



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:53 PM UTC

PDB ID : 3I3Y / pdb_00003i3y
Title : Crystal structure of Ribokinase in Complex with D-Ribose from *Klebsiella pneumoniae*
Authors : Satyanarayana, L.; Burley, S.K.; Swaminathan, S.; New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on : 2009-07-01
Resolution : 2.15 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

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

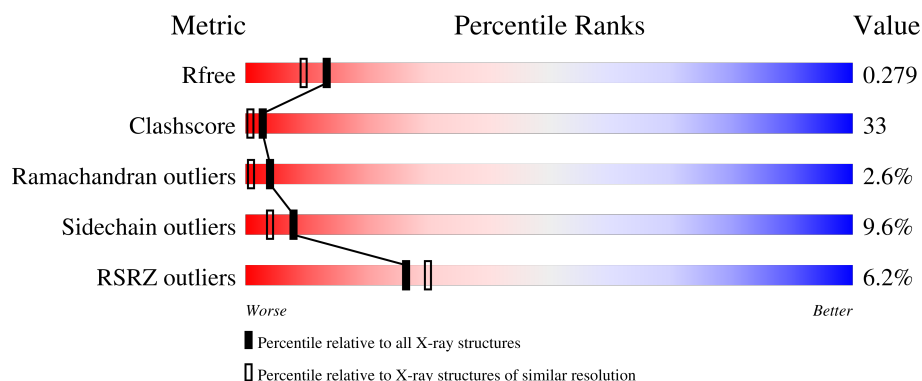
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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	2057 (2.16-2.16)
Clashscore	190562	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)
RSRZ outliers	180081	2059 (2.16-2.16)

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	299	
1	B	299	
1	C	299	
1	D	299	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8707 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 Carbohydrate kinase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	285	Total	C	N	O	S	Se	0	0	0
			2121	1333	372	408	3	5			
1	B	282	Total	C	N	O	S	Se	0	0	0
			2099	1322	368	401	3	5			
1	C	285	Total	C	N	O	S	Se	0	0	0
			2121	1333	372	408	3	5			
1	D	285	Total	C	N	O	S	Se	0	0	0
			2121	1333	372	408	3	5			

There are 44 discrepancies between the modelled and reference sequences:

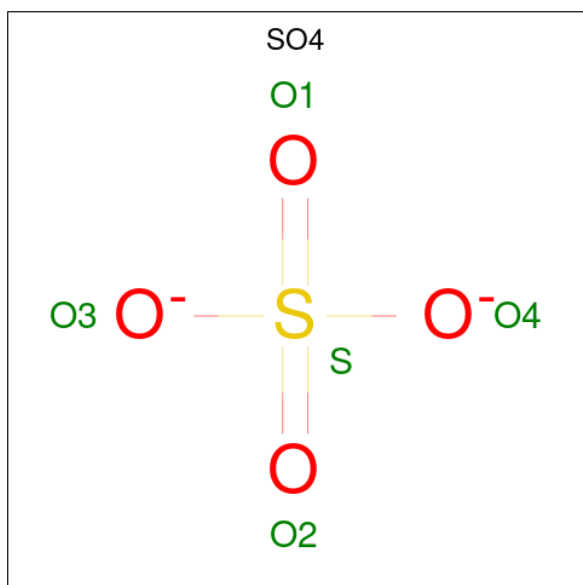
Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	MSE	-	expression tag	UNP A6T989
A	-2	SER	-	expression tag	UNP A6T989
A	-1	LEU	-	expression tag	UNP A6T989
A	290	GLU	-	expression tag	UNP A6T989
A	291	GLY	-	expression tag	UNP A6T989
A	292	HIS	-	expression tag	UNP A6T989
A	293	HIS	-	expression tag	UNP A6T989
A	294	HIS	-	expression tag	UNP A6T989
A	295	HIS	-	expression tag	UNP A6T989
A	296	HIS	-	expression tag	UNP A6T989
A	297	HIS	-	expression tag	UNP A6T989
B	-3	MSE	-	expression tag	UNP A6T989
B	-2	SER	-	expression tag	UNP A6T989
B	-1	LEU	-	expression tag	UNP A6T989
B	290	GLU	-	expression tag	UNP A6T989
B	291	GLY	-	expression tag	UNP A6T989
B	292	HIS	-	expression tag	UNP A6T989
B	293	HIS	-	expression tag	UNP A6T989
B	294	HIS	-	expression tag	UNP A6T989
B	295	HIS	-	expression tag	UNP A6T989
B	296	HIS	-	expression tag	UNP A6T989

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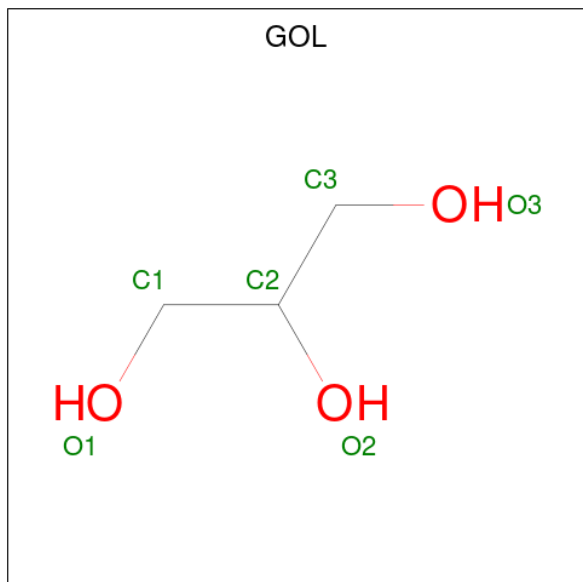
Chain	Residue	Modelled	Actual	Comment	Reference
B	297	HIS	-	expression tag	UNP A6T989
C	-3	MSE	-	expression tag	UNP A6T989
C	-2	SER	-	expression tag	UNP A6T989
C	-1	LEU	-	expression tag	UNP A6T989
C	290	GLU	-	expression tag	UNP A6T989
C	291	GLY	-	expression tag	UNP A6T989
C	292	HIS	-	expression tag	UNP A6T989
C	293	HIS	-	expression tag	UNP A6T989
C	294	HIS	-	expression tag	UNP A6T989
C	295	HIS	-	expression tag	UNP A6T989
C	296	HIS	-	expression tag	UNP A6T989
C	297	HIS	-	expression tag	UNP A6T989
D	-3	MSE	-	expression tag	UNP A6T989
D	-2	SER	-	expression tag	UNP A6T989
D	-1	LEU	-	expression tag	UNP A6T989
D	290	GLU	-	expression tag	UNP A6T989
D	291	GLY	-	expression tag	UNP A6T989
D	292	HIS	-	expression tag	UNP A6T989
D	293	HIS	-	expression tag	UNP A6T989
D	294	HIS	-	expression tag	UNP A6T989
D	295	HIS	-	expression tag	UNP A6T989
D	296	HIS	-	expression tag	UNP A6T989
D	297	HIS	-	expression tag	UNP A6T989

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



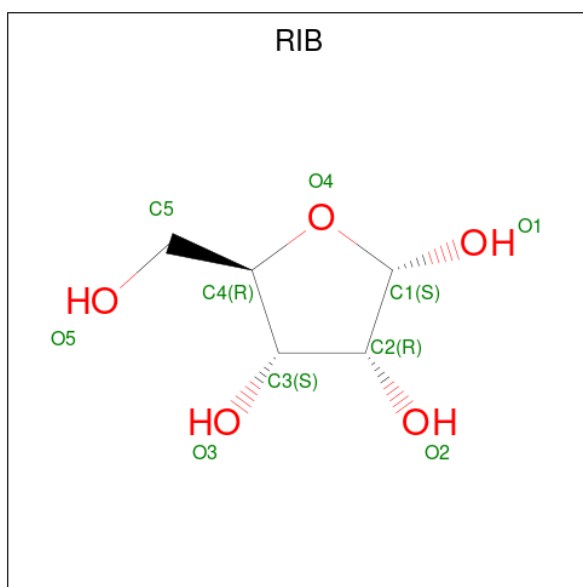
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	C	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is alpha-D-ribofuranose (CCD ID: RIB) (formula: $C_5H_{10}O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	D	1	Total	C	O	0	0
			10	5	5		

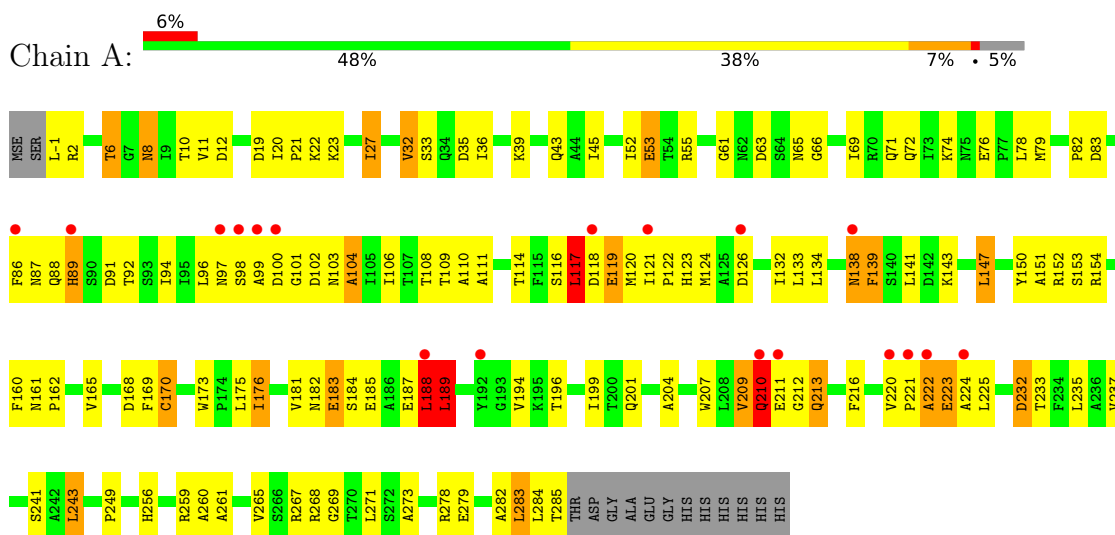
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	60	Total	O	0	0
			60	60		
5	B	41	Total	O	0	0
			41	41		
5	C	60	Total	O	0	0
			60	60		
5	D	38	Total	O	0	0
			38	38		

