



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 02:34 PM EDT

PDB ID : 3WFP / pdb_00003wfp
Title : tRNA processing enzyme (apo form 2)
Authors : Yamashita, S.; Takeshita, D.; Tomita, K.
Deposited on : 2013-07-23
Resolution : 4.00 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

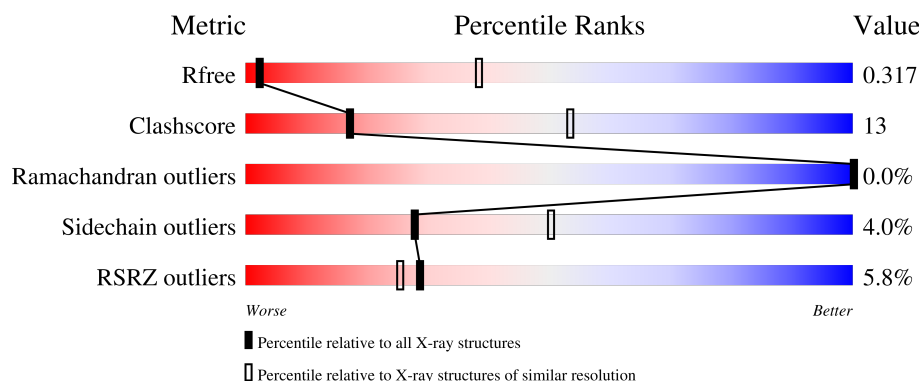
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.00 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	1082 (4.20-3.80)
Clashscore	190562	1129 (4.20-3.80)
Ramachandran outliers	187476	1064 (4.20-3.80)
Sidechain outliers	187428	1055 (4.20-3.80)
RSRZ outliers	180081	1082 (4.20-3.80)

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	497	4% 64% 24% • 8%
1	B	497	5% 67% 23% • 9%
1	C	497	8% 63% 20% • 16%
1	D	497	7% 63% 19% • 16%
1	E	497	2% 60% 21% • 17%

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Mol	Chain	Length	Quality of chain
1	F	497	
1	G	497	
1	H	497	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	C	1001	-	-	X	-
2	SO4	H	1001	-	-	X	-

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 27564 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.

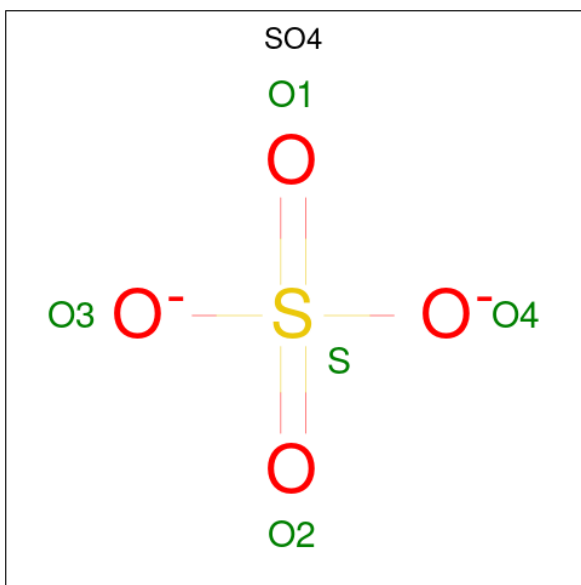
- Molecule 1 is a protein called Poly A polymerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	455	Total	C	N	O	S	0	0	0
			3624	2334	624	659	7			
1	B	450	Total	C	N	O	S	0	0	0
			3568	2296	611	654	7			
1	C	419	Total	C	N	O	S	0	0	0
			3436	2222	588	619	7			
1	D	419	Total	C	N	O	S	0	0	0
			3436	2222	588	619	7			
1	E	411	Total	C	N	O	S	0	0	0
			3365	2175	572	611	7			
1	F	411	Total	C	N	O	S	0	0	0
			3365	2175	572	611	7			
1	G	411	Total	C	N	O	S	0	0	0
			3365	2175	572	611	7			
1	H	411	Total	C	N	O	S	0	0	0
			3365	2175	572	611	7			

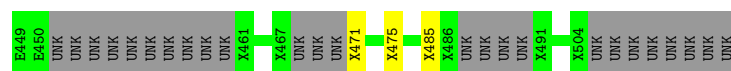
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	16	MET	-	expression tag	UNP O67911
B	16	MET	-	expression tag	UNP O67911
C	16	MET	-	expression tag	UNP O67911
D	16	MET	-	expression tag	UNP O67911
E	16	MET	-	expression tag	UNP O67911
F	16	MET	-	expression tag	UNP O67911
G	16	MET	-	expression tag	UNP O67911
H	16	MET	-	expression tag	UNP O67911

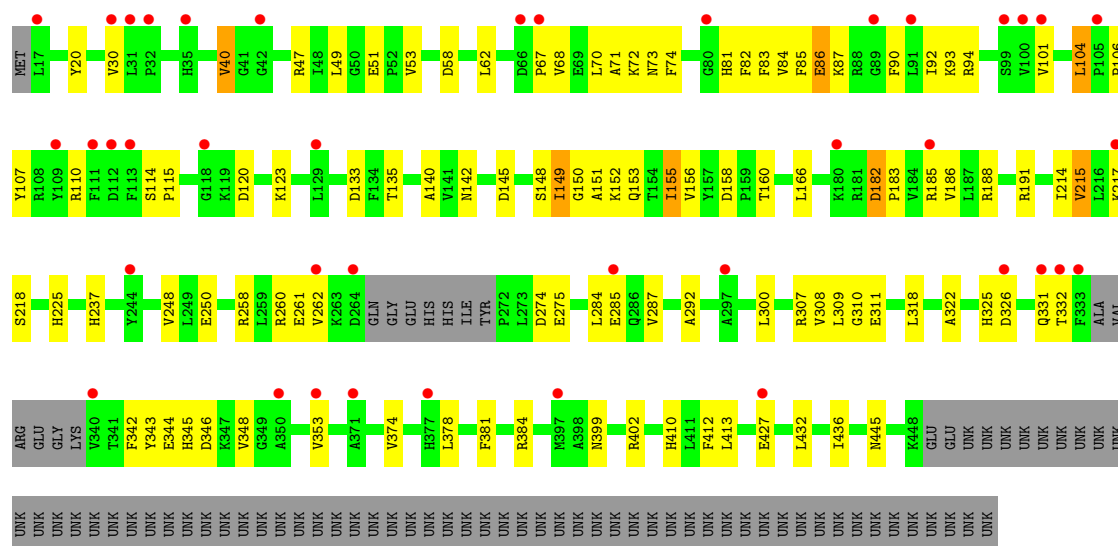
- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



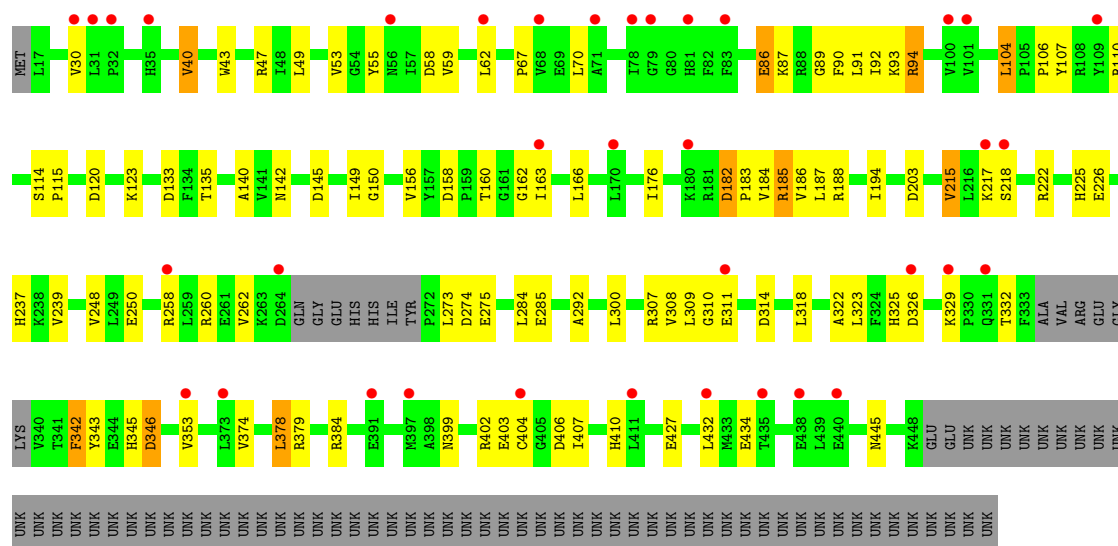
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	F	1	Total	O	S	0	0
			5	4	1		
2	G	1	Total	O	S	0	0
			5	4	1		
2	H	1	Total	O	S	0	0
			5	4	1		



