



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:45 PM UTC

PDB ID : 3DWK / pdb_00003dwk
Title : Identification of Dynamic Structural Motifs Involved in Peptidoglycan Glycosyltransfer
Authors : Lovering, A.L.; De Castro, L.; Strynadka, N.C.J.
Deposited on : 2008-07-22
Resolution : 3.10 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

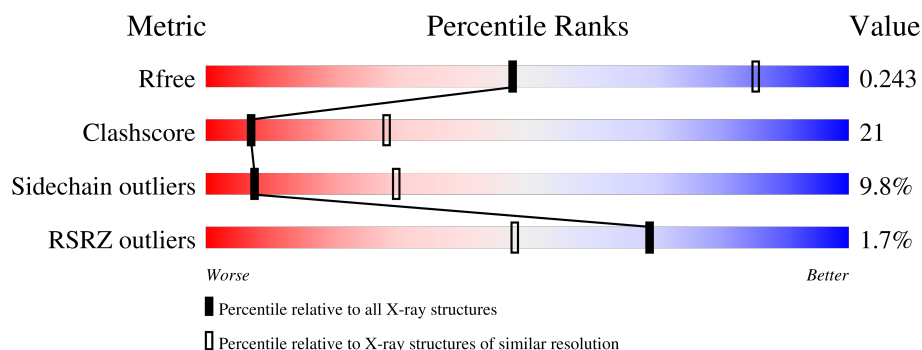
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

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	625	3% 57% 33% 5% .
1	B	625	% 62% 33% 5% .
1	C	625	% 60% 34% 5%
1	D	625	2% 59% 32% 5% .

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	A	11	-	-	X	-
2	SO4	A	15	-	-	X	-
2	SO4	A	17	-	-	X	-
2	SO4	A	41	-	-	X	-
2	SO4	B	38	-	-	X	-
2	SO4	C	31	-	-	X	-
2	SO4	D	39	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 19474 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 Penicillin-binding protein 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	598	Total	C	N	O	S	0	0	0
			4712	2953	809	938	12			
1	B	621	Total	C	N	O	S	0	0	0
			4874	3051	839	972	12			
1	C	623	Total	C	N	O	S	0	0	0
			4891	3060	843	976	12			
1	D	602	Total	C	N	O	S	0	0	0
			4751	2977	817	945	12			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	68	MET	LYS	engineered mutation	UNP Q5HFX3
B	68	MET	LYS	engineered mutation	UNP Q5HFX3
C	68	MET	LYS	engineered mutation	UNP Q5HFX3
D	68	MET	LYS	engineered mutation	UNP Q5HFX3

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



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

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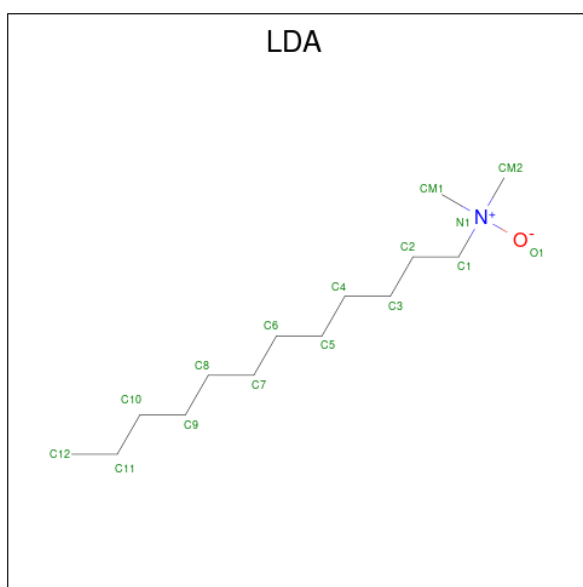
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total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

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

- Molecule 3 is LAURYL DIMETHYLAMINE-N-OXIDE (CCD ID: LDA) (formula: C₁₄H₃₁NO).

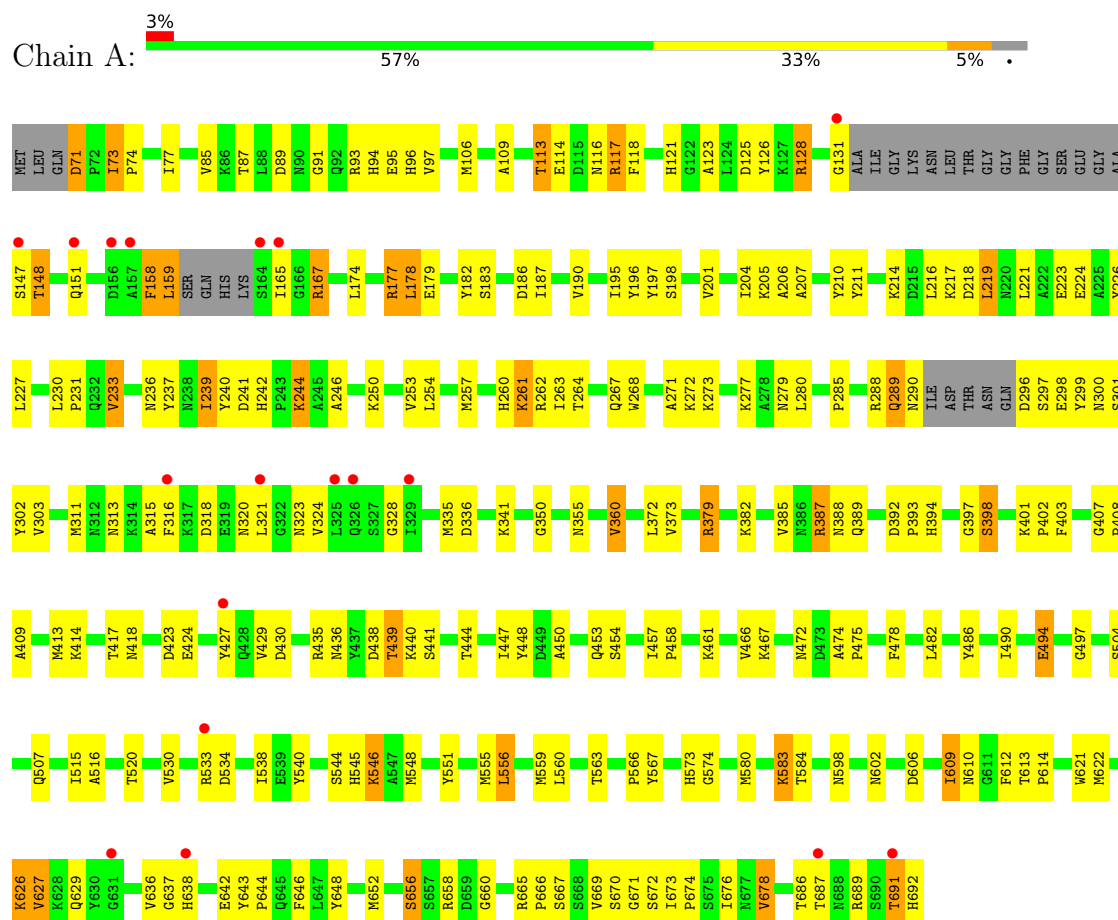


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	D	1	Total	C	N	O	0	0
			16	14	1	1		

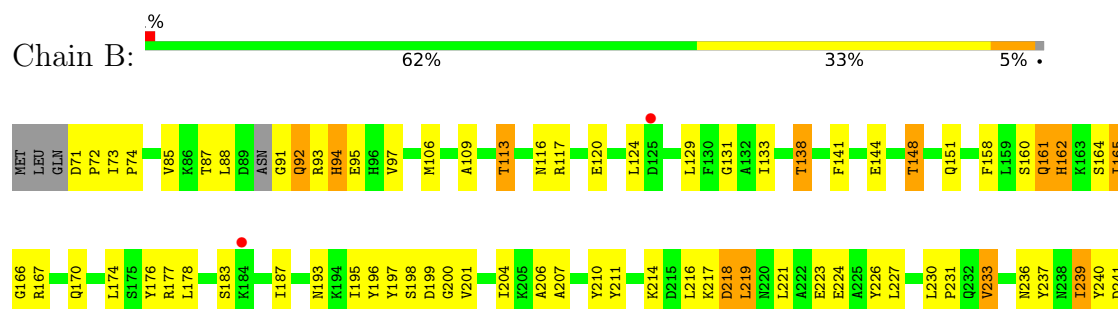
3 Residue-property plots

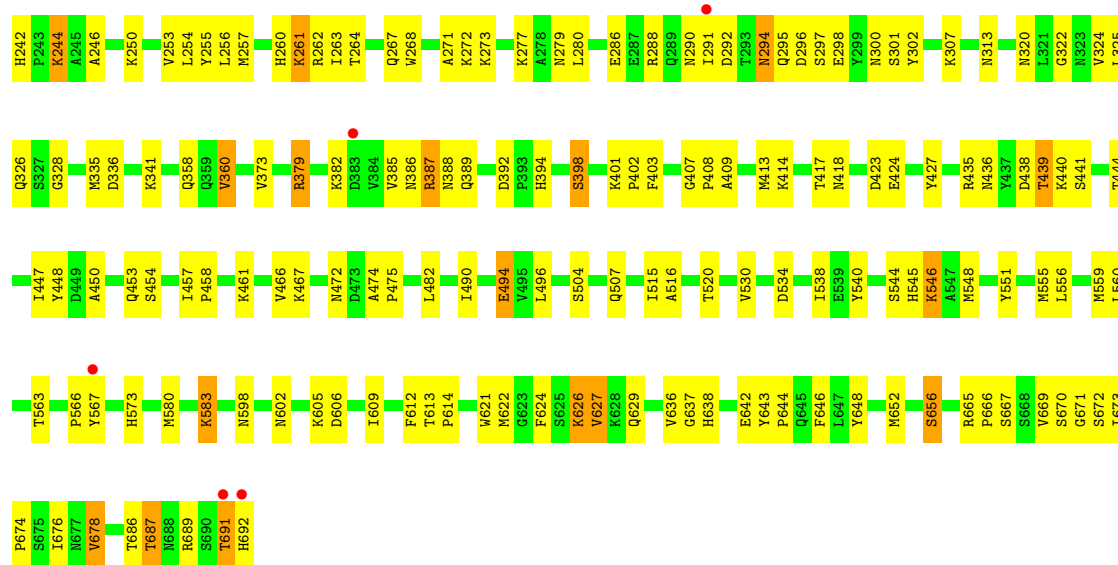
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Penicillin-binding protein 2

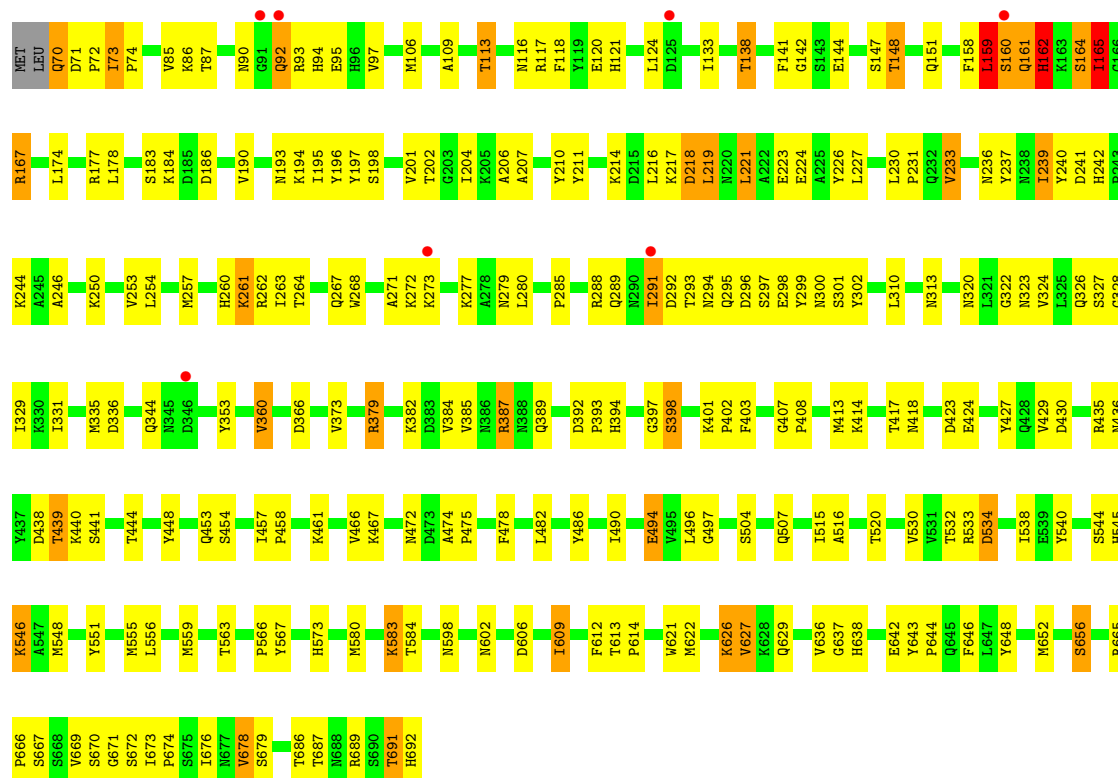


• Molecule 1: Penicillin-binding protein 2





• Molecule 1: Penicillin-binding protein 2



• Molecule 1: Penicillin-binding protein 2





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	85.35Å 217.47Å 95.73Å 90.00° 90.30° 90.00°	Depositor
Resolution (Å)	41.88 – 3.10 41.88 – 3.10	Depositor EDS
% Data completeness (in resolution range)	95.8 (41.88-3.10) 95.7 (41.88-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.92 (at 3.12Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.218 , 0.264 (Not available) , 0.243	Depositor DCC
R_{free} test set	3052 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å ²)	63.1	Xtriage
Anisotropy	0.139	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 67.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	0.125 for h,-k,-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	19474	wwPDB-VP
Average B, all atoms (Å ²)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.56% 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, LDA

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	0/4813	0.82	5/6504 (0.1%)
1	B	0.45	0/4979	0.81	2/6729 (0.0%)
1	C	0.47	0/4997	0.85	11/6755 (0.2%)
1	D	0.46	0/4853	0.82	3/6559 (0.0%)
All	All	0.45	0/19642	0.83	21/26547 (0.1%)

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
1	A	0	1
1	C	0	1
All	All	0	2

There are no bond length outliers.