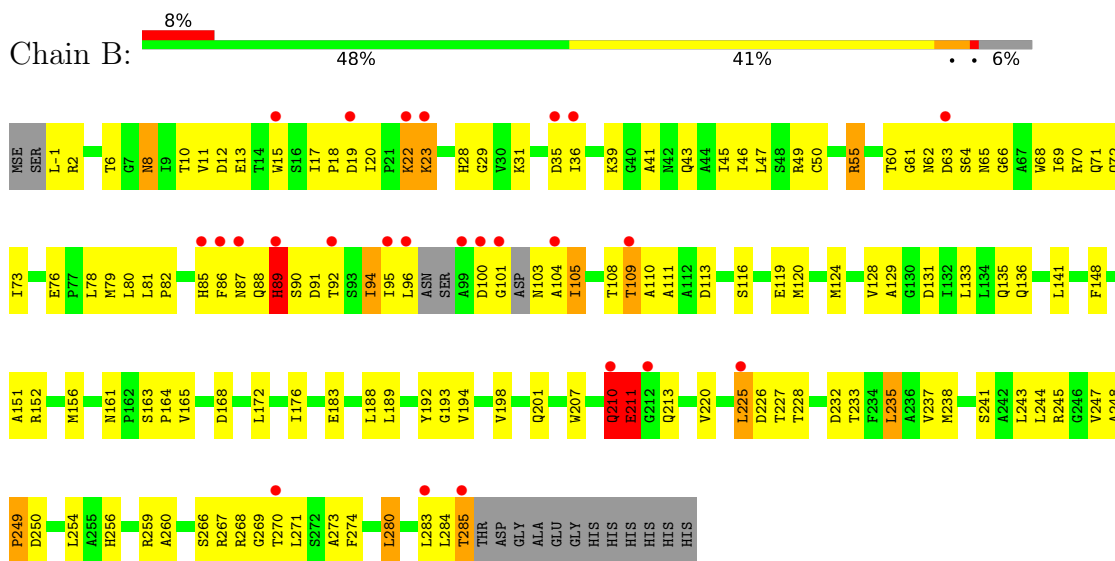
3 Residue-property plots

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: Carbohydrate kinase

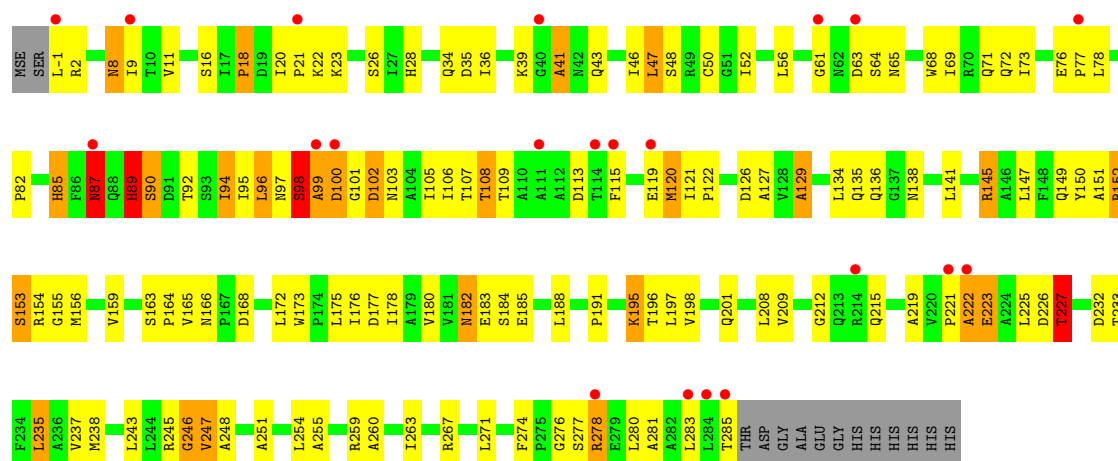


• Molecule 1: Carbohydrate kinase



• Molecule 1: Carbohydrate kinase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	54.49Å 105.90Å 121.15Å 90.00° 99.45° 90.00°	Depositor
Resolution (Å)	34.97 – 2.15 34.97 – 2.15	Depositor EDS
% Data completeness (in resolution range)	91.3 (34.97-2.15) 88.3 (34.97-2.15)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.50 (at 2.05Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.244 , 0.276 0.251 , 0.279	Depositor DCC
R_{free} test set	4236 reflections (2.55%)	wwPDB-VP
Wilson B-factor (Å ²)	33.6	Xtriage
Anisotropy	0.350	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 37.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	8707	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.02% 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: GOL, SO4, RIB

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	0.49	0/2155	1.10	17/2931 (0.6%)
1	B	0.47	0/2131	0.94	4/2895 (0.1%)
1	C	0.46	0/2155	1.03	12/2931 (0.4%)
1	D	0.46	0/2155	1.03	8/2931 (0.3%)
All	All	0.47	0/8596	1.03	41/11688 (0.4%)

There are no bond length outliers.

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	225	LEU	N-CA-C	-11.09	99.26	113.12
1	C	64	SER	N-CA-C	-9.05	100.82	112.23
1	D	176	ILE	N-CA-C	8.85	120.56	108.17
1	A	89	HIS	N-CA-C	7.87	121.71	110.14
1	A	169	PHE	N-CA-C	-7.51	103.85	112.87
1	A	32	VAL	N-CA-C	7.24	117.84	110.82
1	D	152	ARG	N-CA-C	-7.12	100.46	110.50
1	D	41	ALA	N-CA-C	-7.09	103.48	111.14
1	A	102	ASP	N-CA-C	6.74	119.26	110.43
1	D	156	MSE	N-CA-C	6.60	119.80	110.23
1	C	183	GLU	N-CA-C	-6.27	104.52	111.36
1	A	220	VAL	N-CA-C	-6.17	101.95	107.56
1	A	117	LEU	N-CA-C	-6.14	100.21	109.60
1	A	22	LYS	N-CA-C	-6.09	102.68	110.53
1	C	176	ILE	N-CA-C	6.08	117.77	108.71
1	B	176	ILE	N-CA-C	6.05	117.30	108.53
1	C	88	GLN	N-CA-C	-6.03	99.79	108.60
1	C	65	ASN	N-CA-C	-5.95	104.87	111.36
1	D	151	ALA	N-CA-C	-5.88	104.56	110.97
1	A	176	ILE	N-CA-C	5.85	116.36	108.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	233	THR	N-CA-C	-5.65	105.20	111.36
1	B	105	ILE	N-CA-C	5.65	116.61	108.48
1	C	20	ILE	CA-C-N	5.65	125.65	119.89
1	C	20	ILE	C-N-CA	5.65	125.65	119.89
1	D	212	GLY	N-CA-C	-5.64	107.96	115.40
1	D	120	MSE	N-CA-C	5.58	118.44	111.24
1	C	103	ASN	N-CA-C	5.55	117.70	110.43
1	D	227	THR	N-CA-C	5.50	119.09	112.38
1	A	161	ASN	CA-C-N	5.46	126.66	119.84
1	A	161	ASN	C-N-CA	5.46	126.66	119.84
1	C	161	ASN	CA-C-N	5.39	126.58	119.84
1	C	161	ASN	C-N-CA	5.39	126.58	119.84
1	A	27	ILE	N-CA-C	5.37	116.58	108.96
1	A	165	VAL	N-CA-C	5.31	115.90	108.89
1	A	213	GLN	N-CA-C	5.30	117.77	110.35
1	A	104	ALA	N-CA-C	-5.20	101.81	110.17
1	C	53	GLU	N-CA-C	-5.16	102.27	109.96
1	B	89	HIS	N-CA-C	5.16	117.57	110.35
1	A	209	VAL	N-CA-C	5.15	117.25	108.86
1	C	120	MSE	N-CA-C	5.12	119.40	111.56
1	B	210	GLN	CB-CA-C	-5.12	109.00	116.53

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	2121	0	2122	166	0
1	B	2099	0	2105	154	0
1	C	2121	0	2122	106	0
1	D	2121	0	2122	165	0
2	B	15	0	0	0	0
2	C	10	0	0	0	0
2	D	5	0	0	0	0
3	C	6	0	8	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	10	0	0	0	0
5	A	60	0	0	12	0
5	B	41	0	0	8	0
5	C	60	0	0	2	0
5	D	38	0	0	6	0
All	All	8707	0	8479	555	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 33.

