLN:HE21	1:D:333:ARG:HG2	1.73	0.52
1:C:12:VAL:CG1	1:C:401:GLY:HA2	2.40	0.52
1:B:325:LEU:HG	1:B:329:LEU:HD21	1.92	0.52
1:D:41:ASN:HB3	1:D:105:PHE:CE2	2.44	0.51
1:A:393:GLU:OE2	1:A:393:GLU:HA	2.11	0.51
1:B:271:GLU:O	1:B:275:HIS:HD2	1.94	0.51
1:C:326:LYS:HA	1:C:365:VAL:HG11	1.92	0.51
1:C:166:ARG:O	1:C:166:ARG:HD3	2.10	0.51
1:C:233:TYR:C	1:C:235:LEU:H	2.12	0.51
1:B:360:ILE:CG2	1:B:361:LEU:HD13	2.34	0.51
1:C:409:LEU:HD23	1:C:409:LEU:O	2.10	0.51
2:E:4:U:O2	2:E:4:U:O4'	2.29	0.51
1:B:198:ARG:HB2	1:B:198:ARG:HH21	1.75	0.51
1:D:170:VAL:HA	1:D:272:VAL:CG2	2.40	0.51
1:D:160:SER:HB2	1:D:163:LEU:HD11	1.91	0.51
1:A:322:LEU:HB3	1:A:361:LEU:HD11	1.92	0.51
1:C:288:LEU:HD12	1:C:289:GLU:H	1.76	0.51
1:A:165:ASN:C	1:A:165:ASN:HD22	2.14	0.51
1:A:170:VAL:CG2	1:A:230:GLU:HG3	2.40	0.51
1:C:122:GLU:O	1:C:125:GLU:HG3	2.10	0.51
1:D:3:ILE:HD11	1:D:17:HIS:CB	2.41	0.51
1:A:54:ALA:HA	1:A:76:TYR:OH	2.10	0.51
1:D:85:ALA:HB2	1:D:267:TYR:CE2	2.46	0.51
1:D:87:VAL:HG13	1:D:118:LEU:CD1	2.41	0.51
1:A:289:GLU:OE2	1:B:291:VAL:HA	2.10	0.51
1:C:288:LEU:HD12	1:C:289:GLU:N	2.26	0.51
1:B:353:ALA:O	1:B:354:ARG:HB3	2.11	0.51
1:D:216:GLY:O	1:D:306:PRO:HA	2.11	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:222:THR:CG2	1:D:339:VAL:HG21	2.40	0.51
1:A:397:VAL:CG1	1:A:423:ALA:HB2	2.41	0.51
1:C:2:ARG:HH22	1:C:430:PRO:HB3	1.76	0.51
1:B:398:LEU:N	1:B:398:LEU:CD1	2.74	0.51
1:A:84:ARG:HG2	1:A:84:ARG:NH1	2.20	0.51
1:D:386:LEU:HD23	1:D:409:LEU:HD11	1.92	0.51
1:B:128:ARG:O	1:B:129:LEU:HD23	2.10	0.51
1:C:236:TYR:CE2	1:C:282:PRO:HA	2.46	0.50
1:B:88:LEU:HD12	1:B:264:LEU:CD1	2.38	0.50
1:B:57:LEU:HG	1:B:65:VAL:HG22	1.92	0.50
1:A:421:SER:OG	1:A:422:LEU:N	2.45	0.50
1:D:295:GLU:N	1:D:295:GLU:OE2	2.25	0.50
1:A:198:ARG:HH21	1:A:198:ARG:HG3	1.76	0.50
1:B:86:THR:O	1:B:90:MET:HB2	2.10	0.50
1:C:85:ALA:HB2	1:C:267:TYR:CD2	2.46	0.50
1:D:132:LEU:HD22	1:D:134:LEU:HG	1.92	0.50
1:C:134:LEU:HD23	1:C:150:ALA:HB2	1.93	0.50
1:C:28:LEU:O	1:C:29:ASP:HB2	2.11	0.50
1:D:397:VAL:HG21	1:D:429:VAL:HG11	1.92	0.50
1:A:87:VAL:HA	1:A:90:MET:CE	2.42	0.50
1:C:354:ARG:HA	1:C:367:LEU:HD23	1.93	0.50
1:D:227:ARG:NH1	1:D:379:GLY:N	2.60	0.50
1:C:52:VAL:HG12	1:C:76:TYR:CE2	2.47	0.50
1:C:424:ARG:NH1	1:C:424:ARG:HB3	2.25	0.50
1:C:190:GLY:HA3	1:C:409:LEU:HB2	1.93	0.50
1:B:142:LEU:H	1:B:145:SER:HB3	1.76	0.50
1:D:233:TYR:O	1:D:237:THR:HG23	2.12	0.50
1:C:184:LEU:HD11	1:C:399:VAL:HG11	1.94	0.50
1:B:170:VAL:HG12	1:B:171:LEU:HD13	1.94	0.50
1:C:165:ASN:ND2	1:C:385:GLU:OE1	2.45	0.50
1:D:49:PRO:HG3	1:D:74:GLU:HG2	1.94	0.50
1:A:365:VAL:HG23	1:A:365:VAL:O	2.12	0.50
1:C:250:ASP:O	1:C:251:SER:HB2	2.11	0.50
1:A:85:ALA:HB3	1:A:144:GLY:HA3	1.94	0.50
1:C:101:MET:SD	1:C:104:PRO:HA	2.52	0.50
1:A:87:VAL:HA	1:A:90:MET:HE2	1.94	0.50
1:B:1:MET:HG3	1:B:21:ALA:HB2	1.94	0.50
1:C:225:VAL:HG12	1:C:226:GLU:N	2.26	0.50
1:D:84:ARG:NH2	1:D:263:ARG:NH2	2.57	0.50
1:A:295:GLU:OE1	1:B:244:ARG:HB2	2.11	0.50
1:C:302:ARG:HG3	1:C:302:ARG:HH21	1.77	0.50
1:C:236:TYR:CD2	1:C:282:PRO:HA	2.45	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:358:VAL:O	1:D:365:VAL:N	2.44	0.49
1:B:10:ARG:HH11	1:B:10:ARG:HG3	1.77	0.49
1:D:312:GLY:HA2	1:D:313:SER:O	2.12	0.49
1:A:404:GLU:N	1:A:404:GLU:OE2	2.25	0.49
1:A:32:MET:HE3	1:A:66:GLY:CA	2.42	0.49
1:B:147:PHE:HB3	1:B:160:SER:O	2.12	0.49
1:A:20:LEU:HD22	1:A:25:ARG:HG2	1.94	0.49
1:C:322:LEU:HD22	1:C:347:LEU:HD23	1.93	0.49
1:B:347:LEU:HD11	1:B:358:VAL:CG1	2.42	0.49
1:B:41:ASN:HB3	1:B:105:PHE:CE2	2.47	0.49
1:C:170:VAL:HG21	1:C:230:GLU:HG3	1.94	0.49
1:C:406:LEU:O	1:C:408:ALA:N	2.45	0.49
1:B:398:LEU:HD23	1:B:406:LEU:O	2.12	0.49
1:C:210:LYS:O	1:C:210:LYS:HD3	2.12	0.49
1:B:40:ARG:C	1:B:42:HIS:H	2.16	0.49
1:A:129:LEU:O	1:A:132:LEU:HB3	2.13	0.49
1:C:155:ARG:HD2	1:C:431:VAL:O	2.12	0.49
1:A:217:LYS:HG2	1:A:307:MET:HG2	1.95	0.49
1:A:362:GLY:O	1:A:363:GLU:HB2	2.11	0.49
1:C:284:ARG:HA	1:C:288:LEU:CD2	2.43	0.49
1:C:203:GLU:O	1:C:207:ILE:HG13	2.12	0.49
1:A:76:TYR:O	1:A:77:ARG:CD	2.57	0.49
1:B:7:GLY:O	1:B:8:ALA:C	2.50	0.49
1:C:386:LEU:O	1:C:390:LEU:HD13	2.12	0.49
1:A:1:MET:SD	1:A:431:VAL:HG11	2.51	0.49
1:C:387:LEU:CB	1:C:416:ARG:HH12	2.23	0.49
1:B:37:GLU:OE2	1:B:37:GLU:N	2.45	0.49
1:A:220:ILE:HD12	1:A:310:LEU:HD21	1.94	0.49
1:C:236:TYR:OH	1:C:280:LYS:HB3	2.12	0.49
1:D:358:VAL:O	1:D:365:VAL:HG22	2.11	0.49
1:D:225:VAL:HG12	1:D:226:GLU:N	2.27	0.49
1:B:80:VAL:HB	1:B:118:LEU:HD23	1.95	0.49
1:D:65:VAL:HG11	1:D:94:LEU:HD11	1.94	0.49
1:D:55:VAL:HG22	1:D:80:VAL:HA	1.95	0.49
1:D:61:HIS:O	1:D:65:VAL:HG23	2.13	0.49
1:C:248:TYR:CD2	1:C:300:LEU:HD21	2.48	0.49
1:A:396:VAL:HG12	1:A:398:LEU:HD13	1.94	0.49
1:C:202:ARG:O	1:C:206:GLU:HG3	2.13	0.49
1:D:269:SER:HB2	3:D:436:SO4:O3	2.13	0.49
1:A:321:ILE:O	1:A:325:LEU:HD13	2.13	0.49
1:C:206:GLU:C	1:C:208:LEU:H	2.17	0.49
1:D:32:MET:HE1	1:D:105:PHE:HZ	1.77	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:9:ALA:O	1:C:11:GLU:HG2	2.12	0.49
1:D:219:LEU:HD23	1:D:325:LEU:CD1	2.42	0.49
1:C:265:VAL:HG13	1:C:266:ARG:H	1.78	0.48
1:B:409:LEU:HD22	1:B:413:LEU:HG	1.95	0.48
1:A:250:ASP:OD2	1:A:297:SER:OG	2.30	0.48
1:C:424:ARG:HH11	1:C:424:ARG:HB3	1.78	0.48
1:C:409:LEU:HA	1:C:412:LEU:HD12	1.95	0.48
1:B:299:ALA:HA	1:B:302:ARG:HH21	1.78	0.48
1:A:318:GLY:HA2	1:A:322:LEU:HD12	1.95	0.48
1:A:83:THR:O	1:A:87:VAL:HG23	2.12	0.48
1:B:235:LEU:HD13	1:B:247:ILE:HD13	1.95	0.48
1:A:82:ALA:HB1	1:A:86:THR:HB	1.95	0.48
1:C:224:ALA:HB1	1:C:254:ALA:N	2.28	0.48
1:A:167:GLU:HB3	1:A:197:TYR:HB2	1.95	0.48
1:B:48:ASP:OD2	1:B:50:LYS:HB2	2.13	0.48
1:A:391:GLN:HA	1:A:416:ARG:NH2	2.29	0.48
1:A:214:GLN:NE2	1:A:333:ARG:HA	2.28	0.48
1:D:402:GLU:HB2	1:D:405:LYS:CG	2.43	0.48
1:C:141:HIS:HB3	1:C:145:SER:HB2	1.94	0.48
1:D:214:GLN:NE2	1:D:333:ARG:HG2	2.28	0.48
1:A:252:PRO:HD2	2:E:4:U:OP1	2.13	0.48
1:C:165:ASN:C	1:C:167:GLU:H	2.17	0.48
1:C:331:ASP:O	1:C:334:ASN:OD1	2.31	0.48
1:B:239:GLY:C	1:B:241:ARG:N	2.67	0.48
1:C:80:VAL:HB	1:C:118:LEU:HD23	1.96	0.48
1:C:184:LEU:HD12	1:C:397:VAL:O	2.14	0.48
1:D:28:LEU:O	1:D:29:ASP:HB2	2.13	0.48
1:C:25:ARG:NH1	1:C:51:GLU:HB3	2.28	0.48
1:D:219:LEU:HD23	1:D:325:LEU:HD12	1.95	0.48
1:A:43:ALA:HB1	1:A:44:PRO:HD2	1.94	0.48
1:A:62:LEU:HD13	1:A:93:VAL:HG12	1.95	0.48
1:B:37:GLU:HG2	1:B:40:ARG:NH1	2.21	0.48
1:D:102:ASP:CG	1:D:103:GLU:N	2.64	0.48
1:A:318:GLY:HA2	1:A:322:LEU:CD1	2.43	0.48
1:C:398:LEU:CD1	1:C:398:LEU:N	2.76	0.48
1:A:229:GLN:HG3	1:A:261:TYR:CE1	2.49	0.48
1:D:319:GLY:CA	2:H:3:U:H1'	2.44	0.48