• Molecule 1: Poly A polymerase

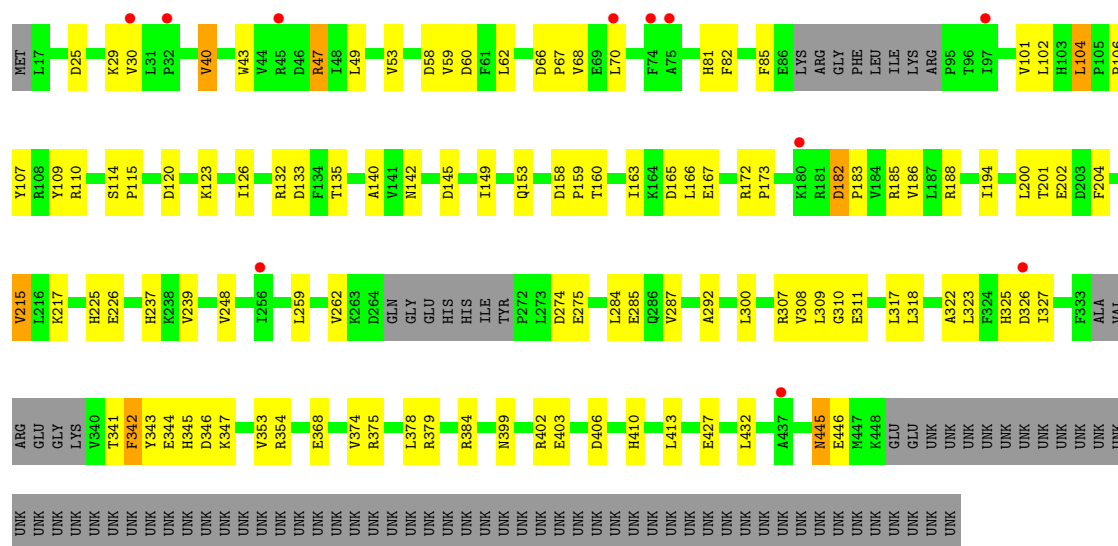


• Molecule 1: Poly A polymerase

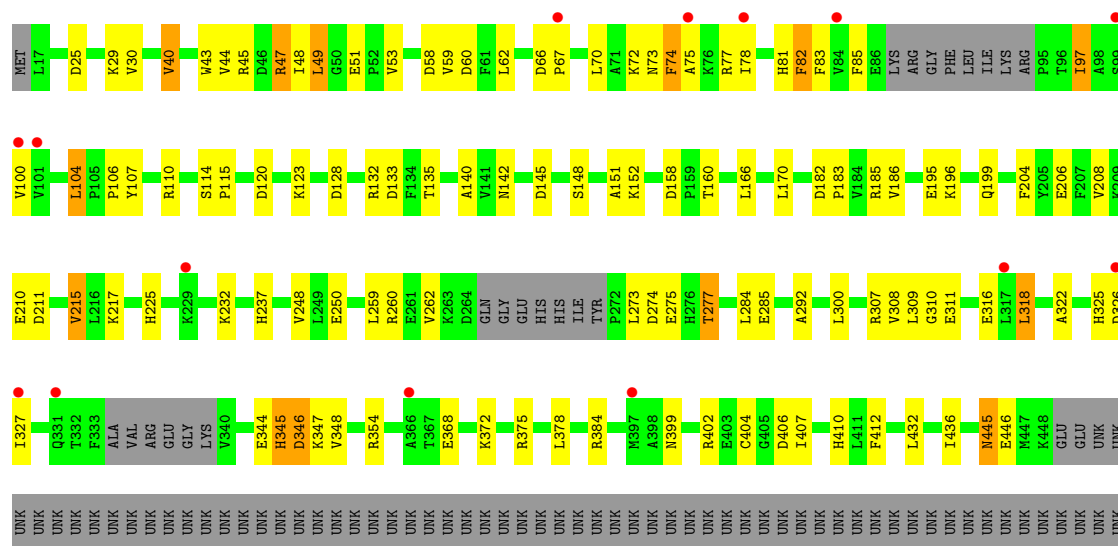


• Molecule 1: Poly A polymerase

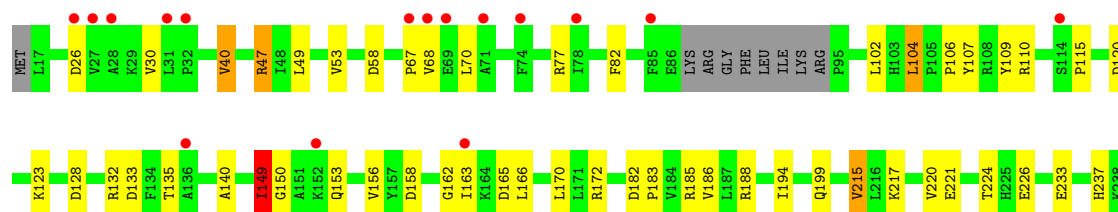


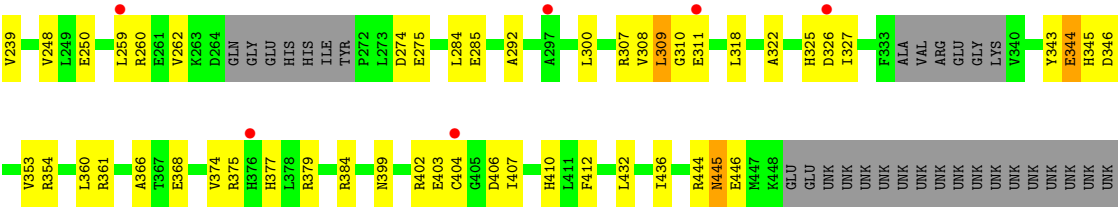


• Molecule 1: Poly A polymerase

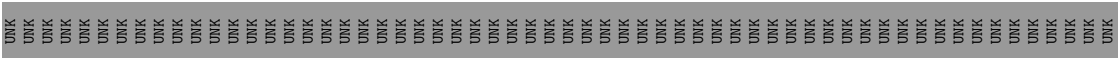
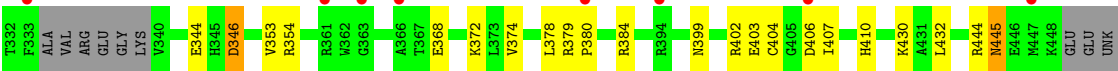
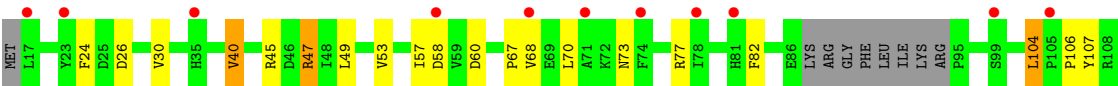


• Molecule 1: Poly A polymerase





● Molecule 1: Poly A polymerase



UNK

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	126.91Å 138.36Å 147.62Å 90.00° 111.04° 90.00°	Depositor
Resolution (Å)	19.97 – 4.00 19.97 – 4.00	Depositor EDS
% Data completeness (in resolution range)	86.8 (19.97-4.00) 86.0 (19.97-4.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.68 (at 4.00Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.258 , 0.314 0.263 , 0.317	Depositor DCC
R_{free} test set	1756 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	68.6	Xtriage
Anisotropy	0.055	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 78.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.38$, $\langle L^2 \rangle = 0.21$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.79	EDS
Total number of atoms	27564	wwPDB-VP
Average B, all atoms (Å ²)	142.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.68% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.31	0/3527	0.78	4/4750 (0.1%)
1	B	0.29	0/3454	0.77	2/4653 (0.0%)
1	C	0.31	0/3509	0.78	3/4726 (0.1%)
1	D	0.33	1/3509 (0.0%)	0.81	8/4726 (0.2%)
1	E	0.28	0/3436	0.74	3/4629 (0.1%)
1	F	0.34	0/3436	0.80	5/4629 (0.1%)
1	G	0.29	0/3436	0.78	4/4629 (0.1%)
1	H	0.28	0/3436	0.75	2/4629 (0.0%)
All	All	0.30	1/27743 (0.0%)	0.78	31/37371 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	94	ARG	C-N	5.90	1.41	1.33

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	343	TYR	N-CA-C	8.85	120.70	111.14
1	B	446	GLU	N-CA-C	8.21	123.14	113.20
1	B	149	ILE	N-CA-C	7.62	118.22	110.82
1	C	182	ASP	CA-C-N	7.48	127.12	119.19
1	C	182	ASP	C-N-CA	7.48	127.12	119.19
1	D	343	TYR	N-CA-C	7.32	119.34	111.36
1	G	150	GLY	N-CA-C	7.21	124.17	111.25
1	F	346	ASP	N-CA-C	-7.04	102.67	111.11
1	D	150	GLY	N-CA-C	7.01	121.67	110.87
1	G	309	LEU	N-CA-C	-6.86	104.49	112.86
1	G	149	ILE	N-CA-C	6.74	120.48	111.44
1	D	94	ARG	CA-C-N	-6.43	113.13	119.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	94	ARG	C-N-CA	-6.43	113.13	119.76
1	A	261	GLU	N-CA-C	6.43	120.23	112.38
1	F	47	ARG	N-CA-C	-6.39	104.40	111.82
1	A	259	LEU	N-CA-C	-6.27	104.90	112.54
1	E	85	PHE	CB-CA-C	-6.21	99.12	111.91
1	F	82	PHE	N-CA-C	6.19	119.03	109.07
1	D	182	ASP	CA-C-N	6.12	125.68	119.19
1	D	182	ASP	C-N-CA	6.12	125.68	119.19
1	H	149	ILE	N-CA-C	6.01	117.55	111.00
1	D	86	GLU	N-CA-C	5.86	119.93	111.56
1	H	152	LYS	N-CA-C	5.85	118.43	108.90
1	A	150	GLY	N-CA-C	5.74	119.97	110.55
1	F	74	PHE	N-CA-C	5.60	117.07	110.97
1	D	185	ARG	N-CA-C	-5.56	105.75	112.54
1	G	153	GLN	N-CA-C	-5.38	100.40	108.96
1	F	49	LEU	N-CA-C	-5.11	107.21	113.50
1	A	308	VAL	N-CA-C	5.04	115.53	108.17
1	E	182	ASP	CA-C-N	5.04	124.53	119.19
1	E	182	ASP	C-N-CA	5.04	124.53	119.19

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	3624	0	3522	108	0
1	B	3568	0	3439	81	0
1	C	3436	0	3470	104	0
1	D	3436	0	3470	107	0
1	E	3365	0	3384	76	0
1	F	3365	0	3384	96	0
1	G	3365	0	3384	84	0
1	H	3365	0	3384	58	0
2	A	5	0	0	0	0
2	B	5	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	5	0	0	2	0
2	D	5	0	0	0	0
2	E	5	0	0	1	0
2	F	5	0	0	1	0
2	G	5	0	0	0	0
2	H	5	0	0	2	0
All	All	27564	0	27437	691	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 13.

