Full wwPDB X-ray Structure Validation Report ⓘ

Jun 3, 2020 – 02:30 pm BST

PDB ID	:	1HSL
Title	:	REFINED 1.89 ANGSTROMS STRUCTURE OF THE HISTIDINE-BINDING PROTEIN COMPLEXED WITH HISTIDINE AND ITS RELATIONSHIP WITH MANY OTHER ACTIVE TRANSPORT(SLASH)CHEMOSENSORY RECEPTORS
Authors	:	Yao, N.; Trakhanov, S.; Quiocho, F.A.
Deposited on	:	1994-01-03
Resolution	:	1.89 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 following versions of software and data (see references ⓘ) were used in the production of this report:

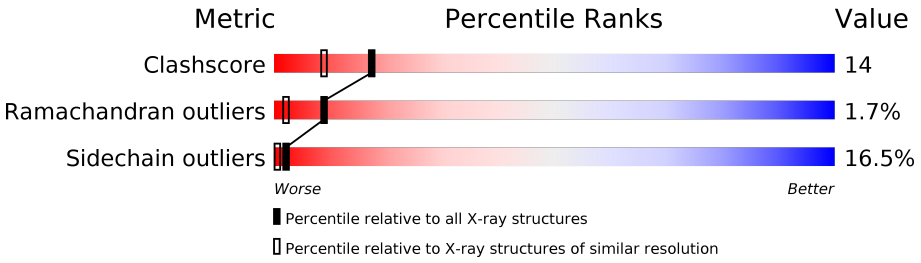
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 1.89 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))
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)

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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	238	59% 29% 11%
1	B	238	61% 29% 9% .

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4001 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.

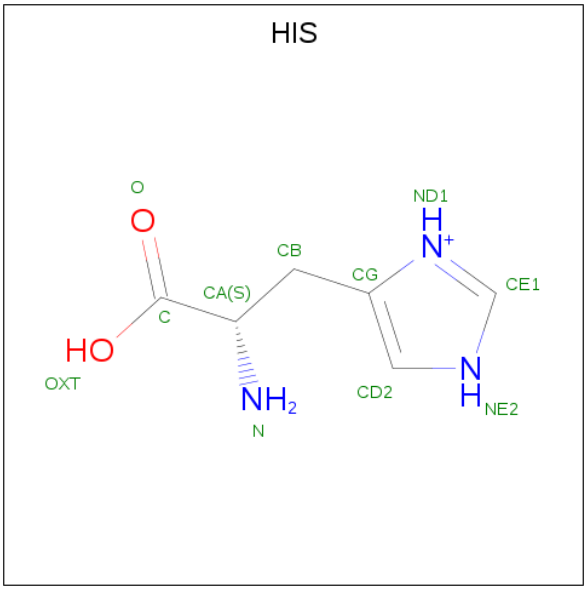
- Molecule 1 is a protein called HISTIDINE-BINDING PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	238	Total	C	N	O	S	0	0	0
			1843	1166	311	361	5			
1	B	238	Total	C	N	O	S	0	0	0
			1843	1166	311	361	5			

- Molecule 2 is CADMIUM ION (three-letter code: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total	Cd	0	0
			2	2		
2	A	5	Total	Cd	0	0
			5	5		

- Molecule 3 is HISTIDINE (three-letter code: HIS) (formula: $C_6H_{10}N_3O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			11	6	3	2		
3	B	1	Total	C	N	O	0	0
			11	6	3	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	161	Total	O	0	0
			161	161		
4	B	125	Total	O	0	0
			125	125		