1:D:165:ASN:C	1:D:167:GLU:H	2.17	0.48
1:C:28:LEU:HD12	1:C:28:LEU:N	2.29	0.48
1:D:61:HIS:CD2	2:H:2:U:OP2	2.67	0.48
1:C:65:VAL:CG1	1:C:94:LEU:HD11	2.44	0.48
1:A:177:PRO:HD3	1:A:389:TRP:NE1	2.28	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:55:VAL:HG21	1:D:80:VAL:HG13	1.93	0.48
1:C:57:LEU:HD21	1:C:68:LEU:HD22	1.96	0.48
1:A:102:ASP:CG	1:A:103:GLU:N	2.67	0.48
1:A:62:LEU:N	2:E:2:U:OP2	2.32	0.48
1:A:313:SER:HB3	2:E:3:U:C6	2.49	0.48
1:C:275:HIS:N	1:C:275:HIS:CD2	2.82	0.48
1:D:43:ALA:HB1	1:D:44:PRO:HD2	1.95	0.48
1:C:351:ILE:HG23	1:C:367:LEU:CD1	2.40	0.48
1:D:383:GLN:NE2	1:D:412:LEU:HD11	2.29	0.48
1:D:61:HIS:ND1	2:H:1:U:H5'	2.29	0.48
1:C:219:LEU:HD21	1:C:324:HIS:O	2.14	0.48
1:D:168:LYS:HA	1:D:197:TYR:CE1	2.48	0.47
1:D:212:LEU:HA	1:D:306:PRO:HB3	1.95	0.47
1:A:358:VAL:CG1	1:A:359:ARG:N	2.76	0.47
1:A:357:ALA:CB	1:A:366:PRO:HA	2.44	0.47
1:C:189:TYR:OH	1:C:341:TYR:HB2	2.14	0.47
1:C:242:LEU:HB3	1:C:243:PRO:HD2	1.96	0.47
1:D:192:ARG:HH21	1:D:405:LYS:NZ	2.12	0.47
1:A:170:VAL:HG12	1:A:171:LEU:HD13	1.95	0.47
2:F:1:U:O2'	2:F:2:U:OP1	2.32	0.47
1:C:177:PRO:HD3	1:C:389:TRP:CE2	2.49	0.47
1:C:13:THR:HB	1:C:33:PHE:HA	1.96	0.47
1:A:229:GLN:H	1:A:229:GLN:HE21	1.60	0.47
1:A:1:MET:HA	1:A:20:LEU:O	2.14	0.47
1:A:265:VAL:HA	1:A:268:PHE:HD2	1.79	0.47
1:A:225:VAL:HG12	1:A:226:GLU:N	2.29	0.47
1:C:7:GLY:HA3	1:C:14:GLY:O	2.14	0.47
1:B:88:LEU:HB3	1:B:260:LEU:HD21	1.96	0.47
1:C:360:ILE:O	1:C:361:LEU:HB2	2.14	0.47
1:D:91:GLU:O	1:D:95:GLU:CG	2.61	0.47
1:C:37:GLU:O	1:C:39:ALA:N	2.47	0.47
1:B:297:SER:O	1:B:300:LEU:HB2	2.14	0.47
1:B:33:PHE:HD2	1:B:41:ASN:ND2	2.12	0.47
1:C:236:TYR:CA	1:C:285:PRO:HB3	2.44	0.47
1:C:225:VAL:HG21	2:G:2:U:OP1	2.14	0.47
1:D:357:ALA:HB1	1:D:365:VAL:O	2.15	0.47
1:B:229:GLN:H	1:B:229:GLN:NE2	2.12	0.47
1:C:141:HIS:HB3	1:C:145:SER:CB	2.45	0.47
2:E:2:U:H1'	2:E:3:U:C5	2.49	0.47
1:B:233:TYR:CE1	1:B:282:PRO:HB2	2.49	0.47
1:A:156:THR:N	1:A:181:ASP:OD1	2.42	0.47
1:D:37:GLU:N	1:D:37:GLU:CD	2.68	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:33:PHE:HD2	1:B:41:ASN:HD22	1.61	0.47
1:A:351:ILE:HG12	1:A:358:VAL:HG21	1.96	0.47
1:D:166:ARG:O	1:D:166:ARG:CG	2.61	0.47
1:D:315:MET:O	1:D:316:LEU:HB2	2.14	0.47
1:C:322:LEU:HD22	1:C:347:LEU:CD2	2.45	0.47
1:C:214:GLN:HE21	1:C:333:ARG:CB	2.28	0.47
1:C:170:VAL:HG13	1:C:283:PHE:HZ	1.79	0.47
1:C:232:LEU:CD2	1:C:288:LEU:HD13	2.42	0.47
1:D:42:HIS:CE1	1:D:105:PHE:HB3	2.50	0.47
1:A:121:LEU:HD12	1:A:125:GLU:HB3	1.97	0.47
1:D:219:LEU:HB2	1:D:336:LEU:HA	1.97	0.47
1:B:9:ALA:O	1:B:10:ARG:HB2	2.15	0.47
1:A:143:PRO:HD3	1:A:226:GLU:HG2	1.96	0.47
1:A:7:GLY:HA3	1:A:14:GLY:O	2.15	0.47
1:D:184:LEU:HD21	1:D:399:VAL:HG21	1.97	0.47
1:D:153:GLU:O	1:D:155:ARG:HG2	2.15	0.47
1:A:4:VAL:HA	1:A:428:GLY:HA2	1.97	0.46
1:C:2:ARG:NH2	1:C:430:PRO:HB3	2.30	0.46
1:C:281:ASN:C	1:C:283:PHE:H	2.19	0.46
1:D:420:VAL:O	1:D:421:SER:HB3	2.15	0.46
1:C:166:ARG:HH21	1:C:166:ARG:HG3	1.80	0.46
1:C:166:ARG:NH2	1:C:166:ARG:HG3	2.29	0.46
1:C:401:GLY:HA3	1:C:406:LEU:CD1	2.45	0.46
1:C:227:ARG:HG2	1:C:227:ARG:HH11	1.80	0.46
1:A:321:ILE:HG13	1:A:325:LEU:HD13	1.98	0.46
1:A:24:ARG:HH11	1:A:130:GLY:HA2	1.79	0.46
1:A:297:SER:OG	1:A:320:ARG:HD3	2.16	0.46
1:C:225:VAL:HG12	1:C:226:GLU:H	1.80	0.46
1:D:220:ILE:HB	1:D:310:LEU:HD23	1.97	0.46
1:A:5:PRO:HG2	1:A:423:ALA:HB1	1.97	0.46
1:C:140:GLY:O	1:C:164:GLY:HA3	2.15	0.46
1:C:58:THR:O	1:C:59:HIS:HB3	2.15	0.46
1:B:32:MET:HA	1:B:67:ARG:HG3	1.96	0.46
1:C:11:GLU:O	1:C:401:GLY:N	2.48	0.46
1:D:55:VAL:CG2	1:D:80:VAL:HA	2.46	0.46
1:D:228:ALA:O	1:D:231:ILE:HB	2.15	0.46
1:C:272:VAL:O	1:C:276:PHE:HD2	1.97	0.46
1:C:108:PRO:HD2	1:C:109:GLU:OE2	2.15	0.46
1:D:177:PRO:HD3	1:D:389:TRP:CD1	2.51	0.46
1:B:45:PHE:HB3	1:B:47:PHE:CE1	2.51	0.46
1:C:329:LEU:HB3	1:C:366:PRO:O	2.15	0.46
1:A:38:GLU:O	1:A:41:ASN:HB2	2.16	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:326:LYS:C	1:D:328:GLY:H	2.19	0.46
1:D:227:ARG:HH11	1:D:379:GLY:N	2.13	0.46
1:B:1:MET:HG3	1:B:21:ALA:CB	2.46	0.46
1:B:5:PRO:HG2	1:B:423:ALA:HB1	1.98	0.46
1:A:28:LEU:N	1:A:28:LEU:CD1	2.78	0.46
1:C:232:LEU:HD13	1:C:288:LEU:CD2	2.46	0.46
1:C:205:LEU:O	1:C:208:LEU:HB2	2.16	0.46
1:D:165:ASN:HB3	1:D:168:LYS:CG	2.42	0.46
1:B:393:GLU:O	1:B:418:GLN:HG2	2.16	0.46
1:D:77:ARG:HG2	1:D:77:ARG:HH11	1.80	0.46
1:D:31:GLY:O	1:D:67:ARG:CD	2.64	0.46
1:C:350:GLU:OE1	1:C:358:VAL:HG13	2.15	0.46
1:C:384:ASP:HA	1:C:387:LEU:CD1	2.44	0.46
1:A:266:ARG:HH21	1:D:273:GLN:HE22	1.63	0.46
1:B:85:ALA:HB3	1:B:144:GLY:HA3	1.98	0.46
1:C:221:PRO:HB3	1:C:321:ILE:CG1	2.38	0.45
1:B:425:PHE:O	1:B:427:GLU:N	2.49	0.45
1:B:37:GLU:CG	1:B:40:ARG:HH11	2.24	0.45
1:D:33:PHE:N	1:D:41:ASN:HD21	1.95	0.45
1:A:10:ARG:NH1	1:A:10:ARG:CG	2.74	0.45
1:D:3:ILE:HD11	1:D:17:HIS:HB3	1.98	0.45
1:B:229:GLN:HG3	1:B:261:TYR:CE1	2.51	0.45
1:D:322:LEU:O	1:D:326:LYS:N	2.49	0.45
1:C:32:MET:CE	1:C:105:PHE:HZ	2.29	0.45
1:A:288:LEU:HD12	1:A:289:GLU:N	2.32	0.45
1:A:354:ARG:NH2	1:A:370:SER:HA	2.31	0.45
1:C:294:THR:HA	1:C:297:SER:HB3	1.98	0.45
1:C:199:GLU:HA	1:C:202:ARG:HG2	1.98	0.45
1:A:229:GLN:H	1:A:229:GLN:CD	2.14	0.45
1:C:3:ILE:HD12	1:C:18:LEU:C	2.36	0.45
1:D:236:TYR:N	1:D:285:PRO:HB3	2.31	0.45
1:B:117:HIS:O	1:B:119:ARG:HG3	2.17	0.45
1:A:238:HIS:O	1:A:241:ARG:HG3	2.17	0.45
1:D:223:PHE:C	1:D:225:VAL:H	2.20	0.45
1:B:27:LEU:HD13	1:B:29:ASP:O	2.15	0.45
1:C:68:LEU:HD11	1:C:72:PHE:HE1	1.82	0.45
1:D:2:ARG:HG2	1:D:20:LEU:HB2	1.99	0.45
1:D:297:SER:HB2	1:D:320:ARG:NH1	2.32	0.45
1:B:47:PHE:HA	3:B:447:SO4:O1	2.16	0.45
1:B:62:LEU:O	1:B:62:LEU:HG	2.16	0.45
1:A:20:LEU:CD2	1:A:25:ARG:HH11	2.23	0.45
1:C:88:LEU:HD12	1:C:264:LEU:HD11	1.98	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:354:ARG:NH1	1:C:369:ALA:O	2.42	0.45
1:D:2:ARG:CZ	3:D:437:SO4:O1	2.64	0.45
1:D:214:GLN:HE21	1:D:333:ARG:CG	2.30	0.45
1:A:278:GLN:O	1:A:280:LYS:HG3	2.17	0.45
1:C:359:ARG:NH1	1:C:359:ARG:HG3	2.31	0.45
1:D:37:GLU:HB2	1:D:40:ARG:NE	2.25	0.45
1:C:320:ARG:HG2	1:C:320:ARG:O	2.15	0.45
1:C:12:VAL:O	1:C:12:VAL:HG23	2.17	0.45
1:C:407:LEU:HD12	1:C:422:LEU:CD2	2.47	0.45
1:C:7:GLY:O	1:C:9:ALA:N	2.50	0.45
1:B:397:VAL:HA	1:B:421:SER:O	2.17	0.45
1:D:73:ARG:NH2	1:D:106:PHE:CA	2.77	0.45
1:B:226:GLU:C	1:B:229:GLN:HE21	2.20	0.45
1:B:31:GLY:HA3	1:B:63:ASP:O	2.16	0.45
1:C:248:TYR:CE2	1:C:300:LEU:HD21	2.51	0.45
1:B:42:HIS:ND1	1:B:105:PHE:HB3	2.32	0.45
1:D:401:GLY:HA3	1:D:406:LEU:HD11	1.99	0.45
1:C:212:LEU:O	1:C:306:PRO:HG3	2.16	0.45
1:C:32:MET:HE1	1:C:105:PHE:CZ	2.51	0.45