All (691) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92:ILE:HD12	1:A:93:LYS:N	1.27	1.41
1:C:345:HIS:HD2	1:C:346:ASP:N	1.30	1.28
1:C:345:HIS:CD2	1:C:346:ASP:H	1.57	1.20
1:A:92:ILE:CD1	1:A:93:LYS:H	1.55	1.19
1:C:345:HIS:CD2	1:C:346:ASP:N	2.10	1.16
1:D:86:GLU:HG3	1:D:94:ARG:HG3	1.28	1.15
1:D:308:VAL:HG12	1:D:309:LEU:HD13	1.27	1.14
1:D:133:ASP:HB3	1:D:185:ARG:HD3	1.25	1.14
1:F:347:LYS:HE3	1:F:375:ARG:HE	0.97	1.09
1:A:90:PHE:O	1:A:91:LEU:HG	1.56	1.05
1:E:308:VAL:HG12	1:E:309:LEU:HD13	1.37	1.05
1:F:49:LEU:HD11	1:F:196:LYS:HB3	1.40	1.04
1:G:325:HIS:CD2	1:G:377:HIS:HE1	1.77	1.03
1:D:90:PHE:CZ	1:D:222:ARG:HD3	1.93	1.03
1:G:221:GLU:HG3	1:G:361:ARG:HH11	1.21	1.02
1:A:92:ILE:CD1	1:A:93:LYS:N	2.20	0.99
1:F:347:LYS:HE3	1:F:375:ARG:NE	1.76	0.99
1:G:308:VAL:HG12	1:G:309:LEU:HD13	1.45	0.99
1:C:152:LYS:HE2	1:C:152:LYS:HA	1.46	0.97
1:D:184:VAL:CG1	1:D:222:ARG:HH21	1.76	0.97
1:C:308:VAL:HG12	1:C:309:LEU:HD13	1.46	0.96
1:E:347:LYS:HG2	1:E:375:ARG:NE	1.80	0.96
1:D:90:PHE:HE1	1:D:218:SER:CB	1.77	0.95
1:D:184:VAL:HG12	1:D:222:ARG:HH21	1.27	0.95
1:F:49:LEU:HD12	1:F:196:LYS:HD2	1.49	0.95
1:A:91:LEU:HB3	1:A:92:ILE:HA	1.49	0.95
1:D:183:PRO:HG3	1:D:217:LYS:HB2	1.46	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:155:ILE:HD12	1:C:156:VAL:H	1.33	0.94
1:G:325:HIS:CD2	1:G:377:HIS:CE1	2.56	0.93
1:D:90:PHE:CE2	1:D:222:ARG:HD3	2.05	0.92
1:C:155:ILE:HD12	1:C:156:VAL:N	1.85	0.91
1:D:90:PHE:CZ	1:D:222:ARG:CD	2.54	0.90
1:C:308:VAL:CG1	1:C:309:LEU:HD13	2.02	0.90
1:D:90:PHE:HE1	1:D:218:SER:HB2	1.38	0.89
1:C:183:PRO:HG3	1:C:217:LYS:HB2	1.53	0.88
1:F:44:VAL:HG12	1:F:48:ILE:HD12	1.56	0.88
1:F:347:LYS:CE	1:F:375:ARG:HE	1.85	0.88
1:D:90:PHE:CZ	1:D:222:ARG:NE	2.42	0.87
1:F:346:ASP:OD1	1:F:347:LYS:N	2.08	0.86
1:G:325:HIS:HD2	1:G:377:HIS:CE1	1.92	0.86
1:F:49:LEU:CD1	1:F:196:LYS:HD2	2.05	0.85
1:F:75:ALA:HB3	1:F:82:PHE:CE1	2.11	0.85
1:D:133:ASP:CB	1:D:185:ARG:HD3	2.07	0.84
1:D:133:ASP:HB3	1:D:185:ARG:CD	2.06	0.84
1:B:341:THR:OG1	1:B:343:TYR:HE2	1.59	0.83
1:D:332:THR:OG1	1:D:342:PHE:HB3	1.79	0.83
1:E:341:THR:HG1	1:E:343:TYR:HE2	0.93	0.83
1:G:344:GLU:N	1:G:344:GLU:OE2	2.13	0.82
1:C:151:ALA:HB2	1:D:427:GLU:HG3	1.61	0.82
1:D:308:VAL:CG1	1:D:309:LEU:HD13	2.08	0.81
1:A:345:HIS:CE1	1:A:346:ASP:OD1	2.34	0.81
1:D:184:VAL:HG12	1:D:222:ARG:NH2	1.96	0.80
1:E:308:VAL:HG12	1:E:309:LEU:CD1	2.12	0.80
1:F:75:ALA:HA	1:F:78:ILE:HG12	1.62	0.80
1:F:345:HIS:O	1:F:346:ASP:C	2.23	0.79
1:D:308:VAL:HG12	1:D:309:LEU:CD1	2.11	0.79
1:D:184:VAL:CG1	1:D:222:ARG:NH2	2.46	0.79
1:E:183:PRO:HG3	1:E:217:LYS:HB2	1.64	0.79
1:D:86:GLU:CG	1:D:94:ARG:HG3	2.11	0.79
1:B:183:PRO:HG3	1:B:217:LYS:HB2	1.65	0.78
1:G:183:PRO:HG3	1:G:217:LYS:HB2	1.65	0.78
1:A:183:PRO:HG3	1:A:217:LYS:HB2	1.66	0.77
1:F:49:LEU:HB3	1:F:51:GLU:HG3	1.67	0.77
1:G:221:GLU:CG	1:G:361:ARG:HH11	1.98	0.77
1:D:90:PHE:HZ	1:D:222:ARG:HD3	1.49	0.77
1:H:183:PRO:HG3	1:H:217:LYS:HB2	1.68	0.76
1:F:44:VAL:HG12	1:F:48:ILE:CD1	2.14	0.76
1:G:343:TYR:C	1:G:344:GLU:OE2	2.29	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:149:ILE:HD13	1:C:149:ILE:H	1.51	0.76
1:B:447:MET:N	1:B:447:MET:SD	2.58	0.76
1:F:347:LYS:HG2	1:F:375:ARG:NE	2.01	0.75
1:G:308:VAL:HG12	1:G:309:LEU:CD1	2.15	0.75
1:A:90:PHE:O	1:A:91:LEU:CG	2.31	0.75
1:B:225:HIS:NE2	1:B:311:GLU:OE2	2.20	0.75
1:E:308:VAL:CG1	1:E:309:LEU:HD13	2.15	0.75
1:G:346:ASP:O	1:G:375:ARG:HA	1.86	0.75
1:E:347:LYS:HG2	1:E:375:ARG:CD	2.16	0.74
1:C:225:HIS:NE2	1:C:311:GLU:OE2	2.21	0.74
1:D:184:VAL:HG23	1:D:187:LEU:HD12	1.70	0.74
1:C:345:HIS:HD2	1:C:346:ASP:H	0.77	0.74
1:D:90:PHE:CE1	1:D:218:SER:HB2	2.22	0.73
1:E:225:HIS:NE2	1:E:311:GLU:OE2	2.21	0.73
1:E:309:LEU:N	1:E:309:LEU:HD12	2.02	0.73
1:C:151:ALA:HB2	1:D:427:GLU:CG	2.19	0.73
1:B:308:VAL:HG12	1:B:309:LEU:HD13	1.70	0.73
1:D:91:LEU:HG	1:D:91:LEU:O	1.89	0.72
1:C:215:VAL:HG21	1:C:248:VAL:HG13	1.72	0.72
1:B:148:SER:OG	1:B:152:LYS:NZ	2.22	0.71
1:A:298:GLU:CD	1:A:444:ARG:HD2	2.16	0.71
1:H:250:GLU:OE2	1:H:260:ARG:NH2	2.20	0.71
1:C:71:ALA:HB3	1:C:82:PHE:HE1	1.56	0.70
1:G:221:GLU:HG3	1:G:361:ARG:NH1	2.03	0.70
1:G:346:ASP:O	1:G:375:ARG:HD2	1.92	0.69
1:D:86:GLU:HG3	1:D:94:ARG:CG	2.17	0.69
1:B:341:THR:OG1	1:B:343:TYR:CE2	2.41	0.69
1:D:90:PHE:CE2	1:D:222:ARG:CD	2.76	0.69
1:D:90:PHE:CD2	1:D:94:ARG:NH2	2.61	0.69
1:B:309:LEU:HD12	1:B:309:LEU:N	2.07	0.68
1:E:308:VAL:CG1	1:E:309:LEU:CD1	2.72	0.68
1:E:341:THR:OG1	1:E:343:TYR:HE2	1.71	0.68
1:D:250:GLU:OE2	1:D:260:ARG:NH2	2.27	0.68
1:F:183:PRO:HG3	1:F:217:LYS:HB2	1.75	0.68
1:F:237:HIS:ND1	1:F:285:GLU:OE1	2.26	0.68
1:F:83:PHE:HB3	1:F:85:PHE:HE2	1.59	0.68
1:F:345:HIS:O	1:F:348:VAL:N	2.27	0.68
1:C:149:ILE:HG12	1:C:150:GLY:N	2.10	0.67
1:F:30:VAL:HG13	1:F:73:ASN:HB2	1.75	0.67
1:G:325:HIS:HB2	1:G:377:HIS:CE1	2.29	0.67
1:A:332:THR:CG2	1:A:345:HIS:HB3	2.24	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:346:ASP:OD1	1:D:346:ASP:N	2.22	0.67
1:D:345:HIS:HD2	1:D:346:ASP:N	1.93	0.67
1:E:354:ARG:NH1	1:E:368:GLU:OE1	2.28	0.67
1:C:82:PHE:CZ	1:C:84:VAL:HG21	2.30	0.67
1:C:151:ALA:O	1:C:152:LYS:HB2	1.95	0.67
1:D:225:HIS:NE2	1:D:311:GLU:OE2	2.27	0.67
1:C:151:ALA:HB2	1:D:427:GLU:CD	2.20	0.67
1:F:49:LEU:HD11	1:F:196:LYS:CB	2.20	0.67
1:G:308:VAL:CG1	1:G:309:LEU:HD13	2.23	0.66
1:D:89:GLY:O	1:D:94:ARG:HD3	1.95	0.66
1:C:309:LEU:N	1:C:309:LEU:HD12	2.11	0.66
1:B:448:LYS:HB3	1:B:448:LYS:HZ2	1.59	0.65
1:C:345:HIS:O	1:C:346:ASP:C	2.37	0.65
1:A:308:VAL:HG12	1:A:309:LEU:HD12	1.79	0.65
1:C:153:GLN:OE1	1:C:153:GLN:HA	1.97	0.64
1:D:215:VAL:HG21	1:D:248:VAL:HG13	1.79	0.64
1:D:90:PHE:CE1	1:D:218:SER:CB	2.70	0.64
1:F:49:LEU:HD12	1:F:51:GLU:CD	2.22	0.64
1:F:347:LYS:HG2	1:F:375:ARG:CD	2.28	0.64
1:D:237:HIS:ND1	1:D:285:GLU:OE1	2.29	0.64
1:A:347:LYS:HG2	1:A:375:ARG:CZ	2.28	0.64
1:A:347:LYS:HG2	1:A:375:ARG:NE	2.13	0.63
1:C:250:GLU:OE2	1:C:260:ARG:NH2	2.27	0.63
1:C:71:ALA:CB	1:C:82:PHE:HE1	2.12	0.63
1:H:30:VAL:HG12	1:H:70:LEU:HD12	1.79	0.63
1:A:92:ILE:O	1:A:93:LYS:C	2.42	0.63
1:D:90:PHE:HZ	1:D:222:ARG:CD	2.07	0.63
1:B:448:LYS:HB3	1:B:448:LYS:NZ	2.13	0.63
1:A:308:VAL:HG11	1:A:366:ALA:HB2	1.81	0.63
1:E:284:LEU:HD22	1:E:322:ALA:HB2	1.81	0.63
1:H:40:VAL:HG13	1:H:140:ALA:HB2	1.81	0.63
1:D:184:VAL:HG11	1:D:222:ARG:HH21	1.61	0.63
1:F:225:HIS:NE2	1:F:311:GLU:OE2	2.32	0.63
1:F:284:LEU:HD22	1:F:322:ALA:HB2	1.80	0.63
1:A:445:ASN:ND2	1:B:77:ARG:O	2.27	0.62
1:B:284:LEU:HD22	1:B:322:ALA:HB2	1.81	0.62
1:G:284:LEU:HD22	1:G:322:ALA:HB2	1.81	0.62
1:C:30:VAL:HG12	1:C:70:LEU:HD12	1.81	0.62
1:F:250:GLU:OE2	1:F:260:ARG:NH2	2.30	0.62
1:F:30:VAL:HG21	1:F:74:PHE:HA	1.81	0.62
1:F:40:VAL:HG13	1:F:140:ALA:HB2	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:128:ASP:OD1	1:A:132:ARG:NH1	2.32	0.61
1:B:30:VAL:HG12	1:B:70:LEU:HD12	1.82	0.61
1:G:237:HIS:ND1	1:G:285:GLU:OE1	2.31	0.61
1:G:343:TYR:HB3	1:G:344:GLU:OE2	2.00	0.61
1:F:44:VAL:O	1:F:48:ILE:HG13	1.99	0.61
1:B:308:VAL:CG1	1:B:309:LEU:HD13	2.31	0.61
1:C:284:LEU:HD22	1:C:322:ALA:HB2	1.81	0.61
1:G:221:GLU:HG3	1:G:361:ARG:HD2	1.83	0.61
1:G:445:ASN:OD1	1:H:77:ARG:NH2	2.34	0.61
1:H:225:HIS:NE2	1:H:311:GLU:OE2	2.34	0.61
1:A:90:PHE:C	1:A:91:LEU:HG	2.25	0.61
1:G:379:ARG:NH1	1:G:403:GLU:OE1	2.29	0.61
1:A:94:ARG:HD3	1:A:95:PRO:HD2	1.83	0.60
1:A:345:HIS:O	1:A:348:VAL:N	2.34	0.60
1:A:26:ASP:OD1	1:B:444:ARG:NH2	2.31	0.60
1:D:30:VAL:HG12	1:D:70:LEU:HD12	1.83	0.60
1:G:250:GLU:OE2	1:G:260:ARG:NH2	2.27	0.60
1:G:346:ASP:HB3	1:G:375:ARG:O	2.01	0.60
1:C:40:VAL:HG13	1:C:140:ALA:HB2	1.81	0.60
1:C:237:HIS:ND1	1:C:285:GLU:OE1	2.32	0.60
1:H:284:LEU:HD22	1:H:322:ALA:HB2	1.83	0.60
1:A:345:HIS:O	1:A:348:VAL:HB	2.02	0.60
1:F:62:LEU:HD23	1:F:114:SER:HB2	1.84	0.60
1:E:237:HIS:ND1	1:E:285:GLU:OE1	2.32	0.60
1:D:284:LEU:HD22	1:D:322:ALA:HB2	1.82	0.60