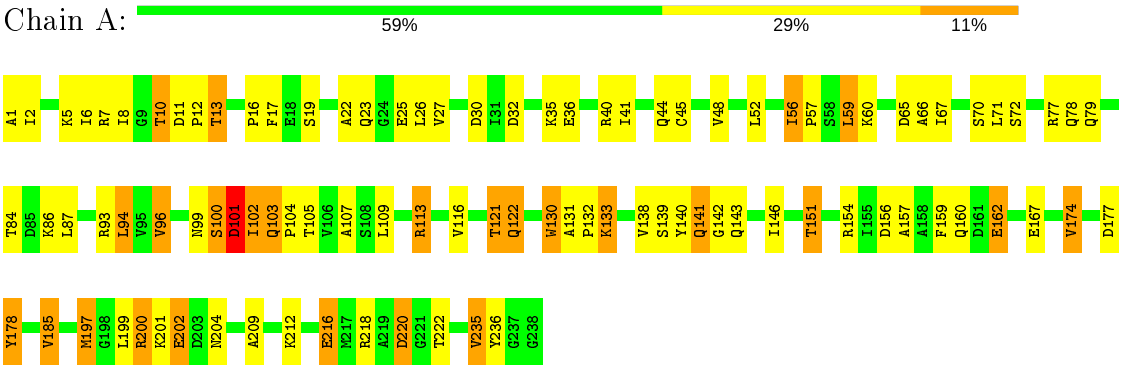
3 Residue-property plots (i)

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. 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. 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.

Note EDS was not executed.

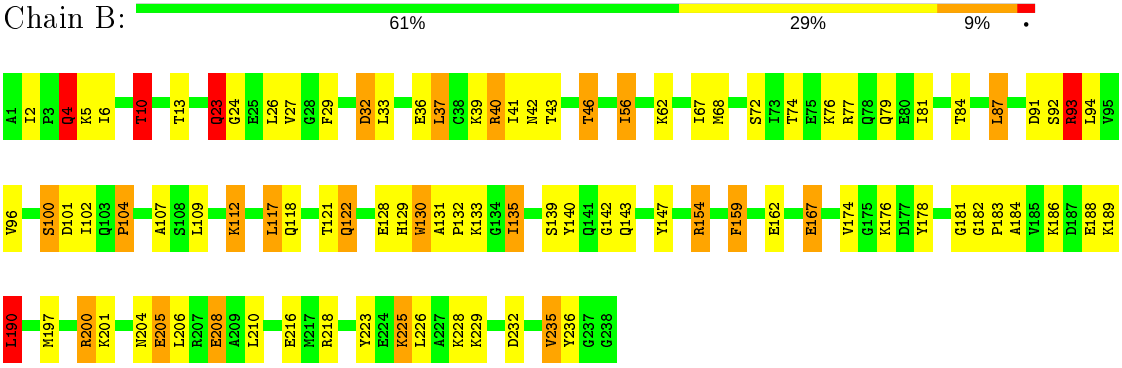
- Molecule 1: HISTIDINE-BINDING PROTEIN

Chain A:



- Molecule 1: HISTIDINE-BINDING PROTEIN

Chain B:



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	39.16Å 102.52Å 64.98Å 90.00° 93.56° 90.00°	Depositor
Resolution (Å)	8.00 – 1.89	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-1.89)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.199 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4001	wwPDB-VP
Average B, all atoms (Å^2)	21.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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	0.98	1/1874 (0.1%)	1.94	45/2522 (1.8%)
1	B	1.01	0/1874	1.89	41/2522 (1.6%)
All	All	0.99	1/3748 (0.0%)	1.91	86/5044 (1.7%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	100	SER	CA-CB	-5.63	1.44	1.52

