Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 10:16 AM GMT

PDB ID	:	3LIE
Title	:	Crystal Structure of the extracellular domain of the putative histidine kinase vpHK1S-Z8
Authors	:	Zhang, Z.; Hendrickson, W.A.
Deposited on	:	2010-01-24
Resolution	:	2.59 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

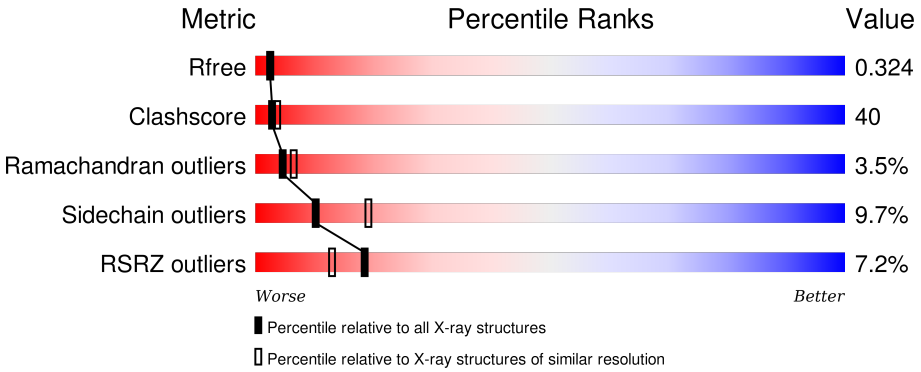
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.59 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}	91344	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

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. 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	295	6% 46% 36% 7% 10%
1	B	295	7% 45% 36% 7% • 11%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4317 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 Putative sensory box/GGDEF family protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	266	Total	C	N	O	S	0	0	0
			2151	1367	367	414	3			
1	B	262	Total	C	N	O	S	0	0	0
			2134	1361	360	410	3			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	26	MET	-	EXPRESSION TAG	UNP Q87SR8
A	27	GLU	-	EXPRESSION TAG	UNP Q87SR8
A	314	GLU	-	EXPRESSION TAG	UNP Q87SR8
A	315	HIS	-	EXPRESSION TAG	UNP Q87SR8
A	316	HIS	-	EXPRESSION TAG	UNP Q87SR8
A	317	HIS	-	EXPRESSION TAG	UNP Q87SR8
A	318	HIS	-	EXPRESSION TAG	UNP Q87SR8
A	319	HIS	-	EXPRESSION TAG	UNP Q87SR8
A	320	HIS	-	EXPRESSION TAG	UNP Q87SR8
B	26	MET	-	EXPRESSION TAG	UNP Q87SR8
B	27	GLU	-	EXPRESSION TAG	UNP Q87SR8
B	314	GLU	-	EXPRESSION TAG	UNP Q87SR8
B	315	HIS	-	EXPRESSION TAG	UNP Q87SR8
B	316	HIS	-	EXPRESSION TAG	UNP Q87SR8
B	317	HIS	-	EXPRESSION TAG	UNP Q87SR8
B	318	HIS	-	EXPRESSION TAG	UNP Q87SR8
B	319	HIS	-	EXPRESSION TAG	UNP Q87SR8
B	320	HIS	-	EXPRESSION TAG	UNP Q87SR8

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Mg 1 1	0	0

- Molecule 3 is water.

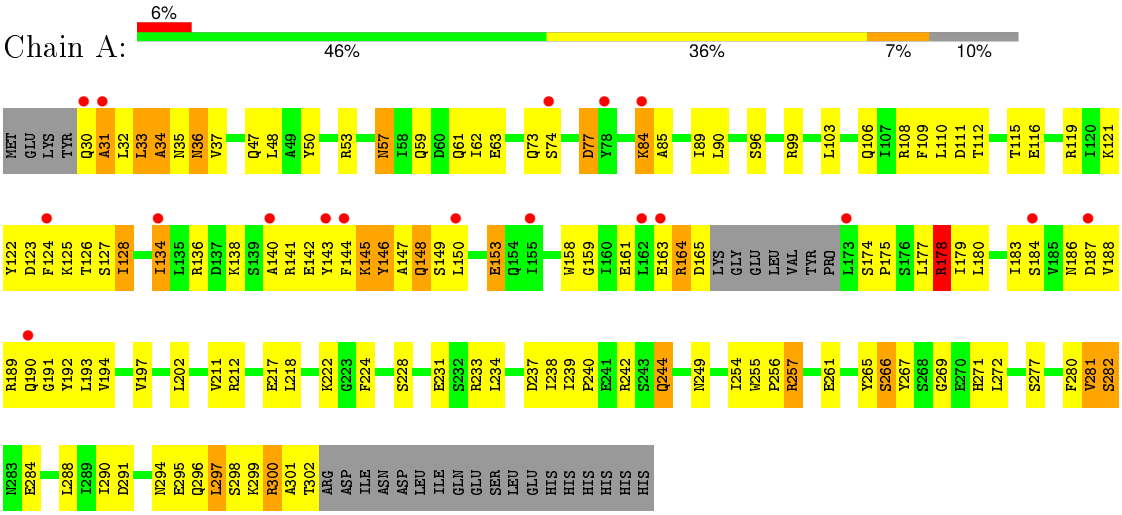
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	16	Total O 16 16	0	0
3	B	14	Total O 14 14	0	0