1:D:182:ASP:OD1	1:D:222:ARG:NH2	2.34	0.59
1:C:49:LEU:HD21	1:C:166:LEU:HD22	1.84	0.59
1:C:90:PHE:HB2	1:C:94:ARG:HB2	1.84	0.59
1:C:427:GLU:HB3	1:D:149:ILE:O	2.01	0.59
1:G:307:ARG:NH2	1:G:310:GLY:O	2.34	0.59
1:B:399:ASN:OD1	1:B:402:ARG:NH2	2.36	0.59
1:G:40:VAL:HG13	1:G:140:ALA:HB2	1.84	0.59
1:C:84:VAL:HG12	1:C:84:VAL:O	2.02	0.59
1:E:347:LYS:CG	1:E:375:ARG:NE	2.63	0.59
1:C:345:HIS:CD2	1:C:346:ASP:OD1	2.56	0.59
1:E:40:VAL:HG13	1:E:140:ALA:HB2	1.85	0.59
1:C:82:PHE:CZ	1:C:84:VAL:CG2	2.85	0.59
1:D:90:PHE:CZ	1:D:222:ARG:CZ	2.85	0.59
1:H:237:HIS:ND1	1:H:285:GLU:OE1	2.34	0.59
1:E:30:VAL:HG12	1:E:70:LEU:HD12	1.84	0.58
1:H:307:ARG:NH2	1:H:310:GLY:O	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:344:GLU:HG3	1:C:344:GLU:O	2.02	0.58
1:F:259:LEU:HD21	1:F:327:ILE:HD12	1.84	0.58
1:B:40:VAL:HG13	1:B:140:ALA:HB2	1.85	0.58
1:G:67:PRO:HG2	1:G:115:PRO:HG3	1.86	0.58
1:H:45:ARG:NH2	2:H:1001:SO4:O1	2.32	0.58
1:F:354:ARG:NH1	1:F:368:GLU:OE1	2.37	0.58
1:C:81:HIS:N	1:C:101:VAL:O	2.35	0.58
1:C:151:ALA:CB	1:D:427:GLU:HG3	2.33	0.58
1:A:308:VAL:HG12	1:A:309:LEU:CD1	2.35	0.57
1:A:444:ARG:NH2	1:B:78:ILE:O	2.37	0.57
1:C:384:ARG:HD3	1:C:432:LEU:HB2	1.86	0.57
1:E:399:ASN:OD1	1:E:402:ARG:NH2	2.37	0.57
1:E:345:HIS:HD2	1:E:346:ASP:H	1.51	0.57
1:C:82:PHE:CE2	1:C:84:VAL:HG23	2.39	0.57
1:C:47:ARG:NH1	1:C:51:GLU:O	2.38	0.57
1:D:307:ARG:NH2	1:D:310:GLY:O	2.34	0.57
1:E:345:HIS:CD2	1:E:346:ASP:N	2.73	0.57
1:D:346:ASP:CG	1:D:378:LEU:HD21	2.29	0.57
1:F:72:LYS:HA	1:F:82:PHE:CE1	2.39	0.57
1:C:345:HIS:O	1:C:348:VAL:N	2.37	0.56
1:B:250:GLU:OE2	1:B:260:ARG:NH2	2.38	0.56
1:A:237:HIS:ND1	1:A:285:GLU:OE1	2.36	0.56
1:D:40:VAL:HG13	1:D:140:ALA:HB2	1.86	0.56
1:D:342:PHE:N	1:D:342:PHE:CD2	2.73	0.56
1:G:30:VAL:HG12	1:G:70:LEU:HD12	1.86	0.56
1:C:82:PHE:CE2	1:C:84:VAL:CG2	2.88	0.56
1:D:90:PHE:CE1	1:D:218:SER:HA	2.40	0.56
1:E:341:THR:OG1	1:E:343:TYR:CE2	2.43	0.56
1:E:342:PHE:N	1:E:342:PHE:CD2	2.73	0.56
1:G:183:PRO:HB2	1:G:215:VAL:HA	1.88	0.56
1:D:345:HIS:CD2	1:D:346:ASP:N	2.73	0.56
1:G:308:VAL:C	1:G:310:GLY:H	2.13	0.56
1:E:307:ARG:NH2	1:E:310:GLY:O	2.36	0.56
1:E:384:ARG:HD3	1:E:432:LEU:HB2	1.87	0.56
1:G:77:ARG:NH2	1:H:445:ASN:OD1	2.38	0.56
1:F:345:HIS:ND1	1:F:346:ASP:N	2.53	0.55
1:A:354:ARG:NH1	1:A:368:GLU:OE1	2.40	0.55
1:C:307:ARG:NH2	1:C:310:GLY:O	2.37	0.55
1:E:67:PRO:HG2	1:E:115:PRO:HG3	1.87	0.55
1:A:133:ASP:OD1	1:A:133:ASP:N	2.40	0.55
1:A:284:LEU:HD22	1:A:322:ALA:HB2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:332:THR:HG21	1:A:345:HIS:HB3	1.88	0.55
1:B:406:ASP:OD1	1:B:406:ASP:N	2.39	0.55
1:F:307:ARG:NH2	1:F:310:GLY:O	2.34	0.55
1:H:399:ASN:OD1	1:H:402:ARG:NH2	2.39	0.55
1:D:309:LEU:HD12	1:D:309:LEU:N	2.21	0.55
1:F:58:ASP:OD2	1:F:110:ARG:HD3	2.07	0.55
1:F:97:ILE:HG22	1:F:114:SER:HA	1.89	0.55
1:B:183:PRO:HB2	1:B:215:VAL:HA	1.89	0.54
1:C:332:THR:OG1	1:C:342:PHE:HB3	2.07	0.54
1:D:156:VAL:HG21	1:D:163:ILE:HD11	1.88	0.54
1:D:318:LEU:HG	1:D:410:HIS:HB3	1.88	0.54
1:D:399:ASN:OD1	1:D:402:ARG:NH2	2.40	0.54
1:F:399:ASN:OD1	1:F:402:ARG:NH2	2.40	0.54
1:A:347:LYS:HD3	1:A:375:ARG:NH2	2.22	0.54
1:C:58:ASP:OD2	1:C:110:ARG:HD3	2.07	0.54
1:B:318:LEU:HG	1:B:410:HIS:HB3	1.89	0.54
1:H:384:ARG:HD3	1:H:432:LEU:HB2	1.89	0.54
1:A:318:LEU:HG	1:A:410:HIS:HB3	1.90	0.54
1:F:384:ARG:HD3	1:F:432:LEU:HB2	1.87	0.54
1:G:345:HIS:O	1:G:346:ASP:HB2	2.07	0.54
1:G:26:ASP:OD1	1:H:444:ARG:NH2	2.41	0.54
1:A:329:LYS:HE3	1:A:342:PHE:CD2	2.42	0.54
1:D:67:PRO:HG2	1:D:115:PRO:HG3	1.89	0.54
1:C:345:HIS:HD2	1:C:346:ASP:CA	2.17	0.54
1:D:353:VAL:HG21	1:D:374:VAL:HG21	1.89	0.54
1:A:329:LYS:HA	1:A:345:HIS:HD2	1.73	0.54
1:F:308:VAL:HG12	1:F:309:LEU:HD13	1.90	0.54
1:G:308:VAL:CG1	1:G:309:LEU:CD1	2.86	0.54
1:A:43:TRP:CD1	1:A:59:VAL:HG22	2.43	0.53
1:B:346:ASP:OD1	1:B:346:ASP:N	2.40	0.53
1:B:49:LEU:HD21	1:B:166:LEU:HD22	1.90	0.53
1:C:345:HIS:NE2	1:C:346:ASP:OD1	2.42	0.53
1:G:399:ASN:OD1	1:G:402:ARG:NH2	2.41	0.53
1:A:91:LEU:HB3	1:A:92:ILE:CA	2.31	0.53
1:A:372:LYS:HG2	1:A:407:ILE:HD13	1.91	0.53
1:D:90:PHE:HE1	1:D:218:SER:CA	2.20	0.53
1:B:394:ARG:HH12	1:B:485:UNK:HA	1.74	0.53
1:F:67:PRO:HG2	1:F:115:PRO:HG3	1.90	0.53
1:G:220:VAL:HG13	1:G:361:ARG:HD2	1.91	0.53
1:F:45:ARG:NH2	2:F:1001:SO4:O2	2.42	0.53
1:F:75:ALA:HB3	1:F:82:PHE:HE1	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:406:ASP:OD1	1:F:406:ASP:N	2.39	0.53
1:H:318:LEU:HG	1:H:410:HIS:HB3	1.90	0.53
1:B:133:ASP:N	1:B:133:ASP:OD1	2.42	0.52
1:C:378:LEU:HD12	1:C:381:PHE:HD2	1.74	0.52
1:D:90:PHE:CE1	1:D:218:SER:CA	2.92	0.52
1:G:224:THR:OG1	1:G:360:LEU:O	2.25	0.52
1:H:49:LEU:HD21	1:H:166:LEU:HD22	1.91	0.52
1:A:40:VAL:HG13	1:A:140:ALA:HB2	1.90	0.52
1:C:133:ASP:OD1	1:C:133:ASP:N	2.42	0.52
1:C:214:ILE:O	1:C:217:LYS:HG2	2.08	0.52
1:D:49:LEU:HD21	1:D:166:LEU:HD22	1.91	0.52
1:H:135:THR:HG22	1:H:160:THR:HB	1.92	0.52
1:A:141:VAL:HG12	1:A:156:VAL:HG12	1.90	0.52
1:B:237:HIS:ND1	1:B:285:GLU:OE1	2.38	0.52
1:C:152:LYS:O	1:C:153:GLN:HG2	2.09	0.52
1:D:104:LEU:HD23	1:D:106:PRO:HD2	1.90	0.52
1:E:133:ASP:OD1	1:E:133:ASP:N	2.42	0.52
1:F:211:ASP:N	1:F:211:ASP:OD1	2.42	0.52
1:H:133:ASP:OD1	1:H:133:ASP:N	2.42	0.52
1:A:104:LEU:HD22	1:A:107:TYR:H	1.74	0.52
1:F:72:LYS:HA	1:F:82:PHE:CZ	2.45	0.52
1:C:309:LEU:N	1:C:309:LEU:CD1	2.73	0.52
1:E:58:ASP:OD2	1:E:110:ARG:HD3	2.08	0.52
1:C:308:VAL:CG1	1:C:309:LEU:CD1	2.83	0.52
1:C:399:ASN:OD1	1:C:402:ARG:NH2	2.41	0.52
1:D:104:LEU:HD22	1:D:107:TYR:H	1.75	0.52
1:D:133:ASP:N	1:D:133:ASP:OD1	2.42	0.52
1:F:104:LEU:HD22	1:F:107:TYR:H	1.75	0.52
1:F:133:ASP:OD1	1:F:133:ASP:N	2.43	0.52
1:A:329:LYS:HE3	1:A:342:PHE:CE2	2.45	0.52
1:A:345:HIS:CE1	1:A:346:ASP:CG	2.88	0.52
1:E:345:HIS:CD2	1:E:346:ASP:H	2.27	0.52
1:B:58:ASP:OD2	1:B:110:ARG:HD3	2.10	0.52
1:C:308:VAL:HG13	1:C:309:LEU:HD13	1.88	0.52
1:D:142:ASN:HB3	1:D:145:ASP:OD2	2.10	0.52
1:G:406:ASP:OD1	1:G:406:ASP:N	2.39	0.52
1:H:379:ARG:NH1	1:H:403:GLU:OE1	2.37	0.51
1:D:92:ILE:HG22	1:D:92:ILE:O	2.10	0.51
1:G:133:ASP:OD1	1:G:133:ASP:N	2.42	0.51
1:B:104:LEU:HD22	1:B:107:TYR:H	1.76	0.51
1:B:379:ARG:NH1	1:B:403:GLU:OE1	2.37	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:308:VAL:C	1:D:310:GLY:H	2.17	0.51
1:F:135:THR:HG22	1:F:160:THR:HB	1.93	0.51
1:H:104:LEU:HD22	1:H:107:TYR:H	1.75	0.51
1:A:391:GLU:CG	1:D:258:ARG:HH12	2.24	0.51
1:D:184:VAL:HG11	1:D:222:ARG:NH2	2.23	0.51
1:F:104:LEU:HD23	1:F:106:PRO:HD2	1.92	0.51
1:B:104:LEU:HD23	1:B:106:PRO:HD2	1.92	0.51
1:C:318:LEU:HG	1:C:410:HIS:HB3	1.92	0.51
1:F:182:ASP:OD2	1:F:185:ARG:HD3	2.11	0.51
1:A:191:ARG:NH1	1:A:195:GLU:OE1	2.44	0.51
1:E:104:LEU:HD23	1:E:106:PRO:HD2	1.91	0.51
1:F:49:LEU:CD1	1:F:51:GLU:OE2	2.58	0.51
1:A:215:VAL:HG21	1:A:248:VAL:HG13	1.92	0.51
1:B:292:ALA:HA	1:B:300:LEU:HD11	1.93	0.51
1:D:188:ARG:HG2	1:D:226:GLU:OE2	2.11	0.51
1:G:104:LEU:HD23	1:G:106:PRO:HD2	1.93	0.51
1:A:30:VAL:HG12	1:A:70:LEU:HD12	1.92	0.51
1:C:104:LEU:HD23	1:C:106:PRO:HD2	1.93	0.51
1:G:346:ASP:O	1:G:375:ARG:CD	2.59	0.51
1:A:345:HIS:O	1:A:349:GLY:N	2.38	0.51
1:F:49:LEU:HD12	1:F:51:GLU:OE2	2.10	0.51
1:G:354:ARG:NH1	1:G:368:GLU:OE1	2.44	0.51
1:A:62:LEU:HD23	1:A:114:SER:HB2	1.93	0.50
1:F:142:ASN:HB3	1:F:145:ASP:OD2	2.10	0.50
1:B:309:LEU:N	1:B:309:LEU:CD1	2.73	0.50
1:C:104:LEU:HD22	1:C:107:TYR:H	1.74	0.50
1:B:67:PRO:HG2	1:B:115:PRO:HG3	1.92	0.50
1:C:185:ARG:HG3	1:C:188:ARG:HD3	1.93	0.50
1:E:309:LEU:CD1	1:E:309:LEU:N	2.73	0.50
1:F:148:SER:HB3	1:F:152:LYS:HD2	1.93	0.50
1:G:353:VAL:HG21	1:G:374:VAL:HG21	1.94	0.50
1:A:90:PHE:O	1:A:91:LEU:CD2	2.60	0.50
1:E:215:VAL:HG21	1:E:248:VAL:HG13	1.91	0.50
1:G:58:ASP:OD2	1:G:110:ARG:HD3	2.12	0.50
1:E:49:LEU:HD21	1:E:166:LEU:HD22	1.94	0.50
1:A:353:VAL:HG21	1:A:374:VAL:HG21	1.92	0.50
1:B:68:VAL:HG13	1:B:82:PHE:HZ	1.76	0.50
1:G:104:LEU:HD22	1:G:107:TYR:H	1.76	0.50