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	291	ILE	N-CA-C	-9.44	101.67	110.82
1	A	71	ASP	CA-C-N	6.41	127.86	119.84
1	A	71	ASP	C-N-CA	6.41	127.86	119.84
1	C	165	ILE	N-CA-C	-6.17	106.42	111.91
1	A	131	GLY	N-CA-C	-5.86	96.29	113.30
1	C	73	ILE	CA-C-N	5.86	126.19	119.92
1	C	73	ILE	C-N-CA	5.86	126.19	119.92
1	D	165	ILE	N-CA-C	-5.84	104.39	112.50
1	C	162	HIS	N-CA-C	5.80	118.85	109.86
1	C	233	VAL	CA-C-N	5.49	125.84	119.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	233	VAL	C-N-CA	5.49	125.84	119.47
1	C	160	SER	N-CA-C	5.45	122.41	110.80
1	B	233	VAL	CA-C-N	5.41	125.75	119.47
1	B	233	VAL	C-N-CA	5.41	125.75	119.47
1	A	233	VAL	CA-C-N	5.32	125.64	119.47
1	A	233	VAL	C-N-CA	5.32	125.64	119.47
1	C	159	LEU	CA-CB-CG	-5.27	97.86	116.30
1	C	92	GLN	CA-C-N	-5.08	115.99	122.79
1	C	92	GLN	C-N-CA	-5.08	115.99	122.79
1	D	233	VAL	CA-C-N	5.01	125.28	119.47
1	D	233	VAL	C-N-CA	5.01	125.28	119.47

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	158	PHE	Peptide
1	C	159	LEU	Peptide

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	4712	0	4518	200	0
1	B	4874	0	4676	198	0
1	C	4891	0	4691	217	0
1	D	4751	0	4562	198	0
2	A	75	0	0	14	0
2	B	65	0	0	8	0
2	C	45	0	0	6	0
2	D	45	0	0	5	0
3	D	16	0	31	7	0
All	All	19474	0	18478	798	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 21.

All (798) close contacts within the same asymmetric unit are listed below, sorted by their clash

magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:162:HIS:CE1	1:B:164:SER:HB2	1.78	1.18
1:C:160:SER:HB2	1:C:167:ARG:NH1	1.61	1.15
1:C:160:SER:CB	1:C:167:ARG:HH11	1.59	1.14
1:C:159:LEU:HD22	1:C:532:THR:HB	1.23	1.11
1:D:118:PHE:HA	1:D:121:HIS:CE1	1.95	1.01
1:A:118:PHE:HA	1:A:121:HIS:CE1	1.99	0.97
1:C:72:PRO:HD3	1:C:94:HIS:CE1	2.00	0.96
1:C:159:LEU:CD2	1:C:532:THR:HB	1.95	0.96
1:C:160:SER:CB	1:C:167:ARG:NH1	2.24	0.95
1:C:160:SER:HB2	1:C:167:ARG:HH11	0.79	0.95
1:C:144:GLU:HB2	1:D:574:GLY:O	1.66	0.95
1:D:164:SER:HB2	1:D:167:ARG:H	1.32	0.95
1:B:605:LYS:HE2	2:B:35:SO4:O4	1.73	0.88
1:B:162:HIS:NE2	1:B:164:SER:HB2	1.87	0.88
1:C:116:ASN:ND2	1:C:262:ARG:NH1	2.21	0.88
1:C:116:ASN:ND2	1:C:262:ARG:HH12	1.72	0.88
1:A:118:PHE:HA	1:A:121:HIS:HE1	1.37	0.87
1:D:118:PHE:HA	1:D:121:HIS:HE1	1.35	0.86
1:A:350:GLY:HA2	1:B:138:THR:HG21	1.57	0.85
1:A:106:MET:HE2	1:A:224:GLU:HG2	1.57	0.85
1:D:162:HIS:HB2	1:D:167:ARG:NE	1.92	0.85
1:B:162:HIS:NE2	1:B:164:SER:CB	2.39	0.84
1:D:580:MET:HB3	1:D:613:THR:HG22	1.57	0.84
1:C:73:ILE:HD12	1:C:74:PRO:HD2	1.59	0.83
1:B:161:GLN:O	1:B:162:HIS:HB2	1.78	0.83
1:C:580:MET:HB3	1:C:613:THR:HG22	1.59	0.83
1:A:580:MET:HB3	1:A:613:THR:HG22	1.60	0.83
1:B:580:MET:HB3	1:B:613:THR:HG22	1.58	0.83
1:D:176:TYR:CD2	3:D:1:LDA:H32	2.15	0.82
1:C:141:PHE:HB2	1:C:148:THR:HG21	1.61	0.81
1:A:574:GLY:O	1:B:144:GLU:HB2	1.81	0.81
1:B:116:ASN:ND2	1:B:262:ARG:NH1	2.28	0.81
1:C:106:MET:HE2	1:C:224:GLU:HG2	1.63	0.81
1:B:687:THR:HG22	2:B:23:SO4:O2	1.81	0.80
1:B:116:ASN:ND2	1:B:262:ARG:HH12	1.77	0.80
1:C:161:GLN:O	1:C:161:GLN:HG2	1.80	0.80
1:B:162:HIS:CE1	1:B:164:SER:CB	2.62	0.79
1:D:313:ASN:HB2	1:D:540:TYR:CE2	2.18	0.78
1:D:679:SER:HA	2:D:9:SO4:O2	1.84	0.77
1:D:382:LYS:HB2	1:D:385:VAL:HB	1.67	0.77
1:A:382:LYS:HB2	1:A:385:VAL:HB	1.66	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:159:LEU:HD22	1:C:532:THR:CB	2.11	0.76
1:A:126:TYR:HB2	2:A:15:SO4:O2	1.84	0.76
1:C:138:THR:HG21	1:D:350:GLY:HA2	1.68	0.76
1:C:382:LYS:HB2	1:C:385:VAL:HB	1.67	0.76
1:B:382:LYS:HB2	1:B:385:VAL:HB	1.68	0.76
1:C:73:ILE:HG23	1:C:328:GLY:HA3	1.68	0.76
1:B:106:MET:HE2	1:B:224:GLU:HG2	1.68	0.75
1:D:626:LYS:HD2	1:D:627:VAL:N	2.02	0.74
1:B:233:VAL:HG22	1:B:237:TYR:CE1	2.22	0.74
1:D:106:MET:HE2	1:D:224:GLU:HG2	1.68	0.74
1:C:313:ASN:HB2	1:C:540:TYR:CE2	2.22	0.74
1:B:530:VAL:HG23	1:B:538:ILE:HD13	1.71	0.73
1:C:233:VAL:HG22	1:C:237:TYR:CE1	2.23	0.73
1:D:159:LEU:HD12	1:D:532:THR:HB	1.70	0.73
1:A:116:ASN:ND2	1:A:262:ARG:HH12	1.87	0.72
1:A:244:LYS:HB2	2:A:17:SO4:O3	1.88	0.72
1:B:427:TYR:CE2	1:B:461:LYS:HE2	2.25	0.72
1:A:567:TYR:CE2	1:A:692:HIS:HB2	2.24	0.72
1:B:92:GLN:O	1:B:93:ARG:HG3	1.90	0.72
1:C:427:TYR:CE2	1:C:461:LYS:HE2	2.25	0.71
1:B:567:TYR:CE2	1:B:692:HIS:HB2	2.26	0.71
1:A:626:LYS:HD2	1:A:627:VAL:N	2.06	0.70
1:C:626:LYS:HD2	1:C:627:VAL:N	2.06	0.70
1:A:177:ARG:NH2	2:A:41:SO4:O1	2.24	0.70
1:C:73:ILE:HG23	1:C:328:GLY:CA	2.21	0.70
1:B:242:HIS:HA	2:B:38:SO4:O4	1.91	0.70
1:B:240:TYR:CD1	1:B:288:ARG:HD3	2.26	0.70
1:B:116:ASN:C	1:B:116:ASN:HD22	1.99	0.69
1:B:161:GLN:HE21	1:B:538:ILE:HA	1.57	0.69
1:D:116:ASN:ND2	1:D:262:ARG:HH12	1.90	0.69
1:D:121:HIS:HD2	1:D:125:ASP:HB2	1.57	0.69
1:A:530:VAL:HG23	1:A:538:ILE:HD13	1.74	0.69
1:C:567:TYR:CE2	1:C:692:HIS:HB2	2.27	0.69
1:C:240:TYR:CD1	1:C:288:ARG:HD3	2.27	0.69
1:A:660:GLY:HA3	1:B:255:TYR:CE2	2.28	0.69
1:D:652:MET:O	1:D:656:SER:HB2	1.92	0.69
1:D:164:SER:HB2	1:D:167:ARG:N	2.07	0.69
1:D:530:VAL:HG23	1:D:538:ILE:HD13	1.73	0.69
1:A:240:TYR:CD1	1:A:288:ARG:HD3	2.26	0.69
1:B:217:LYS:HG3	1:B:218:ASP:H	1.59	0.69
1:C:679:SER:HA	2:C:4:SO4:O1	1.93	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:ASP:C	1:A:91:GLY:H	2.02	0.68
1:A:95:GLU:H	1:A:206:ALA:HB2	1.58	0.68
1:C:474:ALA:HB3	1:C:475:PRO:HD3	1.75	0.68
1:B:626:LYS:HD2	1:B:627:VAL:N	2.08	0.68
1:C:637:GLY:HA2	2:C:31:SO4:O4	1.94	0.68
1:C:652:MET:O	1:C:656:SER:HB2	1.93	0.68
1:A:233:VAL:HG22	1:A:237:TYR:CE1	2.29	0.68
1:C:217:LYS:HG3	1:C:218:ASP:H	1.59	0.68
1:D:233:VAL:HG22	1:D:237:TYR:CE1	2.29	0.68
1:D:427:TYR:CE2	1:D:461:LYS:HE2	2.29	0.68
1:D:457:ILE:HB	1:D:458:PRO:HD3	1.77	0.67
1:A:427:TYR:CE2	1:A:461:LYS:HE2	2.30	0.67
1:A:116:ASN:ND2	1:A:262:ARG:NH1	2.43	0.67
1:A:217:LYS:HG3	1:A:218:ASP:H	1.58	0.67
1:B:665:ARG:NH2	1:B:671:GLY:O	2.28	0.67
1:A:158:PHE:CE1	1:A:159:LEU:HD23	2.29	0.67
1:B:652:MET:O	1:B:656:SER:HB2	1.95	0.67
1:C:530:VAL:HG23	1:C:538:ILE:HD13	1.76	0.67
1:C:389:GLN:HG2	1:C:621:TRP:CZ3	2.30	0.67
1:A:148:THR:HG23	1:A:151:GLN:HB2	1.78	0.66
1:C:71:ASP:HB3	1:C:72:PRO:HD2	1.76	0.66
1:A:389:GLN:HG2	1:A:621:TRP:CZ3	2.30	0.66
1:D:116:ASN:ND2	1:D:262:ARG:NH1	2.44	0.66
1:D:217:LYS:HG3	1:D:218:ASP:H	1.60	0.66
1:D:240:TYR:CD1	1:D:288:ARG:HD3	2.31	0.66
1:A:93:ARG:NH1	1:A:210:TYR:CE2	2.64	0.66
1:A:159:LEU:CD2	1:A:167:ARG:HD3	2.26	0.66
1:B:313:ASN:HB2	1:B:540:TYR:CE2	2.30	0.66
1:D:159:LEU:HD12	1:D:533:ARG:H	1.61	0.66
1:B:389:GLN:HG2	1:B:621:TRP:CZ3	2.31	0.65
1:D:389:GLN:HG2	1:D:621:TRP:CZ3	2.30	0.65
1:D:567:TYR:CE2	1:D:692:HIS:HB2	2.30	0.65
1:A:665:ARG:NH2	1:A:671:GLY:O	2.30	0.65
1:C:72:PRO:CB	1:C:92:GLN:HE22	2.09	0.65
1:A:652:MET:O	1:A:656:SER:HB2	1.97	0.65
1:A:121:HIS:HD2	1:A:125:ASP:HB2	1.62	0.65
1:D:148:THR:HG23	1:D:151:GLN:HB2	1.79	0.65
1:A:242:HIS:HA	2:A:17:SO4:O4	1.97	0.65
1:A:239:ILE:HD12	1:A:280:LEU:HD22	1.78	0.65
1:D:121:HIS:CD2	1:D:125:ASP:HB2	2.32	0.64
1:B:158:PHE:HZ	1:B:170:GLN:HG2	1.63	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:293:THR:HG22	1:C:294:ASN:H	1.60	0.64
1:A:73:ILE:HD12	1:A:74:PRO:HD2	1.80	0.64
1:B:158:PHE:CZ	1:B:170:GLN:HG2	2.32	0.64
1:A:177:ARG:NH2	2:A:41:SO4:O4	2.31	0.63
1:B:161:GLN:NE2	1:B:538:ILE:HA	2.13	0.63
1:C:665:ARG:NH2	1:C:671:GLY:O	2.30	0.63
1:B:162:HIS:CD2	1:B:164:SER:HB2	2.34	0.63
1:D:290:ASN:HB3	1:D:292:ASP:H	1.64	0.63
1:A:201:VAL:HG11	1:A:207:ALA:HA	1.81	0.63
1:B:436:ASN:OD1	1:B:457:ILE:HG12	1.99	0.63
1:C:293:THR:HG22	1:C:294:ASN:N	2.13	0.63
1:D:320:ASN:O	1:D:324:VAL:HG23	2.00	0.62
1:D:665:ARG:NH2	1:D:671:GLY:O	2.32	0.62
1:A:159:LEU:HD22	1:A:167:ARG:HD3	1.81	0.62
1:C:141:PHE:HB2	1:C:148:THR:CG2	2.28	0.62
1:A:95:GLU:N	1:A:206:ALA:HB2	2.13	0.62
1:D:159:LEU:CD1	1:D:533:ARG:H	2.12	0.62
1:D:389:GLN:HG3	1:D:394:HIS:CE1	2.35	0.62
1:D:474:ALA:HB3	1:D:475:PRO:HD3	1.81	0.62
1:A:298:GLU:HG3	1:A:341:LYS:HG2	1.81	0.62
1:A:177:ARG:NH2	2:A:41:SO4:S	2.73	0.62
1:A:350:GLY:HA2	1:B:138:THR:CG2	2.28	0.61
1:A:457:ILE:HB	1:A:458:PRO:HD3	1.82	0.61
1:D:289:GLN:HB3	1:D:384:VAL:HG21	1.81	0.61
1:A:196:TYR:CE1	1:A:198:SER:HA	2.35	0.61
1:A:408:PRO:HB2	1:A:466:VAL:HG11	1.82	0.61
1:C:320:ASN:O	1:C:324:VAL:HG23	2.00	0.61
1:A:253:VAL:HG12	1:A:257:MET:HE2	1.81	0.61
1:B:201:VAL:HG11	1:B:207:ALA:HA	1.81	0.61
1:C:196:TYR:CE1	1:C:198:SER:HA	2.35	0.61
1:A:117:ARG:NH2	2:A:15:SO4:O1	2.30	0.61
1:A:598:ASN:HD22	1:A:629:GLN:HE21	1.47	0.61
1:D:538:ILE:HD12	1:D:538:ILE:H	1.66	0.61
1:D:109:ALA:O	1:D:113:THR:HG22	2.01	0.61
1:D:196:TYR:CE1	1:D:198:SER:HA	2.35	0.61
1:C:116:ASN:HD22	1:C:262:ARG:HH12	1.47	0.61
1:A:474:ALA:HB3	1:A:475:PRO:HD3	1.82	0.61
1:B:386:ASN:HA	2:B:25:SO4:O1	2.01	0.61
1:D:436:ASN:OD1	1:D:457:ILE:HG12	1.99	0.61
1:C:201:VAL:HG11	1:C:207:ALA:HA	1.83	0.61
1:B:196:TYR:CE1	1:B:198:SER:HA	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:121:HIS:HD2	1:D:125:ASP:CB	2.13	0.60
1:B:264:THR:OG1	1:B:267:GLN:HG2	2.01	0.60
1:A:159:LEU:C	1:A:167:ARG:NH2	2.59	0.60
1:C:264:THR:OG1	1:C:267:GLN:HG2	2.01	0.60
1:B:474:ALA:HB3	1:B:475:PRO:HD3	1.82	0.60
1:C:436:ASN:OD1	1:C:457:ILE:HG12	2.02	0.60
1:D:295:GLN:O	1:D:296:ASP:HB2	2.00	0.60
1:D:555:MET:HE1	1:D:678:VAL:HG22	1.82	0.60
1:D:605:LYS:HE2	2:D:7:SO4:O1	2.02	0.60
1:C:116:ASN:HD22	1:C:116:ASN:C	2.07	0.60
1:A:264:THR:OG1	1:A:267:GLN:HG2	2.02	0.60
1:B:389:GLN:HG3	1:B:394:HIS:CE1	2.37	0.60
1:C:148:THR:HG23	1:C:151:GLN:HB2	1.84	0.59
1:C:408:PRO:HB2	1:C:466:VAL:HG11	1.83	0.59
1:D:253:VAL:HG12	1:D:257:MET:HE2	1.84	0.59
1:A:121:HIS:CD2	1:A:125:ASP:HB2	2.36	0.59
1:C:253:VAL:HG12	1:C:257:MET:HE2	1.83	0.59
1:D:201:VAL:HG11	1:D:207:ALA:HA	1.84	0.59
1:B:148:THR:HG23	1:B:151:GLN:HB2	1.83	0.59
1:C:457:ILE:HB	1:C:458:PRO:HD3	1.83	0.59
1:D:293:THR:HG23	1:D:294:ASN:N	2.16	0.59
1:A:73:ILE:HG23	1:A:328:GLY:HA3	1.82	0.59
1:A:109:ALA:O	1:A:113:THR:HG22	2.02	0.59
1:A:389:GLN:HG3	1:A:394:HIS:CE1	2.37	0.59
1:B:424:GLU:C	1:B:441:SER:HB2	2.27	0.59
1:B:298:GLU:HG3	1:B:341:LYS:HG2	1.84	0.59
1:C:666:PRO:HG2	1:C:669:VAL:HG22	1.84	0.59
1:B:183:SER:O	1:B:187:ILE:HG13	2.01	0.59
1:B:320:ASN:O	1:B:324:VAL:HG23	2.02	0.59
1:B:418:ASN:HB3	1:B:674:PRO:O	2.03	0.59
1:C:389:GLN:HG3	1:C:394:HIS:CE1	2.37	0.59
1:D:169:ALA:HB1	3:D:1:LDA:H123	1.84	0.59
1:B:538:ILE:HD12	1:B:538:ILE:H	1.68	0.59
1:B:161:GLN:O	1:B:162:HIS:CB	2.51	0.59
1:D:116:ASN:C	1:D:116:ASN:HD22	2.10	0.59
1:B:239:ILE:HD12	1:B:280:LEU:HD22	1.84	0.58
1:A:73:ILE:HG23	1:A:328:GLY:CA	2.32	0.58
1:A:216:LEU:O	1:A:219:LEU:HD23	2.03	0.58
1:A:233:VAL:O	1:A:233:VAL:HG23	2.04	0.58
1:D:264:THR:OG1	1:D:267:GLN:HG2	2.03	0.58
1:D:216:LEU:O	1:D:219:LEU:HD23	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106:MET:HE1	1:A:224:GLU:HA	1.85	0.58
1:B:71:ASP:CG	1:B:72:PRO:HD2	2.29	0.58
1:C:160:SER:HB3	1:C:167:ARG:NH1	2.16	0.58
1:D:424:GLU:C	1:D:441:SER:HB2	2.29	0.58
1:B:408:PRO:HB2	1:B:466:VAL:HG11	1.86	0.58
1:C:233:VAL:HG23	1:C:233:VAL:O	2.02	0.58
1:C:424:GLU:C	1:C:441:SER:HB2	2.28	0.58
1:C:285:PRO:O	1:C:289:GLN:HG3	2.03	0.58
1:D:389:GLN:HG2	1:D:621:TRP:HZ3	1.67	0.58
1:A:424:GLU:C	1:A:441:SER:HB2	2.29	0.57
1:C:109:ALA:O	1:C:113:THR:HG22	2.04	0.57
1:B:162:HIS:CD2	1:B:164:SER:CB	2.88	0.57
1:D:204:ILE:HD11	1:D:227:LEU:HB3	1.87	0.57
1:A:436:ASN:OD1	1:A:457:ILE:HG12	2.03	0.57
1:C:239:ILE:HD12	1:C:280:LEU:HD22	1.86	0.57
1:C:387:ARG:HG3	1:C:392:ASP:OD2	2.05	0.57
1:C:504:SER:OG	1:C:507:GLN:HG3	2.04	0.57
1:A:285:PRO:HB2	1:A:385:VAL:HG13	1.86	0.57
1:B:457:ILE:HB	1:B:458:PRO:HD3	1.86	0.57
1:D:239:ILE:HD12	1:D:280:LEU:HD22	1.87	0.57
1:B:73:ILE:CG1	1:B:328:GLY:HA3	2.35	0.57
1:C:204:ILE:HD11	1:C:227:LEU:HB3	1.87	0.57
1:D:387:ARG:HG3	1:D:392:ASP:OD2	2.05	0.57
1:A:320:ASN:O	1:A:324:VAL:HG12	2.05	0.57
1:B:91:GLY:HA2	1:B:290:ASN:CG	2.30	0.57
1:A:240:TYR:CE2	1:A:280:LEU:HD11	2.40	0.57
1:A:244:LYS:N	2:A:17:SO4:O3	2.38	0.57
1:B:253:VAL:HG12	1:B:257:MET:HE2	1.86	0.57
1:C:72:PRO:HB2	1:C:92:GLN:HE22	1.69	0.57
1:C:217:LYS:HG3	1:C:218:ASP:N	2.20	0.56
1:C:159:LEU:HD13	1:C:532:THR:HG21	1.87	0.56
1:A:217:LYS:HG3	1:A:218:ASP:N	2.21	0.56
1:B:162:HIS:ND1	1:B:164:SER:HB2	2.19	0.56
1:A:158:PHE:CZ	1:A:159:LEU:HD23	2.41	0.56
1:A:313:ASN:HB2	1:A:540:TYR:CE2	2.40	0.56
1:A:355:ASN:HA	1:D:180:GLN:NE2	2.21	0.56
1:B:216:LEU:O	1:B:219:LEU:HD23	2.05	0.56
1:C:72:PRO:CG	1:C:92:GLN:HE22	2.18	0.56
1:C:230:LEU:HB3	1:C:231:PRO:HD3	1.88	0.56
1:A:555:MET:HE1	1:A:678:VAL:HG22	1.87	0.56
1:B:233:VAL:HG23	1:B:233:VAL:O	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:302:TYR:CZ	1:C:335:MET:HB2	2.40	0.56
1:D:598:ASN:HD22	1:D:629:GLN:HE21	1.54	0.56
1:A:538:ILE:HD12	1:A:538:ILE:H	1.69	0.56
1:C:538:ILE:HD12	1:C:538:ILE:H	1.71	0.56
1:D:217:LYS:HG3	1:D:218:ASP:N	2.21	0.56
1:D:544:SER:O	1:D:545:HIS:HB3	2.06	0.56
1:A:93:ARG:NH1	1:A:210:TYR:HE2	2.04	0.56
1:A:418:ASN:HB3	1:A:674:PRO:O	2.07	0.56
1:A:660:GLY:CA	1:B:255:TYR:CZ	2.89	0.56
1:B:88:LEU:HD12	1:B:325:LEU:HD22	1.89	0.55
1:A:515:ILE:HG12	1:A:548:MET:HE1	1.87	0.55
1:B:387:ARG:HG3	1:B:392:ASP:OD2	2.06	0.55
1:C:418:ASN:HB3	1:C:674:PRO:O	2.07	0.55
1:C:295:GLN:O	1:C:296:ASP:HB2	2.06	0.55
1:C:216:LEU:O	1:C:219:LEU:HD23	2.07	0.55
1:A:389:GLN:HG2	1:A:621:TRP:HZ3	1.68	0.55
1:D:408:PRO:HB2	1:D:466:VAL:HG11	1.89	0.55
1:B:217:LYS:HG3	1:B:218:ASP:N	2.20	0.55
1:C:555:MET:HE1	1:C:678:VAL:HG22	1.87	0.55
1:A:178:LEU:HD23	1:A:182:TYR:HD1	1.71	0.55