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

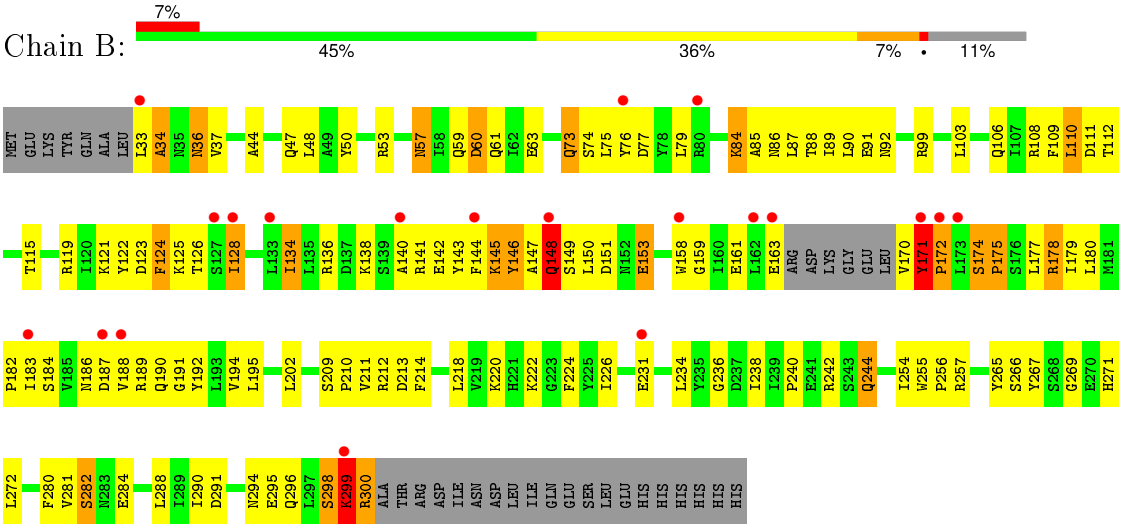
- Molecule 1: Putative sensory box/GGDEF family protein

Chain A:



- Molecule 1: Putative sensory box/GGDEF family protein

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	78.05Å 114.95Å 69.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.03 – 2.59 39.02 – 2.59	Depositor EDS
% Data completeness (in resolution range)	97.2 (39.03-2.59) 97.3 (39.02-2.59)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.13 (at 2.58Å)	Xtriage
Refinement program	REFMAC 5.5.0066	Depositor
R, R_{free}	0.254 , 0.326 0.260 , 0.324	Depositor DCC
R_{free} test set	991 reflections (5.35%)	DCC
Wilson B-factor (Å^2)	52.8	Xtriage
Anisotropy	0.180	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 52.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Outliers	0 of 19500 reflections	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	4317	wwPDB-VP
Average B, all atoms (Å^2)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 31.68 % of the origin peak, indicating pseudo translational symmetry.The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 1.0637e-03.The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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

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	0.82	2/2196 (0.1%)	0.86	2/2974 (0.1%)
1	B	0.85	1/2181 (0.0%)	0.87	3/2955 (0.1%)
All	All	0.83	3/4377 (0.1%)	0.86	5/5929 (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	B	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	50	TYR	CE1-CZ	-6.29	1.30	1.38
1	A	50	TYR	CG-CD2	-5.91	1.31	1.39
1	B	50	TYR	CG-CD1	-5.81	1.31	1.39

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	178	ARG	NE-CZ-NH1	-9.38	115.61	120.30
1	B	178	ARG	NE-CZ-NH2	-8.51	116.05	120.30
1	A	178	ARG	NE-CZ-NH2	8.31	124.45	120.30
1	B	178	ARG	NE-CZ-NH1	6.48	123.54	120.30
1	B	60	ASP	CB-CG-OD2	5.45	123.21	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	299	LYS	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	2151	0	2106	182	0
1	B	2134	0	2095	178	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	16	0	0	3	0
3	B	14	0	0	0	0
All	All	4317	0	4201	339	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 40.