1:G:308:VAL:HG11	1:G:366:ALA:HB2	1.93	0.50
1:F:49:LEU:CB	1:F:51:GLU:HG3	2.39	0.49
1:A:329:LYS:CA	1:A:345:HIS:HD2	2.25	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:73:ASN:O	1:F:77:ARG:HG3	2.12	0.49
1:H:58:ASP:OD2	1:H:110:ARG:HD3	2.11	0.49
1:B:384:ARG:HD3	1:B:432:LEU:HB2	1.93	0.49
1:C:258:ARG:NH1	1:C:331:GLN:HE22	2.11	0.49
1:E:104:LEU:HD22	1:E:107:TYR:H	1.78	0.49
1:G:221:GLU:CG	1:G:361:ARG:HD2	2.42	0.49
1:E:259:LEU:HD21	1:E:327:ILE:HD12	1.95	0.49
1:F:30:VAL:HG12	1:F:70:LEU:HD12	1.95	0.49
1:F:120:ASP:HB3	1:F:123:LYS:HB3	1.94	0.49
1:A:58:ASP:OD2	1:A:110:ARG:HD3	2.13	0.49
1:G:318:LEU:HG	1:G:410:HIS:HB3	1.95	0.49
1:B:344:GLU:O	1:B:346:ASP:N	2.45	0.49
1:F:318:LEU:HG	1:F:410:HIS:HB3	1.93	0.49
1:G:182:ASP:OD2	1:G:185:ARG:HD3	2.13	0.49
1:H:104:LEU:HD23	1:H:106:PRO:HD2	1.94	0.49
1:A:445:ASN:HD21	1:B:77:ARG:C	2.19	0.49
1:C:68:VAL:HG22	1:C:84:VAL:HG11	1.94	0.49
1:D:91:LEU:O	1:D:91:LEU:CG	2.60	0.48
1:F:45:ARG:HA	1:F:48:ILE:HB	1.95	0.48
1:F:49:LEU:HD11	1:F:196:LYS:HD2	1.91	0.48
1:G:384:ARG:HD3	1:G:432:LEU:HB2	1.93	0.48
1:H:215:VAL:HG21	1:H:248:VAL:HG13	1.96	0.48
1:C:151:ALA:CB	1:D:427:GLU:CD	2.85	0.48
1:C:120:ASP:HB3	1:C:123:LYS:HB3	1.94	0.48
1:G:120:ASP:HB3	1:G:123:LYS:HB3	1.95	0.48
1:G:325:HIS:HB2	1:G:377:HIS:ND1	2.29	0.48
1:H:284:LEU:HD21	1:H:318:LEU:HD22	1.95	0.48
1:A:298:GLU:OE1	1:A:444:ARG:HD2	2.13	0.48
1:G:325:HIS:CG	1:G:377:HIS:CE1	3.01	0.48
1:C:182:ASP:OD2	1:C:185:ARG:HD3	2.14	0.48
1:G:308:VAL:C	1:G:310:GLY:N	2.68	0.48
1:H:142:ASN:HB3	1:H:145:ASP:OD2	2.12	0.48
1:C:292:ALA:HA	1:C:300:LEU:HD11	1.96	0.48
1:H:406:ASP:OD1	1:H:406:ASP:N	2.39	0.48
1:D:120:ASP:HB3	1:D:123:LYS:HE3	1.95	0.48
1:E:62:LEU:HD23	1:E:114:SER:HB2	1.95	0.48
1:B:182:ASP:OD2	1:B:185:ARG:HD3	2.14	0.47
1:C:71:ALA:HB3	1:C:82:PHE:CE1	2.42	0.47
1:E:25:ASP:C	1:E:29:LYS:HZ3	2.22	0.47
1:A:347:LYS:HA	1:A:375:ARG:HD3	1.96	0.47
1:B:394:ARG:HH12	1:B:485:UNK:C	2.27	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:67:PRO:HG2	1:C:115:PRO:HG3	1.96	0.47
1:E:68:VAL:HG13	1:E:82:PHE:HZ	1.80	0.47
1:G:47:ARG:HD3	1:G:47:ARG:HA	1.76	0.47
1:A:142:ASN:HB3	1:A:145:ASP:OD2	2.14	0.47
1:A:274:ASP:OD1	1:A:275:GLU:N	2.46	0.47
1:B:274:ASP:OD1	1:B:275:GLU:N	2.48	0.47
1:A:329:LYS:N	1:A:345:HIS:HD2	2.12	0.47
1:D:184:VAL:CG2	1:D:187:LEU:HD12	2.43	0.47
1:A:404:CYS:HB2	1:A:407:ILE:HG12	1.95	0.47
1:C:182:ASP:OD2	1:C:185:ARG:NH1	2.47	0.47
1:F:404:CYS:HB2	1:F:407:ILE:HG12	1.97	0.47
1:G:135:THR:HB	1:G:162:GLY:HA2	1.97	0.47
1:A:298:GLU:OE2	1:A:444:ARG:HD2	2.14	0.47
1:A:444:ARG:NH1	1:B:23:TYR:OH	2.48	0.47
1:B:135:THR:HG22	1:B:160:THR:HB	1.96	0.47
1:F:30:VAL:HG11	1:F:70:LEU:O	2.15	0.47
1:F:215:VAL:HG21	1:F:248:VAL:HG13	1.95	0.47
1:H:353:VAL:HG21	1:H:374:VAL:HG21	1.97	0.47
1:E:292:ALA:HA	1:E:300:LEU:HD11	1.97	0.47
1:C:135:THR:HG22	1:C:160:THR:HB	1.96	0.47
1:C:72:LYS:N	1:C:82:PHE:CE1	2.83	0.47
1:C:353:VAL:HG21	1:C:374:VAL:HG21	1.96	0.46
1:D:62:LEU:HD23	1:D:114:SER:HB2	1.97	0.46
1:F:284:LEU:HD21	1:F:318:LEU:HD22	1.97	0.46
1:D:292:ALA:HA	1:D:300:LEU:HD11	1.96	0.46
1:F:44:VAL:O	1:F:48:ILE:CG1	2.63	0.46
1:H:274:ASP:OD1	1:H:275:GLU:N	2.49	0.46
1:A:244:TYR:OH	1:A:260:ARG:CG	2.63	0.46
1:D:58:ASP:OD2	1:D:110:ARG:HD3	2.15	0.46
1:G:221:GLU:HG3	1:G:361:ARG:CD	2.43	0.46
1:B:443:ASN:HA	1:B:447:MET:SD	2.55	0.46
1:C:142:ASN:HB3	1:C:145:ASP:OD2	2.15	0.46
1:C:185:ARG:HE	1:C:188:ARG:HH11	1.64	0.46
1:B:372:LYS:HG2	1:B:407:ILE:HD13	1.98	0.46
1:D:332:THR:O	1:D:342:PHE:HD1	1.99	0.46
1:H:292:ALA:HA	1:H:300:LEU:HD11	1.97	0.46
1:B:62:LEU:HD23	1:B:114:SER:HB2	1.96	0.46
1:B:142:ASN:HB3	1:B:145:ASP:OD2	2.14	0.46
1:B:471:UNK:O	1:B:475:UNK:N	2.48	0.46
1:G:292:ALA:HA	1:G:300:LEU:HD11	1.98	0.46
1:A:384:ARG:HD3	1:A:432:LEU:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:30:VAL:HG21	1:C:74:PHE:HA	1.98	0.46
1:C:308:VAL:HG13	1:C:309:LEU:CD1	2.43	0.46
1:A:298:GLU:OE1	1:A:444:ARG:NH1	2.49	0.46
1:A:378:LEU:HD12	1:A:381:PHE:HD2	1.81	0.46
1:B:194:ILE:HG13	1:B:239:VAL:HG22	1.97	0.46
1:G:274:ASP:OD1	1:G:275:GLU:N	2.48	0.46
1:D:308:VAL:O	1:D:309:LEU:HB2	2.16	0.46
1:E:308:VAL:O	1:E:309:LEU:HB2	2.15	0.46
1:A:182:ASP:OD2	1:A:185:ARG:HD3	2.15	0.45
1:F:128:ASP:OD1	1:F:132:ARG:NH1	2.49	0.45
1:F:274:ASP:OD1	1:F:275:GLU:N	2.49	0.45
1:A:345:HIS:ND1	1:A:346:ASP:N	2.64	0.45
1:D:86:GLU:HG3	1:D:86:GLU:O	2.15	0.45
1:E:194:ILE:HG13	1:E:239:VAL:HG22	1.97	0.45
1:A:175:SER:OG	1:A:178:ASN:OD1	2.29	0.45
1:B:30:VAL:HG21	1:B:74:PHE:HA	1.98	0.45
1:E:200:LEU:HD13	1:E:204:PHE:CE2	2.51	0.45
1:F:25:ASP:C	1:F:29:LYS:HZ3	2.25	0.45
1:H:184:VAL:HG23	1:H:223:ILE:HD13	1.98	0.45
1:A:75:ALA:HB2	1:A:100:VAL:HG22	1.98	0.45
1:B:259:LEU:HD21	1:B:327:ILE:HD12	1.97	0.45
1:E:142:ASN:HB3	1:E:145:ASP:OD2	2.16	0.45
1:F:195:GLU:OE2	1:F:196:LYS:NZ	2.49	0.45
1:G:284:LEU:HD21	1:G:318:LEU:HD22	1.99	0.45
1:C:86:GLU:OE2	1:C:94:ARG:CZ	2.64	0.45
1:D:194:ILE:HG13	1:D:239:VAL:HG22	1.98	0.45
1:G:259:LEU:HD21	1:G:327:ILE:HD12	1.99	0.45
1:A:158:ASP:OD1	1:A:158:ASP:N	2.50	0.45
1:A:377:HIS:HA	1:A:411:LEU:HD11	1.98	0.45
1:A:406:ASP:OD1	1:A:406:ASP:N	2.43	0.45
1:B:353:VAL:HG21	1:B:374:VAL:HG21	1.97	0.45
1:E:353:VAL:HG21	1:E:374:VAL:HG21	1.99	0.45
1:G:194:ILE:HG13	1:G:239:VAL:HG22	1.98	0.45
1:H:68:VAL:HG13	1:H:82:PHE:HZ	1.82	0.45
1:D:90:PHE:HE2	1:D:222:ARG:HD3	1.74	0.45
1:E:183:PRO:HB2	1:E:215:VAL:HA	1.97	0.45
1:F:325:HIS:CG	1:F:326:ASP:N	2.85	0.45
1:G:165:ASP:OD1	1:G:172:ARG:NH2	2.43	0.45
1:A:332:THR:HG23	1:A:345:HIS:HB3	1.96	0.45
1:A:150:GLY:HA2	1:B:427:GLU:OE1	2.17	0.45
1:A:259:LEU:HD21	1:A:327:ILE:HD12	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:379:ARG:NH1	1:D:403:GLU:OE1	2.43	0.45
1:A:92:ILE:HD12	1:A:92:ILE:C	2.16	0.45
1:C:274:ASP:OD1	1:C:275:GLU:N	2.48	0.45
1:C:284:LEU:HD21	1:C:318:LEU:HD22	1.99	0.45
1:E:347:LYS:CG	1:E:375:ARG:CZ	2.95	0.45
1:F:83:PHE:HB3	1:F:85:PHE:CE2	2.45	0.45
1:H:325:HIS:CG	1:H:326:ASP:N	2.84	0.45
1:B:47:ARG:HA	1:B:47:ARG:HD3	1.71	0.44
1:D:345:HIS:CD2	1:D:346:ASP:OD1	2.70	0.44
1:F:206:GLU:O	1:F:210:GLU:HG3	2.17	0.44
1:A:184:VAL:HG23	1:A:223:ILE:HD13	1.99	0.44
1:C:85:PHE:CD2	1:C:85:PHE:O	2.70	0.44
1:F:232:LYS:HA	1:F:316:GLU:OE2	2.17	0.44
1:A:389:LYS:O	1:D:258:ARG:NH1	2.49	0.44
1:C:82:PHE:CE2	1:C:84:VAL:HG21	2.51	0.44
1:C:152:LYS:HE2	1:C:152:LYS:CA	2.32	0.44
1:D:346:ASP:OD2	1:D:378:LEU:HD21	2.17	0.44
1:E:318:LEU:HG	1:E:410:HIS:HB3	2.00	0.44
1:H:183:PRO:HB2	1:H:215:VAL:HA	2.00	0.44
1:H:194:ILE:HG13	1:H:239:VAL:HG22	1.99	0.44
1:H:308:VAL:HG21	1:H:317:LEU:HD11	1.99	0.44
1:A:347:LYS:HG2	1:A:375:ARG:CD	2.48	0.44
1:E:120:ASP:HB3	1:E:123:LYS:HE3	1.99	0.44
1:G:120:ASP:HB3	1:G:123:LYS:HE3	1.99	0.44
1:A:284:LEU:HD21	1:A:318:LEU:HD22	1.99	0.44
1:A:325:HIS:CG	1:A:326:ASP:N	2.85	0.44
1:D:273:LEU:HD13	1:D:329:LYS:NZ	2.32	0.44
1:D:274:ASP:OD1	1:D:275:GLU:N	2.49	0.44
1:D:404:CYS:HB2	1:D:407:ILE:HG12	1.98	0.44
1:E:325:HIS:CG	1:E:326:ASP:N	2.85	0.44
1:F:292:ALA:HA	1:F:300:LEU:HD11	1.98	0.44
1:G:325:HIS:CG	1:G:326:ASP:N	2.85	0.44
1:H:47:ARG:HD3	1:H:47:ARG:HA	1.77	0.44
1:G:128:ASP:OD1	1:G:132:ARG:NH1	2.50	0.44
1:H:188:ARG:HG2	1:H:226:GLU:OE2	2.17	0.44
1:H:354:ARG:NH1	1:H:368:GLU:OE1	2.50	0.44
1:C:188:ARG:NH2	2:C:1001:SO4:O2	2.50	0.44
1:D:120:ASP:HB3	1:D:123:LYS:HB3	1.99	0.44
1:F:75:ALA:HB2	1:F:100:VAL:CG1	2.48	0.44
1:A:87:LYS:HD3	1:A:87:LYS:HA	1.79	0.44
1:E:188:ARG:NH2	2:E:1001:SO4:O2	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:284:LEU:HD21	1:E:318:LEU:HD22	1.99	0.44
1:F:49:LEU:HD23	1:F:49:LEU:HA	1.86	0.44
1:F:72:LYS:O	1:F:82:PHE:CZ	2.71	0.44
1:G:149:ILE:HA	1:H:430:LYS:HE3	2.00	0.44
1:C:62:LEU:HD23	1:C:114:SER:HB2	2.00	0.44
1:C:325:HIS:CG	1:C:326:ASP:N	2.85	0.44
1:E:120:ASP:HB3	1:E:123:LYS:HB3	1.99	0.44
1:E:135:THR:HG22	1:E:160:THR:HB	1.99	0.44