All (86) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	154	ARG	NE-CZ-NH2	15.83	128.22	120.30
1	A	77	ARG	NE-CZ-NH2	15.11	127.85	120.30
1	B	77	ARG	NE-CZ-NH2	14.77	127.69	120.30
1	A	100	SER	CA-C-N	-10.52	94.06	117.20
1	B	208	GLU	CA-CB-CG	9.85	135.07	113.40
1	A	154	ARG	NE-CZ-NH1	-9.84	115.38	120.30
1	A	218	ARG	NE-CZ-NH1	-9.62	115.49	120.30
1	B	77	ARG	NE-CZ-NH1	-9.11	115.75	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	100	SER	O-C-N	9.04	137.17	122.70
1	B	235	VAL	CB-CA-C	-8.59	95.08	111.40
1	A	93	ARG	NE-CZ-NH2	8.42	124.51	120.30
1	B	93	ARG	NE-CZ-NH1	-8.32	116.14	120.30
1	B	200	ARG	NE-CZ-NH1	-8.29	116.15	120.30
1	B	23	GLN	CA-CB-CG	8.27	131.59	113.40
1	A	218	ARG	NE-CZ-NH2	8.17	124.39	120.30
1	B	181	GLY	CA-C-N	-8.01	100.18	116.20
1	A	141	GLN	CA-CB-CG	-7.99	95.83	113.40
1	B	154	ARG	NE-CZ-NH2	7.94	124.27	120.30
1	B	216	GLU	CA-CB-CG	-7.76	96.34	113.40
1	A	177	ASP	CA-CB-CG	7.72	130.39	113.40
1	A	200	ARG	NE-CZ-NH1	-7.64	116.48	120.30
1	A	130	TRP	CD1-CG-CD2	7.61	112.38	106.30
1	B	200	ARG	NE-CZ-NH2	7.58	124.09	120.30
1	B	40	ARG	NE-CZ-NH1	-7.48	116.56	120.30
1	A	133	LYS	CA-CB-CG	7.23	129.30	113.40
1	B	10	THR	CB-CA-C	-7.22	92.11	111.60
1	B	93	ARG	NE-CZ-NH2	7.08	123.84	120.30
1	A	1	ALA	N-CA-C	7.08	130.12	111.00
1	B	147	TYR	CB-CG-CD2	-7.04	116.78	121.00
1	B	10	THR	N-CA-CB	7.02	123.64	110.30
1	A	185	VAL	CA-C-N	-7.01	101.78	117.20
1	A	10	THR	N-CA-CB	6.86	123.34	110.30
1	A	94	LEU	CA-CB-CG	6.71	130.74	115.30
1	B	130	TRP	CE2-CD2-CG	-6.69	101.95	107.30
1	B	181	GLY	O-C-N	6.57	134.37	123.20
1	A	45	CYS	CA-CB-SG	-6.48	102.33	114.00
1	B	122	GLN	CA-CB-CG	6.46	127.62	113.40
1	A	103	GLN	CA-CB-CG	6.46	127.60	113.40
1	A	10	THR	CB-CA-C	-6.42	94.27	111.60
1	B	87	LEU	CA-CB-CG	6.41	130.05	115.30
1	A	35	LYS	CB-CG-CD	-6.33	95.16	111.60
1	B	130	TRP	CD1-CG-CD2	6.28	111.33	106.30
1	A	162	GLU	N-CA-CB	-6.25	99.35	110.60
1	A	178	TYR	CB-CG-CD2	-6.21	117.28	121.00
1	A	130	TRP	CE2-CD2-CG	-6.20	102.34	107.30
1	A	78	GLN	CA-CB-CG	-6.15	99.88	113.40
1	A	185	VAL	CA-CB-CG1	-6.09	101.76	110.90
1	A	156	ASP	CB-CG-OD2	-6.05	112.86	118.30
1	A	235	VAL	CB-CA-C	-6.04	99.93	111.40
1	B	32	ASP	CB-CG-OD2	6.03	123.72	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	93	ARG	CB-CG-CD	6.00	127.19	111.60
1	B	101	ASP	N-CA-C	5.97	127.13	111.00
1	A	103	GLN	N-CA-C	5.97	127.13	111.00
1	B	223	TYR	CG-CD1-CE1	-5.95	116.54	121.30
1	B	190	LEU	CA-CB-CG	5.92	128.91	115.30
1	A	32	ASP	CB-CG-OD2	-5.90	112.99	118.30
1	A	11	ASP	CB-CG-OD2	5.88	123.59	118.30
1	A	1	ALA	C-N-CA	5.87	136.37	121.70
1	A	100	SER	CA-CB-OG	-5.77	95.62	111.20
1	B	167	GLU	CA-CB-CG	-5.68	100.89	113.40
1	A	96	VAL	N-CA-CB	-5.67	99.02	111.50
1	B	200	ARG	CG-CD-NE	-5.66	99.92	111.80
1	B	40	ARG	CG-CD-NE	-5.61	100.01	111.80
1	A	101	ASP	N-CA-C	5.53	125.94	111.00
1	B	186	LYS	N-CA-C	5.53	125.94	111.00
1	A	197	MET	CG-SD-CE	-5.46	91.47	100.20
1	A	59	LEU	CA-CB-CG	5.44	127.81	115.30
1	A	177	ASP	CB-CA-C	-5.41	99.58	110.40
1	B	130	TRP	CG-CD2-CE3	5.38	138.74	133.90
1	A	235	VAL	CG1-CB-CG2	5.36	119.47	110.90
1	A	77	ARG	NE-CZ-NH1	-5.36	117.62	120.30
1	B	206	LEU	CB-CG-CD2	-5.29	102.01	111.00
1	B	232	ASP	CB-CG-OD1	-5.24	113.59	118.30
1	B	29	PHE	O-C-N	-5.23	114.33	122.70
1	B	23	GLN	OE1-CD-NE2	-5.21	109.92	121.90
1	B	236	TYR	CA-C-N	5.20	126.59	116.20
1	B	174	VAL	CB-CA-C	-5.17	101.58	111.40
1	A	121	THR	CA-CB-CG2	5.17	119.63	112.40
1	A	167	GLU	O-C-N	-5.16	114.42	123.20
1	B	140	TYR	CG-CD1-CE1	-5.10	117.22	121.30
1	B	128	GLU	O-C-N	-5.08	114.57	122.70
1	B	4	GLN	N-CA-CB	-5.06	101.50	110.60
1	B	140	TYR	CB-CG-CD1	-5.05	117.97	121.00
1	A	13	THR	CA-CB-CG2	5.03	119.44	112.40
1	A	200	ARG	NE-CZ-NH2	5.02	122.81	120.30
1	B	162	GLU	N-CA-CB	-5.01	101.58	110.60