All (339) 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:177:LEU:CD2	1:A:179:ILE:HD11	1.63	1.26
1:A:126:THR:OG1	1:A:128:ILE:CD1	1.85	1.25
1:A:177:LEU:CD2	1:A:179:ILE:CD1	2.18	1.21
1:B:177:LEU:CD2	1:B:179:ILE:HD11	1.69	1.20
1:A:126:THR:OG1	1:A:128:ILE:HD11	1.33	1.19
1:A:36:ASN:HD22	1:A:36:ASN:C	1.36	1.18
1:A:244:GLN:NE2	1:A:244:GLN:H	1.45	1.12
1:A:177:LEU:HD22	1:A:179:ILE:HD11	1.15	1.11
1:A:32:LEU:HA	1:A:33:LEU:CB	1.68	1.11
1:B:299:LYS:O	1:B:300:ARG:HB2	1.47	1.10
1:B:177:LEU:CD2	1:B:179:ILE:CD1	2.30	1.10
1:A:244:GLN:HE21	1:A:244:GLN:N	1.49	1.09
1:B:36:ASN:HD22	1:B:36:ASN:C	1.55	1.07
1:A:161:GLU:CD	1:A:178:ARG:NH1	2.08	1.06
1:B:177:LEU:HD22	1:B:179:ILE:HD11	1.33	1.05
1:B:163:GLU:C	1:B:170:VAL:HG11	1.78	1.04
1:A:84:LYS:HB2	1:A:84:LYS:NZ	1.71	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:244:GLN:H	1:B:244:GLN:NE2	1.54	1.02
1:B:163:GLU:C	1:B:170:VAL:CG1	2.26	1.02
1:B:177:LEU:HD21	1:B:179:ILE:CD1	1.92	0.99
1:B:170:VAL:HG12	1:B:170:VAL:O	1.63	0.99
1:A:177:LEU:HD21	1:A:179:ILE:CD1	1.92	0.98
1:B:171:TYR:HB3	1:B:172:PRO:HB3	1.42	0.98
1:A:36:ASN:ND2	1:A:36:ASN:C	2.14	0.97
1:B:84:LYS:HB2	1:B:84:LYS:NZ	1.78	0.97
1:B:244:GLN:HE21	1:B:244:GLN:N	1.64	0.95
1:A:186:ASN:O	1:A:188:VAL:HG23	1.68	0.94
1:B:36:ASN:HD22	1:B:37:VAL:N	1.66	0.93
1:B:177:LEU:HD21	1:B:179:ILE:HD11	1.47	0.93
1:B:134:ILE:N	1:B:134:ILE:HD12	1.84	0.93
1:B:110:LEU:N	1:B:110:LEU:HD12	1.83	0.93
1:A:177:LEU:CD2	1:A:179:ILE:HD13	1.98	0.92
1:A:57:ASN:HD21	1:B:212:ARG:HH12	1.09	0.91
1:A:161:GLU:CD	1:A:178:ARG:HH11	1.73	0.90
1:B:244:GLN:HE21	1:B:244:GLN:H	0.94	0.89
1:B:161:GLU:CD	1:B:178:ARG:HH12	1.76	0.89
1:A:32:LEU:CA	1:A:33:LEU:CB	2.52	0.88
1:A:267:TYR:CE2	1:A:269:GLY:HA2	2.10	0.87
1:B:109:PHE:C	1:B:110:LEU:HD12	1.95	0.86
1:B:36:ASN:ND2	1:B:36:ASN:C	2.28	0.86
1:A:37:VAL:HG22	1:A:297:LEU:HD13	1.58	0.86
1:B:110:LEU:CD1	1:B:110:LEU:N	2.39	0.85
1:A:299:LYS:O	1:A:300:ARG:NH2	2.09	0.85
1:B:299:LYS:HD3	1:B:300:ARG:N	1.92	0.84
1:A:53:ARG:CB	1:B:53:ARG:HG2	2.07	0.84
1:A:212:ARG:HH12	1:B:57:ASN:HD21	1.25	0.84
1:B:145:LYS:HA	1:B:148:GLN:CG	2.08	0.83
1:B:186:ASN:O	1:B:188:VAL:HG23	1.77	0.83
1:A:147:ALA:HA	1:A:150:LEU:HD12	1.60	0.82
1:B:299:LYS:HD3	1:B:299:LYS:C	2.00	0.82
1:B:170:VAL:CG1	1:B:170:VAL:O	2.27	0.82
1:B:180:LEU:HD23	1:B:194:VAL:HG22	1.60	0.81
1:B:267:TYR:OH	1:B:294:ASN:ND2	2.13	0.81
1:B:171:TYR:HB3	1:B:172:PRO:CB	2.11	0.80
1:A:33:LEU:O	1:A:34:ALA:CB	2.29	0.80
1:A:180:LEU:HD23	1:A:194:VAL:HG22	1.62	0.80
1:B:163:GLU:C	1:B:170:VAL:CB	2.49	0.80
1:A:84:LYS:HZ2	1:A:84:LYS:HB2	1.43	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:33:LEU:O	1:B:34:ALA:CB	2.29	0.79
1:A:300:ARG:CZ	1:A:300:ARG:HA	2.12	0.79
1:B:126:THR:OG1	1:B:128:ILE:CD1	2.31	0.79
1:B:84:LYS:HB2	1:B:84:LYS:HZ3	1.48	0.78
1:B:163:GLU:C	1:B:170:VAL:HB	2.04	0.78
1:A:145:LYS:HA	1:A:148:GLN:CG	2.14	0.77
1:A:267:TYR:OH	1:A:294:ASN:ND2	2.18	0.77
1:B:126:THR:OG1	1:B:128:ILE:HD11	1.85	0.77
1:B:145:LYS:HA	1:B:148:GLN:HG2	1.66	0.77
1:B:171:TYR:HD2	1:B:171:TYR:H	1.29	0.76
1:A:84:LYS:HZ3	1:A:84:LYS:HB2	1.47	0.76
1:B:177:LEU:CD2	1:B:179:ILE:HD13	2.15	0.75
1:A:119:ARG:NH2	1:A:121:LYS:NZ	2.34	0.75
1:B:134:ILE:CD1	1:B:134:ILE:N	2.50	0.75
1:A:53:ARG:HG2	1:B:53:ARG:CB	2.16	0.75
1:B:147:ALA:HA	1:B:150:LEU:HD12	1.68	0.74
1:A:85:ALA:O	1:A:89:ILE:HD12	1.89	0.73
1:A:126:THR:OG1	1:A:128:ILE:HD12	1.86	0.73
1:B:295:GLU:O	1:B:298:SER:OG	2.07	0.72
1:B:134:ILE:CD1	1:B:134:ILE:H	2.02	0.72
1:A:184:SER:HB3	1:A:189:ARG:HA	1.72	0.72
1:A:110:LEU:HD12	1:A:110:LEU:N	2.05	0.72
1:B:267:TYR:CE2	1:B:269:GLY:HA2	2.25	0.72
1:A:282:SER:OG	1:A:284:GLU:HB2	1.89	0.72
1:A:296:GLN:C	1:A:298:SER:H	1.94	0.71
1:A:300:ARG:NH1	1:A:300:ARG:HA	2.04	0.71