1:C:411:LYS:O	1:C:414:ALA:HB3	2.17	0.45
1:B:165:ASN:HD22	1:B:165:ASN:C	2.20	0.45
1:B:384:ASP:N	1:B:384:ASP:OD2	2.49	0.45
1:B:32:MET:HE3	1:B:66:GLY:HA3	1.99	0.45
1:C:247:ILE:HA	1:C:308:VAL:HB	1.98	0.45
1:D:235:LEU:O	1:D:239:GLY:N	2.50	0.45
1:A:80:VAL:HB	1:A:118:LEU:HD23	1.98	0.45
1:B:126:TRP:CE3	1:C:178:PRO:HB3	2.51	0.45
1:C:38:GLU:O	1:C:38:GLU:OE2	2.34	0.45
1:C:355:PRO:HD2	1:C:367:LEU:CD2	2.47	0.45
1:D:163:LEU:HD21	1:D:389:TRP:CD2	2.52	0.45
1:D:2:ARG:NH2	3:D:437:SO4:O2	2.49	0.45
1:D:134:LEU:HD23	1:D:150:ALA:HA	1.99	0.45
1:D:113:GLU:OE2	1:D:117:HIS:HE1	2.00	0.45
1:C:359:ARG:HH11	1:C:359:ARG:HG3	1.82	0.45
1:C:294:THR:O	1:C:297:SER:HB3	2.17	0.45
1:B:239:GLY:C	1:B:241:ARG:H	2.19	0.45
1:D:347:LEU:O	1:D:351:ILE:HG13	2.17	0.45
1:B:77:ARG:HH11	1:B:77:ARG:HG3	1.81	0.45
1:B:205:LEU:O	1:B:209:GLU:HG3	2.17	0.45
1:D:59:HIS:CD2	1:D:142:LEU:HD12	2.52	0.44
1:C:396:VAL:HG12	1:C:398:LEU:HD12	1.98	0.44
1:C:165:ASN:O	1:C:167:GLU:N	2.50	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:140:GLY:O	1:B:164:GLY:HA3	2.16	0.44
1:B:2:ARG:HG2	1:B:2:ARG:HH21	1.82	0.44
1:B:32:MET:HB2	1:B:41:ASN:OD1	2.17	0.44
1:C:232:LEU:HB3	1:C:283:PHE:O	2.17	0.44
1:C:192:ARG:NH1	1:C:405:LYS:NZ	2.61	0.44
1:A:81:TYR:HD2	1:A:121:LEU:HB2	1.82	0.44
1:C:195:ARG:HB3	1:C:375:GLY:O	2.16	0.44
1:B:270:GLU:O	1:B:273:GLN:N	2.48	0.44
1:D:192:ARG:HH21	1:D:405:LYS:HZ2	1.64	0.44
1:D:410:GLY:CA	1:D:420:VAL:HG21	2.45	0.44
1:D:229:GLN:HB3	1:D:258:LEU:HD13	1.99	0.44
2:H:3:U:HO2'	2:H:4:U:P	2.40	0.44
1:D:306:PRO:O	1:D:307:MET:HB3	2.17	0.44
1:B:65:VAL:O	1:B:65:VAL:HG12	2.16	0.44
1:C:331:ASP:OD2	1:C:332:PRO:HD2	2.17	0.44
1:D:13:THR:CB	1:D:34:GLN:H	2.30	0.44
1:D:406:LEU:O	1:D:407:LEU:C	2.56	0.44
1:A:171:LEU:HD21	1:A:226:GLU:HG3	1.98	0.44
1:D:350:GLU:HG3	1:D:351:ILE:H	1.82	0.44
1:B:130:GLY:N	3:B:441:SO4:O3	2.50	0.44
1:C:233:TYR:C	1:C:235:LEU:N	2.70	0.44
1:A:168:LYS:HA	1:A:197:TYR:CD1	2.53	0.44
1:C:49:PRO:HB3	1:C:71:LEU:CD1	2.47	0.44
1:D:204:PHE:HD2	1:D:374:LEU:CD1	2.31	0.44
1:C:386:LEU:N	1:C:386:LEU:HD12	2.32	0.44
1:A:28:LEU:N	1:A:28:LEU:HD12	2.33	0.44
1:D:384:ASP:OD2	1:D:384:ASP:N	2.50	0.44
1:D:195:ARG:O	1:D:196:PRO:C	2.56	0.44
1:C:407:LEU:HD12	1:C:422:LEU:HD21	1.99	0.44
1:D:55:VAL:C	1:D:56:LEU:HD12	2.37	0.44
1:D:197:TYR:O	1:D:201:VAL:HG23	2.16	0.44
1:B:312:GLY:CA	1:B:313:SER:C	2.85	0.44
1:D:97:ALA:HA	2:H:2:U:H5	1.81	0.44
1:D:297:SER:O	1:D:324:HIS:HE1	2.01	0.44
1:C:386:LEU:HD12	1:C:386:LEU:H	1.83	0.44
1:C:275:HIS:CD2	1:C:275:HIS:H	2.35	0.44
1:A:284:ARG:NH2	4:A:450:FLC:HA1	2.33	0.44
1:C:232:LEU:HD13	1:C:283:PHE:O	2.17	0.44
1:C:12:VAL:CG1	1:C:401:GLY:CA	2.95	0.44
1:C:405:LYS:O	1:C:408:ALA:HB3	2.17	0.44
1:B:101:MET:HG2	1:B:104:PRO:HA	2.00	0.44
1:B:49:PRO:HG3	1:B:74:GLU:HB3	1.99	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:37:GLU:H	1:B:37:GLU:CD	2.21	0.44
1:B:104:PRO:C	1:B:106:PHE:H	2.20	0.44
1:D:61:HIS:CG	2:H:1:U:H5'	2.53	0.44
1:B:37:GLU:CG	1:B:40:ARG:NH1	2.81	0.43
1:C:62:LEU:O	1:C:66:GLY:N	2.46	0.43
1:C:401:GLY:HA3	1:C:406:LEU:HD11	2.00	0.43
1:B:313:SER:HB3	2:F:3:U:C5	2.53	0.43
1:B:77:ARG:NH1	1:B:113:GLU:OE1	2.42	0.43
1:A:429:VAL:HG13	1:A:430:PRO:HD2	2.00	0.43
1:A:90:MET:HE1	1:A:118:LEU:HD22	2.01	0.43
1:D:358:VAL:HG12	1:D:359:ARG:N	2.33	0.43
1:A:35:GLY:O	1:A:38:GLU:HB2	2.17	0.43
1:D:350:GLU:C	1:D:352:ILE:H	2.21	0.43
1:D:284:ARG:HA	1:D:288:LEU:CD2	2.43	0.43
1:D:3:ILE:HG12	1:D:184:LEU:HD12	1.99	0.43
1:A:341:TYR:CE1	1:A:343:PRO:HA	2.53	0.43
1:A:236:TYR:CD2	1:A:236:TYR:C	2.91	0.43
1:D:404:GLU:H	1:D:404:GLU:CD	2.20	0.43
1:A:70:LYS:O	1:A:74:GLU:HG3	2.18	0.43
1:D:298:LYS:HE2	1:D:323:HIS:ND1	2.32	0.43
1:D:1:MET:HE2	1:D:21:ALA:CB	2.46	0.43
1:C:297:SER:OG	1:C:320:ARG:HD3	2.18	0.43
1:D:128:ARG:C	1:D:129:LEU:HD23	2.38	0.43
1:D:233:TYR:CE1	1:D:282:PRO:HB2	2.53	0.43
1:C:233:TYR:OH	1:C:271:GLU:HG2	2.19	0.43
1:C:231:ILE:HG21	1:C:310:LEU:HD11	2.01	0.43
1:B:60:ALA:O	1:B:61:HIS:C	2.57	0.43
1:A:128:ARG:HH21	1:D:177:PRO:HG2	1.83	0.43
1:A:126:TRP:CE3	1:A:135:ALA:HB2	2.54	0.43
1:B:422:LEU:N	1:B:422:LEU:CD1	2.82	0.43
1:A:48:ASP:HA	1:A:49:PRO:HD2	1.81	0.43
1:C:251:SER:HB3	1:C:254:ALA:HB3	2.01	0.43
1:D:362:GLY:O	1:D:363:GLU:HB2	2.18	0.43
1:D:223:PHE:O	1:D:225:VAL:N	2.46	0.43
1:A:61:HIS:CG	2:E:1:U:H5'	2.53	0.43
1:C:214:GLN:NE2	1:C:333:ARG:HA	2.34	0.43
1:C:390:LEU:HD23	1:C:396:VAL:HG21	2.01	0.43
1:A:90:MET:HE3	1:A:118:LEU:HD13	2.00	0.43
1:B:64:HIS:NE2	1:B:162:ASP:OD1	2.51	0.43
1:D:148:VAL:HG12	1:D:149:VAL:N	2.34	0.43
1:C:344:GLN:HA	1:C:349:ALA:HB2	2.01	0.43
1:C:27:LEU:HD13	1:C:29:ASP:O	2.18	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:212:LEU:HD13	1:D:245:ALA:HB3	2.00	0.43
1:B:261:TYR:HD1	1:B:283:PHE:CE2	2.35	0.43
1:D:389:TRP:HB3	1:D:390:LEU:HD12	2.00	0.43
1:B:200:THR:HG23	1:B:374:LEU:HB3	2.00	0.43
1:C:96:ASP:O	1:C:96:ASP:OD1	2.36	0.43
1:D:34:GLN:HA	1:D:38:GLU:HG2	1.99	0.43
1:D:269:SER:O	1:D:273:GLN:HG3	2.19	0.43
1:D:62:LEU:CD1	1:D:93:VAL:HG12	2.47	0.43
1:C:250:ASP:HA	1:C:291:VAL:CB	2.38	0.43
1:C:202:ARG:CG	1:C:203:GLU:N	2.82	0.43
1:D:223:PHE:HA	2:H:3:U:OP1	2.19	0.43
1:B:398:LEU:O	1:B:399:VAL:HG13	2.18	0.43
1:A:235:LEU:HD13	1:A:247:ILE:CD1	2.41	0.43
1:B:69:PRO:HB2	1:B:106:PHE:CD2	2.54	0.43
1:B:163:LEU:HD21	1:B:389:TRP:CG	2.53	0.43
1:D:236:TYR:OH	1:D:280:LYS:HE2	2.19	0.43
1:C:10:ARG:HH12	1:C:422:LEU:HD13	1.84	0.43
1:A:25:ARG:HG2	1:A:25:ARG:HH11	1.82	0.43
1:D:197:TYR:O	1:D:198:ARG:C	2.58	0.43
1:B:102:ASP:C	1:B:104:PRO:HD3	2.39	0.43
1:D:251:SER:HB3	1:D:254:ALA:CB	2.47	0.43
1:C:84:ARG:HB3	1:C:267:TYR:OH	2.19	0.43
1:D:168:LYS:CE	1:D:230:GLU:OE2	2.58	0.42
1:D:351:ILE:O	1:D:351:ILE:HG22	2.18	0.42
1:A:84:ARG:HH11	1:A:84:ARG:CG	2.26	0.42
1:C:350:GLU:O	1:C:355:PRO:HD3	2.19	0.42
2:F:1:U:O2'	2:F:2:U:P	2.76	0.42
1:D:155:ARG:CZ	1:D:181:ASP:OD1	2.67	0.42
1:B:36:LYS:HB2	1:B:37:GLU:OE2	2.19	0.42
1:C:14:GLY:HA2	1:C:31:GLY:O	2.19	0.42
1:A:316:LEU:C	1:A:318:GLY:H	2.22	0.42
1:C:257:VAL:HG12	1:C:261:TYR:CD2	2.55	0.42
1:D:281:ASN:O	1:D:283:PHE:N	2.51	0.42
1:C:227:ARG:NH2	1:C:378:SER:HA	2.24	0.42
1:D:90:MET:HE1	1:D:118:LEU:HD22	2.02	0.42
1:D:90:MET:O	1:D:94:LEU:HD13	2.19	0.42
1:A:163:LEU:HD21	1:A:389:TRP:CE2	2.54	0.42
1:D:323:HIS:CD2	1:D:323:HIS:N	2.87	0.42
1:C:235:LEU:CD1	1:C:247:ILE:HD13	2.34	0.42
1:D:12:VAL:HG23	1:D:13:THR:N	2.33	0.42
1:C:347:LEU:HD21	1:C:360:ILE:CD1	2.50	0.42
1:A:109:GLU:HG2	1:A:110:ASP:N	2.34	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:424:ARG:NE	1:A:427:GLU:OE2	2.52	0.42