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	178	TYR	Sidechain

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Mol	Chain	Res	Type	Group
1	B	178	TYR	Sidechain

5.2 Too-close contacts (i)

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	1843	0	1840	48	0
1	B	1843	0	1840	50	0
2	A	5	0	0	0	2
2	B	2	0	0	0	0
3	A	11	0	6	1	0
3	B	11	0	6	2	0
4	A	161	0	0	5	0
4	B	125	0	0	6	2
All	All	4001	0	3692	94	2

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 14.

All (94) 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:113:ARG:NH2	1:A:138:VAL:HG21	1.91	0.85
1:B:121:THR:HG21	4:B:249:HOH:O	1.78	0.84
1:B:118:GLN:HG2	1:B:139:SER:HB3	1.70	0.74
1:B:94:LEU:HD11	1:B:130:TRP:HH2	1.52	0.74
1:B:109:LEU:HD13	1:B:135:ILE:HD13	1.70	0.71
1:A:56:ILE:HG13	1:A:57:PRO:HD3	1.74	0.69
1:B:62:LYS:HA	1:B:200:ARG:HH11	1.57	0.68
1:B:72:SER:HG	3:B:239:HIS:N	1.93	0.67
1:A:6:ILE:HG23	1:A:65:ASP:HB2	1.78	0.66
1:B:5:LYS:HE3	1:B:46:THR:HB	1.77	0.65
1:B:104:PRO:HG3	1:B:183:PRO:HD2	1.78	0.64
1:B:92:SER:O	1:B:184:ALA:HA	1.97	0.64
1:A:113:ARG:HH22	1:A:138:VAL:HG21	1.63	0.63
1:B:93:ARG:HG2	1:B:184:ALA:HA	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:7:ARG:HH11	1:A:48:VAL:HG21	1.65	0.61
1:A:41:ILE:HD12	1:A:209:ALA:HB1	1.81	0.61
1:A:113:ARG:HH21	1:A:113:ARG:HB3	1.67	0.60
1:A:94:LEU:HD23	1:A:159:PHE:HB2	1.83	0.59
1:A:84:THR:HG22	1:A:197:MET:H	1.66	0.58
1:A:102:ILE:HG13	1:A:109:LEU:HD23	1.85	0.57
1:B:104:PRO:HD3	1:B:182:GLY:HA3	1.87	0.57
1:B:56:ILE:HD12	1:B:56:ILE:H	1.70	0.57
1:A:122:GLN:HB3	1:A:159:PHE:CD2	2.40	0.56
1:A:121:THR:HG21	4:A:244:HOH:O	2.06	0.56
1:B:62:LYS:HA	1:B:200:ARG:NH1	2.21	0.56
1:B:122:GLN:HE22	3:B:239:HIS:HB2	1.70	0.55
1:B:13:THR:HG21	1:B:142:GLY:HA2	1.89	0.55
1:A:44:GLN:OE1	1:B:225:LYS:HB2	2.07	0.55
1:B:122:GLN:HB2	1:B:159:PHE:CD2	2.43	0.54
1:A:13:THR:O	1:A:143:GLN:HB3	2.08	0.53
1:A:200:ARG:HB3	1:A:202:GLU:HG2	1.89	0.53
1:A:113:ARG:HH21	1:A:138:VAL:HG21	1.70	0.53
1:A:5:LYS:HA	1:A:44:GLN:O	2.08	0.53
1:A:130:TRP:CZ2	1:A:185:VAL:HG11	2.43	0.53
1:A:67:ILE:HG21	1:A:71:LEU:HD22	1.92	0.52
1:B:130:TRP:HB3	1:B:135:ILE:HG12	1.91	0.52
1:B:76:LYS:NZ	1:B:190:LEU:HA	2.25	0.52
1:B:2:ILE:HD11	1:B:41:ILE:HD12	1.90	0.52
1:A:56:ILE:HG12	4:A:439:HOH:O	2.10	0.51
1:A:8:ILE:HG12	1:A:66:ALA:HB3	1.92	0.51
1:B:117:LEU:HD21	4:B:356:HOH:O	2.10	0.51
1:B:76:LYS:HZ2	1:B:190:LEU:HA	1.75	0.51