1:B:146:TYR:HD1	1:B:158:TRP:CZ3	2.09	0.71
1:A:134:ILE:HD12	1:A:134:ILE:N	2.05	0.71
1:B:177:LEU:HD23	1:B:178:ARG:N	2.05	0.71
1:B:161:GLU:CD	1:B:178:ARG:NH1	2.44	0.71
1:A:164:ARG:HG3	1:A:165:ASP:N	2.06	0.71
1:A:128:ILE:HD12	1:A:128:ILE:H	1.55	0.71
1:A:57:ASN:HD21	1:B:212:ARG:NH1	1.87	0.70
1:A:109:PHE:C	1:A:110:LEU:HD12	2.12	0.70
1:B:296:GLN:O	1:B:299:LYS:HG3	1.90	0.70
1:A:57:ASN:HD22	1:B:212:ARG:HH22	1.39	0.70
1:B:222:LYS:HD3	1:B:224:PHE:HD2	1.55	0.70
1:B:134:ILE:H	1:B:134:ILE:HD12	1.55	0.70
1:B:144:PHE:O	1:B:147:ALA:HB3	1.91	0.70
1:A:161:GLU:CD	1:A:178:ARG:HH12	1.94	0.70
1:B:145:LYS:HA	1:B:148:GLN:HG3	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:141:ARG:O	1:B:145:LYS:HD2	1.91	0.69
1:A:110:LEU:CD1	1:A:110:LEU:N	2.55	0.69
1:B:180:LEU:CD2	1:B:194:VAL:HG22	2.22	0.69
1:A:57:ASN:ND2	1:B:212:ARG:HH22	1.91	0.69
1:A:144:PHE:O	1:A:147:ALA:HB3	1.93	0.68
1:A:145:LYS:HA	1:A:148:GLN:HG2	1.75	0.68
1:B:177:LEU:HD21	1:B:179:ILE:HD13	1.76	0.67
1:A:145:LYS:HA	1:A:148:GLN:HG3	1.75	0.67
1:A:126:THR:HG1	1:A:128:ILE:CD1	2.05	0.67
1:B:142:GLU:HA	1:B:145:LYS:HD3	1.74	0.67
1:B:33:LEU:O	1:B:34:ALA:HB2	1.93	0.67
1:B:299:LYS:CD	1:B:300:ARG:N	2.57	0.67
1:A:145:LYS:O	1:A:148:GLN:HB2	1.95	0.66
1:B:145:LYS:O	1:B:148:GLN:HB2	1.95	0.66
1:A:244:GLN:HE21	1:A:244:GLN:H	0.74	0.66
1:B:84:LYS:HZ2	1:B:84:LYS:HB2	1.60	0.65
1:A:177:LEU:HD23	1:A:179:ILE:HD13	1.77	0.65
1:A:30:GLN:O	1:A:31:ALA:HB2	1.96	0.65
1:A:267:TYR:CZ	1:A:269:GLY:HA2	2.32	0.65
1:A:296:GLN:O	1:A:298:SER:N	2.30	0.65
1:A:161:GLU:OE1	1:A:178:ARG:NH1	2.25	0.65
1:A:53:ARG:HG2	1:B:53:ARG:HG2	1.78	0.64
1:A:140:ALA:O	1:A:145:LYS:HE2	1.97	0.64
1:A:36:ASN:HD22	1:A:37:VAL:N	1.91	0.63
1:A:302:THR:CG2	3:A:322:HOH:O	2.46	0.63
1:A:141:ARG:O	1:A:145:LYS:HD2	1.98	0.63
1:A:147:ALA:HA	1:A:150:LEU:CD1	2.27	0.63
1:A:53:ARG:CG	1:B:53:ARG:HG2	2.29	0.63
1:B:85:ALA:O	1:B:89:ILE:HD12	1.98	0.63
1:A:146:TYR:HD1	1:A:158:TRP:CZ3	2.16	0.62
1:A:106:GLN:NE2	1:A:119:ARG:HE	1.97	0.62
1:B:255:TRP:HB3	1:B:256:PRO:HD3	1.81	0.62
1:B:145:LYS:CA	1:B:148:GLN:HG2	2.29	0.62
1:A:212:ARG:HH22	1:B:57:ASN:ND2	1.97	0.61
1:B:265:TYR:HD1	1:B:272:LEU:HD11	1.64	0.61
1:A:119:ARG:NH2	1:A:121:LYS:HZ1	1.99	0.61
1:A:146:TYR:HE2	1:A:150:LEU:HD21	1.65	0.61
1:A:180:LEU:CD2	1:A:194:VAL:HG22	2.29	0.61
1:A:222:LYS:HD3	1:A:224:PHE:HD2	1.64	0.61
1:A:299:LYS:O	1:A:300:ARG:CZ	2.49	0.61
1:A:161:GLU:HG2	1:A:178:ARG:HH12	1.65	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:LEU:O	1:A:34:ALA:HB2	2.00	0.60
1:B:119:ARG:NH2	1:B:121:LYS:NZ	2.48	0.60
1:A:177:LEU:HD21	1:A:179:ILE:HD11	1.61	0.60
1:B:36:ASN:ND2	1:B:37:VAL:N	2.46	0.60
1:B:265:TYR:CD1	1:B:272:LEU:HD11	2.36	0.60
1:A:161:GLU:CG	1:A:178:ARG:HH12	2.13	0.60
1:A:177:LEU:HD22	1:A:179:ILE:CD1	1.99	0.60
1:B:163:GLU:O	1:B:170:VAL:HG21	2.02	0.60
1:A:48:LEU:HD21	1:A:290:ILE:HG13	1.82	0.59
1:A:211:VAL:HG21	1:B:61:GLN:HG2	1.84	0.59
1:A:53:ARG:HG2	1:B:53:ARG:CG	2.32	0.59
1:B:163:GLU:O	1:B:170:VAL:CB	2.50	0.59
1:A:257:ARG:NH2	1:A:261:GLU:OE2	2.35	0.59
1:B:177:LEU:C	1:B:177:LEU:HD23	2.22	0.59
1:B:171:TYR:HB3	1:B:172:PRO:CA	2.33	0.58
1:A:177:LEU:HD21	1:A:179:ILE:HD13	1.75	0.58
1:B:108:ARG:HG2	1:B:119:ARG:HA	1.85	0.58
1:A:103:LEU:HD12	1:A:197:VAL:HG13	1.85	0.58
1:B:147:ALA:HA	1:B:150:LEU:CD1	2.34	0.58
1:A:255:TRP:HB3	1:A:256:PRO:HD3	1.86	0.58
1:B:106:GLN:NE2	1:B:119:ARG:HE	2.02	0.57
1:A:212:ARG:HH22	1:B:57:ASN:HD22	1.49	0.57
1:A:53:ARG:HG2	1:B:53:ARG:HB2	1.87	0.57
1:A:288:LEU:HD12	1:A:288:LEU:N	2.19	0.57
1:B:146:TYR:HD1	1:B:158:TRP:HZ3	1.50	0.57
1:A:217:GLU:OE2	1:A:233:ARG:NH1	2.37	0.57
1:B:144:PHE:O	1:B:148:GLN:HG2	2.05	0.56
1:A:33:LEU:O	1:A:34:ALA:HB3	2.05	0.56
1:A:296:GLN:C	1:A:298:SER:N	2.59	0.56
1:A:280:PHE:C	1:A:281:VAL:HG23	2.25	0.56