All (555) 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:61:GLY:H	1:A:89:HIS:CD2	1.66	1.13
1:A:10:THR:HG23	1:A:91:ASP:HA	1.34	1.10
1:D:195:LYS:H	1:D:195:LYS:HD2	0.95	1.09
1:A:181:VAL:HG13	1:A:185:GLU:HB2	1.42	1.01
1:D:259:ARG:HB3	1:D:283:LEU:HD11	1.45	0.98
1:A:61:GLY:N	1:A:89:HIS:HD2	1.63	0.95
1:C:6:THR:HG21	1:C:147:LEU:HD13	1.43	0.95
1:A:6:THR:HG23	1:A:120:MSE:HE1	1.49	0.93
1:A:61:GLY:H	1:A:89:HIS:HD2	0.93	0.93
1:D:195:LYS:HD2	1:D:195:LYS:N	1.81	0.93
1:B:70:ARG:HD3	1:B:85:HIS:NE2	1.86	0.89
1:B:63:ASP:H	1:B:89:HIS:HE1	1.22	0.87
1:A:188:LEU:O	1:A:189:LEU:HB2	1.71	0.86
1:A:45:ILE:HD13	1:A:271:LEU:HD11	1.56	0.86
1:B:228:THR:HG21	1:B:270:THR:HG22	1.57	0.86
1:A:19:ASP:HA	1:A:97:ASN:HD22	1.40	0.86
1:C:20:ILE:O	1:C:20:ILE:HD12	1.78	0.83
1:A:100:ASP:HB3	1:C:23:LYS:NZ	1.93	0.83
1:D:43:GLN:NE2	1:D:136:GLN:HE21	1.77	0.83
1:B:63:ASP:H	1:B:89:HIS:CE1	1.97	0.83
1:D:195:LYS:H	1:D:195:LYS:CD	1.80	0.83
1:B:63:ASP:HB3	1:B:89:HIS:CE1	2.13	0.82
1:C:79:MSE:HE2	1:C:81:LEU:HD21	1.59	0.82
1:C:166:ASN:HD21	1:C:168:ASP:HB2	1.43	0.82
1:A:20:ILE:HG13	1:A:97:ASN:HD21	1.46	0.80
1:D:177:ASP:HA	1:D:195:LYS:HD3	1.62	0.80
1:A:209:VAL:O	1:A:210:GLN:HB2	1.79	0.80
1:D:141:LEU:HD11	1:D:172:LEU:HD11	1.65	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:66:GLY:CA	1:A:89:HIS:NE2	2.47	0.78
1:D:278:ARG:HG2	5:D:325:HOH:O	1.83	0.78
1:B:8:ASN:HD22	1:B:8:ASN:H	1.31	0.77
1:C:-1:LEU:HD12	1:C:2:ARG:N	2.00	0.77
1:C:152:ARG:CZ	1:C:175:LEU:HA	2.14	0.77
1:B:63:ASP:N	1:B:89:HIS:HE1	1.82	0.76
1:D:11:VAL:HG21	1:D:65:ASN:HB3	1.65	0.76
1:A:194:VAL:O	1:A:210:GLN:HG2	1.86	0.76
1:C:6:THR:HG23	1:C:139:PHE:HE2	1.49	0.76
1:D:145:ARG:CB	1:D:145:ARG:HH11	2.00	0.75
1:A:117:LEU:C	1:A:119:GLU:H	1.94	0.75
1:D:16:SER:HA	1:D:97:ASN:HB3	1.69	0.74
1:B:79:MSE:HE2	1:B:81:LEU:HD21	1.69	0.74
1:B:220:VAL:HG21	1:B:259:ARG:HG3	1.69	0.74
1:B:65:ASN:HB2	1:B:89:HIS:CD2	2.23	0.73
1:C:152:ARG:NH1	1:C:175:LEU:HA	2.03	0.73
1:A:-1:LEU:N	5:A:349:HOH:O	2.20	0.73
1:D:43:GLN:HE22	1:D:136:GLN:HE21	1.37	0.73
1:B:39:LYS:HE2	1:B:232:ASP:OD1	1.86	0.73
1:B:23:LYS:HD3	1:D:101:GLY:HA3	1.71	0.73
1:B:141:LEU:HD11	1:B:172:LEU:HD11	1.71	0.72
1:B:68:TRP:O	1:B:72:GLN:HG2	1.89	0.72
1:C:105:ILE:C	1:C:105:ILE:HD12	2.14	0.72
1:C:225:LEU:HD21	1:C:266:SER:C	2.14	0.72
1:A:183:GLU:CD	1:A:201:GLN:HG2	2.15	0.72
1:C:68:TRP:HE1	1:C:72:GLN:NE2	1.88	0.72
1:B:124:MSE:HE3	1:B:156:MSE:HE1	1.72	0.71
1:B:63:ASP:CG	1:B:64:SER:H	1.99	0.71
1:B:63:ASP:HB3	1:B:89:HIS:NE2	2.06	0.71
1:B:28:HIS:CE1	1:D:138:ASN:HD22	2.09	0.70
1:B:23:LYS:NZ	1:D:101:GLY:HA3	2.06	0.70
1:D:238:MSE:HG3	1:D:254:LEU:HD12	1.72	0.70
1:A:65:ASN:CB	1:A:89:HIS:HE1	2.04	0.70
1:A:282:ALA:O	1:A:285:THR:HG22	1.92	0.70
1:B:210:GLN:HB2	5:B:307:HOH:O	1.91	0.70
1:D:71:GLN:NE2	1:D:72:GLN:HE21	1.90	0.70
1:A:117:LEU:H	1:A:143:LYS:HZ2	1.37	0.70
1:D:141:LEU:HD22	1:D:168:ASP:HB3	1.74	0.69
1:A:224:ALA:HA	1:A:265:VAL:HG12	1.74	0.69
1:D:82:PRO:HD3	1:D:115:PHE:CZ	2.26	0.69
1:C:68:TRP:HE1	1:C:72:GLN:HE22	1.40	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:283:LEU:C	1:A:283:LEU:HD12	2.18	0.69
1:B:285:THR:HG22	5:B:328:HOH:O	1.92	0.69
1:B:95:ILE:HG23	1:B:104:ALA:HB3	1.75	0.68
1:B:70:ARG:HD3	1:B:85:HIS:CE1	2.28	0.68
1:A:196:THR:HG21	1:A:249:PRO:HG2	1.75	0.68
1:A:121:ILE:HD12	1:A:124:MSE:HE3	1.74	0.68
1:D:134:LEU:HA	1:D:159:VAL:HG13	1.74	0.68
1:C:49:ARG:HD2	1:C:76:GLU:OE1	1.93	0.68
1:A:241:SER:OG	1:A:256:HIS:HD2	1.76	0.67
1:B:11:VAL:HG11	1:B:65:ASN:CG	2.19	0.67
1:A:100:ASP:HB3	1:C:23:LYS:HZ2	1.58	0.67
1:A:36:ILE:HD11	1:A:72:GLN:HB2	1.74	0.67
1:D:109:THR:HG23	1:D:113:ASP:OD2	1.95	0.66
1:B:63:ASP:CG	1:B:64:SER:N	2.52	0.66
1:D:121:ILE:HG13	1:D:122:PRO:CD	2.26	0.66
1:B:94:ILE:N	1:B:94:ILE:HD12	2.11	0.66
1:B:60:THR:HG23	1:B:85:HIS:HD1	1.60	0.65
1:A:66:GLY:N	1:A:89:HIS:NE2	2.43	0.65
1:A:117:LEU:HD22	1:A:143:LYS:NZ	2.12	0.65
1:A:210:GLN:O	1:A:211:GLU:HB2	1.97	0.65
1:C:17:ILE:O	1:C:98:SER:HA	1.97	0.65
1:D:61:GLY:HA3	1:D:89:HIS:O	1.97	0.65
1:D:99:ALA:O	1:D:100:ASP:HB3	1.96	0.65
1:B:100:ASP:HB3	1:D:23:LYS:NZ	2.12	0.65
1:B:247:VAL:O	1:B:248:ALA:HB3	1.96	0.64
1:B:19:ASP:HB3	1:B:100:ASP:OD1	1.97	0.64
1:C:154:ARG:HH11	1:C:154:ARG:HG2	1.62	0.64
1:B:70:ARG:CD	1:B:85:HIS:NE2	2.60	0.64
1:B:20:ILE:HD13	1:D:21:PRO:O	1.96	0.64
1:A:108:THR:HG23	1:C:15:TRP:CZ3	2.33	0.64
1:B:109:THR:HG22	1:D:28:HIS:HE1	1.63	0.64
1:A:23:LYS:NZ	1:C:100:ASP:HB2	2.13	0.63
1:A:43:GLN:HG3	1:A:232:ASP:HB2	1.80	0.63
1:A:86:PHE:C	1:A:87:ASN:OD1	2.41	0.63
1:C:225:LEU:H	1:C:225:LEU:CD2	2.12	0.63
1:A:100:ASP:CB	1:C:23:LYS:NZ	2.62	0.63
1:A:187:GLU:O	1:A:188:LEU:HG	1.98	0.63
1:C:6:THR:HG22	1:C:6:THR:O	1.97	0.63
1:C:43:GLN:HE21	1:C:134:LEU:HD21	1.63	0.63
1:D:39:LYS:HB3	1:D:136:GLN:HG2	1.81	0.63
1:B:23:LYS:HZ2	1:D:101:GLY:HA3	1.63	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:28:HIS:HE1	1:D:138:ASN:HD22	1.46	0.62
1:B:63:ASP:CA	1:B:89:HIS:HE1	2.11	0.62
1:A:139:PHE:HB2	5:A:314:HOH:O	1.98	0.62
1:C:115:PHE:HB3	1:C:120:MSE:HE3	1.82	0.62
1:A:61:GLY:N	1:A:89:HIS:CD2	2.47	0.62
1:A:6:THR:HG23	1:A:120:MSE:CE	2.27	0.62
1:B:36:ILE:HD11	1:B:72:GLN:HB2	1.81	0.62
1:B:109:THR:O	1:B:111:ALA:N	2.31	0.61
1:B:165:VAL:HG21	1:B:188:LEU:HD23	1.82	0.61
1:B:60:THR:HG23	1:B:85:HIS:ND1	2.14	0.61
1:D:115:PHE:HB3	1:D:120:MSE:HE3	1.80	0.61
1:D:152:ARG:O	1:D:153:SER:CB	2.46	0.61
1:D:237:VAL:HG21	1:D:260:ALA:CB	2.29	0.61
1:B:124:MSE:CE	1:B:156:MSE:SE	2.99	0.61
1:D:247:VAL:HG22	1:D:248:ALA:H	1.64	0.61
1:D:152:ARG:O	1:D:153:SER:HB3	1.98	0.61
1:A:104:ALA:HB1	1:C:21:PRO:HB2	1.83	0.61
1:D:121:ILE:HG13	1:D:122:PRO:N	2.15	0.61
1:A:121:ILE:HD11	1:A:150:TYR:CE1	2.36	0.61
1:B:17:ILE:HB	1:B:18:PRO:HD2	1.81	0.61
1:B:66:GLY:H	1:B:89:HIS:CE1	2.18	0.61
1:B:225:LEU:HD21	1:B:266:SER:O	2.01	0.60
1:D:8:ASN:HD22	1:D:8:ASN:H	1.47	0.60
1:A:138:ASN:O	1:A:139:PHE:CG	2.54	0.60
1:A:66:GLY:HA2	1:A:89:HIS:NE2	2.15	0.60
1:B:8:ASN:H	1:B:8:ASN:ND2	1.98	0.60
1:B:104:ALA:C	1:B:105:ILE:HD12	2.26	0.60
1:D:36:ILE:CD1	1:D:72:GLN:HG3	2.31	0.60
1:A:117:LEU:O	1:A:119:GLU:N	2.32	0.60