1:B:218:ARG:HD2	4:B:387:HOH:O	2.10	0.50
1:B:104:PRO:CD	1:B:182:GLY:HA3	2.40	0.50
1:A:72:SER:HG	3:A:239:HIS:N	2.10	0.50
1:A:103:GLN:HB2	1:A:104:PRO:HD3	1.93	0.49
1:B:10:THR:HG23	1:B:68:MET:O	2.12	0.49
1:A:84:THR:CG2	1:A:197:MET:H	2.25	0.49
1:B:135:ILE:O	1:B:135:ILE:HG13	2.12	0.49
1:A:40:ARG:HH22	1:A:222:THR:HG21	1.77	0.49
1:A:22:ALA:HB3	1:B:42:ASN:HD21	1.79	0.48
1:A:142:GLY:N	4:A:816:HOH:O	2.47	0.48
1:B:13:THR:O	1:B:143:GLN:HB3	2.13	0.48
1:A:105:THR:HG22	1:A:107:ALA:H	1.77	0.48
1:A:216:GLU:O	1:A:220:ASP:HB3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:109:LEU:HA	1:B:112:LYS:HG3	1.96	0.47
1:B:102:ILE:HG12	1:B:112:LYS:HD3	1.97	0.47
1:B:36:GLU:O	1:B:40:ARG:HG3	2.14	0.47
1:B:205:GLU:CD	1:B:205:GLU:H	2.18	0.47
1:A:140:TYR:CD2	1:A:146:ILE:HG12	2.49	0.47
1:A:84:THR:HG22	1:A:197:MET:N	2.30	0.46
1:A:151:THR:HG22	4:A:833:HOH:O	2.15	0.46
1:B:32:ASP:HB3	1:B:226:LEU:HD22	1.98	0.46
1:A:57:PRO:O	1:A:60:LYS:HG2	2.15	0.46
1:A:23:GLN:HG2	1:B:42:ASN:HD22	1.82	0.44
1:A:17:PHE:O	1:A:30:ASP:HB2	2.17	0.44
1:B:204:ASN:O	1:B:208:GLU:HG3	2.18	0.44
1:A:105:THR:HG22	1:A:107:ALA:N	2.32	0.44
1:B:4:GLN:HG3	1:B:4:GLN:H	1.34	0.44
1:A:130:TRP:HZ2	1:A:185:VAL:HG11	1.82	0.43
1:B:229:LYS:HD3	4:B:864:HOH:O	2.17	0.43
1:B:100:SER:HB3	1:B:102:ILE:HD12	2.00	0.43
1:B:131:ALA:N	1:B:132:PRO:HD2	2.34	0.43
1:A:12:PRO:O	1:A:19:SER:HA	2.18	0.43
1:A:56:ILE:H	1:A:56:ILE:HG12	1.65	0.42
1:B:76:LYS:HB2	1:B:76:LYS:HE2	1.85	0.42
1:B:210:LEU:HA	1:B:210:LEU:HD23	1.87	0.42
1:B:76:LYS:NZ	1:B:189:LYS:O	2.50	0.42
1:B:67:ILE:HG21	1:B:67:ILE:HD13	1.83	0.42
1:B:81:ILE:HA	4:B:801:HOH:O	2.18	0.42
1:B:94:LEU:HD11	1:B:130:TRP:CH2	2.42	0.42
1:A:41:ILE:HD13	1:A:41:ILE:HA	1.69	0.42
1:A:86:LYS:O	1:A:236:TYR:HE2	2.03	0.42
1:A:116:VAL:O	1:A:139:SER:HA	2.21	0.41
1:A:41:ILE:HG23	1:A:41:ILE:HD12	1.82	0.41
1:B:23:GLN:NE2	4:B:386:HOH:O	2.52	0.41
1:B:37:LEU:HD23	1:B:197:MET:CE	2.51	0.41
1:B:74:THR:HB	1:B:76:LYS:HZ3	1.86	0.41
1:B:76:LYS:H	1:B:76:LYS:HD3	1.86	0.40
1:A:131:ALA:N	1:A:132:PRO:HD2	2.36	0.40
1:A:101:ASP:O	1:A:103:GLN:N	2.54	0.40
1:A:102:ILE:HD11	1:A:157:ALA:HB2	2.02	0.40
1:A:174:VAL:HG22	4:A:330:HOH:O	2.21	0.40
1:A:25:GLU:HB2	1:B:39:LYS:HB3	2.04	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:752:CD:CD	4:B:962:HOH:O[2_445]	1.59	0.61
2:A:756:CD:CD	4:B:956:HOH:O[2_445]	1.64	0.56