1:H:120:ASP:HB3	1:H:123:LYS:HB3	2.00	0.44
1:A:378:LEU:HG	1:A:378:LEU:O	2.18	0.43
1:A:471:UNK:O	1:A:475:UNK:N	2.51	0.43
1:C:185:ARG:NE	1:C:188:ARG:HH11	2.14	0.43
1:E:379:ARG:NH1	1:E:403:GLU:OE1	2.42	0.43
1:F:120:ASP:HB3	1:F:123:LYS:HE3	2.00	0.43
1:C:82:PHE:O	1:C:83:PHE:CD1	2.70	0.43
1:F:60:ASP:OD2	1:F:132:ARG:NH2	2.51	0.43
1:F:75:ALA:HB2	1:F:100:VAL:HG13	1.99	0.43
1:A:47:ARG:HD3	1:A:47:ARG:HA	1.72	0.43
1:C:120:ASP:HB3	1:C:123:LYS:HE3	2.00	0.43
1:A:45:ARG:NH1	1:A:192:ILE:HD13	2.33	0.43
1:B:120:ASP:HB3	1:B:123:LYS:HB3	1.99	0.43
1:D:325:HIS:CG	1:D:326:ASP:N	2.85	0.43
1:A:94:ARG:HD3	1:A:94:ARG:HA	1.81	0.43
1:B:120:ASP:HB3	1:B:123:LYS:HE3	1.99	0.43
1:B:224:THR:OG1	1:B:360:LEU:O	2.34	0.43
1:B:325:HIS:CG	1:B:326:ASP:N	2.87	0.43
1:C:92:ILE:HG12	1:C:93:LYS:HD2	2.00	0.43
1:G:188:ARG:HG2	1:G:226:GLU:OE2	2.18	0.43
1:A:347:LYS:O	1:A:350:ALA:HB3	2.18	0.43
1:F:49:LEU:CD1	1:F:196:LYS:CD	2.87	0.43
1:A:194:ILE:HG13	1:A:239:VAL:HG22	2.00	0.43
1:B:43:TRP:CD1	1:B:59:VAL:HG22	2.54	0.43
1:C:30:VAL:HG13	1:C:73:ASN:HB2	2.00	0.43
1:F:170:LEU:HD23	1:F:199:GLN:HB3	2.01	0.43
1:B:164:LYS:HZ2	1:E:81:HIS:CE1	2.36	0.43
1:C:47:ARG:HA	1:C:47:ARG:HD3	1.65	0.43
1:C:92:ILE:HG23	1:C:93:LYS:HD3	2.01	0.43
1:E:427:GLU:HG3	1:F:151:ALA:HA	2.01	0.43
1:A:347:LYS:HD3	1:A:375:ARG:CZ	2.49	0.43
1:C:158:ASP:OD1	1:C:158:ASP:N	2.52	0.43
1:C:378:LEU:O	1:C:378:LEU:HG	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:92:ILE:O	1:D:92:ILE:CG2	2.67	0.43
1:D:135:THR:HB	1:D:162:GLY:HA2	2.00	0.43
1:G:343:TYR:CB	1:G:344:GLU:OE2	2.66	0.43
1:G:377:HIS:O	1:G:377:HIS:CD2	2.71	0.43
1:B:412:PHE:HB3	1:B:436:ILE:HD13	2.01	0.43
1:F:30:VAL:HG21	1:F:74:PHE:CA	2.48	0.43
1:F:158:ASP:OD1	1:F:158:ASP:N	2.52	0.43
1:C:183:PRO:HG2	1:C:218:SER:HB3	2.01	0.42
1:E:182:ASP:OD2	1:E:185:ARG:HD3	2.19	0.42
1:G:404:CYS:HB2	1:G:407:ILE:HG12	2.01	0.42
1:A:183:PRO:HB2	1:A:215:VAL:HA	2.00	0.42
1:B:57:ILE:HD12	1:B:109:TYR:CE2	2.54	0.42
1:C:114:SER:HA	1:C:115:PRO:HD3	1.89	0.42
1:D:135:THR:HG22	1:D:160:THR:HB	2.00	0.42
1:E:102:LEU:HB3	1:E:109:TYR:HB2	2.00	0.42
1:F:372:LYS:HG2	1:F:407:ILE:HD13	2.00	0.42
1:G:156:VAL:HG21	1:G:163:ILE:HD11	2.01	0.42
1:A:244:TYR:OH	1:A:260:ARG:HG2	2.19	0.42
1:A:292:ALA:HA	1:A:300:LEU:HD11	2.01	0.42
1:B:323:LEU:HD23	1:B:323:LEU:HA	1.90	0.42
1:B:326:ASP:OD1	1:B:377:HIS:NE2	2.52	0.42
1:D:92:ILE:O	1:D:93:LYS:CB	2.67	0.42
1:D:384:ARG:HD3	1:D:432:LEU:HB2	2.00	0.42
1:G:215:VAL:HG21	1:G:248:VAL:HG13	2.01	0.42
1:H:30:VAL:HG13	1:H:73:ASN:HB2	2.01	0.42
1:A:134:PHE:HA	1:A:173:PRO:HA	2.01	0.42
1:C:412:PHE:HB3	1:C:436:ILE:HD13	2.01	0.42
1:E:347:LYS:HG2	1:E:375:ARG:CZ	2.45	0.42
1:G:309:LEU:N	1:G:309:LEU:HD12	2.34	0.42
1:H:158:ASP:OD1	1:H:158:ASP:N	2.52	0.42
1:B:204:PHE:O	1:B:208:VAL:HG23	2.20	0.42
1:D:314:ASP:OD1	1:D:314:ASP:N	2.47	0.42
1:E:158:ASP:N	1:E:158:ASP:OD1	2.52	0.42
1:D:323:LEU:HD23	1:D:323:LEU:HA	1.89	0.42
1:E:188:ARG:HG2	1:E:226:GLU:OE2	2.18	0.42
1:F:183:PRO:HB2	1:F:215:VAL:HA	2.01	0.42
1:G:158:ASP:OD1	1:G:158:ASP:N	2.52	0.42
1:B:185:ARG:HE	1:B:188:ARG:HH11	1.67	0.42
1:E:274:ASP:OD1	1:E:275:GLU:N	2.50	0.42
1:G:49:LEU:HD21	1:G:166:LEU:HD22	2.02	0.42
1:H:45:ARG:NH1	1:H:137:ASN:OD1	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:185:ARG:HG3	1:H:188:ARG:HD3	2.00	0.42
1:B:30:VAL:HG13	1:B:73:ASN:HB2	2.02	0.42
1:D:309:LEU:CD1	1:D:309:LEU:N	2.82	0.42
1:E:43:TRP:CD1	1:E:59:VAL:HG22	2.55	0.42
1:H:57:ILE:HD12	1:H:109:TYR:CE2	2.55	0.42
1:D:158:ASP:OD1	1:D:158:ASP:N	2.52	0.42
1:F:43:TRP:CD1	1:F:59:VAL:HG22	2.54	0.42
1:F:204:PHE:O	1:F:208:VAL:HG23	2.20	0.42
1:F:412:PHE:HB3	1:F:436:ILE:HD13	2.02	0.42
1:G:412:PHE:HB3	1:G:436:ILE:HD13	2.01	0.42
1:H:60:ASP:OD2	1:H:132:ARG:NH2	2.53	0.42
1:A:20:TYR:CE1	1:B:434:GLU:HG2	2.54	0.41
1:B:188:ARG:NH2	2:B:1001:SO4:O1	2.53	0.41
1:B:447:MET:HE3	1:B:447:MET:HB3	1.58	0.41
1:F:166:LEU:HD23	1:F:166:LEU:HA	1.81	0.41
1:H:67:PRO:HG2	1:H:115:PRO:HG3	2.01	0.41
1:H:191:ARG:NH2	2:H:1001:SO4:O2	2.47	0.41
1:B:448:LYS:NZ	1:B:448:LYS:CB	2.81	0.41
1:C:20:TYR:CE1	1:D:434:GLU:HG2	2.55	0.41
1:D:92:ILE:O	1:D:93:LYS:HB3	2.19	0.41
1:A:25:ASP:C	1:A:29:LYS:HZ3	2.28	0.41
1:A:227:LEU:HD11	1:A:252:ILE:HG21	2.03	0.41
1:G:221:GLU:CG	1:G:361:ARG:CD	2.99	0.41
1:A:68:VAL:HG13	1:A:84:VAL:HG21	2.01	0.41
1:A:135:THR:HB	1:A:162:GLY:HA2	2.01	0.41
1:B:185:ARG:HG3	1:B:188:ARG:HD3	2.02	0.41
1:C:133:ASP:HB3	1:C:185:ARG:HG2	2.03	0.41
1:D:86:GLU:O	1:D:94:ARG:CG	2.68	0.41
1:E:60:ASP:OD2	1:E:132:ARG:NH2	2.53	0.41
1:E:66:ASP:HA	1:E:67:PRO:HD3	1.92	0.41
1:G:233:GLU:OE2	1:G:239:VAL:HG21	2.20	0.41
1:B:307:ARG:NH2	1:B:310:GLY:O	2.47	0.41
1:D:406:ASP:OD1	1:D:406:ASP:N	2.40	0.41
1:F:273:LEU:O	1:F:277:THR:OG1	2.38	0.41
1:G:311:GLU:O	1:G:311:GLU:HG2	2.20	0.41
1:E:323:LEU:HD23	1:E:323:LEU:HA	1.89	0.41
1:H:346:ASP:OD1	1:H:346:ASP:N	2.39	0.41
1:H:404:CYS:HB2	1:H:407:ILE:HG12	2.03	0.41
1:A:38:PHE:O	1:A:61:PHE:HA	2.21	0.41
1:B:158:ASP:N	1:B:158:ASP:OD1	2.53	0.41
1:B:172:ARG:HA	1:B:173:PRO:HD2	1.94	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:149:ILE:HD13	1:C:149:ILE:N	2.29	0.41
1:E:81:HIS:N	1:E:101:VAL:O	2.33	0.41
1:A:30:VAL:HG13	1:A:73:ASN:HB2	2.02	0.41
1:G:170:LEU:HD23	1:G:199:GLN:HB3	2.03	0.41
1:H:24:PHE:HB3	1:H:143:LEU:HD11	2.03	0.41
1:A:86:GLU:HG2	1:A:95:PRO:O	2.21	0.41
1:A:340:VAL:HG12	1:A:341:THR:HG23	2.02	0.41
1:A:379:ARG:HB3	1:A:380:PRO:HD3	2.03	0.41
1:B:215:VAL:HG21	1:B:248:VAL:HG13	2.03	0.41
1:C:191:ARG:NH2	2:C:1001:SO4:O1	2.47	0.41
1:E:126:ILE:HG23	1:E:159:PRO:HG3	2.03	0.41
1:E:287:VAL:HG12	1:E:413:LEU:HD22	2.03	0.41
1:G:444:ARG:NH2	1:H:26:ASP:OD1	2.54	0.41
1:H:117:LYS:HE2	1:H:117:LYS:HB3	1.93	0.41
1:C:149:ILE:HG12	1:C:150:GLY:H	1.82	0.41
1:D:55:TYR:HB3	1:D:106:PRO:O	2.21	0.41
1:E:173:PRO:HD2	1:E:201:THR:HG22	2.02	0.41
1:G:102:LEU:HB3	1:G:109:TYR:HB2	2.03	0.41
1:H:259:LEU:HD21	1:H:327:ILE:HD12	2.03	0.41
1:A:43:TRP:CZ3	1:A:47:ARG:HG2	2.56	0.40
1:C:258:ARG:O	1:C:261:GLU:HG2	2.21	0.40
1:D:43:TRP:CD1	1:D:59:VAL:HG22	2.56	0.40
1:E:201:THR:OG1	1:E:202:GLU:N	2.54	0.40
1:H:141:VAL:HG12	1:H:156:VAL:HG12	2.02	0.40
1:B:51:GLU:HA	1:B:52:PRO:HD3	1.94	0.40
1:E:163:ILE:O	1:E:167:GLU:HG3	2.21	0.40
1:E:406:ASP:OD1	1:E:406:ASP:N	2.40	0.40
1:G:68:VAL:HG13	1:G:82:PHE:HZ	1.86	0.40
1:A:80:GLY:HA2	1:A:101:VAL:O	2.21	0.40
1:F:66:ASP:HA	1:F:67:PRO:HD3	1.96	0.40
1:A:94:ARG:HA	1:A:95:PRO:HD2	1.90	0.40
1:A:102:LEU:HB3	1:A:109:TYR:HB2	2.03	0.40
1:B:188:ARG:HG2	1:B:226:GLU:OE2	2.22	0.40
1:B:284:LEU:HD21	1:B:318:LEU:HD22	2.03	0.40
1:C:287:VAL:HG12	1:C:413:LEU:HD22	2.04	0.40
1:D:176:ILE:HD11	1:D:203:ASP:HB2	2.03	0.40
1:E:165:ASP:OD1	1:E:172:ARG:NH2	2.44	0.40
1:F:44:VAL:HG12	1:F:48:ILE:HD11	1.99	0.40
1:H:204:PHE:O	1:H:208:VAL:HG23	2.22	0.40
1:A:92:ILE:CG1	1:A:93:LYS:N	2.83	0.40
1:B:273:LEU:HD13	1:B:329:LYS:NZ	2.37	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:394:ARG:HH12	1:B:485:UNK:CA	2.33	0.40
1:E:47:ARG:HD3	1:E:47:ARG:HA	1.70	0.40
1:E:308:VAL:HG21	1:E:317:LEU:HD11	2.04	0.40
1:E:445:ASN:OD1	1:E:446:GLU:HG3	2.22	0.40
1:F:445:ASN:OD1	1:F:446:GLU:HG3	2.20	0.40
1:G:445:ASN:OD1	1:G:446:GLU:HG3	2.22	0.40
1:H:372:LYS:HG2	1:H:407:ILE:HD13	2.04	0.40
1:H:379:ARG:HB3	1:H:380:PRO:HD3	2.04	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	415/497 (84%)	409 (99%)	6 (1%)	0	100	100
1	B	405/497 (82%)	402 (99%)	2 (0%)	1 (0%)	43	75
1	C	413/497 (83%)	407 (98%)	6 (2%)	0	100	100
1	D	413/497 (83%)	407 (98%)	6 (2%)	0	100	100
1	E	403/497 (81%)	402 (100%)	1 (0%)	0	100	100
1	F	403/497 (81%)	400 (99%)	3 (1%)	0	100	100
1	G	403/497 (81%)	400 (99%)	3 (1%)	0	100	100
1	H	403/497 (81%)	399 (99%)	4 (1%)	0	100	100
All	All	3258/3976 (82%)	3226 (99%)	31 (1%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	345	HIS