1:C:68:TRP:NE1	1:C:72:GLN:NE2	2.50	0.60
1:A:65:ASN:HB2	1:A:89:HIS:HE1	1.65	0.59
1:D:43:GLN:NE2	1:D:136:GLN:NE2	2.50	0.59
1:B:105:ILE:HD12	1:B:105:ILE:N	2.18	0.59
1:B:241:SER:OG	1:B:256:HIS:HD2	1.85	0.59
1:B:244:LEU:HD12	1:B:284:LEU:HD13	1.83	0.59
1:B:100:ASP:C	1:D:23:LYS:HZ2	2.10	0.59
1:A:43:GLN:HG3	1:A:232:ASP:CB	2.32	0.59
1:C:141:LEU:HD22	1:C:168:ASP:HB3	1.84	0.59
1:B:17:ILE:HG22	1:B:29:GLY:HA3	1.84	0.59
1:A:12:ASP:OD1	1:A:92:THR:HG22	2.03	0.58
1:B:28:HIS:NE2	1:D:164:PRO:HG3	2.18	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:-1:LEU:CD1	1:C:131:ASP:HA	2.32	0.58
1:D:245:ARG:O	1:D:246:GLY:C	2.46	0.58
1:A:82:PRO:HB3	1:A:123:HIS:NE2	2.18	0.58
1:C:21:PRO:HG3	1:C:27:ILE:CD1	2.32	0.58
1:C:165:VAL:HG23	1:C:189:LEU:HD11	1.84	0.58
1:D:149:GLN:O	1:D:152:ARG:O	2.21	0.58
1:C:39:LYS:HB3	1:C:136:GLN:HG2	1.84	0.58
1:D:121:ILE:HG13	1:D:122:PRO:HD3	1.84	0.58
1:D:135:GLN:HE22	1:D:147:LEU:HD12	1.68	0.58
1:D:247:VAL:HG22	1:D:248:ALA:N	2.18	0.58
1:A:10:THR:HG22	1:A:11:VAL:N	2.17	0.58
1:B:201:GLN:HE21	1:B:207:TRP:HD1	1.52	0.58
1:D:87:ASN:N	1:D:87:ASN:HD22	2.01	0.58
1:A:10:THR:CG2	1:A:11:VAL:N	2.67	0.57
1:B:15:TRP:CE2	1:D:94:ILE:HD11	2.40	0.57
1:C:6:THR:HG22	1:C:135:GLN:HG2	1.85	0.57
1:A:100:ASP:CB	1:C:23:LYS:HZ3	2.17	0.57
1:D:9:ILE:HG21	1:D:69:ILE:HG21	1.86	0.57
1:C:235:LEU:HD12	1:C:235:LEU:O	2.04	0.57
1:A:222:ALA:O	1:A:223:GLU:HB2	2.05	0.57
1:B:109:THR:CG2	1:D:28:HIS:HE1	2.17	0.57
1:C:115:PHE:O	1:C:120:MSE:HE3	2.04	0.57
1:A:121:ILE:HD11	1:A:150:TYR:CZ	2.40	0.57
1:A:106:ILE:HD11	1:C:21:PRO:HG2	1.86	0.57
1:A:222:ALA:O	1:A:223:GLU:CB	2.53	0.57
1:A:2:ARG:HD2	5:A:308:HOH:O	2.04	0.56
1:A:20:ILE:HG13	1:A:97:ASN:ND2	2.18	0.56
1:B:141:LEU:HD11	1:B:172:LEU:CD1	2.35	0.56
1:C:87:ASN:HD22	1:C:87:ASN:H	1.53	0.56
1:D:2:ARG:HH11	1:D:2:ARG:HG2	1.70	0.56
1:D:43:GLN:O	1:D:47:LEU:HB2	2.05	0.56
1:D:36:ILE:HD11	1:D:72:GLN:HG3	1.87	0.56
1:A:173:TRP:CE3	1:A:176:ILE:HD12	2.40	0.56
1:B:8:ASN:HD22	1:B:8:ASN:N	1.94	0.56
1:B:211:GLU:H	1:B:211:GLU:CD	2.10	0.56
1:A:261:ALA:O	1:A:265:VAL:HG23	2.04	0.56
1:A:121:ILE:HD11	1:A:150:TYR:CD1	2.40	0.56
1:A:182:ASN:OD1	1:A:185:GLU:HG3	2.05	0.56
1:B:23:LYS:HD3	1:D:102:ASP:H	1.69	0.56
1:A:98:SER:O	1:A:99:ALA:C	2.49	0.56
1:B:95:ILE:HG22	1:B:104:ALA:O	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:180:VAL:HG21	1:C:235:LEU:HD13	1.88	0.56
1:B:65:ASN:O	1:B:69:ILE:HG13	2.06	0.56
1:C:8:ASN:H	1:C:8:ASN:HD22	1.53	0.56
1:A:237:VAL:HG21	1:A:260:ALA:CB	2.36	0.56
1:B:22:LYS:HB2	1:B:22:LYS:NZ	2.20	0.56
1:D:98:SER:HB2	1:D:100:ASP:H	1.71	0.55
1:D:141:LEU:HD11	1:D:172:LEU:CD1	2.35	0.55
1:A:181:VAL:HG12	1:A:182:ASN:O	2.06	0.55
1:D:99:ALA:O	1:D:100:ASP:CB	2.54	0.55
1:B:210:GLN:HE21	1:B:210:GLN:HA	1.72	0.55
1:D:105:ILE:HG22	1:D:106:ILE:N	2.22	0.55
1:D:165:VAL:HG21	1:D:188:LEU:HD23	1.89	0.55
1:D:255:ALA:O	1:D:259:ARG:HD3	2.07	0.55
1:A:116:SER:C	1:A:117:LEU:O	2.49	0.55
1:A:168:ASP:C	1:A:170:CYS:H	2.15	0.55
1:B:17:ILE:HD13	1:B:95:ILE:HD11	1.88	0.55
1:B:61:GLY:O	1:B:85:HIS:ND1	2.40	0.55
1:A:8:ASN:H	1:A:8:ASN:HD22	1.55	0.54
1:A:11:VAL:HG23	1:A:69:ILE:HD11	1.89	0.54
1:C:166:ASN:ND2	1:C:168:ASP:HB2	2.17	0.54
1:B:63:ASP:HB3	1:B:89:HIS:HE2	1.72	0.54
1:D:115:PHE:CG	1:D:120:MSE:HE3	2.42	0.54
1:D:127:ALA:O	1:D:154:ARG:NH2	2.41	0.54
1:B:63:ASP:CB	1:B:89:HIS:CE1	2.87	0.54
1:A:23:LYS:O	1:C:103:ASN:O	2.26	0.54
1:B:245:ARG:NH2	1:B:250:ASP:OD2	2.40	0.54
1:A:221:PRO:O	1:A:222:ALA:HB2	2.08	0.54
1:D:182:ASN:N	1:D:182:ASN:ND2	2.54	0.54
1:A:222:ALA:O	1:A:223:GLU:HG3	2.09	0.53
1:B:105:ILE:O	1:D:26:SER:HA	2.08	0.53
1:D:150:TYR:CZ	1:D:154:ARG:HD3	2.43	0.53
1:A:184:SER:O	1:A:187:GLU:O	2.26	0.53
1:B:226:ASP:HB3	1:B:267:ARG:O	2.08	0.53
1:D:152:ARG:HG2	1:D:152:ARG:HH11	1.72	0.53
1:A:188:LEU:O	1:A:189:LEU:CB	2.50	0.53
1:B:100:ASP:HB3	1:D:23:LYS:HZ2	1.72	0.53
1:B:136:GLN:HA	1:B:161:ASN:O	2.08	0.53
1:B:270:THR:OG1	1:B:271:LEU:N	2.42	0.53
1:D:227:THR:HG21	5:D:323:HOH:O	2.09	0.53
1:A:121:ILE:HG23	1:A:122:PRO:HD3	1.88	0.53
1:A:52:ILE:HD12	1:A:243:LEU:HD23	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:105:ILE:N	1:D:105:ILE:HD12	2.24	0.53
1:A:152:ARG:NH1	1:A:175:LEU:HA	2.23	0.52
1:A:2:ARG:HG2	1:A:53:GLU:HB3	1.91	0.52
1:A:117:LEU:C	1:A:119:GLU:N	2.62	0.52
1:A:87:ASN:OD1	1:A:87:ASN:N	2.43	0.52
1:A:168:ASP:C	1:A:170:CYS:N	2.61	0.52
1:B:66:GLY:N	1:B:89:HIS:ND1	2.57	0.52
1:C:6:THR:O	1:C:6:THR:CG2	2.56	0.52
1:A:6:THR:HG22	1:A:6:THR:O	2.08	0.52
1:B:20:ILE:HG21	1:D:20:ILE:HG22	1.92	0.52
1:A:65:ASN:O	1:A:69:ILE:HG13	2.10	0.52
1:B:65:ASN:HB2	1:B:89:HIS:CG	2.45	0.52
1:C:43:GLN:NE2	1:C:136:GLN:HE21	2.08	0.52
1:B:41:ALA:O	1:B:45:ILE:HG13	2.10	0.51
1:D:107:THR:HG22	1:D:108:THR:O	2.09	0.51
1:B:271:LEU:HA	1:B:274:PHE:CD2	2.45	0.51
1:D:182:ASN:ND2	1:D:185:GLU:OE1	2.44	0.51
1:A:20:ILE:HD11	5:A:313:HOH:O	2.11	0.51
1:A:39:LYS:HE3	5:A:355:HOH:O	2.10	0.51
1:A:141:LEU:HD22	1:A:168:ASP:HB3	1.91	0.51
1:B:23:LYS:CD	1:D:101:GLY:HA3	2.39	0.51
1:B:95:ILE:CG2	1:B:104:ALA:HB3	2.38	0.51
1:B:116:SER:HB2	1:B:119:GLU:OE2	2.10	0.51
1:C:6:THR:CG2	1:C:139:PHE:HE2	2.22	0.51
1:D:2:ARG:NH1	5:D:304:HOH:O	2.42	0.51
1:B:124:MSE:HE2	1:B:156:MSE:SE	2.60	0.51
1:C:244:LEU:CD1	1:C:284:LEU:HD13	2.41	0.51
1:A:117:LEU:CD2	1:A:143:LYS:HD3	2.41	0.51
1:B:101:GLY:O	1:B:103:ASN:ND2	2.44	0.51
1:B:201:GLN:NE2	1:B:207:TRP:CD1	2.79	0.51
1:C:166:ASN:HB3	1:C:169:PHE:CD1	2.46	0.51
1:C:177:ASP:HA	1:C:195:LYS:HZ2	1.76	0.51
1:B:109:THR:HG22	1:D:28:HIS:CE1	2.44	0.51
1:A:117:LEU:HA	5:A:336:HOH:O	2.10	0.51
1:B:95:ILE:HG23	1:B:95:ILE:O	2.10	0.51
1:D:2:ARG:NH2	1:D:126:ASP:O	2.44	0.51
1:D:82:PRO:HD3	1:D:115:PHE:HZ	1.73	0.51
1:D:182:ASN:ND2	1:D:185:GLU:CD	2.69	0.51
1:B:6:THR:OG1	1:B:135:GLN:HG2	2.10	0.50
1:D:87:ASN:ND2	5:D:318:HOH:O	2.44	0.50
1:D:173:TRP:CZ2	1:D:191:PRO:HG3	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:114:THR:HG22	1:A:114:THR:O	2.10	0.50
1:A:117:LEU:O	1:A:118:ASP:HB2	2.11	0.50
1:A:121:ILE:HB	5:A:336:HOH:O	2.10	0.50
1:C:79:MSE:CE	1:C:81:LEU:HD21	2.35	0.50
1:D:46:ILE:CD1	1:D:233:THR:HA	2.40	0.50
1:D:129:ALA:O	1:D:155:GLY:O	2.29	0.50