1:A:387:ARG:HG3	1:A:392:ASP:OD2	2.07	0.55
1:A:660:GLY:HA3	1:B:255:TYR:CZ	2.41	0.55
1:B:555:MET:HE1	1:B:678:VAL:HG22	1.89	0.54
1:A:197:TYR:CE2	1:A:231:PRO:HG3	2.41	0.54
1:C:324:VAL:HA	1:C:327:SER:OG	2.07	0.54
1:A:121:HIS:HD2	1:A:125:ASP:CB	2.20	0.54
1:D:233:VAL:HG23	1:D:233:VAL:O	2.08	0.54
1:D:666:PRO:HG2	1:D:669:VAL:HG22	1.89	0.54
1:A:666:PRO:HG2	1:A:669:VAL:HG22	1.89	0.54
1:B:241:ASP:CG	1:B:288:ARG:HH22	2.15	0.54
1:C:544:SER:O	1:C:545:HIS:HB3	2.06	0.54
1:D:196:TYR:OH	1:D:322:GLY:HA3	2.07	0.54
1:A:504:SER:OG	1:A:507:GLN:HG3	2.08	0.54
1:B:573:HIS:HE1	1:B:646:PHE:CE2	2.25	0.54
1:C:160:SER:OG	1:C:162:HIS:CD2	2.61	0.54
1:D:195:ILE:HD12	1:D:231:PRO:HB3	1.90	0.54
1:D:290:ASN:O	1:D:291:ILE:HG22	2.07	0.54
1:C:162:HIS:CD2	1:C:162:HIS:H	2.26	0.54
1:C:389:GLN:HG2	1:C:621:TRP:HZ3	1.71	0.54
1:D:427:TYR:HB3	1:D:457:ILE:HD12	1.90	0.54
1:B:204:ILE:HD11	1:B:227:LEU:HB3	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:598:ASN:HD22	1:B:629:GLN:HE21	1.55	0.54
1:A:241:ASP:CG	1:A:288:ARG:HH22	2.16	0.53
1:B:260:HIS:C	1:B:261:LYS:HG2	2.34	0.53
1:B:544:SER:O	1:B:545:HIS:HB3	2.07	0.53
1:A:230:LEU:HB3	1:A:231:PRO:HD3	1.89	0.53
1:A:389:GLN:HE21	1:A:394:HIS:HE1	1.56	0.53
1:B:141:PHE:HB2	1:B:148:THR:HG21	1.90	0.53
1:C:427:TYR:HB3	1:C:457:ILE:HD12	1.90	0.53
1:A:355:ASN:HA	1:D:180:GLN:HE22	1.72	0.53
1:C:133:ILE:HD11	1:C:141:PHE:HB3	1.90	0.53
1:A:515:ILE:CG1	1:A:548:MET:HE1	2.37	0.53
1:C:197:TYR:CE2	1:C:231:PRO:HG3	2.43	0.53
1:A:93:ARG:CZ	1:A:210:TYR:HE2	2.21	0.53
1:A:116:ASN:C	1:A:116:ASN:HD22	2.16	0.53
1:A:637:GLY:HA2	2:A:11:SO4:O3	2.08	0.53
1:B:133:ILE:HD11	1:B:141:PHE:HB3	1.90	0.53
1:B:389:GLN:HG2	1:B:621:TRP:HZ3	1.71	0.53
1:B:453:GLN:OE1	1:B:691:THR:HG21	2.09	0.53
1:C:638:HIS:N	2:C:31:SO4:O4	2.42	0.53
1:D:197:TYR:CE2	1:D:231:PRO:HG3	2.44	0.53
1:D:230:LEU:HB3	1:D:231:PRO:HD3	1.91	0.53
1:B:666:PRO:HG2	1:B:669:VAL:HG22	1.89	0.53
1:C:194:LYS:NZ	1:C:533:ARG:NH2	2.57	0.53
1:C:467:LYS:HG2	1:C:472:ASN:HA	1.91	0.53
1:D:398:SER:HB3	1:D:401:LYS:HE3	1.89	0.53
1:C:95:GLU:H	1:C:206:ALA:HB2	1.74	0.53
1:C:196:TYR:OH	1:C:322:GLY:HA3	2.09	0.53
1:C:573:HIS:HE1	1:C:646:PHE:CE2	2.27	0.53
1:D:123:ALA:HA	1:D:179:GLU:HG3	1.90	0.53
1:D:292:ASP:O	1:D:293:THR:HB	2.08	0.52
1:C:196:TYR:CG	1:C:323:ASN:HB2	2.44	0.52
1:C:423:ASP:O	1:C:424:GLU:HG3	2.09	0.52
1:D:607:VAL:HG23	1:D:644:PRO:HG3	1.92	0.52
1:B:116:ASN:ND2	1:B:116:ASN:C	2.63	0.52
1:C:162:HIS:C	1:C:164:SER:H	2.18	0.52
1:C:289:GLN:HB2	1:C:384:VAL:HG11	1.90	0.52
1:A:177:ARG:NH1	2:A:41:SO4:O4	2.42	0.52
1:D:467:LYS:HG2	1:D:472:ASN:HA	1.91	0.52
1:A:427:TYR:HB3	1:A:457:ILE:HD12	1.92	0.52
1:A:448:TYR:HA	1:A:559:MET:CE	2.40	0.52
1:C:389:GLN:HE21	1:C:394:HIS:HE1	1.56	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:116:ASN:HD21	1:B:262:ARG:NH1	2.08	0.52
1:B:197:TYR:CE2	1:B:231:PRO:HG3	2.44	0.52
1:C:159:LEU:HD11	1:C:534:ASP:OD2	2.09	0.52
1:D:268:TRP:O	1:D:272:LYS:HG2	2.10	0.52
1:B:691:THR:HG22	1:B:692:HIS:CE1	2.44	0.52
1:C:453:GLN:OE1	1:C:691:THR:HG21	2.09	0.52
1:C:598:ASN:HD22	1:C:629:GLN:HE21	1.57	0.52
1:D:538:ILE:HD12	1:D:538:ILE:N	2.24	0.52
1:D:602:ASN:ND2	2:D:5:SO4:O4	2.42	0.52
1:D:241:ASP:CG	1:D:288:ARG:HH22	2.17	0.52
1:D:389:GLN:HE21	1:D:394:HIS:HE1	1.56	0.52
1:B:165:ILE:HD12	1:D:176:TYR:CE1	2.45	0.52
1:B:196:TYR:OH	1:B:322:GLY:HA3	2.10	0.52
1:A:544:SER:O	1:A:545:HIS:HB3	2.10	0.51
1:B:109:ALA:O	1:B:113:THR:HG22	2.10	0.51
1:B:161:GLN:HG2	1:B:538:ILE:HG13	1.91	0.51
1:D:123:ALA:HB2	1:D:179:GLU:HG3	1.92	0.51
1:C:165:ILE:HG13	1:C:165:ILE:O	2.10	0.51
1:C:241:ASP:CG	1:C:288:ARG:HH22	2.19	0.51
1:C:448:TYR:HA	1:C:559:MET:CE	2.41	0.51
1:B:131:GLY:HA3	1:D:130:PHE:CZ	2.44	0.51
1:D:260:HIS:C	1:D:261:LYS:HG2	2.35	0.51
1:A:106:MET:CE	1:A:224:GLU:HG2	2.34	0.51
1:A:467:LYS:HG2	1:A:472:ASN:HA	1.92	0.51
1:C:453:GLN:HG2	1:C:567:TYR:O	2.10	0.51
1:A:573:HIS:HE1	1:A:646:PHE:CE2	2.29	0.51
1:C:93:ARG:NH1	1:C:210:TYR:CE2	2.78	0.51
1:B:438:ASP:O	1:B:439:THR:HG22	2.10	0.51
1:C:106:MET:CE	1:C:224:GLU:HG2	2.36	0.51
1:B:240:TYR:CE2	1:B:280:LEU:HD11	2.45	0.51
1:C:233:VAL:HG23	1:C:236:ASN:HB2	1.92	0.51
1:C:293:THR:CG2	1:C:294:ASN:H	2.24	0.51
1:D:226:TYR:CE2	1:D:246:ALA:HB1	2.45	0.51
1:A:93:ARG:HD3	1:A:210:TYR:CD2	2.46	0.51
1:D:453:GLN:OE1	1:D:691:THR:HG21	2.10	0.51
1:B:226:TYR:CE2	1:B:246:ALA:HB1	2.46	0.50
1:D:551:TYR:HD2	1:D:555:MET:CE	2.24	0.50
1:A:244:LYS:CB	2:A:17:SO4:O3	2.59	0.50
1:C:116:ASN:ND2	1:C:116:ASN:C	2.70	0.50
1:D:555:MET:O	1:D:559:MET:HG3	2.10	0.50
1:A:204:ILE:HD11	1:A:227:LEU:HB3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:691:THR:HG22	1:A:692:HIS:CE1	2.46	0.50
1:D:302:TYR:CZ	1:D:335:MET:HB2	2.46	0.50
1:D:448:TYR:HA	1:D:559:MET:CE	2.42	0.50
1:A:453:GLN:OE1	1:A:691:THR:HG21	2.11	0.50
1:B:241:ASP:OD2	1:B:288:ARG:NH2	2.41	0.50
1:C:254:LEU:HD23	1:C:257:MET:HE3	1.93	0.50
1:D:178:LEU:HD23	1:D:182:TYR:HD1	1.76	0.50
1:A:551:TYR:HD2	1:A:555:MET:CE	2.25	0.50
1:B:97:VAL:HG12	1:B:193:ASN:OD1	2.11	0.50
1:A:555:MET:O	1:A:559:MET:HG3	2.11	0.50
1:B:230:LEU:HB3	1:B:231:PRO:HD3	1.92	0.50
1:B:244:LYS:N	2:B:38:SO4:O1	2.40	0.50
1:D:515:ILE:CG1	1:D:548:MET:HE1	2.42	0.50
1:D:289:GLN:HB2	1:D:384:VAL:HG11	1.92	0.50
1:D:418:ASN:HB3	1:D:674:PRO:O	2.12	0.50
1:C:538:ILE:HD12	1:C:538:ILE:N	2.27	0.49
1:D:118:PHE:CD2	1:D:149:LEU:HB2	2.47	0.49
1:D:691:THR:HG22	1:D:692:HIS:CE1	2.47	0.49
1:B:250:LYS:HD2	1:B:250:LYS:C	2.38	0.49
1:D:214:LYS:HD3	1:D:218:ASP:O	2.12	0.49
1:D:504:SER:OG	1:D:507:GLN:HG3	2.12	0.49
1:B:268:TRP:O	1:B:272:LYS:HG2	2.13	0.49
1:C:90:ASN:HB3	1:C:293:THR:OG1	2.12	0.49
1:B:423:ASP:O	1:B:424:GLU:HG3	2.12	0.49
1:B:427:TYR:HB3	1:B:457:ILE:HD12	1.93	0.49
1:C:515:ILE:CG1	1:C:548:MET:HE1	2.42	0.49
1:A:268:TRP:O	1:A:272:LYS:HG2	2.12	0.49
1:B:116:ASN:HD22	1:B:262:ARG:HH12	1.58	0.49
1:B:515:ILE:CG1	1:B:548:MET:HE1	2.43	0.49
1:C:268:TRP:O	1:C:272:LYS:HG2	2.11	0.49
1:A:538:ILE:HD12	1:A:538:ILE:N	2.27	0.49
1:C:260:HIS:C	1:C:261:LYS:HG2	2.37	0.49
1:A:71:ASP:N	1:A:533:ARG:HH22	2.11	0.49
1:A:123:ALA:HA	1:A:179:GLU:HG3	1.94	0.49
1:B:398:SER:HB3	1:B:401:LYS:HE3	1.94	0.49
1:B:448:TYR:HA	1:B:559:MET:CE	2.43	0.49
1:B:538:ILE:HD12	1:B:538:ILE:N	2.28	0.49
1:C:164:SER:HB3	1:C:167:ARG:H	1.78	0.49
1:D:310:LEU:HD13	1:D:331:ILE:HD13	1.95	0.49
1:D:573:HIS:HE1	1:D:646:PHE:CE2	2.30	0.49
1:B:129:LEU:HD11	3:D:1:LDA:H111	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:277:LYS:HG2	1:D:280:LEU:HD23	1.95	0.48
1:B:141:PHE:HB2	1:B:148:THR:CG2	2.43	0.48
1:C:195:ILE:HD12	1:C:231:PRO:HB3	1.94	0.48
1:D:106:MET:HE1	1:D:224:GLU:HA	1.95	0.48
1:D:515:ILE:HG12	1:D:548:MET:HE1	1.94	0.48
1:A:398:SER:HB3	1:A:401:LYS:HE3	1.96	0.48
1:D:106:MET:CE	1:D:224:GLU:HG2	2.41	0.48
1:D:244:LYS:HB2	2:D:39:SO4:O2	2.13	0.48
1:A:214:LYS:CE	1:A:279:ASN:HD22	2.27	0.48
1:B:398:SER:O	1:B:583:LYS:HE3	2.14	0.48
1:B:467:LYS:HG2	1:B:472:ASN:HA	1.94	0.48
1:C:159:LEU:O	1:C:160:SER:CB	2.61	0.48
1:D:116:ASN:ND2	1:D:116:ASN:C	2.72	0.48
1:B:360:VAL:HG13	1:B:622:MET:HG2	1.95	0.48
1:A:566:PRO:O	1:A:567:TYR:HB2	2.14	0.48
1:B:164:SER:HB3	1:B:166:GLY:H	1.78	0.48
1:A:148:THR:HG23	1:A:151:GLN:CB	2.42	0.48
1:A:226:TYR:CE2	1:A:246:ALA:HB1	2.48	0.48
1:A:448:TYR:HA	1:A:559:MET:HE3	1.96	0.48
1:C:72:PRO:HD3	1:C:94:HIS:ND1	2.27	0.48
1:C:398:SER:O	1:C:583:LYS:HE3	2.13	0.48
1:C:515:ILE:HG12	1:C:548:MET:HE1	1.95	0.48
1:A:159:LEU:HD21	1:A:167:ARG:HD3	1.96	0.48
1:A:311:MET:SD	1:A:324:VAL:HG11	2.54	0.48
1:B:613:THR:HB	1:B:614:PRO:HD2	1.95	0.48
1:C:219:LEU:HD12	1:C:223:GLU:HB3	1.95	0.48
1:D:115:ASP:CG	1:D:118:PHE:HB2	2.39	0.48
1:D:298:GLU:HA	1:D:344:GLN:HG2	1.94	0.48
1:A:423:ASP:O	1:A:424:GLU:HG3	2.14	0.48
1:B:389:GLN:HE21	1:B:394:HIS:HE1	1.61	0.48
1:B:551:TYR:HD2	1:B:555:MET:CE	2.27	0.48
1:A:85:VAL:HG13	1:A:299:TYR:CE1	2.49	0.48
1:A:195:ILE:HD12	1:A:231:PRO:HB3	1.96	0.47
1:C:116:ASN:HD21	1:C:262:ARG:NH1	2.06	0.47
1:C:427:TYR:CB	1:C:457:ILE:HD12	2.43	0.47
1:B:515:ILE:HG12	1:B:548:MET:HE1	1.96	0.47
1:A:260:HIS:C	1:A:261:LYS:HG2	2.38	0.47
1:B:161:GLN:HE21	1:B:538:ILE:HG13	1.78	0.47
1:B:242:HIS:CA	2:B:38:SO4:O4	2.61	0.47
1:A:96:HIS:ND1	2:A:3:SO4:O4	2.41	0.47
1:C:414:LYS:HB3	1:C:678:VAL:HG21	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:555:MET:O	1:C:559:MET:HG3	2.13	0.47
1:A:567:TYR:CD2	1:A:692:HIS:HB2	2.50	0.47
1:C:691:THR:HG22	1:C:692:HIS:CE1	2.50	0.47
1:B:93:ARG:NH1	1:B:210:TYR:CE2	2.82	0.47
1:B:638:HIS:O	1:B:642:GLU:HB2	2.14	0.47
1:C:161:GLN:O	1:C:161:GLN:CG	2.57	0.47
1:C:194:LYS:HZ1	1:C:533:ARG:HH22	1.61	0.47
1:D:109:ALA:O	1:D:113:THR:CG2	2.62	0.47
1:D:159:LEU:CD1	1:D:532:THR:HB	2.41	0.47
1:A:97:VAL:HB	1:A:205:LYS:HB2	1.97	0.47
1:A:409:ALA:O	1:A:413:MET:HG2	2.15	0.47
1:B:95:GLU:H	1:B:206:ALA:HB2	1.79	0.47
1:B:214:LYS:CE	1:B:279:ASN:HD22	2.28	0.47
1:C:194:LYS:NZ	1:C:533:ARG:HH22	2.13	0.47
1:C:202:THR:CG2	1:C:326:GLN:OE1	2.62	0.47
1:C:214:LYS:CE	1:C:279:ASN:HD22	2.28	0.47
1:C:546:LYS:HB3	1:C:546:LYS:HE3	1.63	0.47
1:D:123:ALA:CB	1:D:179:GLU:HG3	2.44	0.47
1:D:162:HIS:HB2	1:D:167:ARG:CD	2.45	0.47
1:D:438:ASP:O	1:D:439:THR:HG22	2.15	0.47
1:A:613:THR:HB	1:A:614:PRO:HD2	1.97	0.47
1:A:427:TYR:CB	1:A:457:ILE:HD12	2.44	0.47
1:B:402:PRO:O	1:B:407:GLY:HA3	2.14	0.47
1:C:602:ASN:O	1:C:636:VAL:HA	2.15	0.47
1:D:197:TYR:O	1:D:230:LEU:HD21	2.15	0.47
1:D:398:SER:O	1:D:583:LYS:HE3	2.15	0.47
1:D:427:TYR:CB	1:D:457:ILE:HD12	2.45	0.47
1:C:94:HIS:C	1:C:94:HIS:CD2	2.92	0.47
1:C:438:ASP:O	1:C:439:THR:HG22	2.15	0.47
1:B:490:ILE:HA	1:B:494:GLU:HG3	1.97	0.46
1:C:240:TYR:CE2	1:C:280:LEU:HD11	2.50	0.46
1:C:73:ILE:CG2	1:C:328:GLY:HA3	2.44	0.46
1:C:214:LYS:HE3	1:C:279:ASN:HD22	1.80	0.46
1:D:613:THR:HB	1:D:614:PRO:HD2	1.96	0.46
1:A:214:LYS:HD3	1:A:218:ASP:O	2.16	0.46
1:A:277:LYS:HG2	1:A:280:LEU:HD23	1.97	0.46
1:A:602:ASN:O	1:A:636:VAL:HA	2.15	0.46
1:C:194:LYS:HZ2	1:C:533:ARG:NH2	2.14	0.46
1:C:268:TRP:CE2	1:C:272:LYS:HE2	2.50	0.46
1:C:297:SER:HA	1:C:300:ASN:OD1	2.15	0.46
1:A:109:ALA:O	1:A:113:THR:CG2	2.63	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:297:SER:HA	1:B:300:ASN:OD1	2.16	0.46
1:C:567:TYR:CD2	1:C:692:HIS:HB2	2.50	0.46
1:D:408:PRO:HD3	1:D:478:PHE:CD1	2.51	0.46
1:B:162:HIS:CG	1:B:164:SER:HB2	2.51	0.46
1:C:97:VAL:HG12	1:C:193:ASN:OD1	2.16	0.46
1:C:226:TYR:CE2	1:C:246:ALA:HB1	2.50	0.46
1:C:457:ILE:O	1:C:461:LYS:HG2	2.15	0.46
1:C:551:TYR:HD2	1:C:555:MET:CE	2.28	0.46
1:D:123:ALA:CA	1:D:179:GLU:HG3	2.45	0.46
1:D:250:LYS:C	1:D:250:LYS:HD2	2.40	0.46
1:B:106:MET:CE	1:B:224:GLU:HG2	2.43	0.46
1:B:302:TYR:CZ	1:B:335:MET:HB2	2.50	0.46
1:C:117:ARG:O	1:C:121:HIS:CD2	2.69	0.46
1:C:516:ALA:HB2	1:C:612:PHE:HB2	1.98	0.46
1:C:613:THR:HB	1:C:614:PRO:HD2	1.98	0.46
1:D:95:GLU:H	1:D:206:ALA:HB2	1.80	0.46
1:D:546:LYS:HB3	1:D:546:LYS:HE3	1.63	0.46
1:A:398:SER:O	1:A:583:LYS:HE3	2.15	0.46
1:D:297:SER:HA	1:D:300:ASN:OD1	2.15	0.46
1:A:159:LEU:C	1:A:167:ARG:HH21	2.23	0.46
1:A:219:LEU:HD12	1:A:223:GLU:HB3	1.98	0.46
1:A:264:THR:HG23	1:A:267:GLN:OE1	2.16	0.46
1:C:398:SER:HB3	1:C:401:LYS:HE3	1.98	0.46
1:D:242:HIS:HA	2:D:39:SO4:O3	2.16	0.46
1:D:261:LYS:HB3	1:D:261:LYS:HE2	1.65	0.46
1:A:660:GLY:HA2	1:B:255:TYR:OH	2.16	0.46
1:B:214:LYS:HE3	1:B:279:ASN:HD22	1.81	0.46
1:D:241:ASP:OD2	1:D:288:ARG:NH2	2.45	0.46
1:B:210:TYR:HD1	1:B:211:TYR:CD1	2.34	0.45
1:B:277:LYS:HG2	1:B:280:LEU:HD23	1.96	0.45
1:C:277:LYS:HG2	1:C:280:LEU:HD23	1.98	0.45
1:D:423:ASP:O	1:D:424:GLU:HG3	2.16	0.45
1:D:516:ALA:HB2	1:D:612:PHE:HB2	1.98	0.45
1:A:389:GLN:HG3	1:A:394:HIS:HE1	1.80	0.45
1:B:73:ILE:HG13	1:B:328:GLY:CA	2.46	0.45
1:B:566:PRO:O	1:B:567:TYR:HB2	2.16	0.45
1:C:250:LYS:HD2	1:C:250:LYS:C	2.41	0.45
1:C:322:GLY:N	2:C:19:SO4:O3	2.44	0.45
1:D:360:VAL:HG13	1:D:622:MET:HG2	1.98	0.45
1:A:94:HIS:CD2	1:A:94:HIS:C	2.94	0.45