1:A:108:ARG:HG2	1:A:119:ARG:HA	1.86	0.56
1:B:282:SER:OG	1:B:284:GLU:HB2	2.05	0.55
1:B:140:ALA:O	1:B:145:LYS:HE2	2.05	0.55
1:B:136:ARG:HB2	1:B:138:LYS:HE2	1.88	0.55
1:B:177:LEU:HD22	1:B:179:ILE:CD1	2.13	0.55
1:A:36:ASN:ND2	1:A:36:ASN:O	2.30	0.55
1:A:85:ALA:O	1:A:89:ILE:CD1	2.54	0.55
1:A:145:LYS:CA	1:A:148:GLN:HG2	2.36	0.54
1:B:148:GLN:O	1:B:150:LEU:N	2.35	0.54
1:A:134:ILE:N	1:A:134:ILE:CD1	2.71	0.54
1:B:111:ASP:OD2	1:B:115:THR:HB	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:136:ARG:HB2	1:A:138:LYS:HE2	1.89	0.54
1:A:144:PHE:O	1:A:148:GLN:HG2	2.08	0.54
1:B:184:SER:HB3	1:B:189:ARG:HA	1.90	0.54
1:A:161:GLU:CG	1:A:178:ARG:NH1	2.70	0.53
1:B:171:TYR:CD2	1:B:171:TYR:N	2.71	0.53
1:B:244:GLN:N	1:B:244:GLN:NE2	2.35	0.53
1:B:280:PHE:C	1:B:281:VAL:HG23	2.28	0.53
1:A:53:ARG:HB2	1:B:53:ARG:HG2	1.89	0.53
1:B:163:GLU:O	1:B:170:VAL:HB	2.08	0.52
1:B:299:LYS:O	1:B:300:ARG:CB	2.33	0.52
1:B:145:LYS:O	1:B:148:GLN:CB	2.57	0.52
1:A:53:ARG:HB3	1:B:53:ARG:HG2	1.88	0.52
1:A:146:TYR:CE2	1:A:150:LEU:HD21	2.45	0.52
1:B:143:TYR:HB3	1:B:158:TRP:CE2	2.45	0.52
1:A:61:GLN:HG2	1:B:211:VAL:HG21	1.91	0.52
1:B:238:ILE:O	1:B:240:PRO:HD3	2.10	0.52
1:B:119:ARG:NH2	1:B:121:LYS:HZ1	2.08	0.52
1:B:48:LEU:HD21	1:B:290:ILE:HG13	1.92	0.52
1:B:209:SER:O	1:B:213:ASP:N	2.41	0.51
1:A:212:ARG:NH1	1:B:57:ASN:HD21	2.02	0.51
1:B:99:ARG:HA	1:B:122:TYR:CE1	2.45	0.51
1:B:186:ASN:O	1:B:188:VAL:N	2.44	0.51
1:A:146:TYR:HD2	1:A:146:TYR:C	2.14	0.51
1:B:148:GLN:C	1:B:150:LEU:H	2.15	0.51
1:B:106:GLN:NE2	1:B:121:LYS:HE2	2.26	0.51
1:B:146:TYR:HE2	1:B:150:LEU:HD21	1.76	0.50
1:A:126:THR:OG1	1:A:128:ILE:CG1	2.57	0.50
1:B:299:LYS:CD	1:B:300:ARG:H	2.22	0.50
1:B:163:GLU:O	1:B:170:VAL:CG2	2.60	0.50
1:A:186:ASN:O	1:A:188:VAL:N	2.44	0.50
1:B:153:GLU:OE2	1:B:183:ILE:HA	2.12	0.50
1:B:158:TRP:CG	1:B:159:GLY:N	2.79	0.50
1:A:298:SER:O	1:A:298:SER:OG	2.29	0.50
1:B:210:PRO:O	1:B:211:VAL:C	2.49	0.50
1:A:183:ILE:HD11	1:A:193:LEU:HB2	1.93	0.50
1:A:145:LYS:O	1:A:148:GLN:CB	2.60	0.49
1:A:158:TRP:HD1	1:A:178:ARG:HE	1.58	0.49
1:A:161:GLU:O	1:A:175:PRO:HA	2.11	0.49
1:A:119:ARG:HH21	1:A:121:LYS:HZ3	1.60	0.49
1:B:85:ALA:O	1:B:89:ILE:CD1	2.59	0.49
1:A:143:TYR:HB3	1:A:158:TRP:CE2	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:146:TYR:CD2	1:A:146:TYR:C	2.86	0.49
1:A:158:TRP:CG	1:A:159:GLY:N	2.79	0.49
1:B:224:PHE:CD1	1:B:236:GLY:HA3	2.48	0.49
1:B:146:TYR:HD1	1:B:158:TRP:CE3	2.31	0.49
1:A:295:GLU:O	1:A:298:SER:HB3	2.13	0.48
1:B:158:TRP:CD1	1:B:178:ARG:HD2	2.48	0.48
1:B:112:THR:HG22	1:B:189:ARG:HG2	1.96	0.48
1:A:59:GLN:HA	1:A:62:ILE:HD12	1.93	0.48
1:A:211:VAL:HG23	3:A:20:HOH:O	2.12	0.48
1:B:146:TYR:CD1	1:B:158:TRP:CE3	3.02	0.48
1:B:288:LEU:N	1:B:288:LEU:HD12	2.28	0.48
1:A:112:THR:HG22	1:A:189:ARG:HG2	1.96	0.47
1:A:222:LYS:HD3	1:A:224:PHE:CD2	2.48	0.47
1:B:59:GLN:O	1:B:63:GLU:HG3	2.14	0.47
1:A:126:THR:HG1	1:A:128:ILE:HD12	1.73	0.47
1:B:161:GLU:O	1:B:175:PRO:HA	2.15	0.47
1:B:33:LEU:O	1:B:34:ALA:HB3	2.10	0.47
1:B:74:SER:HB2	1:B:90:LEU:HA	1.95	0.47
1:A:146:TYR:HD1	1:A:158:TRP:HZ3	1.62	0.47
1:A:177:LEU:HD23	1:A:179:ILE:CD1	2.30	0.47
1:A:116:GLU:HG3	1:A:136:ARG:O	2.15	0.47
1:B:124:PHE:O	1:B:124:PHE:CD1	2.68	0.47
1:A:300:ARG:HA	1:A:300:ARG:NE	2.27	0.46
1:A:110:LEU:O	1:A:192:TYR:N	2.44	0.46
1:B:147:ALA:O	1:B:150:LEU:HB2	2.15	0.46
1:B:123:ASP:C	1:B:123:ASP:OD2	2.54	0.46
1:B:161:GLU:CG	1:B:178:ARG:HH12	2.29	0.46
1:B:161:GLU:OE1	1:B:178:ARG:NH1	2.48	0.46
1:A:134:ILE:HD12	1:A:134:ILE:H	1.81	0.46
1:A:244:GLN:NE2	1:A:244:GLN:N	2.28	0.45
1:A:163:GLU:O	1:A:164:ARG:O	2.34	0.45
1:A:30:GLN:O	1:A:31:ALA:CB	2.64	0.45
1:A:143:TYR:O	1:A:146:TYR:HB3	2.17	0.45
1:B:150:LEU:O	1:B:189:ARG:NH2	2.48	0.45
1:A:217:GLU:HG2	1:A:228:SER:HB2	1.98	0.45