1:C:188:LEU:O	1:C:188:LEU:HD23	2.11	0.50
1:A:183:GLU:OE1	1:A:201:GLN:HG2	2.11	0.50
1:C:32:VAL:HG22	1:C:32:VAL:O	2.12	0.50
1:D:180:VAL:HG21	1:D:235:LEU:CD2	2.41	0.50
1:A:108:THR:HG22	1:C:29:GLY:O	2.12	0.50
1:A:279:GLU:HG3	5:B:329:HOH:O	2.12	0.49
1:A:133:LEU:HD22	1:A:151:ALA:HB2	1.93	0.49
1:B:192:TYR:O	1:B:194:VAL:N	2.42	0.49
1:C:154:ARG:HG2	1:C:154:ARG:NH1	2.27	0.49
1:D:9:ILE:HG21	1:D:69:ILE:CG2	2.41	0.49
1:A:20:ILE:N	1:A:97:ASN:ND2	2.60	0.49
1:A:268:ARG:HG2	1:A:269:GLY:N	2.26	0.49
1:D:87:ASN:N	1:D:87:ASN:ND2	2.58	0.49
1:D:276:GLY:O	1:D:277:SER:C	2.55	0.49
1:A:278:ARG:NH2	1:B:131:ASP:OD1	2.44	0.49
1:B:109:THR:OG1	1:B:113:ASP:CG	2.56	0.49
1:A:117:LEU:HD22	1:A:143:LYS:HZ3	1.78	0.49
1:A:121:ILE:CG2	1:A:122:PRO:HD3	2.42	0.49
1:B:10:THR:HB	1:B:91:ASP:HA	1.94	0.49
1:B:11:VAL:CG1	1:B:91:ASP:HB3	2.43	0.49
1:B:135:GLN:HB2	1:B:148:PHE:CZ	2.47	0.49
1:D:267:ARG:HG2	1:D:267:ARG:HH11	1.78	0.49
1:B:245:ARG:O	1:B:247:VAL:HG13	2.13	0.49
1:C:63:ASP:HB3	1:C:66:GLY:H	1.77	0.49
1:D:52:ILE:N	1:D:52:ILE:HD12	2.28	0.49
1:D:177:ASP:HA	1:D:195:LYS:CD	2.39	0.49
1:C:87:ASN:HD22	1:C:87:ASN:N	2.09	0.49
1:A:210:GLN:O	1:A:213:GLN:HG2	2.12	0.48
1:D:76:GLU:C	1:D:78:LEU:H	2.20	0.48
1:D:178:ILE:HG12	1:D:196:THR:HB	1.94	0.48
1:A:10:THR:CG2	1:A:91:ASP:HA	2.24	0.48
1:D:98:SER:O	1:D:99:ALA:CB	2.61	0.48
1:B:13:GLU:OE2	1:B:31:LYS:HE3	2.13	0.48
1:C:79:MSE:HE2	1:C:81:LEU:HD11	1.96	0.48
1:C:225:LEU:H	1:C:225:LEU:HD22	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:36:ILE:N	1:D:36:ILE:HD12	2.28	0.48
1:D:71:GLN:NE2	1:D:72:GLN:NE2	2.60	0.48
1:D:182:ASN:HD21	1:D:185:GLU:CD	2.21	0.48
1:A:20:ILE:N	1:A:97:ASN:HD21	2.10	0.48
1:B:-1:LEU:C	1:B:-1:LEU:HD23	2.38	0.48
1:B:141:LEU:HD22	1:B:168:ASP:HB3	1.95	0.48
1:D:141:LEU:CD1	1:D:172:LEU:HD11	2.42	0.48
1:D:182:ASN:ND2	1:D:182:ASN:H	2.11	0.48
1:B:225:LEU:HD23	1:B:225:LEU:H	1.76	0.48
1:D:9:ILE:HG12	1:D:41:ALA:HB2	1.96	0.48
1:B:267:ARG:HB2	1:B:273:ALA:HB1	1.95	0.48
1:D:9:ILE:HD11	1:D:56:LEU:HD21	1.96	0.48
1:D:50:CYS:SG	1:D:280:LEU:HD13	2.53	0.48
1:D:61:GLY:C	1:D:63:ASP:H	2.22	0.48
1:A:138:ASN:O	1:A:139:PHE:CD1	2.67	0.48
1:A:181:VAL:O	1:A:199:ILE:HA	2.14	0.48
1:C:248:ALA:O	1:C:249:PRO:C	2.55	0.48
1:D:183:GLU:OE1	1:D:201:GLN:HG2	2.14	0.48
1:A:117:LEU:HD22	1:A:143:LYS:HD3	1.96	0.48
1:A:121:ILE:HD11	1:A:150:TYR:CE2	2.49	0.48
1:B:201:GLN:HE21	1:B:207:TRP:CD1	2.30	0.48
1:B:226:ASP:OD2	1:B:269:GLY:N	2.44	0.48
1:A:10:THR:HG23	1:A:91:ASP:CA	2.23	0.47
1:A:117:LEU:CA	5:A:336:HOH:O	2.62	0.47
1:A:181:VAL:HG13	1:A:185:GLU:CB	2.29	0.47
1:B:46:ILE:HD13	1:B:233:THR:HA	1.96	0.47
1:C:152:ARG:NH1	1:C:175:LEU:HD23	2.28	0.47
1:D:180:VAL:HG11	1:D:235:LEU:HD23	1.96	0.47
1:A:117:LEU:HD22	1:A:143:LYS:CD	2.45	0.47
1:A:187:GLU:O	1:A:188:LEU:O	2.32	0.47
1:B:225:LEU:HD21	1:B:266:SER:C	2.38	0.47
1:C:105:ILE:HD12	1:C:106:ILE:N	2.29	0.47
1:C:121:ILE:HG12	1:C:122:PRO:HD3	1.95	0.47
1:D:36:ILE:HD11	1:D:68:TRP:CE2	2.49	0.47
1:A:65:ASN:HB2	1:A:89:HIS:CE1	2.47	0.47
1:B:225:LEU:HD12	1:B:268:ARG:NH2	2.29	0.47
1:A:33:SER:CB	1:A:268:ARG:NH2	2.78	0.47
1:A:11:VAL:O	1:A:91:ASP:HB2	2.14	0.47
1:B:22:LYS:NZ	1:B:22:LYS:CB	2.78	0.47
1:B:43:GLN:HE22	1:B:161:ASN:HD22	1.62	0.47
1:D:8:ASN:HD22	1:D:8:ASN:N	2.08	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:65:ASN:O	1:D:69:ILE:HG13	2.15	0.47
1:D:115:PHE:CB	1:D:120:MSE:HE3	2.42	0.47
1:A:235:LEU:C	1:A:235:LEU:HD23	2.40	0.47
1:B:94:ILE:N	1:B:94:ILE:CD1	2.76	0.47
1:C:152:ARG:NH2	1:C:174:PRO:O	2.47	0.47
1:D:165:VAL:HG22	1:D:166:ASN:N	2.30	0.47
1:A:65:ASN:HB3	1:A:89:HIS:HE1	1.77	0.47
1:A:188:LEU:HD12	1:A:188:LEU:C	2.40	0.47
1:A:204:ALA:O	1:A:216:PHE:HZ	1.98	0.47
1:B:213:GLN:HB2	5:B:307:HOH:O	2.14	0.47
1:D:175:LEU:N	1:D:175:LEU:HD22	2.30	0.47
1:B:20:ILE:CG2	1:D:20:ILE:CG2	2.93	0.46
1:B:238:MSE:HE3	1:B:249:PRO:HG3	1.96	0.46
1:A:55:ARG:HD3	1:A:79:MSE:HE2	1.97	0.46
1:C:-1:LEU:HD12	1:C:-1:LEU:C	2.40	0.46
1:D:134:LEU:HD13	1:D:159:VAL:HG13	1.98	0.46
1:B:63:ASP:N	1:B:89:HIS:CE1	2.68	0.46
1:C:135:GLN:HE22	1:C:144:THR:HA	1.79	0.46
1:D:9:ILE:HD11	1:D:56:LEU:CD2	2.45	0.46
1:D:119:GLU:HG2	5:D:305:HOH:O	2.16	0.46
1:D:183:GLU:H	1:D:183:GLU:HG2	1.55	0.46
1:A:188:LEU:O	1:A:188:LEU:HG	2.14	0.46
1:B:11:VAL:HG12	1:B:91:ASP:HB3	1.97	0.46
1:D:215:GLN:OE1	1:D:251:ALA:HB2	2.14	0.46
1:B:22:LYS:O	1:B:23:LYS:O	2.34	0.46
1:B:87:ASN:OD1	1:B:88:GLN:N	2.38	0.46
1:C:6:THR:HG23	1:C:139:PHE:CE2	2.39	0.46
1:D:267:ARG:HG2	1:D:267:ARG:NH1	2.31	0.46
1:C:-1:LEU:HD12	1:C:2:ARG:H	1.76	0.46
1:C:94:ILE:HG22	1:C:96:LEU:HD22	1.97	0.46
1:C:245:ARG:HH22	1:C:250:ASP:CG	2.24	0.46
1:C:235:LEU:HD12	1:C:235:LEU:C	2.41	0.46
1:D:226:ASP:HB3	1:D:267:ARG:O	2.15	0.46
1:B:70:ARG:CD	1:B:85:HIS:CE1	2.97	0.46
1:B:82:PRO:HG3	1:B:86:PHE:CZ	2.50	0.46
1:B:210:GLN:C	5:B:307:HOH:O	2.58	0.46
1:C:121:ILE:N	1:C:122:PRO:CD	2.79	0.46
1:D:150:TYR:OH	1:D:154:ARG:NH1	2.49	0.46
1:B:15:TRP:CZ2	1:D:94:ILE:HD11	2.52	0.45
1:B:235:LEU:HD12	1:B:235:LEU:C	2.41	0.45
1:D:219:ALA:O	1:D:221:PRO:HD3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2:ARG:HG2	1:D:2:ARG:NH1	2.31	0.45
1:D:90:SER:O	1:D:92:THR:HG23	2.17	0.45
1:A:121:ILE:HD11	1:A:150:TYR:CG	2.51	0.45
1:C:152:ARG:HH11	1:C:175:LEU:HD23	1.82	0.45
1:D:163:SER:HB2	1:D:185:GLU:OE2	2.17	0.45
1:D:235:LEU:HD13	1:D:235:LEU:C	2.41	0.45
1:D:281:ALA:O	1:D:285:THR:HG23	2.16	0.45
1:A:121:ILE:HG23	1:A:122:PRO:CD	2.46	0.45
1:A:124:MSE:HE1	1:A:147:LEU:HD12	1.99	0.45
1:A:160:PHE:CD2	1:A:176:ILE:HD13	2.52	0.45
1:D:145:ARG:HH11	1:D:145:ARG:HB2	1.77	0.45
1:D:271:LEU:HA	1:D:274:PHE:CD2	2.52	0.45
1:A:132:ILE:HD11	1:A:243:LEU:HD11	1.98	0.45
1:A:194:VAL:HG12	1:A:196:THR:H	1.82	0.45
1:D:129:ALA:O	1:D:155:GLY:C	2.60	0.45
1:D:276:GLY:C	1:D:278:ARG:N	2.70	0.45
1:C:237:VAL:HG21	1:C:260:ALA:CB	2.47	0.45
1:C:267:ARG:HB2	1:C:273:ALA:HB1	1.97	0.45
1:A:96:LEU:HD12	1:A:96:LEU:C	2.41	0.45
1:A:150:TYR:O	1:A:153:SER:HB3	2.17	0.45
1:A:212:GLY:N	5:A:320:HOH:O	2.46	0.45
1:B:39:LYS:CE	1:B:232:ASP:OD1	2.61	0.45
1:B:124:MSE:HE3	1:B:156:MSE:CE	2.43	0.45
1:C:152:ARG:NH2	5:C:357:HOH:O	2.31	0.45