1:B:254:LEU:HD23	1:B:257:MET:HE3	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:95:GLU:N	1:C:206:ALA:HB2	2.31	0.45
1:C:389:GLN:HG3	1:C:394:HIS:HE1	1.82	0.45
1:D:389:GLN:HG3	1:D:394:HIS:HE1	1.78	0.45
1:D:414:LYS:HB3	1:D:678:VAL:HG21	1.98	0.45
1:A:490:ILE:HA	1:A:494:GLU:HG3	1.98	0.45
1:B:504:SER:OG	1:B:507:GLN:HG3	2.16	0.45
1:C:70:GLN:N	1:C:194:LYS:HD2	2.31	0.45
1:A:289:GLN:O	1:A:290:ASN:O	2.34	0.45
1:A:302:TYR:CZ	1:A:335:MET:HB2	2.52	0.45
1:A:637:GLY:O	1:A:638:HIS:C	2.60	0.45
1:B:148:THR:HG23	1:B:151:GLN:CB	2.47	0.45
1:B:214:LYS:HD3	1:B:218:ASP:O	2.17	0.45
1:D:93:ARG:NH1	1:D:210:TYR:CE2	2.85	0.45
1:D:240:TYR:CE2	1:D:280:LEU:HD11	2.52	0.45
1:D:429:VAL:O	1:D:430:ASP:HB2	2.17	0.45
1:A:321:LEU:C	1:A:323:ASN:H	2.25	0.45
1:D:292:ASP:O	1:D:293:THR:CB	2.64	0.45
1:D:417:THR:CG2	1:D:676:ILE:HB	2.47	0.45
1:B:427:TYR:CB	1:B:457:ILE:HD12	2.47	0.45
1:C:402:PRO:O	1:C:407:GLY:HA3	2.17	0.45
1:C:448:TYR:HA	1:C:559:MET:HE3	1.99	0.45
1:C:486:TYR:CD1	1:C:490:ILE:HD11	2.52	0.45
1:C:691:THR:HB	1:C:692:HIS:H	1.62	0.45
1:A:598:ASN:HD22	1:A:629:GLN:NE2	2.14	0.45
1:C:360:VAL:HG13	1:C:622:MET:HE2	1.98	0.45
1:B:264:THR:HG23	1:B:267:GLN:OE1	2.17	0.44
1:B:448:TYR:HA	1:B:559:MET:HE3	1.98	0.44
1:B:457:ILE:O	1:B:461:LYS:HG2	2.17	0.44
1:C:254:LEU:HD23	1:C:257:MET:CE	2.46	0.44
1:D:264:THR:HG23	1:D:267:GLN:OE1	2.18	0.44
1:A:444:THR:O	1:A:689:ARG:HD3	2.18	0.44
1:B:94:HIS:CD2	1:B:94:HIS:C	2.95	0.44
1:C:293:THR:CG2	1:C:294:ASN:N	2.79	0.44
1:D:263:ILE:HB	1:D:267:GLN:HG3	1.99	0.44
1:A:413:MET:HE1	1:A:466:VAL:HA	1.99	0.44
1:B:195:ILE:HD12	1:B:231:PRO:HB3	1.98	0.44
1:D:214:LYS:HD2	1:D:219:LEU:HB2	1.99	0.44
1:D:289:GLN:O	1:D:290:ASN:C	2.60	0.44
1:D:486:TYR:CD1	1:D:490:ILE:HD11	2.53	0.44
1:D:648:TYR:CE1	1:D:652:MET:HG3	2.53	0.44
1:B:555:MET:O	1:B:559:MET:HG3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:310:LEU:HD13	1:C:331:ILE:HD13	1.99	0.44
1:C:336:ASP:HB2	1:C:373:VAL:HG13	1.99	0.44
1:A:297:SER:HA	1:A:300:ASN:OD1	2.18	0.44
1:B:129:LEU:CD1	3:D:1:LDA:H111	2.48	0.44
1:B:242:HIS:CB	2:B:38:SO4:O4	2.66	0.44
1:B:261:LYS:HB3	1:B:261:LYS:HE2	1.61	0.44
1:B:648:TYR:CE1	1:B:652:MET:HG3	2.51	0.44
1:C:298:GLU:HA	1:C:344:GLN:HG2	1.99	0.44
1:A:214:LYS:HE3	1:A:279:ASN:HD22	1.83	0.44
1:A:254:LEU:HD23	1:A:257:MET:HE3	1.99	0.44
1:B:233:VAL:HG23	1:B:236:ASN:HB2	2.00	0.44
1:B:244:LYS:HB2	2:B:38:SO4:O1	2.18	0.44
1:B:567:TYR:CD2	1:B:692:HIS:HB2	2.52	0.44
1:D:219:LEU:HD12	1:D:223:GLU:HB3	2.00	0.44
1:D:438:ASP:OD1	1:D:440:LYS:HB2	2.18	0.44
1:A:438:ASP:O	1:A:439:THR:HG22	2.18	0.44
1:B:162:HIS:CD2	1:B:164:SER:HB3	2.53	0.44
1:C:429:VAL:O	1:C:430:ASP:HB2	2.18	0.44
1:C:648:TYR:CE1	1:C:652:MET:HG3	2.52	0.44
1:B:268:TRP:CD2	1:B:272:LYS:HE2	2.53	0.43
1:C:261:LYS:HE2	1:C:261:LYS:HB3	1.64	0.43
1:C:417:THR:CG2	1:C:676:ILE:HB	2.48	0.43
1:D:163:LYS:HB3	1:D:163:LYS:HE2	1.60	0.43
1:D:566:PRO:O	1:D:567:TYR:HB2	2.18	0.43
1:A:438:ASP:OD1	1:A:440:LYS:HB2	2.18	0.43
1:A:556:LEU:HD12	1:A:556:LEU:HA	1.86	0.43
1:A:626:LYS:HD2	1:A:626:LYS:C	2.43	0.43
1:B:379:ARG:H	1:B:379:ARG:HG2	1.60	0.43
1:D:490:ILE:HA	1:D:494:GLU:HG3	1.99	0.43
1:D:602:ASN:O	1:D:636:VAL:HA	2.18	0.43
1:B:358:GLN:HB2	1:B:624:PHE:CE2	2.54	0.43
1:C:387:ARG:HA	1:C:387:ARG:NE	2.33	0.43
1:C:444:THR:O	1:C:689:ARG:HD3	2.18	0.43
1:D:409:ALA:O	1:D:413:MET:HG2	2.18	0.43
1:A:241:ASP:OD2	1:A:288:ARG:NH2	2.44	0.43
1:A:388:ASN:OD1	1:A:388:ASN:C	2.61	0.43
1:A:397:GLY:O	1:A:497:GLY:HA3	2.19	0.43
1:B:92:GLN:C	1:B:93:ARG:HG3	2.43	0.43
1:B:263:ILE:HB	1:B:267:GLN:HG3	2.01	0.43
1:B:389:GLN:HG3	1:B:394:HIS:HE1	1.81	0.43
1:C:72:PRO:HD3	1:C:94:HIS:NE2	2.30	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:138:THR:CG2	1:D:350:GLY:HA2	2.45	0.43
1:C:638:HIS:O	1:C:642:GLU:HB2	2.18	0.43
1:A:360:VAL:HG13	1:A:622:MET:HG2	2.00	0.43
1:A:638:HIS:O	1:A:642:GLU:HB2	2.18	0.43
1:C:263:ILE:HB	1:C:267:GLN:HG3	2.00	0.43
1:D:567:TYR:CD2	1:D:692:HIS:HB2	2.53	0.43
1:A:210:TYR:HD1	1:A:211:TYR:CD1	2.36	0.43
1:A:447:ILE:HA	1:A:450:ALA:HB3	2.01	0.43
1:A:648:TYR:CE1	1:A:652:MET:HG3	2.54	0.43
1:B:230:LEU:N	1:B:231:PRO:CD	2.82	0.43
1:C:109:ALA:O	1:C:113:THR:CG2	2.66	0.43
1:C:148:THR:HG23	1:C:151:GLN:CB	2.49	0.43
1:C:408:PRO:HD3	1:C:478:PHE:CD1	2.53	0.43
1:D:311:MET:HE2	1:D:320:ASN:HA	2.01	0.43
1:D:638:HIS:O	1:D:642:GLU:HB2	2.17	0.43
1:A:355:ASN:CA	1:D:180:GLN:HE22	2.31	0.43
1:B:388:ASN:OD1	1:B:388:ASN:C	2.62	0.43
1:A:261:LYS:HE2	1:A:261:LYS:HB3	1.65	0.43
1:B:176:TYR:OH	1:D:165:ILE:HD13	2.18	0.43
1:C:159:LEU:O	1:C:160:SER:HB3	2.19	0.43
1:D:94:HIS:CD2	1:D:94:HIS:C	2.96	0.43
1:D:254:LEU:HD23	1:D:257:MET:HE3	2.00	0.43
1:A:691:THR:HB	1:A:692:HIS:H	1.61	0.43
1:B:414:LYS:HB3	1:B:678:VAL:HG21	2.01	0.43
1:C:268:TRP:CD2	1:C:272:LYS:HE2	2.54	0.43
1:D:336:ASP:HB2	1:D:373:VAL:HG13	2.01	0.43
1:D:360:VAL:HG13	1:D:622:MET:HE2	2.00	0.43
1:A:183:SER:O	1:A:187:ILE:HG13	2.19	0.43
1:A:250:LYS:HD2	1:A:250:LYS:C	2.44	0.43
1:A:414:LYS:HB3	1:A:678:VAL:HG21	2.00	0.43
1:B:73:ILE:HB	1:B:74:PRO:HD2	2.00	0.43
1:C:117:ARG:HG2	1:C:120:GLU:OE1	2.19	0.43
1:C:186:ASP:O	1:C:190:VAL:HG23	2.19	0.43
1:C:264:THR:HG23	1:C:267:GLN:OE1	2.19	0.43
1:D:121:HIS:HD2	1:D:125:ASP:CA	2.31	0.43
1:D:148:THR:HG23	1:D:151:GLN:CB	2.46	0.43
1:D:233:VAL:HG23	1:D:236:ASN:HB2	2.00	0.43
1:A:263:ILE:HB	1:A:267:GLN:HG3	2.00	0.42
1:A:546:LYS:HE3	1:A:546:LYS:HB3	1.62	0.42
1:B:546:LYS:HB3	1:B:546:LYS:HE3	1.63	0.42
1:D:298:GLU:HG3	1:D:341:LYS:HG2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:523:ASN:O	1:D:525:HIS:HD2	2.01	0.42
1:A:298:GLU:OE2	1:A:341:LYS:HE2	2.19	0.42
1:B:214:LYS:HD2	1:B:219:LEU:HB2	2.00	0.42
1:B:516:ALA:HB2	1:B:612:PHE:HB2	2.01	0.42
1:B:560:LEU:HD23	1:B:560:LEU:HA	1.88	0.42
1:B:602:ASN:O	1:B:636:VAL:HA	2.19	0.42
1:C:637:GLY:O	1:C:638:HIS:C	2.62	0.42
1:A:214:LYS:HD2	1:A:219:LEU:HB2	2.00	0.42
1:A:429:VAL:O	1:A:430:ASP:HB2	2.19	0.42
1:B:409:ALA:O	1:B:413:MET:HG2	2.19	0.42
1:C:353:TYR:CZ	1:C:379:ARG:HD2	2.54	0.42
1:D:289:GLN:CB	1:D:384:VAL:HG11	2.48	0.42
1:D:447:ILE:HG13	1:D:559:MET:HE1	2.01	0.42
1:B:117:ARG:NH1	1:B:120:GLU:OE2	2.50	0.42
1:B:438:ASP:OD1	1:B:440:LYS:HB2	2.19	0.42
1:C:86:LYS:HE3	1:C:295:GLN:O	2.19	0.42
1:C:366:ASP:OD1	1:C:366:ASP:C	2.62	0.42
1:D:214:LYS:HE3	1:D:279:ASN:HD22	1.85	0.42
1:D:230:LEU:N	1:D:231:PRO:CD	2.82	0.42
1:B:219:LEU:HD12	1:B:223:GLU:HB3	2.01	0.42
1:C:241:ASP:OD2	1:C:288:ARG:NH2	2.45	0.42
1:B:95:GLU:N	1:B:206:ALA:HB2	2.35	0.42
1:B:417:THR:CG2	1:B:676:ILE:HB	2.49	0.42
1:C:204:ILE:CD1	1:C:227:LEU:HB3	2.50	0.42
1:C:242:HIS:HB3	2:C:18:SO4:O2	2.20	0.42
1:D:214:LYS:CE	1:D:279:ASN:HD22	2.33	0.42
1:A:271:ALA:C	1:A:273:LYS:H	2.27	0.42
1:A:417:THR:CG2	1:A:676:ILE:HB	2.50	0.42
1:A:643:TYR:N	1:A:644:PRO:HD2	2.35	0.42
1:B:73:ILE:HG13	1:B:328:GLY:HA3	2.00	0.42
1:C:490:ILE:HA	1:C:494:GLU:HG3	2.02	0.42
1:C:566:PRO:O	1:C:567:TYR:HB2	2.20	0.42
1:A:516:ALA:HB2	1:A:612:PHE:HB2	2.01	0.42
1:B:164:SER:C	1:B:166:GLY:N	2.77	0.42
1:C:162:HIS:HB3	1:C:167:ARG:NH1	2.34	0.42
1:C:292:ASP:O	1:C:293:THR:CB	2.67	0.42
1:C:438:ASP:OD1	1:C:440:LYS:HB2	2.19	0.42
1:A:116:ASN:ND2	1:A:116:ASN:C	2.76	0.42
1:A:186:ASP:O	1:A:190:VAL:HG23	2.19	0.42
1:A:227:LEU:HD23	1:A:227:LEU:HA	1.89	0.42
1:A:230:LEU:N	1:A:231:PRO:CD	2.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:486:TYR:CD1	1:A:490:ILE:HD11	2.55	0.42
1:C:93:ARG:CZ	1:C:210:TYR:HE2	2.32	0.42
1:C:637:GLY:CA	2:C:31:SO4:O4	2.67	0.42
1:D:210:TYR:HD1	1:D:211:TYR:CD1	2.37	0.42
1:D:388:ASN:OD1	1:D:388:ASN:C	2.63	0.42
1:B:496:LEU:HD23	1:B:496:LEU:HA	1.87	0.42
1:B:637:GLY:O	1:B:638:HIS:C	2.61	0.42
1:C:117:ARG:O	1:C:121:HIS:CG	2.72	0.42
1:C:397:GLY:O	1:C:497:GLY:HA3	2.20	0.42
1:D:293:THR:O	1:D:294:ASN:CB	2.67	0.42
1:D:673:ILE:HD13	1:D:674:PRO:HA	2.02	0.42
1:A:302:TYR:CE2	1:A:372:LEU:HG	2.54	0.41
1:C:413:MET:HE1	1:C:466:VAL:HA	2.02	0.41
1:A:336:ASP:HB2	1:A:373:VAL:HG13	2.02	0.41
1:A:403:PHE:CD2	1:A:482:LEU:HD13	2.55	0.41
1:B:447:ILE:HA	1:B:450:ALA:HB3	2.02	0.41
1:A:116:ASN:HD21	1:A:262:ARG:NH1	2.15	0.41
1:A:408:PRO:HD3	1:A:478:PHE:CD1	2.55	0.41
1:B:165:ILE:H	1:B:165:ILE:HG12	1.60	0.41
1:B:444:THR:O	1:B:689:ARG:HD3	2.20	0.41
1:C:401:LYS:N	1:C:402:PRO:CD	2.83	0.41
1:C:423:ASP:C	1:C:424:GLU:HG3	2.46	0.41
1:C:643:TYR:N	1:C:644:PRO:HD2	2.36	0.41
1:D:237:TYR:O	1:D:246:ALA:HB2	2.20	0.41
1:B:199:ASP:OD1	1:B:288:ARG:HD2	2.21	0.41
1:B:307:LYS:HB3	1:B:307:LYS:HE2	1.71	0.41
1:B:401:LYS:N	1:B:402:PRO:CD	2.83	0.41
1:C:106:MET:HE1	1:C:224:GLU:HA	2.02	0.41
1:D:126:TYR:HE2	3:D:1:LDA:CM1	2.33	0.41
1:D:182:TYR:HB3	1:D:186:ASP:HB2	2.03	0.41
1:D:221:LEU:HD23	1:D:221:LEU:HA	1.75	0.41
1:A:389:GLN:CG	1:A:621:TRP:CZ3	3.03	0.41
1:A:658:ARG:HG2	1:B:256:LEU:HD21	2.03	0.41
1:B:85:VAL:HG11	1:B:335:MET:HE1	2.02	0.41
1:C:142:GLY:HA3	1:C:147:SER:O	2.20	0.41
1:C:202:THR:HG23	1:C:326:GLN:OE1	2.21	0.41
1:D:413:MET:HE1	1:D:466:VAL:HA	2.01	0.41
3:D:1:LDA:H91	3:D:1:LDA:H122	1.70	0.41
1:B:200:GLY:CA	1:B:326:GLN:HE22	2.33	0.41
1:B:268:TRP:CE2	1:B:272:LYS:HE2	2.55	0.41
1:B:336:ASP:HB2	1:B:373:VAL:HG13	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:71:ASP:HB3	1:C:72:PRO:CD	2.48	0.41
1:C:221:LEU:HD23	1:C:221:LEU:HA	1.78	0.41
1:C:496:LEU:HD23	1:C:496:LEU:HA	1.89	0.41
1:C:584:THR:HG22	1:C:609:ILE:HG13	2.02	0.41
1:D:227:LEU:HD23	1:D:227:LEU:HA	1.92	0.41
3:D:1:LDA:H22	3:D:1:LDA:HM13	1.68	0.41
1:A:298:GLU:HG3	1:A:341:LYS:CG	2.49	0.41
1:B:227:LEU:HD23	1:B:227:LEU:HA	1.90	0.41
1:B:254:LEU:HD23	1:B:257:MET:CE	2.50	0.41
1:C:292:ASP:O	1:C:293:THR:HB	2.21	0.41
1:D:307:LYS:HB3	1:D:307:LYS:HE2	1.74	0.41
1:D:448:TYR:HA	1:D:559:MET:HE2	2.03	0.41
1:A:114:GLU:O	1:A:128:ARG:NH2	2.54	0.41
1:A:233:VAL:HG23	1:A:236:ASN:HB2	2.02	0.41
1:A:392:ASP:HA	1:A:393:PRO:HD3	1.85	0.41
1:A:560:LEU:HA	1:A:560:LEU:HD23	1.86	0.41
1:A:584:THR:HG22	1:A:609:ILE:HG13	2.02	0.41
1:B:109:ALA:O	1:B:113:THR:CG2	2.68	0.41
1:C:271:ALA:C	1:C:273:LYS:H	2.29	0.41
1:C:324:VAL:HG12	1:C:329:ILE:HD13	2.03	0.41
1:D:159:LEU:HD12	1:D:533:ARG:N	2.31	0.41
1:D:444:THR:O	1:D:689:ARG:HD3	2.21	0.41
1:D:447:ILE:HA	1:D:450:ALA:HB3	2.03	0.41
1:D:551:TYR:HB2	1:D:555:MET:HE2	2.03	0.41
1:A:457:ILE:O	1:A:461:LYS:HG2	2.21	0.41
1:B:387:ARG:HA	1:B:387:ARG:NE	2.36	0.41
1:C:210:TYR:HD1	1:C:211:TYR:CD1	2.39	0.41
1:D:115:ASP:HB3	1:D:149:LEU:HG	2.03	0.41
1:A:177:ARG:CZ	2:A:41:SO4:O4	2.69	0.40
1:A:602:ASN:ND2	2:A:11:SO4:O4	2.54	0.40
1:C:118:PHE:HA	1:C:121:HIS:CD2	2.56	0.40
1:C:403:PHE:CD2	1:C:482:LEU:HD13	2.56	0.40
1:D:220:ASN:O	1:D:224:GLU:HG3	2.21	0.40
1:D:417:THR:HG23	1:D:676:ILE:HB	2.03	0.40
1:D:448:TYR:HA	1:D:559:MET:HE3	2.03	0.40
1:D:457:ILE:O	1:D:461:LYS:HG2	2.21	0.40
1:A:77:ILE:CD1	1:A:303:VAL:HG22	2.52	0.40
1:A:315:ALA:C	1:A:316:PHE:CD1	2.99	0.40
1:A:379:ARG:H	1:A:379:ARG:HG2	1.61	0.40
1:B:294:ASN:OD1	1:B:382:LYS:HD2	2.21	0.40
1:D:271:ALA:C	1:D:273:LYS:H	2.30	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:563:THR:HG22	1:D:570:ALA:HB3	2.03	0.40
1:A:440:LYS:HE3	1:A:441:SER:H	1.86	0.40
1:B:403:PHE:CD2	1:B:482:LEU:HD13	2.55	0.40
1:C:392:ASP:HA	1:C:393:PRO:HD3	1.86	0.40
1:D:254:LEU:HD23	1:D:257:MET:CE	2.52	0.40
1:D:387:ARG:NE	1:D:387:ARG:HA	2.37	0.40
1:D:563:THR:CG2	1:D:570:ALA:HB3	2.51	0.40
1:A:402:PRO:O	1:A:407:GLY:HA3	2.21	0.40
1:B:643:TYR:N	1:B:644:PRO:HD2	2.36	0.40
1:C:72:PRO:HG3	1:C:92:GLN:HE22	1.87	0.40
1:C:360:VAL:HG13	1:C:622:MET:HG2	2.04	0.40
1:D:403:PHE:CD2	1:D:482:LEU:HD13	2.57	0.40
1:D:560:LEU:HA	1:D:560:LEU:HD23	1.85	0.40
1:B:197:TYR:O	1:B:230:LEU:HD21	2.21	0.40
1:B:271:ALA:C	1:B:273:LYS:H	2.30	0.40
1:B:286:GLU:HB3	1:B:291:ILE:HD11	2.02	0.40
1:B:295:GLN:O	1:B:296:ASP:HB2	2.22	0.40
1:C:85:VAL:HG13	1:C:299:TYR:CZ	2.57	0.40
1:C:183:SER:O	1:C:184:LYS:C	2.65	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	506/526 (96%)	456 (90%)	50 (10%)	7	29
1	B	522/526 (99%)	471 (90%)	51 (10%)	7	29