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	367/378 (97%)	339 (92%)	28 (8%)	12	36
1	B	360/378 (95%)	347 (96%)	13 (4%)	31	53
1	C	365/378 (97%)	353 (97%)	12 (3%)	33	56
1	D	365/378 (97%)	353 (97%)	12 (3%)	33	56
1	E	358/378 (95%)	345 (96%)	13 (4%)	31	53
1	F	358/378 (95%)	343 (96%)	15 (4%)	26	49
1	G	358/378 (95%)	348 (97%)	10 (3%)	38	60
1	H	358/378 (95%)	345 (96%)	13 (4%)	31	53
All	All	2889/3024 (96%)	2773 (96%)	116 (4%)	28	50

All (116) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	VAL
1	A	47	ARG
1	A	53	VAL
1	A	82	PHE
1	A	83	PHE
1	A	85	PHE
1	A	86	GLU
1	A	88	ARG
1	A	90	PHE
1	A	92	ILE
1	A	93	LYS
1	A	94	ARG
1	A	104	LEU
1	A	152	LYS
1	A	153	GLN
1	A	186	VAL
1	A	211	ASP
1	A	215	VAL
1	A	262	VAL

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Mol	Chain	Res	Type
1	A	264	ASP
1	A	277	THR
1	A	309	LEU
1	A	318	LEU
1	A	323	LEU
1	A	344	GLU
1	A	345	HIS
1	A	377	HIS
1	A	446	GLU
1	B	40	VAL
1	B	47	ARG
1	B	53	VAL
1	B	104	LEU
1	B	149	ILE
1	B	154	THR
1	B	186	VAL
1	B	215	VAL
1	B	262	VAL
1	B	277	THR
1	B	378	LEU
1	B	445	ASN
1	B	448	LYS
1	C	40	VAL
1	C	53	VAL
1	C	86	GLU
1	C	87	LYS
1	C	104	LEU
1	C	148	SER
1	C	149	ILE
1	C	155	ILE
1	C	186	VAL
1	C	215	VAL
1	C	262	VAL
1	C	445	ASN
1	D	40	VAL
1	D	47	ARG
1	D	53	VAL
1	D	87	LYS
1	D	104	LEU
1	D	186	VAL
1	D	215	VAL
1	D	262	VAL