1:A:23:LYS:NZ	1:C:100:ASP:CB	2.79	0.45
1:A:232:ASP:HB3	5:A:355:HOH:O	2.17	0.45
1:B:76:GLU:C	1:B:78:LEU:H	2.25	0.45
1:D:71:GLN:HE22	1:D:72:GLN:HE21	1.60	0.45
1:A:43:GLN:OE1	1:A:134:LEU:HD21	2.18	0.44
1:A:76:GLU:C	1:A:78:LEU:H	2.23	0.44
1:A:209:VAL:CG1	1:A:210:GLN:N	2.80	0.44
1:C:56:LEU:HD23	1:C:80:LEU:HD13	2.00	0.44
1:C:61:GLY:C	1:C:63:ASP:H	2.24	0.44
1:C:105:ILE:C	1:C:105:ILE:CD1	2.82	0.44
1:C:63:ASP:OD1	1:C:89:HIS:HA	2.17	0.44
1:D:11:VAL:CG2	1:D:65:ASN:HB3	2.42	0.44
1:D:152:ARG:HG2	1:D:152:ARG:NH1	2.33	0.44
1:A:282:ALA:HB3	5:A:311:HOH:O	2.16	0.44
1:B:211:GLU:N	5:B:307:HOH:O	2.51	0.44
1:C:166:ASN:HB3	1:C:169:PHE:CE1	2.52	0.44
1:D:43:GLN:HG3	1:D:232:ASP:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:197:LEU:HB3	1:D:209:VAL:HB	1.99	0.44
1:D:221:PRO:O	1:D:222:ALA:HB2	2.17	0.44
1:B:86:PHE:HB2	1:B:87:ASN:H	1.49	0.44
1:D:152:ARG:HE	1:D:175:LEU:HA	1.83	0.44
1:A:224:ALA:CB	1:A:265:VAL:CG1	2.96	0.44
1:B:11:VAL:HG11	1:B:65:ASN:OD1	2.18	0.44
1:B:128:VAL:HG12	1:B:129:ALA:O	2.17	0.44
1:C:132:ILE:HG12	1:C:157:THR:HB	2.00	0.44
1:D:98:SER:O	1:D:99:ALA:HB2	2.17	0.44
1:D:145:ARG:HH11	1:D:145:ARG:CG	2.29	0.44
1:A:141:LEU:O	1:A:141:LEU:HD12	2.18	0.44
1:B:55:ARG:HE	1:B:55:ARG:HB2	1.61	0.44
1:B:247:VAL:O	1:B:248:ALA:CB	2.61	0.44
1:C:163:SER:HA	1:C:164:PRO:C	2.43	0.44
1:A:121:ILE:HD11	1:A:150:TYR:CD2	2.53	0.44
1:B:237:VAL:HG21	1:B:260:ALA:CB	2.48	0.44
1:C:145:ARG:O	1:C:149:GLN:HG3	2.18	0.44
1:A:43:GLN:CG	1:A:232:ASP:HB2	2.47	0.43
1:A:106:ILE:CD1	1:C:21:PRO:HG2	2.48	0.43
1:C:135:GLN:HB2	1:C:148:PHE:CZ	2.53	0.43
1:D:154:ARG:HE	1:D:154:ARG:HB3	1.54	0.43
1:D:237:VAL:HG21	1:D:260:ALA:HB1	1.99	0.43
1:C:31:LYS:NZ	1:C:31:LYS:HB2	2.33	0.43
1:A:194:VAL:O	1:A:210:GLN:CG	2.63	0.43
1:B:10:THR:HG22	1:B:90:SER:HB2	2.00	0.43
1:C:13:GLU:OE2	1:C:31:LYS:HD3	2.18	0.43
1:A:63:ASP:OD1	1:A:89:HIS:NE2	2.52	0.43
1:B:163:SER:HA	1:B:164:PRO:C	2.44	0.43
1:D:145:ARG:HH11	1:D:145:ARG:HB3	1.82	0.43
1:D:208:LEU:HB2	1:D:254:LEU:CD2	2.49	0.43
1:B:285:THR:C	5:B:328:HOH:O	2.62	0.43
1:C:173:TRP:N	1:C:174:PRO:HD2	2.34	0.43
1:C:197:LEU:HB3	1:C:209:VAL:HB	2.01	0.43
1:C:225:LEU:H	1:C:225:LEU:HD23	1.82	0.43
1:C:17:ILE:HD13	1:C:96:LEU:HD12	2.00	0.43
1:A:21:PRO:HD3	1:A:27:ILE:HD11	2.00	0.43
1:A:109:THR:O	1:A:110:ALA:HB3	2.18	0.43
1:B:11:VAL:O	1:B:11:VAL:HG13	2.19	0.43
1:C:115:PHE:CB	1:C:120:MSE:HE3	2.49	0.43
1:D:18:PRO:HA	1:D:99:ALA:HB2	2.01	0.43
1:D:94:ILE:HG22	1:D:96:LEU:HD22	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:187:GLU:O	1:A:188:LEU:CG	2.67	0.42
1:D:198:VAL:HG21	1:D:238:MSE:SE	2.69	0.42
1:C:259:ARG:HB3	1:C:283:LEU:HD11	2.00	0.42
1:A:106:ILE:HD12	1:A:106:ILE:N	2.34	0.42
1:A:259:ARG:HD2	1:A:283:LEU:HB2	2.01	0.42
1:B:116:SER:O	1:B:120:MSE:HG3	2.19	0.42
1:C:8:ASN:HD22	1:C:8:ASN:N	2.14	0.42
1:C:141:LEU:HD11	1:C:172:LEU:HD13	2.00	0.42
1:C:230:ALA:HB2	1:C:265:VAL:CG1	2.49	0.42
1:A:267:ARG:HD2	1:A:273:ALA:O	2.20	0.42
1:B:49:ARG:HD3	1:B:76:GLU:OE1	2.19	0.42
1:D:105:ILE:CG2	1:D:106:ILE:N	2.83	0.42
1:A:109:THR:O	1:A:111:ALA:N	2.47	0.42
1:A:185:GLU:O	1:A:189:LEU:HB2	2.19	0.42
1:B:22:LYS:HB2	1:B:22:LYS:HZ2	1.83	0.42
1:D:46:ILE:HD12	1:D:233:THR:HA	2.00	0.42
1:D:135:GLN:HE22	1:D:147:LEU:CD1	2.33	0.42
1:A:12:ASP:OD1	1:A:92:THR:CG2	2.67	0.42
1:A:12:ASP:HB3	1:A:94:ILE:HD11	2.02	0.42
1:A:209:VAL:HG12	1:A:210:GLN:N	2.33	0.42
1:B:43:GLN:O	1:B:47:LEU:HB2	2.20	0.42
1:D:63:ASP:OD1	1:D:64:SER:N	2.49	0.42
1:B:50:CYS:SG	1:B:280:LEU:HG	2.59	0.42
1:B:198:VAL:HG21	1:B:238:MSE:SE	2.70	0.42
1:D:48:SER:OG	1:D:77:PRO:HG2	2.19	0.42
1:D:225:LEU:C	1:D:225:LEU:HD23	2.44	0.42
1:B:28:HIS:NE2	1:D:164:PRO:CG	2.82	0.42
1:B:20:ILE:HG21	1:D:20:ILE:CG2	2.48	0.42
1:C:188:LEU:C	5:C:315:HOH:O	2.62	0.42
1:C:107:THR:HG22	1:C:108:THR:O	2.20	0.42
1:D:35:ASP:OD1	1:D:36:ILE:N	2.51	0.42
1:D:121:ILE:N	1:D:122:PRO:HD2	2.34	0.42
1:B:20:ILE:H	1:B:20:ILE:HG13	1.58	0.41
1:B:228:THR:CG2	1:B:270:THR:HG22	2.40	0.41
1:D:9:ILE:HD13	1:D:73:ILE:CD1	2.50	0.41
1:D:22:LYS:O	1:D:23:LYS:C	2.63	0.41
1:A:121:ILE:CG2	1:A:122:PRO:CD	2.97	0.41
1:B:45:ILE:O	1:B:49:ARG:HG3	2.20	0.41
1:B:213:GLN:N	5:B:307:HOH:O	2.43	0.41
1:C:79:MSE:HE2	1:C:81:LEU:CD2	2.41	0.41
1:C:87:ASN:O	1:C:87:ASN:ND2	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:95:ILE:CG2	1:D:103:ASN:HD22	2.33	0.41
1:B:12:ASP:OD2	1:B:92:THR:CG2	2.68	0.41
1:D:182:ASN:N	1:D:182:ASN:HD22	2.18	0.41
1:A:121:ILE:HA	1:A:124:MSE:HE3	2.02	0.41
1:A:96:LEU:HD12	1:A:97:ASN:N	2.35	0.41
1:A:150:TYR:CZ	1:A:154:ARG:HD2	2.56	0.41
1:C:225:LEU:HD23	1:C:226:ASP:N	2.36	0.41
1:D:43:GLN:HE21	1:D:134:LEU:HD21	1.86	0.41
1:D:85:HIS:CD2	1:D:85:HIS:H	2.38	0.41
1:A:96:LEU:HA	1:A:103:ASN:OD1	2.21	0.41
1:B:55:ARG:HG2	1:B:81:LEU:HD12	2.02	0.41
1:B:133:LEU:HD22	1:B:151:ALA:HB2	2.02	0.41
1:D:263:ILE:O	1:D:267:ARG:HD3	2.21	0.41
1:A:108:THR:HG22	1:C:29:GLY:C	2.45	0.41
1:A:183:GLU:H	1:A:183:GLU:HG2	1.52	0.41
1:A:222:ALA:O	1:A:223:GLU:CG	2.69	0.41
1:B:-1:LEU:HD23	1:B:2:ARG:N	2.36	0.41
1:B:73:ILE:HG13	1:B:80:LEU:HD22	2.03	0.41
1:B:238:MSE:HG3	1:B:254:LEU:HD12	2.02	0.41
1:C:169:PHE:O	1:C:172:LEU:HB2	2.21	0.41
1:C:22:LYS:O	1:C:23:LYS:C	2.63	0.41
1:D:180:VAL:HG21	1:D:235:LEU:HD22	2.02	0.41
1:A:6:THR:HG21	1:A:147:LEU:HG	2.02	0.40
1:A:207:TRP:CZ3	1:A:216:PHE:HB2	2.57	0.40
1:B:210:GLN:HB2	1:B:211:GLU:OE1	2.21	0.40
1:D:135:GLN:HG3	5:D:300:HOH:O	2.20	0.40
1:C:150:TYR:OH	1:C:154:ARG:HD2	2.21	0.40
1:A:212:GLY:CA	5:A:320:HOH:O	2.69	0.40
1:A:283:LEU:HD12	1:A:284:LEU:N	2.36	0.40
1:B:12:ASP:OD2	1:B:92:THR:HG22	2.22	0.40
1:C:21:PRO:HG3	1:C:27:ILE:HG12	2.03	0.40
1:D:223:GLU:CD	1:D:223:GLU:C	2.90	0.40
1:A:173:TRP:CE3	1:A:173:TRP:HA	2.56	0.40
1:B:192:TYR:C	1:B:194:VAL:H	2.28	0.40
1:C:201:GLN:HE21	1:C:201:GLN:HB2	1.65	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	283/299 (95%)	247 (87%)	27 (10%)	9 (3%)	3	0
1	B	276/299 (92%)	252 (91%)	19 (7%)	5 (2%)	6	2
1	C	283/299 (95%)	268 (95%)	12 (4%)	3 (1%)	11	7
1	D	283/299 (95%)	253 (89%)	18 (6%)	12 (4%)	2	0
All	All	1125/1196 (94%)	1020 (91%)	76 (7%)	29 (3%)	4	1