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	524/526 (100%)	473 (90%)	51 (10%)	8	30
1	D	511/526 (97%)	461 (90%)	50 (10%)	7	29
All	All	2063/2104 (98%)	1861 (90%)	202 (10%)	7	29

All (202) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	73	ILE
1	A	87	THR
1	A	113	THR
1	A	117	ARG
1	A	128	ARG
1	A	147	SER
1	A	148	THR
1	A	159	LEU
1	A	165	ILE
1	A	167	ARG
1	A	174	LEU
1	A	177	ARG
1	A	178	LEU
1	A	219	LEU
1	A	221	LEU
1	A	239	ILE
1	A	244	LYS
1	A	261	LYS
1	A	289	GLN
1	A	296	ASP
1	A	301	SER
1	A	318	ASP
1	A	360	VAL
1	A	379	ARG
1	A	387	ARG
1	A	398	SER
1	A	435	ARG
1	A	439	THR
1	A	454	SER
1	A	494	GLU
1	A	520	THR
1	A	534	ASP
1	A	546	LYS
1	A	556	LEU

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Mol	Chain	Res	Type
1	A	563	THR
1	A	583	LYS
1	A	606	ASP
1	A	609	ILE
1	A	610	ASN
1	A	626	LYS
1	A	627	VAL
1	A	656	SER
1	A	667	SER
1	A	670	SER
1	A	672	SER
1	A	673	ILE
1	A	678	VAL
1	A	686	THR
1	A	687	THR
1	A	691	THR
1	B	87	THR
1	B	92	GLN
1	B	94	HIS
1	B	113	THR
1	B	124	LEU
1	B	138	THR
1	B	148	THR
1	B	160	SER
1	B	161	GLN
1	B	162	HIS
1	B	165	ILE
1	B	167	ARG
1	B	174	LEU
1	B	177	ARG
1	B	178	LEU
1	B	218	ASP
1	B	219	LEU
1	B	221	LEU
1	B	239	ILE
1	B	244	LYS
1	B	261	LYS
1	B	292	ASP
1	B	294	ASN
1	B	301	SER
1	B	360	VAL
1	B	379	ARG

