Full wwPDB X-ray Structure Validation Report (i)

May 15, 2020 – 04:20 am BST

PDB ID : 3DEV

Title : Crystal structure of SH1221 protein from Staphylococcus haemolyticus, Northeast Structural Genomics Consortium Target ShR87

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Deposited on : 2008-06-10

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 (i) symbol.

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

|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

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	Percentile Ranks	Value
Rfree		0.260
Clashscore		42
Ramachandran outliers		3.2%
Sidechain outliers		16.0%
RSRZ outliers		1.5%

Worse   *Better*

▊ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
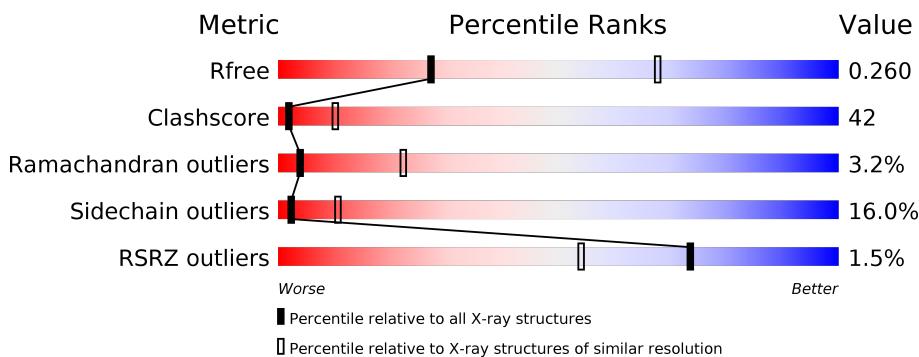
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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 on 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 <=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	320	2% 37% 52% 8% ••
1	B	320	% 40% 51% 8% ••
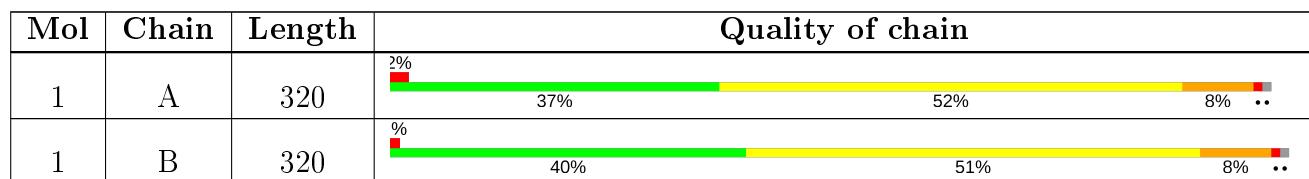
2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 5089 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 SH1221.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	316	Total 2518	C 1590	N 425	O 494	S 3	Se 6	0	0	0
1	B	316	Total 2518	C 1590	N 425	O 494	S 3	Se 6	0	0	0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	313	LEU	-	expression tag	UNP Q4L745
A	314	GLU	-	expression tag	UNP Q4L745
A	315	HIS	-	expression tag	UNP Q4L745
A	316	HIS	-	expression tag	UNP Q4L745
A	317	HIS	-	expression tag	UNP Q4L745
A	318	HIS	-	expression tag	UNP Q4L745
A	319	HIS	-	expression tag	UNP Q4L745
A	320	HIS	-	expression tag	UNP Q4L745
B	313	LEU	-	expression tag	UNP Q4L745
B	314	GLU	-	expression tag	UNP Q4L745
B	315	HIS	-	expression tag	UNP Q4L745
B	316	HIS	-	expression tag	UNP Q4L745
B	317	HIS	-	expression tag	UNP Q4L745
B	318	HIS	-	expression tag	UNP Q4L745
B	319	HIS	-	expression tag	UNP Q4L745
B	320	HIS	-	expression tag	UNP Q4L745

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).

SO4

O1

O3 O4

S

O2
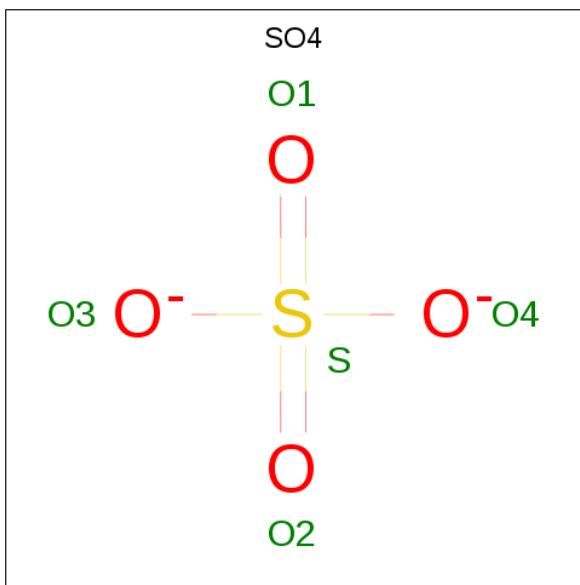
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total 5	O 4	S 1	0	0
2	A	1	Total 5	O 4	S 1	0	0
2	B	1	Total 5	O 4	S 1	0	0

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total 1	Mg 1	0	0
3	A	1	Total 1	Mg 1	0	0

- Molecule 4 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	16	Total 16	O 16	0	0
4	B	20	Total 20	O 20	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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: SH1221

- Molecule 1: SH1221
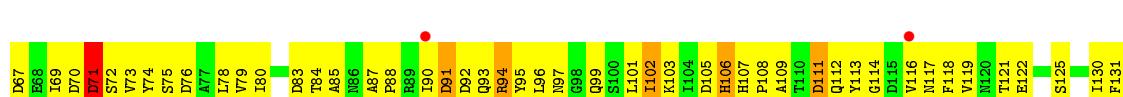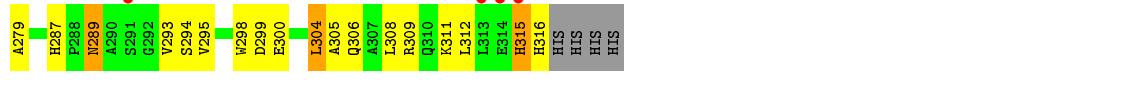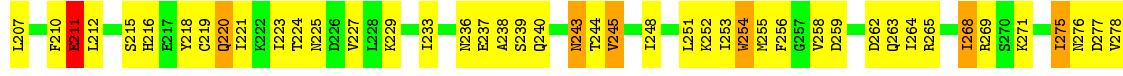
4   Data and refinement statistics (i)