All (29) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	101	GLY
1	A	210	GLN
1	A	222	ALA
1	A	223	GLU
1	B	23	LYS
1	B	110	ALA
1	D	98	SER
1	D	99	ALA
1	D	100	ASP
1	A	88	GLN
1	A	189	LEU
1	B	193	GLY
1	C	101	GLY
1	D	246	GLY
1	C	100	ASP
1	D	129	ALA
1	D	222	ALA
1	D	278	ARG
1	A	139	PHE
1	A	162	PRO
1	A	188	LEU
1	D	87	ASN

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Mol	Chain	Res	Type
1	D	89	HIS
1	B	211	GLU
1	C	162	PRO
1	D	153	SER
1	B	249	PRO
1	D	247	VAL
1	D	18	PRO

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	223/228 (98%)	202 (91%)	21 (9%)	8	4
1	B	220/228 (96%)	197 (90%)	23 (10%)	6	3
1	C	223/228 (98%)	203 (91%)	20 (9%)	9	5
1	D	223/228 (98%)	202 (91%)	21 (9%)	8	4
All	All	889/912 (98%)	804 (90%)	85 (10%)	8	4

All (85) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	THR
1	A	8	ASN
1	A	32	VAL
1	A	35	ASP
1	A	53	GLU
1	A	71	GLN
1	A	74	LYS
1	A	83	ASP
1	A	117	LEU
1	A	119	GLU
1	A	126	ASP
1	A	138	ASN
1	A	147	LEU
1	A	170	CYS