1:A:265:TYR:CD1	1:A:272:LEU:HD11	2.52	0.45
1:A:212:ARG:HH21	1:B:60:ASP:CG	2.20	0.45
1:B:222:LYS:HD3	1:B:224:PHE:CD2	2.44	0.45
1:A:148:GLN:C	1:A:150:LEU:H	2.20	0.45
1:A:302:THR:HG21	3:A:322:HOH:O	2.14	0.45
1:B:146:TYR:HD2	1:B:146:TYR:C	2.20	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:271:HIS:HD2	1:B:291:ASP:OD1	1.99	0.45
1:A:150:LEU:O	1:A:189:ARG:NH2	2.45	0.45
1:A:99:ARG:HA	1:A:122:TYR:CE1	2.52	0.45
1:A:57:ASN:ND2	1:B:212:ARG:NH2	2.63	0.45
1:B:146:TYR:CD2	1:B:146:TYR:C	2.90	0.44
1:A:239:ILE:HB	1:A:242:ARG:HD2	1.99	0.44
1:A:146:TYR:HD1	1:A:158:TRP:CE3	2.34	0.44
1:A:254:ILE:HG12	1:A:266:SER:HB3	1.99	0.44
1:B:191:GLY:C	1:B:192:TYR:CD2	2.91	0.44
1:A:147:ALA:O	1:A:150:LEU:HB2	2.18	0.44
1:B:151:ASP:O	1:B:182:PRO:HG2	2.17	0.44
1:B:254:ILE:O	1:B:255:TRP:C	2.56	0.44
1:A:143:TYR:CD1	1:A:144:PHE:N	2.85	0.44
1:B:143:TYR:O	1:B:146:TYR:HB3	2.18	0.44
1:A:224:PHE:CD2	1:A:237:ASP:HB3	2.53	0.44
1:B:220:LYS:HE2	1:B:226:ILE:CG2	2.48	0.44
1:A:142:GLU:HA	1:A:145:LYS:CD	2.48	0.43
1:A:146:TYR:CD1	1:A:158:TRP:CE3	3.06	0.43
1:A:177:LEU:HD23	1:A:178:ARG:N	2.33	0.43
1:A:134:ILE:CD1	1:A:134:ILE:H	2.31	0.43
1:A:218:LEU:CD2	1:A:288:LEU:HG	2.48	0.43
1:A:234:LEU:O	1:A:242:ARG:HD3	2.19	0.43
1:B:87:LEU:O	1:B:88:THR:C	2.57	0.43
1:A:191:GLY:C	1:A:192:TYR:CD2	2.92	0.43
1:B:119:ARG:NH2	1:B:121:LYS:CE	2.82	0.43
1:A:271:HIS:HD2	1:A:291:ASP:OD1	2.01	0.43
1:A:77:ASP:OD1	1:A:77:ASP:N	2.52	0.43
1:A:147:ALA:HB1	1:A:192:TYR:CD1	2.54	0.43
1:A:280:PHE:CD2	1:A:281:VAL:HG23	2.54	0.43
1:B:179:ILE:HB	1:B:195:LEU:HB2	2.01	0.43
1:B:170:VAL:O	1:B:171:TYR:O	2.37	0.43
1:B:147:ALA:O	1:B:148:GLN:C	2.57	0.42
1:A:57:ASN:ND2	1:B:212:ARG:HH12	1.93	0.42
1:B:87:LEU:O	1:B:90:LEU:N	2.53	0.42
1:B:174:SER:HA	1:B:175:PRO:HD3	1.78	0.42
1:B:47:GLN:OE1	1:B:212:ARG:HD2	2.19	0.42
1:B:103:LEU:O	1:B:103:LEU:HD12	2.20	0.42
1:A:238:ILE:O	1:A:240:PRO:HD3	2.19	0.42
1:A:164:ARG:O	1:A:165:ASP:C	2.58	0.42
1:B:146:TYR:CE2	1:B:150:LEU:HD21	2.55	0.42
1:B:109:PHE:CZ	1:B:191:GLY:HA3	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:75:LEU:O	1:B:79:LEU:HG	2.20	0.42
1:B:177:LEU:CD2	1:B:177:LEU:C	2.88	0.41
1:A:302:THR:O	1:A:302:THR:OG1	2.30	0.41
1:B:86:ASN:HA	1:B:89:ILE:HD12	2.01	0.41
1:B:73:GLN:O	1:B:76:TYR:N	2.54	0.41
1:A:111:ASP:OD2	1:A:115:THR:HB	2.20	0.41
1:A:202:LEU:HD23	1:A:202:LEU:HA	1.67	0.41
1:B:150:LEU:HB2	1:B:182:PRO:HG3	2.01	0.41
1:A:300:ARG:HB3	1:A:301:ALA:H	1.52	0.41
1:A:146:TYR:HD2	1:A:146:TYR:O	2.03	0.41
1:B:119:ARG:HH21	1:B:121:LYS:NZ	2.18	0.41
1:A:148:GLN:HA	1:A:148:GLN:HE21	1.86	0.41
1:A:47:GLN:OE1	1:A:212:ARG:HD2	2.19	0.41
1:B:218:LEU:CD2	1:B:288:LEU:HG	2.51	0.41
1:B:202:LEU:HD23	1:B:202:LEU:HA	1.81	0.41
1:A:123:ASP:O	1:A:127:SER:N	2.37	0.41
1:B:112:THR:HG23	1:B:190:GLN:C	2.41	0.41
1:A:297:LEU:HA	1:A:297:LEU:HD23	1.64	0.41
1:A:119:ARG:NH2	1:A:121:LYS:CE	2.84	0.41
1:A:59:GLN:O	1:A:63:GLU:HG3	2.21	0.41
1:B:44:ALA:HA	1:B:214:PHE:CE2	2.56	0.41
1:A:106:GLN:HE22	1:A:119:ARG:HE	1.66	0.41
1:B:91:GLU:O	1:B:92:ASN:C	2.57	0.41
1:B:234:LEU:O	1:B:242:ARG:HD3	2.20	0.41
1:A:148:GLN:CA	1:A:148:GLN:HE21	2.33	0.40
1:B:222:LYS:HE2	1:B:222:LYS:HB2	1.51	0.40
1:A:161:GLU:OE2	1:A:178:ARG:NH1	2.52	0.40
1:A:126:THR:CB	1:A:128:ILE:HD11	2.41	0.40
1:A:74:SER:HB2	1:A:90:LEU:HA	2.03	0.40
1:A:148:GLN:O	1:A:150:LEU:N	2.50	0.40
1:B:158:TRP:O	1:B:159:GLY:O	2.38	0.40
1:B:158:TRP:HD1	1:B:178:ARG:HD2	1.87	0.40
1:B:106:GLN:HE21	1:B:121:LYS:HE2	1.86	0.40
1:A:153:GLU:OE2	1:A:183:ILE:HA	2.20	0.40
1:A:112:THR:HG23	1:A:190:GLN:C	2.42	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	262/295 (89%)	232 (88%)	20 (8%)	10 (4%)	4	5
1	B	258/295 (88%)	228 (88%)	22 (8%)	8 (3%)	5	8
All	All	520/590 (88%)	460 (88%)	42 (8%)	18 (4%)	4	6