Property	Value	Source
Space group	P 3	Depositor
Cell constants a, b, c, α, β, γ	106.09Å 106.09Å 86.09Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.94 – 3.10 28.85 – 3.10	Depositor EDS
% Data completeness (in resolution range)	82.7 (19.94-3.10) 99.0 (28.85-3.10)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	2.24 (at 3.11Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.193 , 0.245 0.215 , 0.260	Depositor DCC
R_{free} test set	3689 reflections (9.64%)	wwPDB-VP
Wilson B-factor (Å^2)	59.0	Xtriage
Anisotropy	0.590	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 34.5	EDS
L-test for twinning[2]	$< |L| > = 0.50, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.028 for -h,-k,l 0.419 for h,-h-k,-l 0.023 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	5089	wwPDB-VP
Average B, all atoms (Å^2)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.42% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: MG, SO4

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$|Z|$>5	RMSZ	#$|Z|$>5
1	A	0.47	0/2568	0.60	0/3473
1	B	0.47	0/2568	0.60	0/3473
All	All	0.47	0/5136	0.60	0/6946

There are no bond length outliers.

There are no bond angle outliers.

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	2518	0	2417	215	0
1	B	2518	0	2417	202	0
2	A	10	0	0	0	0
2	B	5	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	16	0	0	3	0
4	B	20	0	0	0	0
All	All	5089	0	4834	412	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 42.