1:C:406:LEU:O	1:C:407:LEU:C	2.58	0.42
1:D:201:VAL:O	1:D:205:LEU:HG	2.20	0.42
1:B:8:ALA:HA	1:B:11:GLU:HG3	2.01	0.42
1:D:408:ALA:O	1:D:409:LEU:C	2.58	0.42
1:B:86:THR:HG22	1:B:90:MET:HE3	2.00	0.42
1:A:57:LEU:CD2	1:A:65:VAL:HG22	2.49	0.42
1:D:281:ASN:C	1:D:283:PHE:H	2.22	0.42
1:D:398:LEU:N	1:D:398:LEU:HD12	2.34	0.42
1:A:312:GLY:O	1:A:321:ILE:HG22	2.19	0.42
1:A:24:ARG:NH1	1:A:130:GLY:HA2	2.34	0.42
1:D:133:SER:C	1:D:134:LEU:HG	2.39	0.42
1:C:399:VAL:HG12	1:C:423:ALA:HB3	2.00	0.42
1:D:77:ARG:HG2	1:D:77:ARG:NH1	2.35	0.42
1:D:414:ALA:C	1:D:416:ARG:H	2.22	0.42
1:B:189:TYR:CD2	1:B:194:HIS:HE1	2.37	0.42
1:B:96:ASP:O	1:B:99:LYS:N	2.48	0.42
1:C:253:MET:O	1:C:257:VAL:HG23	2.20	0.42
1:C:33:PHE:O	1:C:38:GLU:HA	2.20	0.42
1:D:191:ASP:OD1	1:D:405:LYS:HD3	2.19	0.42
1:D:48:ASP:HA	1:D:49:PRO:HD2	1.90	0.42
1:C:100:VAL:O	1:C:100:VAL:HG12	2.19	0.42
1:B:42:HIS:CE1	1:B:105:PHE:HB3	2.55	0.42
2:G:2:U:O2	2:G:2:U:C2'	2.68	0.42
1:A:41:ASN:HD22	1:A:41:ASN:HA	1.53	0.42
1:D:325:LEU:HG	1:D:329:LEU:CD1	2.50	0.42
1:A:265:VAL:HA	1:A:268:PHE:CD2	2.55	0.42
1:C:4:VAL:HG22	1:C:428:GLY:HA3	2.02	0.42
1:D:346:GLY:H	1:D:349:ALA:HB3	1.85	0.42
1:C:260:LEU:CD1	1:C:263:ARG:HH21	2.33	0.42
1:D:212:LEU:CD2	1:D:306:PRO:HB2	2.48	0.42
1:D:59:HIS:HD2	1:D:61:HIS:H	1.67	0.42
1:C:165:ASN:HB2	1:C:380:ALA:O	2.19	0.42
1:D:21:ALA:O	1:D:23:GLY:N	2.53	0.42
1:C:323:HIS:HD2	1:C:361:LEU:HD21	1.83	0.42
1:B:102:ASP:C	1:B:104:PRO:CD	2.88	0.42
1:B:68:LEU:N	1:B:69:PRO:CD	2.79	0.42
1:D:360:ILE:O	1:D:361:LEU:HB2	2.18	0.42
1:D:224:ALA:HB3	1:D:253:MET:HE3	1.99	0.42
1:B:3:ILE:HG23	1:B:3:ILE:O	2.20	0.42
1:D:208:LEU:CD2	1:D:218:VAL:HG11	2.48	0.42
1:A:361:LEU:N	1:A:361:LEU:HD12	2.35	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:413:LEU:HD22	1:D:418:GLN:OE1	2.19	0.41
1:C:235:LEU:HD13	1:C:247:ILE:CD1	2.34	0.41
1:B:229:GLN:O	1:B:232:LEU:HB2	2.20	0.41
1:D:312:GLY:HA2	1:D:313:SER:C	2.40	0.41
1:C:388:ASP:O	1:C:391:GLN:CB	2.67	0.41
1:D:181:ASP:O	1:D:182:LEU:HB2	2.20	0.41
1:C:73:ARG:NH2	1:C:110:ASP:OD2	2.50	0.41
1:C:236:TYR:HB2	1:C:285:PRO:CA	2.51	0.41
1:A:25:ARG:HD2	1:A:51:GLU:O	2.21	0.41
1:D:211:THR:HG21	1:D:335:ALA:CB	2.44	0.41
1:D:348:GLY:O	1:D:352:ILE:HG13	2.20	0.41
1:C:322:LEU:CD2	1:C:347:LEU:HD23	2.49	0.41
1:B:196:PRO:HD2	1:B:199:GLU:CD	2.40	0.41
1:B:77:ARG:HD2	1:B:77:ARG:N	2.34	0.41
1:D:250:ASP:OD1	1:D:320:ARG:NH1	2.54	0.41
1:C:224:ALA:HA	1:C:254:ALA:CB	2.50	0.41
1:C:231:ILE:O	1:C:233:TYR:N	2.50	0.41
1:B:77:ARG:NH1	1:B:77:ARG:HG3	2.36	0.41
1:D:61:HIS:CD2	1:D:142:LEU:HD11	2.56	0.41
1:C:341:TYR:CD1	1:C:341:TYR:C	2.93	0.41
1:B:425:PHE:C	1:B:427:GLU:H	2.24	0.41
1:C:202:ARG:HG3	1:C:203:GLU:H	1.86	0.41
1:D:12:VAL:HG12	1:D:401:GLY:HA2	2.02	0.41
1:B:75:GLY:O	1:B:77:ARG:CD	2.69	0.41
1:D:321:ILE:O	1:D:325:LEU:HD13	2.19	0.41
1:C:273:GLN:HA	1:C:276:PHE:HB2	2.02	0.41
1:A:424:ARG:HH11	1:A:424:ARG:HG2	1.84	0.41
1:A:8:ALA:HA	1:A:11:GLU:HG3	2.02	0.41
1:B:398:LEU:HD13	1:B:420:VAL:HG23	2.02	0.41
1:C:295:GLU:HG3	1:C:296:ALA:N	2.36	0.41
1:B:72:PHE:CE2	1:B:117:HIS:ND1	2.84	0.41
1:A:329:LEU:HA	1:A:329:LEU:HD12	1.87	0.41
1:C:186:GLU:HA	1:C:399:VAL:O	2.21	0.41
1:A:140:GLY:O	1:A:164:GLY:HA3	2.21	0.41
1:A:331:ASP:OD2	1:A:331:ASP:C	2.58	0.41
1:C:425:PHE:C	1:C:425:PHE:CD2	2.93	0.41
1:C:347:LEU:O	1:C:351:ILE:HG13	2.20	0.41
1:A:422:LEU:O	1:A:423:ALA:C	2.58	0.41
1:C:302:ARG:CZ	1:C:302:ARG:HB2	2.51	0.41
1:C:36:LYS:O	1:C:37:GLU:HG2	2.20	0.41
1:D:385:GLU:O	1:D:388:ASP:HB2	2.20	0.41
1:C:35:GLY:C	1:C:37:GLU:H	2.24	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:323:HIS:O	1:A:327:HIS:HD2	2.04	0.41
1:C:221:PRO:HG3	1:C:316:LEU:HD21	2.01	0.41
1:C:321:ILE:O	1:C:325:LEU:HD13	2.21	0.41
1:C:280:LYS:O	1:C:282:PRO:CD	2.68	0.41
1:C:223:PHE:C	1:C:225:VAL:H	2.24	0.41
1:A:165:ASN:C	1:A:165:ASN:ND2	2.73	0.41
1:A:10:ARG:HH11	1:A:10:ARG:CG	2.18	0.41
1:B:420:VAL:HG22	1:B:421:SER:N	2.35	0.41
1:C:190:GLY:HA2	1:C:409:LEU:HD12	2.02	0.41
1:B:261:TYR:HD1	1:B:283:PHE:CD2	2.38	0.41
1:D:360:ILE:CG2	1:D:361:LEU:HD13	2.48	0.41
1:D:210:LYS:H	1:D:210:LYS:CD	2.34	0.41
1:D:224:ALA:HB1	1:D:254:ALA:N	2.35	0.41
1:D:312:GLY:O	1:D:320:ARG:N	2.54	0.41
1:D:293:HIS:HB3	1:D:295:GLU:OE2	2.20	0.41
1:C:160:SER:HB3	1:C:185:ALA:HA	2.02	0.41
1:A:326:LYS:HG2	1:A:326:LYS:O	2.21	0.41
1:B:36:LYS:HB2	1:B:36:LYS:HE3	1.84	0.41
1:D:165:ASN:HD22	1:D:165:ASN:HA	1.55	0.41
1:B:28:LEU:O	1:B:29:ASP:HB2	2.20	0.41
1:D:244:ARG:O	1:D:245:ALA:HB2	2.21	0.41
1:C:413:LEU:HD22	1:C:418:GLN:HE22	1.86	0.41
1:C:32:MET:HE2	1:C:32:MET:HB3	1.92	0.41
1:B:83:THR:O	1:B:87:VAL:HG23	2.21	0.41
1:C:31:GLY:HA3	1:C:63:ASP:C	2.42	0.40
1:A:403:GLU:O	1:A:407:LEU:HB2	2.21	0.40
1:D:399:VAL:HG22	1:D:423:ALA:HB3	2.03	0.40
1:B:226:GLU:O	1:B:229:GLN:HG2	2.21	0.40
1:B:178:PRO:HB3	1:C:126:TRP:CD2	2.56	0.40
1:C:312:GLY:HA2	1:C:313:SER:C	2.41	0.40
1:B:165:ASN:C	1:B:165:ASN:ND2	2.74	0.40
1:D:402:GLU:HB2	1:D:405:LYS:HG3	2.02	0.40
1:D:100:VAL:HG13	2:H:3:U:O4	2.21	0.40
1:C:88:LEU:CD1	1:C:264:LEU:HD11	2.51	0.40
1:B:312:GLY:O	1:B:321:ILE:HG22	2.21	0.40
1:D:97:ALA:HA	2:H:2:U:C5	2.56	0.40
1:D:97:ALA:O	1:D:101:MET:N	2.39	0.40
1:C:32:MET:HE1	1:C:105:PHE:HZ	1.84	0.40
1:D:235:LEU:CD1	1:D:247:ILE:HD13	2.50	0.40
1:C:231:ILE:HG21	1:C:310:LEU:HD21	2.03	0.40
1:A:402:GLU:O	1:A:403:GLU:C	2.58	0.40
1:C:336:LEU:CD1	1:C:351:ILE:HG21	2.51	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:354:ARG:HA	1:C:367:LEU:CD2	2.51	0.40
1:C:387:LEU:O	1:C:416:ARG:NH2	2.49	0.40
1:B:48:ASP:HB3	1:B:51:GLU:CG	2.51	0.40
1:A:163:LEU:HD12	1:A:163:LEU:HA	1.70	0.40
1:D:393:GLU:HA	1:D:394:PRO:HD2	1.92	0.40
1:D:189:TYR:OH	1:D:341:TYR:HB2	2.21	0.40
1:C:207:ILE:CG2	1:C:207:ILE:O	2.69	0.40
1:D:358:VAL:CG1	1:D:359:ARG:N	2.84	0.40
1:D:420:VAL:CG2	1:D:421:SER:H	2.22	0.40
1:D:258:LEU:HD21	1:D:283:PHE:O	2.21	0.40
1:D:45:PHE:CE2	1:D:70:LYS:HG2	2.57	0.40
1:A:266:ARG:NH2	1:D:273:GLN:NE2	2.68	0.40
1:C:197:TYR:O	1:C:198:ARG:C	2.60	0.40
1:D:396:VAL:HG12	1:D:397:VAL:N	2.36	0.40
1:D:49:PRO:HB3	1:D:71:LEU:HD12	2.03	0.40
1:C:195:ARG:O	1:C:196:PRO:C	2.60	0.40
1:C:315:MET:HE3	1:C:317:ALA:HB3	2.03	0.40
1:A:277:LEU:C	1:A:279:GLY:H	2.24	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%)	393 (92%)	31 (7%)	5 (1%)	19	54
1	B	429/431 (100%)	374 (87%)	46 (11%)	9 (2%)	11	36
1	C	429/431 (100%)	334 (78%)	73 (17%)	22 (5%)	3	9
1	D	429/431 (100%)	345 (80%)	58 (14%)	26 (6%)	2	5
All	All	1716/1724 (100%)	1446 (84%)	208 (12%)	62 (4%)	5	19