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Mol	Chain	Res	Type
1	B	387	ARG
1	B	398	SER
1	B	435	ARG
1	B	439	THR
1	B	454	SER
1	B	494	GLU
1	B	520	THR
1	B	534	ASP
1	B	546	LYS
1	B	556	LEU
1	B	563	THR
1	B	583	LYS
1	B	606	ASP
1	B	609	ILE
1	B	626	LYS
1	B	627	VAL
1	B	656	SER
1	B	667	SER
1	B	670	SER
1	B	672	SER
1	B	673	ILE
1	B	678	VAL
1	B	686	THR
1	B	687	THR
1	B	691	THR
1	C	70	GLN
1	C	87	THR
1	C	113	THR
1	C	124	LEU
1	C	138	THR
1	C	148	THR
1	C	158	PHE
1	C	159	LEU
1	C	161	GLN
1	C	162	HIS
1	C	164	SER
1	C	165	ILE
1	C	167	ARG
1	C	174	LEU
1	C	177	ARG
1	C	178	LEU
1	C	218	ASP

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Mol	Chain	Res	Type
1	C	219	LEU
1	C	221	LEU
1	C	239	ILE
1	C	244	LYS
1	C	261	LYS
1	C	291	ILE
1	C	301	SER
1	C	360	VAL
1	C	379	ARG
1	C	387	ARG
1	C	398	SER
1	C	435	ARG
1	C	439	THR
1	C	454	SER
1	C	494	GLU
1	C	520	THR
1	C	534	ASP
1	C	546	LYS
1	C	556	LEU
1	C	563	THR
1	C	583	LYS
1	C	606	ASP
1	C	609	ILE
1	C	626	LYS
1	C	627	VAL
1	C	656	SER
1	C	667	SER
1	C	670	SER
1	C	672	SER
1	C	673	ILE
1	C	678	VAL
1	C	686	THR
1	C	687	THR
1	C	691	THR
1	D	73	ILE
1	D	87	THR
1	D	94	HIS
1	D	113	THR
1	D	128	ARG
1	D	148	THR
1	D	158	PHE
1	D	163	LYS

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Mol	Chain	Res	Type
1	D	164	SER
1	D	167	ARG
1	D	174	LEU
1	D	177	ARG
1	D	178	LEU
1	D	219	LEU
1	D	221	LEU
1	D	239	ILE
1	D	244	LYS
1	D	261	LYS
1	D	262	ARG
1	D	291	ILE
1	D	301	SER
1	D	347	VAL
1	D	359	GLN
1	D	360	VAL
1	D	379	ARG
1	D	387	ARG
1	D	398	SER
1	D	435	ARG
1	D	439	THR
1	D	454	SER
1	D	494	GLU
1	D	520	THR
1	D	534	ASP
1	D	546	LYS
1	D	556	LEU
1	D	563	THR
1	D	583	LYS
1	D	606	ASP
1	D	610	ASN
1	D	626	LYS
1	D	627	VAL
1	D	656	SER
1	D	667	SER
1	D	670	SER
1	D	672	SER
1	D	673	ILE
1	D	678	VAL
1	D	686	THR
1	D	687	THR
1	D	691	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (71) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	94	HIS
1	A	116	ASN
1	A	121	HIS
1	A	232	GLN
1	A	258	HIS
1	A	279	ASN
1	A	320	ASN
1	A	334	ASN
1	A	389	GLN
1	A	468	GLN
1	A	472	ASN
1	A	525	HIS
1	A	542	HIS
1	A	598	ASN
1	A	615	GLN
1	A	692	HIS
1	B	116	ASN
1	B	161	GLN
1	B	232	GLN
1	B	258	HIS
1	B	279	ASN
1	B	295	GLN
1	B	323	ASN
1	B	326	GLN
1	B	334	ASN
1	B	389	GLN
1	B	468	GLN
1	B	472	ASN
1	B	525	HIS
1	B	542	HIS
1	B	573	HIS
1	B	598	ASN
1	B	615	GLN
1	B	692	HIS
1	C	90	ASN
1	C	92	GLN
1	C	94	HIS
1	C	121	HIS
1	C	162	HIS
1	C	232	GLN
1	C	258	HIS