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	31	ALA
1	A	33	LEU
1	A	34	ALA
1	A	164	ARG
1	A	187	ASP
1	A	297	LEU
1	B	34	ALA
1	B	172	PRO
1	B	187	ASP
1	B	149	SER
1	B	282	SER
1	A	35	ASN
1	A	149	SER
1	A	282	SER
1	B	175	PRO
1	B	148	GLN
1	B	171	TYR
1	A	281	VAL

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	237/269 (88%)	214 (90%)	23 (10%)	10	19
1	B	238/269 (88%)	215 (90%)	23 (10%)	10	19
All	All	475/538 (88%)	429 (90%)	46 (10%)	10	19

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	ASN
1	A	57	ASN
1	A	73	GLN
1	A	77	ASP
1	A	84	LYS
1	A	96	SER
1	A	124	PHE
1	A	125	LYS
1	A	128	ILE
1	A	134	ILE
1	A	145	LYS
1	A	146	TYR
1	A	148	GLN
1	A	153	GLU
1	A	174	SER
1	A	178	ARG
1	A	231	GLU
1	A	244	GLN
1	A	249	ASN
1	A	257	ARG
1	A	266	SER
1	A	277	SER
1	A	300	ARG
1	B	36	ASN
1	B	57	ASN
1	B	73	GLN
1	B	77	ASP
1	B	84	LYS
1	B	110	LEU
1	B	124	PHE
1	B	125	LYS
1	B	128	ILE
1	B	134	ILE