All (62) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	8	ALA
1	B	38	GLU
1	B	316	LEU
1	B	354	ARG
1	C	166	ARG
1	C	292	GLU
1	A	225	VAL
1	A	423	ALA
1	B	74	GLU
1	C	8	ALA
1	C	38	GLU
1	C	225	VAL
1	C	232	LEU
1	C	363	GLU
1	C	407	LEU
1	D	22	GLY
1	D	166	ARG
1	D	182	LEU
1	D	198	ARG
1	D	228	ALA
1	D	307	MET
1	D	421	SER
1	C	196	PRO
1	C	328	GLY
1	D	196	PRO
1	D	210	LYS
1	D	224	ALA
1	D	328	GLY
1	D	330	SER
1	D	363	GLU
1	D	408	ALA
1	A	363	GLU
1	A	403	GLU
1	A	428	GLY
1	B	426	GLY
1	C	66	GLY
1	C	313	SER
1	D	38	GLU
1	D	102	ASP
1	D	400	HIS
1	B	45	PHE
1	B	399	VAL
1	C	160	SER

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Mol	Chain	Res	Type
1	C	226	GLU
1	C	271	GLU
1	C	344	GLN
1	D	30	CYS
1	D	193	PRO
1	D	282	PRO
1	D	292	GLU
1	D	394	PRO
1	B	377	PHE
1	C	224	ALA
1	C	251	SER
1	C	282	PRO
1	D	366	PRO
1	C	399	VAL
1	D	354	ARG
1	C	281	ASN
1	D	187	GLY
1	C	207	ILE
1	D	351	ILE