All (412) 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:18:ILE:HG22	1:A:78:LEU:HB3	1.33	1.04
1:B:18:ILE:HG22	1:B:78:LEU:HB3	1.35	1.03
1:B:69:ILE:HG23	1:B:94:ARG:HH12	1.42	0.84
1:A:255:MSE:HE1	1:A:304:LEU:HD13	1.62	0.82
1:A:69:ILE:HG23	1:A:94:ARG:HH12	1.43	0.82
1:A:145:GLU:HG2	1:A:182:PRO:HG2	1.61	0.82
1:B:145:GLU:HG2	1:B:182:PRO:HG2	1.61	0.81
1:B:253:ILE:HD11	1:B:308:LEU:HD22	1.62	0.80
1:A:253:ILE:HD11	1:A:308:LEU:HD22	1.63	0.79
1:B:71:ASP:HB2	1:B:94:ARG:HE	1.47	0.79
1:B:255:MSE:HE1	1:B:304:LEU:HD13	1.64	0.78
1:A:221:ILE:HD13	1:A:256:PHE:HD1	1.48	0.78
1:B:243:ASN:HD22	1:B:243:ASN:N	1.83	0.77
1:B:221:ILE:HD13	1:B:256:PHE:HD1	1.49	0.77
1:A:19:ILE:HG22	1:A:51:TYR:HB2	1.67	0.77
1:A:243:ASN:HD22	1:A:243:ASN:N	1.83	0.76
1:A:71:ASP:HB2	1:A:94:ARG:HE	1.49	0.76
1:A:268:ILE:C	1:A:268:ILE:HD13	2.07	0.76
1:A:4:ILE:H	1:A:4:ILE:HD12	1.51	0.75
1:A:278:VAL:HG21	1:A:308:LEU:HD23	1.69	0.75
1:B:268:ILE:HD13	1:B:268:ILE:C	2.07	0.75
1:A:53:THR:HG21	1:A:92:ASP:OD2	1.87	0.75
1:B:53:THR:HG21	1:B:92:ASP:OD2	1.88	0.74
1:B:19:ILE:HG22	1:B:51:TYR:HB2	1.67	0.74
1:B:278:VAL:HG21	1:B:308:LEU:HD23	1.70	0.74
1:B:4:ILE:HD12	1:B:4:ILE:H	1.54	0.73
1:B:225:ASN:HB2	1:B:259:ASP:OD2	1.89	0.73
1:A:225:ASN:HB2	1:A:259:ASP:OD2	1.88	0.73
1:A:268:ILE:HD13	1:A:269:ARG:N	2.04	0.72
1:A:69:ILE:HG12	1:A:74:TYR:HE1	1.55	0.72
1:B:200:MSE:N	1:B:201:PRO:HD2	2.05	0.72
1:A:18:ILE:HD11	1:A:50:ILE:HG13	1.72	0.72
1:A:200:MSE:N	1:A:201:PRO:HD2	2.05	0.72
1:A:237:GLU:O	1:A:240:GLN:HG2	1.90	0.72
1:B:35:LEU:O	1:B:39:LEU:HD23	1.90	0.72
1:A:211:GLU:HB3	1:A:220:GLN:HG3	1.71	0.71
1:B:69:ILE:HG23	1:B:94:ARG:NH1	2.05	0.71
1:A:35:LEU:O	1:A:39:LEU:HD23	1.90	0.71
1:B:102:ILE:HD13	1:B:103:LYS:N	2.06	0.70
1:B:268:ILE:HD13	1:B:269:ARG:N	2.06	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:212:LEU:HD21	1:A:248:ILE:HG21	1.73	0.70
1:A:69:ILE:HG23	1:A:94:ARG:NH1	2.06	0.70
1:B:211:GLU:HB3	1:B:220:GLN:HG3	1.71	0.70
1:B:166:ASN:N	1:B:166:ASN:HD22	1.89	0.70
1:B:18:ILE:HD11	1:B:50:ILE:HG13	1.73	0.70
1:B:164:PHE:HB2	1:B:166:ASN:HD21	1.56	0.70
1:B:212:LEU:HD21	1:B:248:ILE:HG21	1.74	0.70
1:B:69:ILE:HG12	1:B:74:TYR:HE1	1.56	0.70
1:B:237:GLU:O	1:B:240:GLN:HG2	1.91	0.69
1:B:255:MSE:HE3	1:B:268:ILE:HB	1.74	0.69
1:B:139:ASP:HA	1:B:142:ILE:HD13	1.73	0.69
1:A:102:ILE:HD13	1:A:103:LYS:N	2.07	0.69
1:A:168:SER:HB2	1:A:169:PRO:HD2	1.75	0.69
1:B:164:PHE:HB2	1:B:166:ASN:ND2	2.08	0.69
1:A:139:ASP:HA	1:A:142:ILE:HD13	1.74	0.68
1:B:74:TYR:HB3	1:B:97:ASN:O	1.93	0.68
1:B:71:ASP:N	1:B:94:ARG:HH11	1.91	0.68
1:A:164:PHE:HB2	1:A:166:ASN:HD21	1.57	0.68
1:A:164:PHE:HB2	1:A:166:ASN:ND2	2.08	0.68
1:A:71:ASP:N	1:A:94:ARG:HH11	1.91	0.67
1:A:74:TYR:HB3	1:A:97:ASN:O	1.93	0.67
1:A:102:ILE:HD13	1:A:102:ILE:C	2.15	0.67
1:A:166:ASN:HD22	1:A:166:ASN:N	1.90	0.67
1:B:102:ILE:HD13	1:B:102:ILE:C	2.15	0.66
1:B:168:SER:HB2	1:B:169:PRO:HD2	1.77	0.66
1:A:32:GLY:HA2	1:A:150:VAL:HB	1.78	0.66
1:B:149:ARG:HG2	1:B:183:PHE:HD2	1.61	0.66
1:A:92:ASP:OD2	1:A:94:ARG:NH2	2.29	0.65
1:A:149:ARG:HG2	1:A:183:PHE:HD2	1.61	0.65
1:A:255:MSE:HE3	1:A:268:ILE:HB	1.78	0.65
1:B:19:ILE:HD11	1:B:79:VAL:HG22	1.79	0.65
1:B:92:ASP:OD1	1:B:94:ARG:HG2	1.97	0.65
1:A:278:VAL:HG21	1:A:308:LEU:CD2	2.28	0.64
1:A:92:ASP:OD1	1:A:94:ARG:HG2	1.97	0.64
1:B:92:ASP:OD2	1:B:94:ARG:NH2	2.30	0.64
1:B:32:GLY:HA2	1:B:150:VAL:HB	1.80	0.64
1:B:54:GLY:HA2	1:B:91:ASP:OD1	1.99	0.63
1:A:19:ILE:HD11	1:A:79:VAL:HG22	1.80	0.63
1:B:152:TYR:O	1:B:156:VAL:HG23	1.99	0.62
1:A:54:GLY:HA2	1:A:91:ASP:OD1	1.99	0.62
1:B:278:VAL:HG21	1:B:308:LEU:CD2	2.28	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:18:ILE:CG2	1:A:78:LEU:HB3	2.20	0.62