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Mol	Chain	Res	Type
1	D	342	PHE
1	D	346	ASP
1	D	378	LEU
1	D	445	ASN
1	E	40	VAL
1	E	47	ARG
1	E	53	VAL
1	E	104	LEU
1	E	149	ILE
1	E	153	GLN
1	E	186	VAL
1	E	215	VAL
1	E	262	VAL
1	E	342	PHE
1	E	344	GLU
1	E	378	LEU
1	E	445	ASN
1	F	40	VAL
1	F	47	ARG
1	F	53	VAL
1	F	81	HIS
1	F	97	ILE
1	F	104	LEU
1	F	186	VAL
1	F	215	VAL
1	F	262	VAL
1	F	277	THR
1	F	318	LEU
1	F	344	GLU
1	F	345	HIS
1	F	378	LEU
1	F	445	ASN
1	G	40	VAL
1	G	47	ARG
1	G	53	VAL
1	G	104	LEU
1	G	149	ILE
1	G	186	VAL
1	G	215	VAL
1	G	262	VAL
1	G	344	GLU
1	G	445	ASN

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Mol	Chain	Res	Type
1	H	40	VAL
1	H	47	ARG
1	H	53	VAL
1	H	104	LEU
1	H	149	ILE
1	H	154	THR
1	H	186	VAL
1	H	215	VAL
1	H	262	VAL
1	H	344	GLU
1	H	346	ASP
1	H	378	LEU
1	H	445	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	168	GLN
1	A	225	HIS
1	A	331	GLN
1	A	345	HIS
1	B	103	HIS
1	B	168	GLN
1	B	345	HIS
1	C	345	HIS
1	D	81	HIS
1	D	103	HIS
1	D	168	GLN
1	D	345	HIS
1	E	276	HIS
1	E	345	HIS
1	F	73	ASN
1	G	225	HIS
1	G	325	HIS
1	G	377	HIS
1	H	81	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

8 ligands are modelled in this entry.

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	G	1001	-	4,4,4	1.05	0	6,6,6	1.38	1 (16%)
2	SO4	H	1001	-	4,4,4	0.23	0	6,6,6	0.08	0
2	SO4	A	1001	-	4,4,4	0.23	0	6,6,6	0.07	0
2	SO4	B	1001	-	4,4,4	0.23	0	6,6,6	0.07	0
2	SO4	D	1001	-	4,4,4	0.24	0	6,6,6	0.08	0
2	SO4	C	1001	-	4,4,4	0.24	0	6,6,6	0.08	0
2	SO4	E	1001	-	4,4,4	0.23	0	6,6,6	0.07	0
2	SO4	F	1001	-	4,4,4	0.23	0	6,6,6	0.06	0

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	1001	SO4	O4-S-O3	3.05	125.37	108.54

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	1001	SO4	2	0
2	B	1001	SO4	1	0
2	C	1001	SO4	2	0
2	E	1001	SO4	1	0
2	F	1001	SO4	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	421/497 (84%)	0.61	20 (4%)	35	29	51, 113, 166, 211	0
1	B	413/497 (83%)	0.67	23 (5%)	30	26	62, 116, 177, 218	0
1	C	419/497 (84%)	0.80	40 (9%)	14	16	71, 139, 209, 259	0
1	D	419/497 (84%)	0.88	36 (8%)	16	17	75, 133, 193, 243	0
1	E	411/497 (82%)	0.61	11 (2%)	56	41	83, 146, 198, 249	0
1	F	411/497 (82%)	0.59	14 (3%)	48	35	65, 125, 176, 190	0
1	G	411/497 (82%)	0.73	22 (5%)	31	27	118, 167, 230, 259	0
1	H	411/497 (82%)	0.78	25 (6%)	27	24	102, 177, 223, 266	0
All	All	3316/3976 (83%)	0.71	191 (5%)	29	25	51, 140, 209, 266	0

All (191) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	80	GLY	5.0
1	H	23	TYR	4.9
1	A	101	VAL	4.7
1	H	366	ALA	4.7
1	B	68	VAL	4.4
1	A	331	GLN	4.3
1	E	32	PRO	4.2
1	B	297	ALA	4.1
1	D	101	VAL	4.0
1	D	78	ILE	4.0
1	C	353	VAL	4.0
1	H	99	SER	4.0
1	C	99	SER	3.9
1	G	68	VAL	3.9
1	G	71	ALA	3.8
1	A	68	VAL	3.8

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Mol	Chain	Res	Type	RSRZ
1	G	32	PRO	3.8
1	C	105	PRO	3.7
1	G	27	VAL	3.7
1	G	67	PRO	3.7
1	H	78	ILE	3.7
1	H	74	PHE	3.6
1	H	361	ARG	3.5
1	C	264	ASP	3.5
1	D	31	LEU	3.5
1	B	350	ALA	3.5
1	G	326	ASP	3.5
1	G	163	ILE	3.4
1	C	262	VAL	3.4
1	D	397	MET	3.4
1	A	71	ALA	3.3
1	B	75	ALA	3.3
1	D	32	PRO	3.3
1	H	68	VAL	3.3
1	D	326	ASP	3.3
1	B	326	ASP	3.3
1	C	333	PHE	3.3
1	G	297	ALA	3.2
1	C	17	LEU	3.2
1	H	105	PRO	3.2
1	E	180	LYS	3.2
1	B	311	GLU	3.2
1	G	259	LEU	3.2
1	C	377	HIS	3.1
1	E	75	ALA	3.0
1	D	440	GLU	3.0
1	D	329	LYS	3.0
1	D	331	GLN	3.0
1	G	376	HIS	2.9
1	D	264	ASP	2.9
1	G	69	GLU	2.9
1	C	427	GLU	2.9
1	C	42	GLY	2.9
1	B	251	ALA	2.9
1	G	78	ILE	2.9
1	F	99	SER	2.9
1	E	326	ASP	2.9
1	C	112	ASP	2.8

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Mol	Chain	Res	Type	RSRZ
1	F	101	VAL	2.8
1	D	432	LEU	2.8
1	D	83	PHE	2.8
1	C	30	VAL	2.8
1	B	351	GLN	2.8
1	D	109	TYR	2.8
1	F	229	LYS	2.8
1	D	35	HIS	2.7
1	C	101	VAL	2.7
1	D	391	GLU	2.7
1	E	45	ARG	2.7
1	D	217	LYS	2.7
1	G	31	LEU	2.7
1	D	71	ALA	2.7
1	B	32	PRO	2.7
1	A	185	ARG	2.7
1	E	74	PHE	2.7
1	D	180	LYS	2.7
1	G	74	PHE	2.7
1	H	71	ALA	2.6
1	B	436	ILE	2.6
1	A	32	PRO	2.6
1	F	78	ILE	2.6
1	D	170	LEU	2.6
1	D	311	GLU	2.6
1	D	163	ILE	2.6
1	C	66	ASP	2.6
1	D	435	THR	2.6
1	H	331	GLN	2.6
1	C	89	GLY	2.5
1	B	285	GLU	2.5
1	H	221	GLU	2.5
1	B	329	LYS	2.5
1	C	109	TYR	2.5
1	H	333	PHE	2.5
1	F	327	ILE	2.5
1	B	60	ASP	2.5
1	B	432	LEU	2.5
1	A	27	VAL	2.5
1	E	30	VAL	2.5
1	H	394	ARG	2.5
1	H	406	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
1	E	437	ALA	2.5
1	F	75	ALA	2.4
1	B	278	LEU	2.4
1	C	31	LEU	2.4
1	D	258	ARG	2.4
1	C	371	ALA	2.4
1	G	404	CYS	2.4
1	A	26	ASP	2.4
1	C	340	VAL	2.4
1	B	37	CYS	2.4
1	B	215	VAL	2.4
1	C	244	TYR	2.4
1	H	81	HIS	2.4
1	G	85	PHE	2.4
1	H	297	ALA	2.4
1	C	326	ASP	2.4
1	C	180	LYS	2.4
1	G	311	GLU	2.4
1	G	114	SER	2.4
1	C	397	MET	2.4
1	A	62	LEU	2.3
1	D	79	GLY	2.3
1	H	35	HIS	2.3
1	D	56	ASN	2.3
1	A	67	PRO	2.3
1	E	256	ILE	2.3
1	F	366	ALA	2.3
1	A	188	ARG	2.3
1	F	67	PRO	2.3
1	H	363	GLY	2.3
1	B	81	HIS	2.3
1	H	144	ASP	2.3
1	C	113	PHE	2.2
1	H	380	PRO	2.2
1	F	326	ASP	2.2
1	B	36	TYR	2.2
1	G	26	ASP	2.2
1	C	32	PRO	2.2
1	E	70	LEU	2.2
1	D	100	VAL	2.2
1	C	129	LEU	2.2
1	C	285	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	H	17	LEU	2.2
1	B	73	ASN	2.2
1	A	327	ILE	2.2
1	F	317	LEU	2.2
1	F	331	GLN	2.2
1	A	34	GLU	2.2
1	C	100	VAL	2.2
1	G	136	ALA	2.2
1	D	411	LEU	2.2
1	H	168	GLN	2.2
1	H	294	TYR	2.2
1	C	111	PHE	2.1
1	C	217	LYS	2.1
1	D	68	VAL	2.1
1	D	218	SER	2.1
1	A	397	MET	2.1
1	F	397	MET	2.1
1	C	297	ALA	2.1
1	A	60	ASP	2.1
1	A	443	ASN	2.1
1	D	353	VAL	2.1
1	C	331	GLN	2.1
1	D	438	GLU	2.1
1	A	436	ILE	2.1
1	D	404	CYS	2.1
1	B	264	ASP	2.1
1	D	81	HIS	2.1
1	C	350	ALA	2.1
1	F	100	VAL	2.1
1	C	35	HIS	2.1
1	A	366	ALA	2.1
1	G	152	LYS	2.1
1	E	97	ILE	2.1
1	C	332	THR	2.1
1	B	331	GLN	2.1
1	A	36	TYR	2.1
1	C	91	LEU	2.1
1	C	185	ARG	2.0
1	D	62	LEU	2.0
1	D	373	LEU	2.0
1	G	28	ALA	2.0
1	C	67	PRO	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	30	VAL	2.0
1	B	185	ARG	2.0
1	A	364	ASP	2.0
1	C	118	GLY	2.0
1	F	84	VAL	2.0
1	H	447	MET	2.0
1	H	58	ASP	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SO4	H	1001	5/5	0.79	0.19	152,157,161,166	0
2	SO4	G	1001	5/5	0.80	0.17	172,174,178,186	0
2	SO4	F	1001	5/5	0.84	0.13	81,81,91,105	0
2	SO4	C	1001	5/5	0.86	0.15	162,165,166,172	0
2	SO4	D	1001	5/5	0.87	0.11	104,115,144,156	0
2	SO4	E	1001	5/5	0.90	0.13	133,135,137,145	0
2	SO4	A	1001	5/5	0.90	0.12	119,122,146,154	0
2	SO4	B	1001	5/5	0.91	0.14	126,131,139,141	0

6.5 Other polymers [i](#)

There are no such residues in this entry.