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%)	315 (92%)	26 (8%)	19	47
1	B	341/341 (100%)	316 (93%)	25 (7%)	20	49
1	C	341/341 (100%)	324 (95%)	17 (5%)	34	71
1	D	341/341 (100%)	326 (96%)	15 (4%)	39	76
All	All	1364/1364 (100%)	1281 (94%)	83 (6%)	26	59

All (83) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	SER
1	A	27	LEU
1	A	34	GLN

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Mol	Chain	Res	Type
1	A	38	GLU
1	A	41	ASN
1	A	55	VAL
1	A	94	LEU
1	A	163	LEU
1	A	165	ASN
1	A	171	LEU
1	A	186	GLU
1	A	195	ARG
1	A	219	LEU
1	A	226	GLU
1	A	229	GLN
1	A	241	ARG
1	A	264	LEU
1	A	336	LEU
1	A	364	GLU
1	A	386	LEU
1	A	388	ASP
1	A	390	LEU
1	A	398	LEU
1	A	406	LEU
1	A	407	LEU
1	A	409	LEU
1	B	12	VAL
1	B	27	LEU
1	B	28	LEU
1	B	37	GLU
1	B	57	LEU
1	B	74	GLU
1	B	77	ARG
1	B	102	ASP
1	B	128	ARG
1	B	165	ASN
1	B	171	LEU
1	B	175	SER
1	B	186	GLU
1	B	211	THR
1	B	219	LEU
1	B	226	GLU
1	B	227	ARG
1	B	229	GLN
1	B	302	ARG

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Mol	Chain	Res	Type
1	B	329	LEU
1	B	336	LEU
1	B	344	GLN
1	B	365	VAL
1	B	390	LEU
1	B	409	LEU
1	C	13	THR
1	C	27	LEU
1	C	36	LYS
1	C	38	GLU
1	C	57	LEU
1	C	74	GLU
1	C	155	ARG
1	C	165	ASN
1	C	166	ARG
1	C	196	PRO
1	C	227	ARG
1	C	276	PHE
1	C	293	HIS
1	C	315	MET
1	C	389	TRP
1	C	398	LEU
1	C	422	LEU
1	D	27	LEU
1	D	37	GLU
1	D	74	GLU
1	D	96	ASP
1	D	132	LEU
1	D	165	ASN
1	D	166	ARG
1	D	196	PRO
1	D	226	GLU
1	D	229	GLN
1	D	264	LEU
1	D	325	LEU
1	D	359	ARG
1	D	391	GLN
1	D	415	LEU

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

Mol	Chain	Res	Type
1	A	41	ASN
1	A	59	HIS
1	A	151	GLN
1	A	165	ASN
1	A	229	GLN
1	A	301	ASN
1	B	41	ASN
1	B	151	GLN
1	B	165	ASN
1	B	229	GLN
1	B	238	HIS
1	B	275	HIS
1	B	344	GLN
1	B	383	GLN
1	C	41	ASN
1	C	165	ASN
1	C	194	HIS
1	C	214	GLN
1	C	273	GLN
1	C	275	HIS
1	C	278	GLN
1	C	323	HIS
1	C	327	HIS
1	D	34	GLN
1	D	41	ASN
1	D	59	HIS
1	D	117	HIS
1	D	165	ASN
1	D	214	GLN
1	D	229	GLN
1	D	273	GLN
1	D	327	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	E	3/4 (75%)	3 (100%)	0
2	F	4/4 (100%)	3 (75%)	1 (25%)
2	G	1/4 (25%)	1 (100%)	0
2	H	4/4 (100%)	2 (50%)	2 (50%)
All	All	12/16 (75%)	9 (75%)	3 (25%)

All (9) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	E	2	U
2	E	3	U
2	E	4	U
2	F	2	U
2	F	3	U
2	F	4	U
2	G	2	U
2	H	2	U
2	H	4	U

All (3) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	F	1	U
2	H	1	U
2	H	3	U