1:A:255:MSE:HE1	1:A:304:LEU:CD1	2.30	0.62
1:A:145:GLU:CG	1:A:182:PRO:HG2	2.29	0.61
1:B:145:GLU:CG	1:B:182:PRO:HG2	2.29	0.61
1:B:253:ILE:HD12	1:B:275:ILE:HD11	1.82	0.61
1:A:57:GLU:HG3	1:A:59:SER:HB3	1.82	0.61
1:B:131:PHE:O	1:B:135:SER:HB2	2.01	0.60
1:B:18:ILE:H	1:B:18:ILE:HD13	1.65	0.60
1:B:18:ILE:CG2	1:B:78:LEU:HB3	2.21	0.60
1:A:21:HIS:HD1	1:A:95:TYR:HB3	1.65	0.60
1:A:152:TYR:O	1:A:156:VAL:HG23	2.01	0.60
1:B:21:HIS:ND1	1:B:95:TYR:HB3	2.17	0.60
1:A:253:ILE:HD12	1:A:275:ILE:HD11	1.82	0.59
1:B:69:ILE:HG13	1:B:71:ASP:H	1.67	0.59
1:A:21:HIS:ND1	1:A:95:TYR:HB3	2.17	0.59
1:A:131:PHE:O	1:A:135:SER:HB2	2.02	0.59
1:B:218:TYR:CE1	1:B:220:GLN:HG2	2.38	0.59
1:B:9:MSE:HE2	1:B:137:PHE:CD2	2.38	0.59
1:A:18:ILE:HD13	1:A:18:ILE:H	1.66	0.59
1:B:109:ALA:HB2	1:B:119:VAL:HG21	1.85	0.59
1:B:19:ILE:O	1:B:19:ILE:HD12	2.03	0.59
1:B:255:MSE:HE1	1:B:304:LEU:CD1	2.32	0.58
1:B:57:GLU:HG3	1:B:59:SER:HB3	1.83	0.58
1:A:109:ALA:HB2	1:A:119:VAL:HG21	1.85	0.58
1:B:27:ASP:HB2	1:B:28:PRO:HD2	1.85	0.58
1:A:69:ILE:HG13	1:A:71:ASP:H	1.68	0.58
1:A:27:ASP:HB2	1:A:28:PRO:HD2	1.86	0.58
1:A:218:TYR:CE1	1:A:220:GLN:HG2	2.39	0.57
1:A:245:VAL:HG12	1:A:248:ILE:CD1	2.34	0.57
1:A:22:ARG:HG3	1:A:22:ARG:HH21	1.70	0.57
1:B:295:VAL:CG1	1:B:300:GLU:HG2	2.35	0.57
1:A:57:GLU:CG	1:A:59:SER:HB3	2.35	0.57
1:A:69:ILE:HG23	1:A:94:ARG:HH22	1.69	0.57
1:A:9:MSE:HE2	1:A:137:PHE:CD2	2.39	0.57
1:B:28:PRO:HG3	1:B:157:GLY:HA3	1.87	0.57
1:A:17:THR:HG23	1:A:49:ASN:O	2.05	0.57
1:B:221:ILE:N	1:B:221:ILE:HD12	2.19	0.57
1:A:43:ARG:HG2	1:A:142:ILE:O	2.04	0.57
1:A:295:VAL:CG1	1:A:300:GLU:HG2	2.35	0.56
1:A:172:MSE:HB2	1:B:176:SER:HB2	1.87	0.56
1:A:19:ILE:HD12	1:A:19:ILE:O	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:22:ARG:HG3	1:B:22:ARG:HH21	1.70	0.56
1:A:221:ILE:HD12	1:A:221:ILE:N	2.21	0.56
1:A:22:ARG:HG3	1:A:22:ARG:NH2	2.21	0.56
1:B:69:ILE:HG23	1:B:94:ARG:HH22	1.69	0.56
1:B:106:HIS:CE1	1:B:125:SER:HA	2.41	0.56
1:B:184:ASN:ND2	1:B:187:ALA:HB2	2.20	0.56
1:B:57:GLU:CG	1:B:59:SER:HB3	2.35	0.56
1:B:71:ASP:H	1:B:94:ARG:HH11	1.53	0.56
1:A:202:PHE:O	1:A:205:TYR:HB3	2.05	0.56
1:A:71:ASP:H	1:A:94:ARG:HH11	1.52	0.56
1:B:202:PHE:O	1:B:205:TYR:HB3	2.05	0.56
1:A:184:ASN:ND2	1:A:187:ALA:HB2	2.21	0.56
1:A:28:PRO:HG3	1:A:157:GLY:HA3	1.88	0.56
1:A:70:ASP:O	1:A:72:SER:N	2.39	0.56
1:B:8:ILE:O	1:B:12:VAL:HG23	2.06	0.56
1:A:106:HIS:CE1	1:A:125:SER:HA	2.41	0.56
1:A:253:ILE:CG2	1:A:312:LEU:HD11	2.36	0.56
1:A:21:HIS:CE1	1:A:95:TYR:HB3	2.40	0.55
1:B:79:VAL:HG11	1:B:95:TYR:HB2	1.88	0.55
1:A:268:ILE:CD1	1:A:268:ILE:C	2.75	0.55
1:B:253:ILE:CG2	1:B:312:LEU:HD11	2.36	0.55
1:B:69:ILE:CG2	1:B:94:ARG:HH22	2.20	0.55
1:A:253:ILE:HG21	1:A:312:LEU:HD11	1.88	0.55
1:B:245:VAL:HG12	1:B:248:ILE:CD1	2.36	0.55
1:B:253:ILE:HG21	1:B:312:LEU:HD11	1.89	0.55
1:B:43:ARG:HG2	1:B:142:ILE:O	2.06	0.55
1:B:147:VAL:O	1:B:150:VAL:HG22	2.07	0.55
1:B:161:ARG:HH21	1:B:161:ARG:HG3	1.72	0.55
1:B:21:HIS:CE1	1:B:95:TYR:HB3	2.41	0.55
1:A:243:ASN:ND2	1:A:243:ASN:N	2.54	0.55
1:A:1:MSE:HE2	4:A:326:HOH:O	2.07	0.55
1:B:18:ILE:HD13	1:B:18:ILE:N	2.21	0.55
1:A:38:LYS:HE3	1:A:67:ASP:OD2	2.08	0.54
1:A:44:LYS:HD3	1:A:45:PHE:CZ	2.42	0.54
1:A:69:ILE:CG2	1:A:94:ARG:HH22	2.20	0.54
1:A:161:ARG:HG3	1:A:161:ARG:HH21	1.70	0.54
1:A:79:VAL:HG11	1:A:95:TYR:HB2	1.89	0.54
1:B:112:GLN:OE1	1:B:112:GLN:HA	2.08	0.54
1:B:145:GLU:HB3	1:B:182:PRO:O	2.07	0.54
1:A:101:LEU:HD23	1:A:114:GLY:HA2	1.89	0.54
1:A:176:SER:HB2	1:B:172:MSE:HB2	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:22:ARG:HG3	1:B:22:ARG:NH2	2.21	0.54
1:B:268:ILE:CD1	1:B:268:ILE:C	2.76	0.54
1:B:87:ALA:N	1:B:88:PRO:HD2	2.22	0.54