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Mol	Chain	Res	Type
1	C	279	ASN
1	C	290	ASN
1	C	295	GLN
1	C	323	ASN
1	C	359	GLN
1	C	389	GLN
1	C	468	GLN
1	C	472	ASN
1	C	525	HIS
1	C	542	HIS
1	C	598	ASN
1	C	615	GLN
1	C	692	HIS
1	D	94	HIS
1	D	121	HIS
1	D	180	GLN
1	D	232	GLN
1	D	258	HIS
1	D	279	ASN
1	D	294	ASN
1	D	334	ASN
1	D	389	GLN
1	D	468	GLN
1	D	472	ASN
1	D	525	HIS
1	D	542	HIS
1	D	598	ASN
1	D	615	GLN
1	D	638	HIS
1	D	692	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

47 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	B	42	-	4,4,4	0.24	0	6,6,6	0.21	0
2	SO4	A	26	-	4,4,4	0.26	0	6,6,6	0.15	0
2	SO4	D	39	-	4,4,4	0.21	0	6,6,6	0.12	0
2	SO4	B	23	-	4,4,4	0.25	0	6,6,6	0.25	0
2	SO4	A	46	-	4,4,4	0.24	0	6,6,6	0.12	0
2	SO4	B	35	-	4,4,4	0.25	0	6,6,6	0.16	0
2	SO4	A	22	-	4,4,4	0.29	0	6,6,6	0.20	0
2	SO4	A	3	-	4,4,4	0.23	0	6,6,6	0.36	0
2	SO4	A	15	-	4,4,4	0.25	0	6,6,6	0.36	0
2	SO4	C	19	-	4,4,4	0.29	0	6,6,6	0.42	0
2	SO4	D	5	-	4,4,4	0.23	0	6,6,6	0.31	0
2	SO4	B	34	-	4,4,4	0.24	0	6,6,6	0.16	0
2	SO4	C	6	-	4,4,4	0.26	0	6,6,6	0.25	0
2	SO4	C	31	-	4,4,4	0.25	0	6,6,6	0.45	0
2	SO4	B	32	-	4,4,4	0.27	0	6,6,6	0.24	0
2	SO4	C	18	-	4,4,4	0.28	0	6,6,6	0.23	0
2	SO4	D	10	-	4,4,4	0.26	0	6,6,6	0.26	0
2	SO4	A	41	-	4,4,4	0.26	0	6,6,6	0.32	0
2	SO4	A	24	-	4,4,4	0.27	0	6,6,6	0.29	0
2	SO4	B	25	-	4,4,4	0.24	0	6,6,6	0.22	0
2	SO4	A	43	-	4,4,4	0.26	0	6,6,6	0.26	0
2	SO4	C	28	-	4,4,4	0.21	0	6,6,6	0.24	0
2	SO4	B	8	-	4,4,4	0.26	0	6,6,6	0.28	0
2	SO4	D	14	-	4,4,4	0.22	0	6,6,6	0.26	0
2	SO4	D	40	-	4,4,4	0.24	0	6,6,6	0.23	0
2	SO4	A	16	-	4,4,4	0.23	0	6,6,6	0.21	0
3	LDA	D	1	-	13,15,15	2.50	2 (15%)	14,17,17	0.66	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SO4	A	17	-	4,4,4	0.25	0	6,6,6	0.19	0
2	SO4	B	37	-	4,4,4	0.24	0	6,6,6	0.14	0
2	SO4	A	11	-	4,4,4	0.23	0	6,6,6	0.42	0
2	SO4	A	29	-	4,4,4	0.26	0	6,6,6	0.16	0
2	SO4	C	4	-	4,4,4	0.24	0	6,6,6	0.35	0
2	SO4	B	44	-	4,4,4	0.26	0	6,6,6	0.16	0
2	SO4	D	30	-	4,4,4	0.26	0	6,6,6	0.06	0
2	SO4	D	13	-	4,4,4	0.23	0	6,6,6	0.20	0
2	SO4	B	38	-	4,4,4	0.30	0	6,6,6	0.31	0
2	SO4	A	45	-	4,4,4	0.26	0	6,6,6	0.07	0
2	SO4	C	33	-	4,4,4	0.25	0	6,6,6	0.27	0
2	SO4	A	27	-	4,4,4	0.31	0	6,6,6	0.15	0
2	SO4	B	21	-	4,4,4	0.32	0	6,6,6	0.23	0
2	SO4	C	2	-	4,4,4	0.24	0	6,6,6	0.21	0
2	SO4	D	9	-	4,4,4	0.28	0	6,6,6	0.38	0
2	SO4	A	12	-	4,4,4	0.22	0	6,6,6	0.19	0
2	SO4	B	20	-	4,4,4	0.25	0	6,6,6	0.15	0
2	SO4	C	1	-	4,4,4	0.21	0	6,6,6	0.21	0
2	SO4	D	7	-	4,4,4	0.24	0	6,6,6	0.23	0
2	SO4	B	36	-	4,4,4	0.22	0	6,6,6	0.35	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	LDA	D	1	-	-	8/13/13/13	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1	LDA	O1-N1	-6.77	1.25	1.42
3	D	1	LDA	C1-N1	-5.93	1.45	1.51

There are no bond angle outliers.

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	1	LDA	C2-C1-N1-O1

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Mol	Chain	Res	Type	Atoms
3	D	1	LDA	C2-C1-N1-CM1
3	D	1	LDA	C9-C10-C11-C12
3	D	1	LDA	C7-C8-C9-C10
3	D	1	LDA	C3-C4-C5-C6
3	D	1	LDA	C4-C5-C6-C7
3	D	1	LDA	C1-C2-C3-C4
3	D	1	LDA	C2-C1-N1-CM2

There are no ring outliers.

18 monomers are involved in 40 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	39	SO4	2	0
2	B	23	SO4	1	0
2	B	35	SO4	1	0
2	A	3	SO4	1	0
2	A	15	SO4	2	0
2	C	19	SO4	1	0
2	D	5	SO4	1	0
2	C	31	SO4	3	0
2	C	18	SO4	1	0
2	A	41	SO4	5	0
2	B	25	SO4	1	0
3	D	1	LDA	7	0
2	A	17	SO4	4	0
2	A	11	SO4	2	0
2	C	4	SO4	1	0
2	B	38	SO4	5	0
2	D	9	SO4	1	0
2	D	7	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	598/625 (95%)	0.16	18 (3%)	52 31	30, 74, 136, 217	0
1	B	621/625 (99%)	-0.03	7 (1%)	78 59	24, 68, 118, 219	0
1	C	623/625 (99%)	-0.16	7 (1%)	78 59	14, 60, 112, 317	0
1	D	602/625 (96%)	-0.07	10 (1%)	69 48	24, 64, 129, 183	0
All	All	2444/2500 (97%)	-0.03	42 (1%)	69 48	14, 66, 125, 317	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	91	GLY	4.3
1	B	691	THR	3.9
1	A	164	SER	3.8
1	A	157	ALA	3.4
1	B	692	HIS	3.4
1	C	291	ILE	3.2
1	A	156	ASP	3.0
1	D	203	GLY	2.9
1	A	147	SER	2.9
1	A	326	GLN	2.9
1	A	151	GLN	2.8
1	D	130	PHE	2.7
1	D	437	TYR	2.7
1	A	329	ILE	2.6
1	C	92	GLN	2.5
1	C	125	ASP	2.5
1	D	691	THR	2.5
1	A	131	GLY	2.5
1	C	160	SER	2.4
1	B	291	ILE	2.3
1	B	567	TYR	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	89	ASP	2.3
1	A	687	THR	2.3
1	A	325	LEU	2.3
1	C	346	ASP	2.3
1	A	691	THR	2.3
1	A	316	PHE	2.3
1	A	165	ILE	2.3
1	B	125	ASP	2.2
1	A	631	GLY	2.2
1	D	692	HIS	2.2
1	A	638	HIS	2.2
1	B	184	LYS	2.1
1	B	383	ASP	2.1
1	A	533	ARG	2.1
1	D	326	GLN	2.1
1	A	427	TYR	2.1
1	D	285	PRO	2.1
1	A	321	LEU	2.1
1	C	273	LYS	2.0
1	D	146	ALA	2.0
1	D	346	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	A	43	5/5	0.60	0.11	129,129,129,129	0
2	SO4	A	46	5/5	0.67	0.09	151,151,151,151	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SO4	B	20	5/5	0.72	0.12	119,119,119,119	0
2	SO4	B	37	5/5	0.76	0.10	123,123,123,123	0
2	SO4	B	44	5/5	0.77	0.09	118,118,118,118	0
2	SO4	D	39	5/5	0.78	0.09	123,123,123,123	0
2	SO4	C	31	5/5	0.79	0.14	81,81,81,81	0
2	SO4	A	29	5/5	0.79	0.12	112,112,112,112	0
2	SO4	A	12	5/5	0.83	0.10	108,108,108,108	0
2	SO4	B	32	5/5	0.83	0.12	104,104,104,104	0
2	SO4	C	33	5/5	0.83	0.10	101,101,101,101	0
2	SO4	A	11	5/5	0.83	0.12	90,90,90,90	0
2	SO4	B	38	5/5	0.84	0.09	91,91,91,91	0
2	SO4	A	45	5/5	0.85	0.12	115,115,115,115	0
2	SO4	B	36	5/5	0.85	0.10	94,94,94,94	0
2	SO4	D	13	5/5	0.86	0.09	102,102,102,102	0
2	SO4	B	25	5/5	0.87	0.09	100,100,100,100	0
2	SO4	B	21	5/5	0.87	0.12	87,87,87,87	0
2	SO4	A	16	5/5	0.88	0.09	108,108,108,108	0
2	SO4	C	2	5/5	0.88	0.10	106,106,106,106	0
2	SO4	A	41	5/5	0.90	0.12	91,91,91,91	0
2	SO4	C	28	5/5	0.90	0.11	120,120,120,120	0
2	SO4	D	30	5/5	0.90	0.11	112,112,112,112	0
2	SO4	A	26	5/5	0.90	0.10	101,101,101,101	0
2	SO4	D	7	5/5	0.91	0.09	81,81,81,81	0
2	SO4	B	42	5/5	0.91	0.08	94,94,94,94	0
2	SO4	A	22	5/5	0.91	0.09	77,77,77,77	0
2	SO4	D	5	5/5	0.91	0.08	85,85,85,85	0
2	SO4	D	40	5/5	0.91	0.08	104,104,104,104	0
2	SO4	C	1	5/5	0.92	0.08	82,82,82,82	0
2	SO4	D	14	5/5	0.92	0.10	105,105,105,105	0
2	SO4	B	23	5/5	0.92	0.07	95,95,95,95	0
2	SO4	C	4	5/5	0.92	0.08	79,79,79,79	0
2	SO4	A	27	5/5	0.92	0.15	101,101,101,101	0
2	SO4	B	35	5/5	0.93	0.08	102,102,102,102	0
2	SO4	C	18	5/5	0.93	0.07	75,75,75,75	0
2	SO4	A	24	5/5	0.93	0.08	79,79,79,79	0
2	SO4	D	9	5/5	0.94	0.09	75,75,75,75	0
2	SO4	A	17	5/5	0.95	0.06	88,88,88,88	0
2	SO4	B	8	5/5	0.95	0.09	70,70,70,70	0
2	SO4	B	34	5/5	0.96	0.07	69,69,69,69	0
2	SO4	C	19	5/5	0.96	0.06	58,58,58,58	0
2	SO4	A	3	5/5	0.96	0.06	79,79,79,79	0
2	SO4	C	6	5/5	0.96	0.08	77,77,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SO4	D	10	5/5	0.96	0.06	53,53,53,53	0
3	LDA	D	1	16/16	0.97	0.10	49,49,49,49	0
2	SO4	A	15	5/5	0.99	0.04	50,50,50,50	0

6.5 Other polymers [i](#)

There are no such residues in this entry.