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 64 ligands modelled in this entry, 8 are monoatomic - leaving 56 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	$\# Z > 2$
3	SO4	A	432	-	4,4,4	1.72	0	6,6,6	0.82	0
3	SO4	A	433	-	4,4,4	1.64	0	6,6,6	1.13	1 (16%)
3	SO4	A	434	-	4,4,4	1.61	0	6,6,6	0.89	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SO4	A	435	-	4,4,4	1.58	0	6,6,6	0.91	0
3	SO4	A	436	-	4,4,4	1.60	0	6,6,6	0.91	0
3	SO4	A	437	-	4,4,4	1.60	0	6,6,6	0.93	0
3	SO4	A	438	-	4,4,4	1.44	0	6,6,6	0.96	0
3	SO4	A	439	-	4,4,4	1.59	0	6,6,6	0.91	0
3	SO4	A	440	-	4,4,4	1.61	0	6,6,6	0.87	0
3	SO4	A	441	-	4,4,4	1.54	0	6,6,6	0.93	0
3	SO4	A	442	-	4,4,4	1.60	0	6,6,6	0.90	0
3	SO4	A	443	-	4,4,4	1.54	0	6,6,6	0.92	0
3	SO4	A	444	-	4,4,4	1.61	0	6,6,6	0.89	0
3	SO4	A	445	-	4,4,4	1.59	0	6,6,6	0.91	0
3	SO4	A	446	-	4,4,4	1.60	0	6,6,6	0.91	0
3	SO4	A	447	-	4,4,4	1.63	0	6,6,6	0.83	0
3	SO4	A	448	-	4,4,4	1.58	0	6,6,6	0.92	0
3	SO4	A	449	-	4,4,4	1.58	0	6,6,6	0.91	0
4	FLC	A	450	-	5,12,12	4.88	2 (40%)	7,17,17	0.41	0
4	FLC	A	451	-	5,12,12	5.61	2 (40%)	7,17,17	0.39	0
3	SO4	B	432	-	4,4,4	1.58	0	6,6,6	0.92	0
3	SO4	B	433	-	4,4,4	1.59	0	6,6,6	0.95	0
3	SO4	B	434	-	4,4,4	1.56	0	6,6,6	0.92	0
3	SO4	B	435	-	4,4,4	1.62	0	6,6,6	0.90	0
3	SO4	B	436	-	4,4,4	1.66	0	6,6,6	0.87	0
3	SO4	B	437	-	4,4,4	1.60	0	6,6,6	0.91	0
3	SO4	B	438	-	4,4,4	1.62	0	6,6,6	0.90	0
3	SO4	B	439	-	4,4,4	1.56	0	6,6,6	0.91	0
3	SO4	B	440	-	4,4,4	1.54	0	6,6,6	0.91	0
3	SO4	B	441	-	4,4,4	1.64	0	6,6,6	0.88	0
3	SO4	B	442	-	4,4,4	1.57	0	6,6,6	0.92	0
3	SO4	B	443	-	4,4,4	1.62	0	6,6,6	0.90	0
3	SO4	B	444	-	4,4,4	1.68	0	6,6,6	0.91	0
3	SO4	B	445	-	4,4,4	1.57	0	6,6,6	0.92	0
3	SO4	B	446	-	4,4,4	1.60	0	6,6,6	0.89	0
3	SO4	B	447	-	4,4,4	1.56	0	6,6,6	0.91	0
3	SO4	B	448	-	4,4,4	1.67	1 (25%)	6,6,6	0.88	0
3	SO4	C	432	-	4,4,4	1.59	0	6,6,6	0.92	0
3	SO4	C	433	-	4,4,4	1.58	0	6,6,6	0.91	0
3	SO4	C	434	-	4,4,4	1.59	0	6,6,6	0.91	0
3	SO4	C	435	-	4,4,4	1.57	0	6,6,6	0.93	0
3	SO4	C	436	-	4,4,4	1.62	0	6,6,6	0.88	0
3	SO4	C	437	-	4,4,4	1.57	0	6,6,6	0.89	0
3	SO4	C	438	-	4,4,4	1.57	0	6,6,6	0.94	0
3	SO4	C	439	-	4,4,4	1.59	0	6,6,6	0.93	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SO4	C	440	-	4,4,4	1.57	0	6,6,6	0.91	0
3	SO4	C	441	-	4,4,4	1.62	0	6,6,6	0.88	0
3	SO4	D	432	-	4,4,4	1.63	0	6,6,6	0.90	0
3	SO4	D	433	-	4,4,4	1.60	0	6,6,6	0.93	0
3	SO4	D	434	-	4,4,4	1.55	0	6,6,6	0.92	0
3	SO4	D	435	-	4,4,4	1.60	0	6,6,6	0.90	0
3	SO4	D	436	-	4,4,4	1.57	0	6,6,6	0.91	0
3	SO4	D	437	-	4,4,4	1.61	0	6,6,6	0.86	0
3	SO4	D	438	-	4,4,4	1.63	0	6,6,6	0.86	0
3	SO4	D	439	-	4,4,4	1.63	0	6,6,6	0.87	0
3	SO4	D	440	-	4,4,4	1.57	0	6,6,6	0.92	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	SO4	A	432	-	-	0/0/0/0	0/0/0/0
3	SO4	A	433	-	-	0/0/0/0	0/0/0/0
3	SO4	A	434	-	-	0/0/0/0	0/0/0/0
3	SO4	A	435	-	-	0/0/0/0	0/0/0/0
3	SO4	A	436	-	-	0/0/0/0	0/0/0/0
3	SO4	A	437	-	-	0/0/0/0	0/0/0/0
3	SO4	A	438	-	-	0/0/0/0	0/0/0/0
3	SO4	A	439	-	-	0/0/0/0	0/0/0/0
3	SO4	A	440	-	-	0/0/0/0	0/0/0/0
3	SO4	A	441	-	-	0/0/0/0	0/0/0/0
3	SO4	A	442	-	-	0/0/0/0	0/0/0/0
3	SO4	A	443	-	-	0/0/0/0	0/0/0/0
3	SO4	A	444	-	-	0/0/0/0	0/0/0/0
3	SO4	A	445	-	-	0/0/0/0	0/0/0/0
3	SO4	A	446	-	-	0/0/0/0	0/0/0/0
3	SO4	A	447	-	-	0/0/0/0	0/0/0/0
3	SO4	A	448	-	-	0/0/0/0	0/0/0/0
3	SO4	A	449	-	-	0/0/0/0	0/0/0/0
4	FLC	A	450	-	-	0/6/16/16	0/0/0/0
4	FLC	A	451	-	-	0/6/16/16	0/0/0/0
3	SO4	B	432	-	-	0/0/0/0	0/0/0/0
3	SO4	B	433	-	-	0/0/0/0	0/0/0/0
3	SO4	B	434	-	-	0/0/0/0	0/0/0/0
3	SO4	B	435	-	-	0/0/0/0	0/0/0/0
3	SO4	B	436	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SO4	B	437	-	-	0/0/0/0	0/0/0/0
3	SO4	B	438	-	-	0/0/0/0	0/0/0/0
3	SO4	B	439	-	-	0/0/0/0	0/0/0/0
3	SO4	B	440	-	-	0/0/0/0	0/0/0/0
3	SO4	B	441	-	-	0/0/0/0	0/0/0/0
3	SO4	B	442	-	-	0/0/0/0	0/0/0/0
3	SO4	B	443	-	-	0/0/0/0	0/0/0/0
3	SO4	B	444	-	-	0/0/0/0	0/0/0/0
3	SO4	B	445	-	-	0/0/0/0	0/0/0/0
3	SO4	B	446	-	-	0/0/0/0	0/0/0/0
3	SO4	B	447	-	-	0/0/0/0	0/0/0/0
3	SO4	B	448	-	-	0/0/0/0	0/0/0/0
3	SO4	C	432	-	-	0/0/0/0	0/0/0/0
3	SO4	C	433	-	-	0/0/0/0	0/0/0/0
3	SO4	C	434	-	-	0/0/0/0	0/0/0/0
3	SO4	C	435	-	-	0/0/0/0	0/0/0/0
3	SO4	C	436	-	-	0/0/0/0	0/0/0/0
3	SO4	C	437	-	-	0/0/0/0	0/0/0/0
3	SO4	C	438	-	-	0/0/0/0	0/0/0/0
3	SO4	C	439	-	-	0/0/0/0	0/0/0/0
3	SO4	C	440	-	-	0/0/0/0	0/0/0/0
3	SO4	C	441	-	-	0/0/0/0	0/0/0/0
3	SO4	D	432	-	-	0/0/0/0	0/0/0/0
3	SO4	D	433	-	-	0/0/0/0	0/0/0/0
3	SO4	D	434	-	-	0/0/0/0	0/0/0/0
3	SO4	D	435	-	-	0/0/0/0	0/0/0/0
3	SO4	D	436	-	-	0/0/0/0	0/0/0/0
3	SO4	D	437	-	-	0/0/0/0	0/0/0/0
3	SO4	D	438	-	-	0/0/0/0	0/0/0/0
3	SO4	D	439	-	-	0/0/0/0	0/0/0/0
3	SO4	D	440	-	-	0/0/0/0	0/0/0/0

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	451	FLC	CG-CGC	9.25	1.55	1.49
4	A	451	FLC	CA-CAC	8.10	1.54	1.49
4	A	450	FLC	CG-CGC	7.81	1.54	1.49
4	A	450	FLC	CA-CAC	7.44	1.54	1.49
3	B	448	SO4	O1-S	2.08	1.53	1.47

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	433	SO4	O2-S-O1	-2.48	101.32	109.53

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	431/431 (100%)	-0.10	4 (0%) 81 87	25, 46, 69, 83	0
1	B	431/431 (100%)	-0.06	8 (1%) 64 72	24, 46, 84, 103	0
1	C	431/431 (100%)	1.12	98 (22%) 1 2	34, 94, 165, 167	0
1	D	431/431 (100%)	0.94	76 (17%) 2 2	40, 88, 152, 163	0
2	E	4/4 (100%)	1.64	2 (50%) 0 0	70, 76, 81, 95	0
2	F	4/4 (100%)	1.36	1 (25%) 1 1	83, 90, 98, 100	0
2	G	2/4 (50%)	1.60	0 100 100	145, 145, 145, 151	0
2	H	4/4 (100%)	2.02	3 (75%) 0 0	118, 125, 139, 151	0
All	All	1738/1740 (99%)	0.48	192 (11%) 6 7	24, 62, 155, 167	0

All (192) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	335	ALA	12.9
1	C	337	VAL	10.3
1	C	322	LEU	9.1
1	C	219	LEU	9.0
1	C	218	VAL	8.3
1	C	336	LEU	7.9
1	C	326	LYS	7.7
1	C	307	MET	7.4
1	C	329	LEU	7.3
1	C	242	LEU	7.3
1	C	338	PHE	7.0
1	D	294	THR	6.9
1	C	371	VAL	6.8
1	C	205	LEU	6.8
1	C	300	LEU	6.7
1	C	213	SER	6.7

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Mol	Chain	Res	Type	RSRZ
1	C	308	VAL	6.5
1	D	335	ALA	6.2
1	D	360	ILE	6.0
1	C	325	LEU	5.9
1	C	209	GLU	5.7
1	C	250	ASP	5.7
1	C	214	GLN	5.6
1	D	298	LYS	5.5
1	D	322	LEU	5.5
1	D	208	LEU	5.4
1	C	247	ILE	5.4
1	D	300	LEU	5.4
1	D	245	ALA	5.3
1	C	376	GLY	5.3
1	D	334	ASN	5.2
1	C	245	ALA	5.1
1	C	309	VAL	5.1
1	C	241	ARG	5.1
1	C	288	LEU	5.0
1	D	291	VAL	5.0
1	C	248	TYR	5.0
1	C	217	LYS	4.9
1	D	308	VAL	4.8
1	D	218	VAL	4.8
1	D	216	GLY	4.8
1	D	212	LEU	4.8
1	D	283	PHE	4.7
1	C	215	GLY	4.7
1	D	336	LEU	4.6
1	C	301	ASN	4.6
1	C	360	ILE	4.6
1	C	194	HIS	4.6
1	C	324	HIS	4.5
1	C	167	GLU	4.5
1	C	367	LEU	4.4
1	D	297	SER	4.4
1	C	208	LEU	4.4
1	D	363	GLU	4.3
1	C	297	SER	4.3
1	D	324	HIS	4.2
1	D	250	ASP	4.2
1	D	249	LEU	4.2