1:A:39:LEU:HB3	1:A:147:VAL:HG22	1.90	0.54
1:A:69:ILE:HG12	1:A:74:TYR:CE1	2.40	0.54
1:B:101:LEU:HD23	1:B:114:GLY:HA2	1.90	0.54
1:B:39:LEU:HB3	1:B:147:VAL:HG22	1.89	0.54
1:A:149:ARG:CG	1:A:183:PHE:HD2	2.20	0.54
1:A:239:SER:OG	1:A:258:VAL:HG11	2.08	0.54
1:B:17:THR:HG23	1:B:49:ASN:O	2.07	0.54
1:B:38:LYS:HE3	1:B:67:ASP:OD2	2.08	0.54
1:A:18:ILE:HD13	1:A:18:ILE:N	2.22	0.54
1:B:9:MSE:HE2	1:B:137:PHE:CE2	2.43	0.54
1:B:69:ILE:HG12	1:B:74:TYR:CE1	2.41	0.54
1:A:87:ALA:N	1:A:88:PRO:HD2	2.23	0.54
1:B:239:SER:OG	1:B:258:VAL:HG11	2.08	0.53
1:B:149:ARG:CG	1:B:183:PHE:HD2	2.20	0.53
1:A:262:ASP:OD1	1:A:263:GLN:HG2	2.08	0.53
1:A:166:ASN:H	1:A:166:ASN:HD22	1.56	0.53
1:A:145:GLU:HB3	1:A:182:PRO:O	2.09	0.53
1:A:55:GLU:O	1:A:56:ALA:HB3	2.09	0.53
1:A:8:ILE:O	1:A:12:VAL:HG23	2.08	0.53
1:A:9:MSE:HE2	1:A:137:PHE:CE2	2.44	0.53
1:B:262:ASP:OD1	1:B:263:GLN:HG2	2.09	0.53
1:A:112:GLN:HA	1:A:112:GLN:OE1	2.08	0.53
1:A:150:VAL:HG23	1:A:151:LEU:N	2.24	0.53
1:B:70:ASP:O	1:B:72:SER:N	2.40	0.53
1:A:60:LEU:HB3	1:A:63:ILE:HD12	1.90	0.53
1:A:174:VAL:O	1:A:178:LEU:HD22	2.09	0.52
1:A:207:LEU:HD22	1:B:200:MSE:HG2	1.91	0.52
1:B:55:GLU:O	1:B:56:ALA:HB3	2.09	0.52
1:B:105:ASP:OD2	1:B:107:HIS:HB2	2.09	0.52
1:B:60:LEU:HB3	1:B:63:ILE:HD12	1.91	0.52
1:B:9:MSE:HE3	1:B:44:LYS:HE2	1.92	0.52
1:A:147:VAL:O	1:A:150:VAL:HG22	2.08	0.52
1:A:41:LEU:N	1:A:41:LEU:HD23	2.24	0.52
1:B:166:ASN:HD22	1:B:166:ASN:H	1.54	0.52
1:A:143:ILE:HG13	1:A:147:VAL:HB	1.92	0.52
1:B:44:LYS:HD3	1:B:45:PHE:CZ	2.43	0.52
1:A:69:ILE:HG23	1:A:94:ARG:NH2	2.25	0.51
1:B:9:MSE:HB2	1:B:137:PHE:CZ	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:9:MSE:HB2	1:A:137:PHE:CZ	2.45	0.51
1:A:9:MSE:HE3	1:A:44:LYS:HE2	1.91	0.51
1:B:41:LEU:N	1:B:41:LEU:HD23	2.24	0.51
1:A:212:LEU:HD21	1:A:248:ILE:HD13	1.93	0.51
1:B:143:ILE:HG13	1:B:147:VAL:HB	1.91	0.51
1:B:174:VAL:O	1:B:178:LEU:HD22	2.11	0.51
1:B:150:VAL:HG23	1:B:151:LEU:N	2.26	0.51
1:B:211:GLU:CB	1:B:220:GLN:HG3	2.41	0.51
1:B:69:ILE:HG23	1:B:94:ARG:NH2	2.25	0.51
1:A:101:LEU:HD23	1:A:114:GLY:CA	2.41	0.51
1:A:105:ASP:OD2	1:A:107:HIS:HB2	2.10	0.51
1:B:166:ASN:N	1:B:166:ASN:ND2	2.59	0.51
1:A:44:LYS:HG2	1:A:45:PHE:CE1	2.47	0.50
1:B:44:LYS:HG2	1:B:45:PHE:CE1	2.47	0.50
1:B:28:PRO:CG	1:B:157:GLY:HA3	2.41	0.50
1:B:295:VAL:HB	1:B:300:GLU:HG2	1.93	0.50
1:B:84:THR:HG21	1:B:90:ILE:CG1	2.41	0.50
1:A:84:THR:HG21	1:A:90:ILE:CG1	2.41	0.50
1:B:70:ASP:C	1:B:72:SER:H	2.15	0.50
1:B:244:THR:O	1:B:244:THR:HG22	2.12	0.50
1:A:211:GLU:O	1:A:219:CYS:HA	2.11	0.50
1:B:74:TYR:CE2	1:B:94:ARG:O	2.65	0.50
1:A:219:CYS:SG	1:A:245:VAL:HG11	2.51	0.50
1:A:70:ASP:C	1:A:72:SER:H	2.14	0.49
1:A:295:VAL:HB	1:A:300:GLU:HG2	1.94	0.49
1:A:200:MSE:HG2	1:B:207:LEU:HD22	1.93	0.49
1:A:40:TYR:CD2	1:A:41:LEU:HD23	2.47	0.49
1:B:101:LEU:HD23	1:B:114:GLY:CA	2.42	0.49
1:B:220:GLN:HA	1:B:255:MSE:O	2.13	0.49
1:A:130:ILE:O	1:A:134:ILE:HG23	2.13	0.49
1:B:212:LEU:HD21	1:B:248:ILE:HD13	1.94	0.49
1:A:244:THR:O	1:A:244:THR:HG22	2.13	0.49
1:A:20:ILE:HD12	1:A:38:LYS:HB2	1.95	0.49
1:B:219:CYS:SG	1:B:245:VAL:HG11	2.52	0.49
1:B:223:ILE:HB	1:B:258:VAL:HA	1.95	0.49
1:B:308:LEU:O	1:B:311:LYS:HB2	2.13	0.49
1:A:223:ILE:HB	1:A:258:VAL:HA	1.95	0.48
1:A:28:PRO:CG	1:A:157:GLY:HA3	2.43	0.48
1:B:200:MSE:N	1:B:201:PRO:CD	2.76	0.48
1:A:211:GLU:CB	1:A:220:GLN:HG3	2.41	0.48
1:A:264:ILE:HB	1:A:295:VAL:HG23	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:84:THR:HG21	1:A:90:ILE:HG12	1.96	0.48
1:B:40:TYR:CD2	1:B:41:LEU:HD23	2.48	0.48
1:A:220:GLN:HA	1:A:255:MSE:O	2.14	0.48
1:A:224:THR:O	1:A:227:VAL:HG22	2.14	0.48
1:A:245:VAL:HG12	1:A:248:ILE:HD11	1.96	0.48