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Mol	Chain	Res	Type
1	B	145	LYS
1	B	146	TYR
1	B	148	GLN
1	B	153	GLU
1	B	171	TYR
1	B	174	SER
1	B	231	GLU
1	B	244	GLN
1	B	257	ARG
1	B	266	SER
1	B	298	SER
1	B	299	LYS
1	B	300	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	36	ASN
1	A	57	ASN
1	A	61	GLN
1	A	101	GLN
1	A	106	GLN
1	A	148	GLN
1	A	244	GLN
1	A	271	HIS
1	A	294	ASN
1	B	36	ASN
1	B	57	ASN
1	B	61	GLN
1	B	101	GLN
1	B	106	GLN
1	B	148	GLN
1	B	244	GLN
1	B	271	HIS
1	B	294	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	266/295 (90%)	0.57	18 (6%)	20	15	20, 55, 82, 86	0
1	B	262/295 (88%)	0.64	20 (7%)	17	12	34, 55, 82, 86	0
All	All	528/590 (89%)	0.60	38 (7%)	18	13	20, 55, 82, 86	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	171	TYR	5.8
1	B	172	PRO	5.2
1	B	140	ALA	4.6
1	B	128	ILE	4.6
1	B	80	ARG	4.2
1	B	76	TYR	3.9
1	B	173	LEU	3.9
1	A	144	PHE	3.5
1	B	133	LEU	3.4
1	B	162	LEU	3.4
1	A	78	TYR	3.3
1	A	140	ALA	3.2
1	B	187	ASP	3.1
1	A	74	SER	3.0
1	A	187	ASP	2.9
1	B	158	TRP	2.9
1	B	148	GLN	2.8
1	A	124	PHE	2.8
1	B	188	VAL	2.7
1	A	162	LEU	2.7
1	A	31	ALA	2.6
1	A	155	ILE	2.6
1	B	163	GLU	2.6
1	B	33	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	134	ILE	2.5
1	B	127	SER	2.5
1	A	190	GLN	2.5
1	A	184	SER	2.4
1	B	144	PHE	2.4
1	A	173	LEU	2.3
1	A	163	GLU	2.3
1	A	150	LEU	2.3
1	B	231	GLU	2.3
1	B	299	LYS	2.3
1	A	143	TYR	2.1
1	A	84	LYS	2.1
1	A	30	GLN	2.0
1	B	183	ILE	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} 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	LLDF	B-factors(Å^2)	Q<0.9
2	MG	A	2	1/1	0.94	0.61	-	63,63,63,63	0
2	MG	B	1	1/1	0.93	0.56	-	55,55,55,55	0

6.5 Other polymers (i)

There are no such residues in this entry.