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Mol	Chain	Res	Type	RSRZ
1	D	361	LEU	4.2
1	D	106	PHE	4.2
1	C	235	LEU	4.2
1	D	207	ILE	4.2
1	D	316	LEU	4.2
1	D	211	THR	4.1
1	B	77	ARG	4.1
1	D	290	VAL	4.1
1	C	353	ALA	4.0
1	C	377	PHE	4.0
1	C	415	LEU	4.0
1	C	211	THR	3.9
1	C	303	ALA	3.9
1	C	291	VAL	3.9
1	C	204	PHE	3.9
1	B	78	GLY	3.9
1	D	333	ARG	3.8
1	C	294	THR	3.8
1	C	327	HIS	3.7
1	D	358	VAL	3.7
1	C	302	ARG	3.7
1	C	201	VAL	3.6
1	D	362	GLY	3.6
1	C	243	PRO	3.6
1	D	325	LEU	3.6
1	D	307	MET	3.5
1	C	333	ARG	3.5
1	B	72	PHE	3.5
1	C	192	ARG	3.5
1	D	99	LYS	3.5
1	C	239	GLY	3.5
1	D	209	GLU	3.5
1	C	220	ILE	3.4
1	C	354	ARG	3.4
1	D	204	PHE	3.3
1	C	361	LEU	3.3
1	D	326	LYS	3.3
1	D	213	SER	3.3
1	D	247	ILE	3.2
1	C	207	ILE	3.2
1	C	372	HIS	3.2
1	C	298	LYS	3.2

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Mol	Chain	Res	Type	RSRZ
1	D	292	GLU	3.1
1	D	332	PRO	3.1
1	C	358	VAL	3.1
1	C	365	VAL	3.1
1	C	418	GLN	3.1
1	D	374	LEU	3.1
1	D	288	LEU	3.1
1	C	316	LEU	3.1
1	C	352	ILE	3.1
1	D	214	GLN	3.0
1	D	8	ALA	3.0
1	D	309	VAL	3.0
1	C	238	HIS	3.0
1	D	306	PRO	3.0
2	H	4	U	3.0
1	D	339	VAL	2.9
1	C	193	PRO	2.9
1	C	246	PRO	2.9
1	C	210	LYS	2.9
1	D	190	GLY	2.9
1	C	276	PHE	2.9
1	D	301	ASN	2.9
1	D	98	LEU	2.9
1	C	370	SER	2.8
1	C	216	GLY	2.8
1	D	286	ALA	2.8
1	C	364	GLU	2.8
1	C	222	THR	2.8
1	D	219	LEU	2.8
1	D	201	VAL	2.8
1	D	344	GLN	2.7
1	D	329	LEU	2.7
1	C	295	GLU	2.7
1	C	234	VAL	2.7
1	D	312	GLY	2.7
1	C	197	TYR	2.7
1	D	248	TYR	2.7
1	D	246	PRO	2.6
1	C	304	PRO	2.6
1	C	306	PRO	2.6
1	D	205	LEU	2.6
1	B	105	PHE	2.6

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Mol	Chain	Res	Type	RSRZ
2	H	3	U	2.6
1	D	197	TYR	2.6
1	D	293	HIS	2.6
1	C	244	ARG	2.6
1	D	338	PHE	2.6
2	E	2	U	2.5
1	B	71	LEU	2.5
1	C	212	LEU	2.5
1	C	283	PHE	2.5
1	D	240	HIS	2.5
1	D	337	VAL	2.5
1	C	339	VAL	2.4
1	D	96	ASP	2.4
1	C	332	PRO	2.4
1	A	358	VAL	2.4
1	D	102	ASP	2.4
1	B	39	ALA	2.4
1	C	249	LEU	2.4
1	C	359	ARG	2.3
1	C	198	ARG	2.3
1	D	377	PHE	2.3
2	H	2	U	2.3
1	C	296	ALA	2.3
1	C	321	ILE	2.3
1	C	190	GLY	2.3
1	D	328	GLY	2.2
1	A	360	ILE	2.2
1	C	290	VAL	2.2
1	B	50	LYS	2.2
1	C	351	ILE	2.2
1	D	356	PRO	2.2
1	D	251	SER	2.2
1	D	224	ALA	2.2
1	C	305	GLY	2.2
1	C	414	ALA	2.2
1	D	10	ARG	2.1
1	C	185	ALA	2.1
1	D	318	GLY	2.1
1	C	231	ILE	2.1
1	A	361	LEU	2.1
1	C	328	GLY	2.1
2	E	3	U	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	71	LEU	2.1
1	C	221	PRO	2.1
1	B	6	PHE	2.1
1	D	244	ARG	2.1
2	F	2	U	2.0
1	D	319	GLY	2.0
1	C	368	ARG	2.0
1	D	310	LEU	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	SO4	B	432	5/5	0.42	10.88	137,138,138,139	0
3	SO4	B	436	5/5	0.35	9.57	143,143,144,144	0
4	FLC	A	450	13/13	0.39	6.87	122,124,126,128	0
3	SO4	A	432	5/5	0.31	6.15	140,140,141,141	0
3	SO4	A	444	5/5	0.44	5.27	134,134,134,135	0
3	SO4	B	444	5/5	0.24	3.65	78,79,80,80	0
3	SO4	A	436	5/5	0.29	3.41	171,171,171,171	0
3	SO4	A	449	5/5	0.22	3.12	124,124,125,125	0
3	SO4	C	434	5/5	0.30	3.04	137,137,137,137	0
4	FLC	A	451	13/13	0.29	2.87	71,76,85,86	0
3	SO4	A	442	5/5	0.24	2.74	139,140,140,140	0
3	SO4	A	448	5/5	0.26	2.54	126,126,126,127	0
3	SO4	B	435	5/5	0.21	2.22	116,116,116,117	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	SO4	B	447	5/5	0.38	2.01	153,153,153,153	0
3	SO4	A	446	5/5	0.26	1.92	117,118,118,118	0
3	SO4	B	442	5/5	0.24	1.90	116,116,117,117	0
3	SO4	A	445	5/5	0.23	1.60	109,110,110,111	0
3	SO4	B	438	5/5	0.22	1.22	96,97,97,98	0
3	SO4	D	433	5/5	0.18	0.99	135,136,136,136	0
3	SO4	D	434	5/5	0.23	0.89	139,139,139,140	0
3	SO4	C	433	5/5	0.22	0.67	95,95,96,96	0
3	SO4	A	438	5/5	0.18	0.54	61,62,63,65	0
3	SO4	D	436	5/5	0.21	0.49	86,86,87,87	0
3	SO4	B	440	5/5	0.18	0.48	66,67,69,72	0
3	SO4	A	433	5/5	0.17	0.47	53,54,55,58	0
3	SO4	C	435	5/5	0.18	0.21	110,110,110,111	0
3	SO4	C	441	5/5	0.18	0.17	125,125,126,126	0
3	SO4	A	437	5/5	0.19	-0.01	152,152,152,152	0
3	SO4	D	437	5/5	0.19	-0.22	114,114,115,115	0
3	SO4	A	439	5/5	0.16	-0.34	135,135,136,136	0
3	SO4	D	432	5/5	0.18	-0.48	130,130,130,130	0
5	ZN	C	443	1/1	0.14	-0.71	104,104,104,104	0
3	SO4	B	441	5/5	0.12	-0.72	98,98,98,99	0
5	ZN	C	442	1/1	0.15	-0.73	109,109,109,109	0
3	SO4	D	438	5/5	0.14	-0.75	80,81,83,83	0
3	SO4	C	432	5/5	0.21	-0.75	131,132,132,132	0
3	SO4	B	434	5/5	0.19	-0.79	129,129,130,130	0
3	SO4	B	439	5/5	0.14	-0.93	104,104,104,104	0
3	SO4	B	446	5/5	0.11	-1.00	104,104,105,105	0
5	ZN	B	450	1/1	0.11	-1.03	65,65,65,65	0
3	SO4	A	447	5/5	0.12	-1.09	41,41,43,47	0
3	SO4	D	439	5/5	0.14	-1.09	99,99,100,101	0
3	SO4	B	448	5/5	0.12	-1.12	54,59,60,60	0
3	SO4	C	437	5/5	0.19	-1.12	119,119,120,120	0
3	SO4	A	443	5/5	0.13	-1.18	88,88,89,89	0
5	ZN	D	442	1/1	0.12	-1.25	86,86,86,86	0
3	SO4	B	443	5/5	0.15	-1.39	94,95,95,96	0
5	ZN	A	453	1/1	0.10	-1.44	59,59,59,59	0
3	SO4	D	440	5/5	0.16	-1.46	148,148,148,149	0
3	SO4	A	434	5/5	0.15	-1.46	94,95,95,95	0
3	SO4	C	439	5/5	0.13	-1.46	74,75,76,77	0
3	SO4	C	440	5/5	0.11	-1.47	116,116,117,117	0
5	ZN	D	441	1/1	0.13	-1.64	88,88,88,88	0
5	ZN	A	452	1/1	0.09	-1.82	58,58,58,58	0
3	SO4	B	437	5/5	0.14	-1.87	132,132,132,132	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	SO4	C	436	5/5	0.09	-1.99	128,128,128,128	0
5	ZN	B	449	1/1	0.06	-2.15	61,61,61,61	0
3	SO4	B	433	5/5	0.16	-2.21	105,105,105,106	0
3	SO4	C	438	5/5	0.14	-4.94	116,117,118,118	0
3	SO4	A	440	5/5	0.18	-9.71	132,132,133,133	0
3	SO4	A	441	5/5	0.17	-	118,118,119,119	0
3	SO4	D	435	5/5	0.30	-	152,152,153,153	0
3	SO4	B	445	5/5	0.20	-	130,131,131,131	0
3	SO4	A	435	5/5	0.20	-	148,148,149,149	0

6.5 Other polymers ⓘ

There are no such residues in this entry.