1:B:130:ILE:O	1:B:134:ILE:HG23	2.13	0.48
1:A:233:ILE:HD12	1:A:238:ALA:HB2	1.95	0.48
1:B:20:ILE:HD12	1:B:38:LYS:HB2	1.94	0.48
1:A:205:TYR:CZ	1:A:227:VAL:HG11	2.49	0.48
1:A:74:TYR:CE2	1:A:94:ARG:O	2.67	0.48
1:B:243:ASN:ND2	1:B:243:ASN:N	2.54	0.48
1:A:243:ASN:ND2	1:A:254:TRP:CH2	2.82	0.48
1:B:264:ILE:HB	1:B:295:VAL:HG23	1.96	0.48
1:A:106:HIS:ND1	1:A:125:SER:HA	2.28	0.47
1:A:107:HIS:HB3	1:A:108:PRO:HD2	1.96	0.47
1:B:84:THR:HG21	1:B:90:ILE:HG12	1.96	0.47
1:A:24:VAL:HG23	1:A:25:ARG:H	1.79	0.47
1:B:106:HIS:ND1	1:B:125:SER:HA	2.29	0.47
1:B:211:GLU:O	1:B:219:CYS:HA	2.14	0.47
1:A:71:ASP:H	1:A:94:ARG:NH1	2.13	0.47
1:B:243:ASN:ND2	1:B:254:TRP:CH2	2.82	0.47
1:A:293:VAL:HG12	1:A:294:SER:N	2.29	0.47
1:B:107:HIS:HB3	1:B:108:PRO:HD2	1.97	0.47
1:B:136:HIS:O	1:B:136:HIS:CG	2.68	0.47
1:B:205:TYR:CZ	1:B:227:VAL:HG11	2.49	0.47
1:A:289:ASN:HD22	1:A:289:ASN:HA	1.52	0.47
1:B:224:THR:O	1:B:227:VAL:HG22	2.14	0.47
1:B:74:TYR:HE2	1:B:95:TYR:HA	1.79	0.47
1:B:24:VAL:HG23	1:B:25:ARG:H	1.80	0.47
1:A:102:ILE:HG12	1:A:116:VAL:HB	1.96	0.47
1:A:103:LYS:HD3	1:A:113:TYR:CE2	2.50	0.46
1:A:43:ARG:HE	1:A:43:ARG:HB2	1.32	0.46
1:B:102:ILE:HG12	1:B:116:VAL:HB	1.96	0.46
1:B:60:LEU:N	1:B:60:LEU:HD22	2.31	0.46
1:A:74:TYR:HE2	1:A:95:TYR:HA	1.80	0.46
1:B:103:LYS:HD3	1:B:113:TYR:CE2	2.50	0.46
1:A:145:GLU:CD	1:A:145:GLU:H	2.19	0.46
1:B:233:ILE:HD12	1:B:238:ALA:HB2	1.95	0.46
1:B:71:ASP:H	1:B:94:ARG:NH1	2.14	0.46
1:B:293:VAL:HG12	1:B:294:SER:N	2.30	0.46
1:B:69:ILE:HG23	1:B:94:ARG:CZ	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:69:ILE:CG2	1:B:94:ARG:NH2	2.78	0.46
1:A:136:HIS:CG	1:A:136:HIS:O	2.68	0.46
1:B:245:VAL:HG12	1:B:248:ILE:HD11	1.98	0.46
1:A:308:LEU:O	1:A:311:LYS:HB2	2.16	0.46
1:A:21:HIS:NE2	1:A:74:TYR:OH	2.49	0.46
1:A:71:ASP:CA	1:A:94:ARG:HH11	2.29	0.46
1:B:142:ILE:HD12	1:B:142:ILE:H	1.80	0.46
1:A:102:ILE:C	1:A:102:ILE:CD1	2.84	0.45
1:A:200:MSE:N	1:A:201:PRO:CD	2.76	0.45
1:B:21:HIS:NE2	1:B:74:TYR:OH	2.48	0.45
1:B:255:MSE:CE	1:B:304:LEU:HD13	2.43	0.45
1:A:275:ILE:HD12	1:A:275:ILE:HA	1.70	0.45
1:A:69:ILE:HG23	1:A:94:ARG:CZ	2.46	0.45
1:B:162:PHE:CG	1:B:172:MSE:HE3	2.52	0.45
1:A:207:LEU:HD12	1:B:207:LEU:HD12	1.97	0.45
1:A:11:ARG:HE	1:A:11:ARG:HB2	1.58	0.45
1:A:166:ASN:ND2	1:A:166:ASN:N	2.60	0.45
1:A:245:VAL:O	1:A:248:ILE:HG13	2.17	0.45
1:A:277:ASP:HB3	1:A:311:LYS:NZ	2.31	0.45
1:B:275:ILE:C	1:B:277:ASP:N	2.70	0.45
1:B:275:ILE:C	1:B:277:ASP:H	2.19	0.45
1:A:69:ILE:CG2	1:A:94:ARG:NH2	2.79	0.45
1:B:277:ASP:HB3	1:B:311:LYS:NZ	2.32	0.45
1:B:215:SER:O	1:B:216:HIS:HB2	2.17	0.45
1:B:228:LEU:HD23	1:B:228:LEU:HA	1.84	0.45
1:B:275:ILE:O	1:B:278:VAL:HG22	2.17	0.45
1:A:142:ILE:H	1:A:142:ILE:HD12	1.82	0.45
1:A:268:ILE:HD12	1:A:275:ILE:HG21	1.99	0.45
1:A:275:ILE:C	1:A:277:ASP:N	2.71	0.45
1:B:10:GLN:O	1:B:14:GLU:HG2	2.17	0.45
1:B:71:ASP:CA	1:B:94:ARG:HH11	2.30	0.45
1:B:21:HIS:CE1	1:B:74:TYR:OH	2.70	0.44
1:A:221:ILE:HB	1:A:256:PHE:CD1	2.53	0.44
1:A:252:LYS:NZ	4:A:332:HOH:O	2.42	0.44
1:A:173:GLU:O	1:A:176:SER:HB3	2.17	0.44
1:A:305:ALA:HB1	1:A:309:ARG:HH21	1.82	0.44
1:A:80:ILE:HG23	1:A:102:ILE:HG23	1.99	0.44
1:A:276:ASN:HB3	1:A:287:HIS:O	2.18	0.44
1:B:142:ILE:HD12	1:B:142:ILE:N	2.32	0.44
1:B:54:GLY:HA3	1:B:66:LEU:HD13	2.00	0.44
1:B:166:ASN:ND2	1:B:166:ASN:H	2.15	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:162:PHE:CG	1:A:172:MSE:HE3	2.52	0.44
1:A:21:HIS:CE1	1:A:74:TYR:OH	2.71	0.44
1:B:80:ILE:HG23	1:B:102:ILE:HG23	1.99	0.44
1:B:111:ASP:HB3	1:B:113:TYR:HD2	1.83	0.44
1:B:173:GLU:O	1:B:176:SER:HB3	2.17	0.44
1:B:221:ILE:HB	1:B:256:PHE:CD1	2.52	0.44
1:B:305:ALA:HB1	1:B:309:ARG:HH21	1.82	0.44