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	236/238 (99%)	215 (91%)	17 (7%)	4 (2%)	9 2
1	B	236/238 (99%)	214 (91%)	18 (8%)	4 (2%)	9 2
All	All	472/476 (99%)	429 (91%)	35 (7%)	8 (2%)	9 2

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	99	ASN
1	A	101	ASP
1	A	100	SER
1	A	102	ILE
1	B	104	PRO
1	B	107	ALA
1	B	84	THR
1	B	24	GLY

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	193/193 (100%)	164 (85%)	29 (15%)	3 1
1	B	193/193 (100%)	160 (83%)	33 (17%)	2 0
All	All	386/386 (100%)	324 (84%)	62 (16%)	2 0

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ILE
1	A	10	THR
1	A	16	PRO
1	A	26	LEU
1	A	27	VAL
1	A	36	GLU
1	A	52	LEU
1	A	56	ILE
1	A	59	LEU
1	A	70	SER
1	A	79	GLN
1	A	87	LEU
1	A	96	VAL
1	A	113	ARG
1	A	122	GLN
1	A	133	LYS
1	A	141	GLN
1	A	151	THR
1	A	160	GLN
1	A	162	GLU
1	A	174	VAL
1	A	199	LEU
1	A	201	LYS
1	A	202	GLU
1	A	204	ASN
1	A	212	LYS
1	A	216	GLU
1	A	220	ASP
1	A	235	VAL
1	B	4	GLN
1	B	6	ILE
1	B	10	THR
1	B	23	GLN
1	B	26	LEU
1	B	27	VAL

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Mol	Chain	Res	Type
1	B	33	LEU
1	B	37	LEU
1	B	43	THR
1	B	46	THR
1	B	56	ILE
1	B	79	GLN
1	B	87	LEU
1	B	91	ASP
1	B	93	ARG
1	B	96	VAL
1	B	100	SER
1	B	112	LYS
1	B	117	LEU
1	B	129	HIS
1	B	133	LYS
1	B	135	ILE
1	B	154	ARG
1	B	159	PHE
1	B	167	GLU
1	B	176	LYS
1	B	188	GLU
1	B	190	LEU
1	B	201	LYS
1	B	205	GLU
1	B	225	LYS
1	B	228	LYS
1	B	235	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	79	GLN
1	A	122	GLN
1	A	160	GLN
1	B	4	GLN
1	B	42	ASN
1	B	122	GLN
1	B	143	GLN
1	B	204	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 9 ligands modelled in this entry, 7 are monoatomic - leaving 2 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

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.