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Mol	Chain	Res	Type
1	A	183	GLU
1	A	188	LEU
1	A	189	LEU
1	A	210	GLN
1	A	232	ASP
1	A	243	LEU
1	A	283	LEU
1	B	8	ASN
1	B	22	LYS
1	B	35	ASP
1	B	55	ARG
1	B	62	ASN
1	B	71	GLN
1	B	89	HIS
1	B	94	ILE
1	B	96	LEU
1	B	108	THR
1	B	109	THR
1	B	152	ARG
1	B	183	GLU
1	B	189	LEU
1	B	210	GLN
1	B	211	GLU
1	B	225	LEU
1	B	227	THR
1	B	235	LEU
1	B	243	LEU
1	B	280	LEU
1	B	283	LEU
1	B	285	THR
1	C	-1	LEU
1	C	6	THR
1	C	8	ASN
1	C	31	LYS
1	C	47	LEU
1	C	53	GLU
1	C	63	ASP
1	C	72	GLN
1	C	87	ASN
1	C	100	ASP
1	C	102	ASP
1	C	105	ILE

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Mol	Chain	Res	Type
1	C	121	ILE
1	C	172	LEU
1	C	183	GLU
1	C	213	GLN
1	C	225	LEU
1	C	227	THR
1	C	235	LEU
1	C	243	LEU
1	D	-1	LEU
1	D	8	ASN
1	D	34	GLN
1	D	47	LEU
1	D	85	HIS
1	D	87	ASN
1	D	89	HIS
1	D	90	SER
1	D	94	ILE
1	D	96	LEU
1	D	98	SER
1	D	102	ASP
1	D	108	THR
1	D	145	ARG
1	D	182	ASN
1	D	184	SER
1	D	195	LYS
1	D	223	GLU
1	D	227	THR
1	D	235	LEU
1	D	243	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (49) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	ASN
1	A	28	HIS
1	A	71	GLN
1	A	85	HIS
1	A	97	ASN
1	A	138	ASN
1	A	161	ASN
1	A	190	GLN
1	A	215	GLN

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Mol	Chain	Res	Type
1	A	256	HIS
1	B	8	ASN
1	B	62	ASN
1	B	71	GLN
1	B	88	GLN
1	B	89	HIS
1	B	135	GLN
1	B	161	ASN
1	B	171	HIS
1	B	201	GLN
1	B	210	GLN
1	B	256	HIS
1	C	8	ASN
1	C	43	GLN
1	C	72	GLN
1	C	85	HIS
1	C	87	ASN
1	C	88	GLN
1	C	97	ASN
1	C	135	GLN
1	C	161	ASN
1	C	166	ASN
1	C	190	GLN
1	C	201	GLN
1	C	215	GLN
1	D	8	ASN
1	D	28	HIS
1	D	34	GLN
1	D	43	GLN
1	D	71	GLN
1	D	85	HIS
1	D	87	ASN
1	D	88	GLN
1	D	103	ASN
1	D	135	GLN
1	D	138	ASN
1	D	161	ASN
1	D	171	HIS
1	D	182	ASN
1	D	210	GLN

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	B	299	-	4,4,4	0.39	0	6,6,6	0.07	0
2	SO4	D	298	-	4,4,4	0.40	0	6,6,6	0.14	0
2	SO4	B	300	-	4,4,4	0.36	0	6,6,6	0.13	0
3	GOL	C	501	-	5,5,5	0.31	0	5,5,5	0.40	0
2	SO4	C	298	-	4,4,4	0.34	0	6,6,6	0.13	0
4	RIB	D	311	-	10,10,10	1.34	2 (20%)	13,14,14	1.50	2 (15%)
2	SO4	B	298	-	4,4,4	0.37	0	6,6,6	0.09	0
2	SO4	C	1	-	4,4,4	0.34	0	6,6,6	0.16	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
4	RIB	D	311	-	-	0/2/18/18	0/1/1/1
3	GOL	C	501	-	-	0/4/4/4	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	311	RIB	O1-C1	2.41	1.47	1.39
4	D	311	RIB	O4-C1	2.31	1.45	1.43

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	311	RIB	C1-C2-C3	3.13	106.14	102.29
4	D	311	RIB	O4-C4-C3	2.64	110.39	105.15

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	280/299 (93%)	0.48	18 (6%) 25 28	25, 39, 57, 71	0
1	B	277/299 (92%)	0.58	25 (9%) 15 16	26, 39, 61, 83	0
1	C	280/299 (93%)	0.34	5 (1%) 67 71	27, 38, 52, 62	0
1	D	280/299 (93%)	0.69	21 (7%) 20 23	27, 43, 64, 80	0
All	All	1117/1196 (93%)	0.52	69 (6%) 26 30	25, 39, 60, 83	0

All (69) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	99	ALA	4.8
1	B	99	ALA	4.3
1	B	96	LEU	3.8
1	A	89	HIS	3.8
1	B	87	ASN	3.8
1	A	210	GLN	3.7
1	A	98	SER	3.6
1	B	104	ALA	3.4
1	D	40	GLY	3.4
1	B	285	THR	3.2
1	D	87	ASN	3.2
1	D	21	PRO	3.2
1	A	118	ASP	3.2
1	A	126	ASP	3.2
1	A	221	PRO	3.2
1	B	225	LEU	3.1
1	B	15	TRP	3.1
1	C	100	ASP	3.1
1	A	100	ASP	3.0
1	A	99	ALA	3.0
1	D	119	GLU	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	152	ARG	2.9
1	B	35	ASP	2.9
1	A	138	ASN	2.9
1	B	22	LYS	2.9
1	A	188	LEU	2.9
1	D	221	PRO	2.9
1	B	95	ILE	2.8
1	D	100	ASP	2.8
1	B	92	THR	2.8
1	D	222	ALA	2.8
1	D	283	LEU	2.7
1	B	89	HIS	2.7
1	B	85	HIS	2.7
1	C	182	ASN	2.7
1	B	36	ILE	2.6
1	C	171	HIS	2.6
1	A	220	VAL	2.6
1	A	222	ALA	2.6
1	B	212	GLY	2.5
1	B	63	ASP	2.5
1	B	100	ASP	2.5
1	B	283	LEU	2.5
1	D	284	LEU	2.5
1	D	115	PHE	2.5
1	B	101	GLY	2.5
1	D	214	ARG	2.5
1	A	121	ILE	2.4
1	B	109	THR	2.4
1	D	77	PRO	2.4
1	A	211	GLU	2.3
1	D	278	ARG	2.3
1	A	224	ALA	2.3
1	A	192	TYR	2.2
1	D	-1	LEU	2.2
1	D	63	ASP	2.2
1	B	210	GLN	2.2
1	A	86	PHE	2.1
1	B	86	PHE	2.1
1	D	114	THR	2.1
1	D	285	THR	2.1
1	D	61	GLY	2.1
1	C	268	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	97	ASN	2.1
1	B	19	ASP	2.1
1	B	23	LYS	2.1
1	D	111	ALA	2.1
1	D	9	ILE	2.0
1	B	270	THR	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(Å ²)	Q<0.9
4	RIB	D	311	10/10	0.79	0.15	53,55,58,59	0
2	SO4	B	299	5/5	0.80	0.10	82,83,83,84	0
2	SO4	B	300	5/5	0.85	0.15	89,90,90,91	0
2	SO4	C	1	5/5	0.86	0.18	74,74,76,77	0
2	SO4	B	298	5/5	0.87	0.13	72,72,73,74	0
3	GOL	C	501	6/6	0.88	0.14	41,43,44,48	0
2	SO4	D	298	5/5	0.88	0.12	62,62,64,64	0
2	SO4	C	298	5/5	0.95	0.07	42,45,46,48	0

6.5 Other polymers [i](#)

There are no such residues in this entry.