1:A:276:ASN:O	1:A:279:ALA:HB3	2.17	0.44
1:A:60:LEU:N	1:A:60:LEU:HD22	2.32	0.44
1:B:245:VAL:O	1:B:248:ILE:HG13	2.18	0.44
1:A:103:LYS:HG3	1:A:103:LYS:O	2.18	0.43
1:A:18:ILE:CD1	1:A:50:ILE:HG13	2.45	0.43
1:A:199:LEU:C	1:A:201:PRO:HD2	2.38	0.43
1:A:275:ILE:C	1:A:277:ASP:H	2.20	0.43
1:B:268:ILE:HD12	1:B:275:ILE:HG21	2.00	0.43
1:B:145:GLU:H	1:B:145:GLU:CD	2.20	0.43
1:A:10:GLN:O	1:A:14:GLU:HG2	2.17	0.43
1:A:166:ASN:H	1:A:166:ASN:ND2	2.16	0.43
1:A:215:SER:O	1:A:216:HIS:HB2	2.19	0.43
1:A:111:ASP:HB3	1:A:113:TYR:HD2	1.84	0.43
1:A:113:TYR:O	1:A:117:ASN:OD1	2.37	0.43
1:A:271:LYS:HD2	1:A:271:LYS:HA	1.90	0.43
1:B:199:LEU:C	1:B:201:PRO:HD2	2.38	0.43
1:B:210:PHE:HB3	1:B:211:GLU:H	1.48	0.43
1:A:142:ILE:HD12	1:A:142:ILE:N	2.33	0.43
1:A:275:ILE:O	1:A:278:VAL:HG22	2.17	0.43
1:B:276:ASN:HB3	1:B:287:HIS:O	2.19	0.43
1:A:54:GLY:HA3	1:A:66:LEU:HD13	2.01	0.43
1:B:105:ASP:O	1:B:119:VAL:HA	2.19	0.43
1:B:276:ASN:O	1:B:279:ALA:HB3	2.19	0.43
1:A:253:ILE:HG21	1:A:312:LEU:CD1	2.48	0.43
1:B:253:ILE:HG21	1:B:312:LEU:CD1	2.48	0.43
1:A:93:GLN:NE2	1:A:95:TYR:HE2	2.17	0.43
1:B:80:ILE:HA	1:B:102:ILE:O	2.19	0.42
1:B:289:ASN:HD22	1:B:289:ASN:HA	1.53	0.42
1:A:163:LEU:O	1:A:163:LEU:HD12	2.19	0.42
1:B:163:LEU:O	1:B:163:LEU:HD12	2.19	0.42
1:A:105:ASP:O	1:A:119:VAL:HA	2.19	0.42
1:A:17:THR:OG1	1:A:49:ASN:HB2	2.19	0.42
1:B:143:ILE:CG1	1:B:147:VAL:HB	2.49	0.42
1:A:143:ILE:CG1	1:A:147:VAL:HB	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:174:VAL:HG12	1:A:178:LEU:CD2	2.49	0.42
1:A:315:HIS:N	1:A:315:HIS:ND1	2.67	0.42
1:B:130:ILE:HA	1:B:130:ILE:HD13	1.91	0.42
1:B:40:TYR:CE2	1:B:134:ILE:HG22	2.55	0.42
1:A:210:PHE:O	1:A:211:GLU:HB2	2.19	0.42
1:A:210:PHE:HB3	1:A:211:GLU:H	1.47	0.42
1:B:174:VAL:HG12	1:B:178:LEU:CD2	2.50	0.42
1:B:221:ILE:HD13	1:B:256:PHE:CD1	2.41	0.42
1:A:80:ILE:HA	1:A:102:ILE:O	2.20	0.42
1:B:103:LYS:O	1:B:103:LYS:HG3	2.19	0.42
1:B:162:PHE:CG	1:B:172:MSE:CE	3.03	0.42
1:B:50:ILE:N	1:B:50:ILE:HD12	2.35	0.41
1:A:161:ARG:HG3	1:A:161:ARG:NH2	2.35	0.41
1:A:243:ASN:ND2	1:A:254:TRP:HH2	2.18	0.41
1:A:229:LYS:HD3	1:A:229:LYS:HA	1.84	0.41
1:B:19:ILE:CD1	1:B:79:VAL:HG13	2.51	0.41
1:B:4:ILE:HG21	1:B:118:PHE:HB2	2.03	0.41
1:B:243:ASN:ND2	1:B:254:TRP:HH2	2.18	0.41
1:B:113:TYR:O	1:B:117:ASN:OD1	2.38	0.41
1:B:17:THR:OG1	1:B:49:ASN:HB2	2.20	0.41
1:A:150:VAL:CG2	1:A:151:LEU:N	2.84	0.41
1:A:62:PHE:HB2	1:A:191:LYS:HE3	2.02	0.41
1:A:264:ILE:HD13	1:A:298:TRP:CD2	2.56	0.41
1:A:4:ILE:HG21	1:A:118:PHE:HB2	2.03	0.41
1:B:156:VAL:HG13	1:B:161:ARG:HG2	2.02	0.41
1:B:44:LYS:NZ	1:B:139:ASP:OD1	2.50	0.41
1:A:295:VAL:CB	1:A:300:GLU:HG2	2.51	0.41
1:B:18:ILE:CD1	1:B:50:ILE:HG13	2.46	0.41
1:A:201:PRO:HG2	1:A:202:PHE:H	1.86	0.41
1:A:306:GLN:NE2	4:A:336:HOH:O	2.54	0.41
1:B:62:PHE:HB2	1:B:191:LYS:HE3	2.02	0.41
1:A:162:PHE:CG	1:A:172:MSE:CE	3.03	0.41
1:A:19:ILE:CD1	1:A:79:VAL:HG13	2.51	0.41
1:A:40:TYR:CE2	1:A:134:ILE:HG22	2.55	0.40
1:A:252:LYS:HA	1:A:271:LYS:HB2	2.03	0.40
1:A:255:MSE:CE	1:A:304:LEU:HD13	2.41	0.40
1:A:130:ILE:HA	1:A:130:ILE:HD13	1.91	0.40
1:B:264:ILE:HD13	1:B:298:TRP:CD2	2.56	0.40
1:A:218:TYR:HA	1:A:253:ILE:O	2.21	0.40
1:A:236:ASN:HD22	1:A:236:ASN:HA	1.65	0.40
1:A:42:GLU:HG2	1:A:50:ILE:HD13	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:102:ILE:C	1:B:102:ILE:CD1	2.84	0.40
1:B:218:TYR:HA	1:B:253:ILE:O	2.22	0.40
1:B:93:GLN:NE2	1:B:95:TYR:HE2	2.19	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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	314/320 (98%)	269 (86%)	35 (11%)	10 (3%)	4	22
1	B	314/320 (98%)	269 (86%)	35 (11%)	10 (3%)	4	22
All	All	628/640 (98%)	538 (86%)	70 (11%)	20 (3%)	4	22

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	24	VAL
1	A	71	ASP
1	A	91	ASP
1	A	211	GLU
1	B	24	VAL
1	B	71	ASP
1	B	91	ASP
1	B	211	GLU
1	B	183	PHE
1	A	83	ASP
1	A	85	ALA
1	A	183	PHE
1	A	184	ASN
1	B	83	ASP
1	B	85	ALA

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Mol	Chain	Res	Type
1	B	184	ASN
1	A	56	ALA
1	A	75	SER
1	B	56	ALA
1	B	75	SER

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	278/276 (101%)	232 (84%)	46 (16%)	2	10
1	B	278/276 (101%)	235 (84%)	43 (16%)	2	11
All	All	556/552 (101%)	467 (84%)	89 (16%)	2	11

All (89) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	GLU
1	A	11	ARG
1	A	18	ILE
1	A	31	TYR
1	A	37	LEU
1	A	41	LEU
1	A	43	ARG
1	A	47	GLU
1	A	61	SER
1	A	71	ASP
1	A	73	VAL
1	A	76	ASP
1	A	94	ARG
1	A	96	LEU
1	A	99	GLN
1	A	102	ILE
1	A	106	HIS
1	A	111	ASP

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Mol	Chain	Res	Type
1	A	121	THR
1	A	122	GLU
1	A	135	SER
1	A	138	ASN
1	A	141	SER
1	A	153	LEU
1	A	158	ASP
1	A	161	ARG
1	A	166	ASN
1	A	172	MSE
1	A	178	LEU
1	A	183	PHE
1	A	186	ASN
1	A	200	MSE
1	A	211	GLU
1	A	220	GLN
1	A	243	ASN
1	A	245	VAL
1	A	251	LEU
1	A	254	TRP
1	A	265	ARG
1	A	268	ILE
1	A	275	ILE
1	A	289	ASN
1	A	299	ASP
1	A	304	LEU
1	A	315	HIS
1	A	316	HIS
1	B	3	GLU
1	B	11	ARG
1	B	18	ILE
1	B	31	TYR
1	B	37	LEU
1	B	41	LEU
1	B	43	ARG
1	B	47	GLU
1	B	61	SER
1	B	71	ASP
1	B	73	VAL
1	B	76	ASP
1	B	94	ARG
1	B	96	LEU

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Mol	Chain	Res	Type
1	B	99	GLN
1	B	102	ILE
1	B	106	HIS
1	B	111	ASP
1	B	121	THR
1	B	122	GLU
1	B	135	SER
1	B	138	ASN
1	B	153	LEU
1	B	158	ASP
1	B	161	ARG
1	B	166	ASN
1	B	178	LEU
1	B	183	PHE
1	B	186	ASN
1	B	200	MSE
1	B	211	GLU
1	B	220	GLN
1	B	243	ASN
1	B	245	VAL
1	B	251	LEU
1	B	254	TRP
1	B	265	ARG
1	B	268	ILE
1	B	275	ILE
1	B	289	ASN
1	B	299	ASP
1	B	304	LEU
1	B	316	HIS

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

Mol	Chain	Res	Type
1	A	6	ASN
1	A	93	GLN
1	A	97	ASN
1	A	106	HIS
1	A	166	ASN
1	A	186	ASN
1	A	190	ASN
1	A	203	GLN
1	A	208	GLN

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Mol	Chain	Res	Type
1	A	220	GLN
1	A	230	GLN
1	A	236	ASN
1	A	243	ASN
1	A	280	ASN
1	A	289	ASN
1	A	306	GLN
1	A	310	GLN
1	B	6	ASN
1	B	93	GLN
1	B	97	ASN
1	B	106	HIS
1	B	166	ASN
1	B	186	ASN
1	B	190	ASN
1	B	208	GLN
1	B	220	GLN
1	B	230	GLN
1	B	236	ASN
1	B	243	ASN
1	B	280	ASN
1	B	289	ASN
1	B	306	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 5 ligands modelled in this entry, 2 are monoatomic - leaving 3 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#|Z| > 2$	Counts	RMSZ	$\#|Z| > 2$
2	SO4	A	321	-	4,4,4	0.31	0	6,6,6	0.12	0
2	SO4	A	322	-	4,4,4	0.36	0	6,6,6	0.08	0
2	SO4	B	321	-	4,4,4	0.40	0	6,6,6	0.07	0

There are no bond length outliers.

There are no bond angle outliers.

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 (i)

6.1 Protein, DNA and RNA chains (i)

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	310/320 (96%)	0.29	7 (2%)	60	39	30, 66, 91, 115	0
1	B	310/320 (96%)	0.28	2 (0%)	89	78	30, 67, 91, 113	0
All	All	620/640 (96%)	0.28	9 (1%)	73	54	30, 66, 92, 115	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	116	VAL	4.1
1	A	313	LEU	3.4
1	A	314	GLU	3.1
1	A	315	HIS	2.9
1	B	90	ILE	2.5
1	A	70	ASP	2.3
1	A	47	GLU	2.2
1	A	291	SER	2.2
1	A	62	PHE	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 carbohydrates 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
2	SO4	A	321	5/5	0.86	0.25	102,109,110,112	0
2	SO4	A	322	5/5	0.92	0.19	96,96,104,107	0
2	SO4	B	321	5/5	0.94	0.19	86,93,98,102	0
3	MG	B	322	1/1	0.95	0.14	28,28,28,28	0
3	MG	A	323	1/1	0.98	0.22	27,27,27,27	0

6.5　Other polymers (i)

There are no such residues in this entry.