Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 11:38 PM GMT

PDB ID	:	1Y3T
Title	:	Crystal structure of YxaG, a dioxygenase from Bacillus subtilis
Authors	:	Gopal, B.; Madan, L.L.; Betz, S.F.; Kossiakoff, A.A.
Deposited on	:	2004-11-26
Resolution	:	2.40 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:

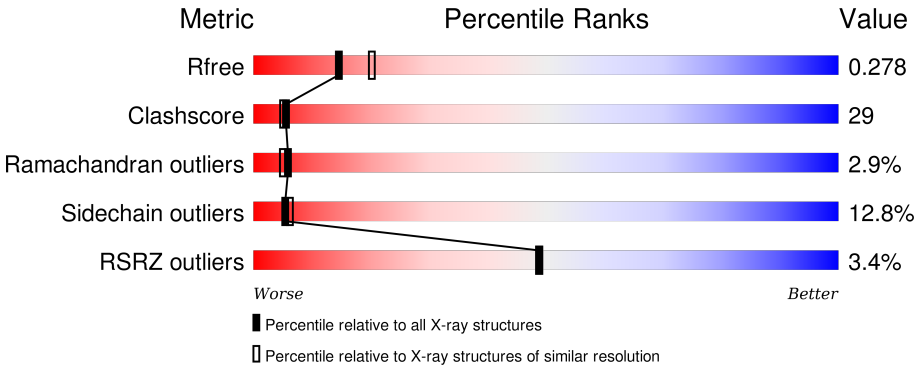
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.40 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	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (2.40-2.40)

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	337	3% 48% 31% 14% 5%
1	B	337	3% 48% 31% 12% 7%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5508 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 Hypothetical protein yxaG.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	330	Total	C	N	O	S	65	0	0
			2570	1630	444	485	11			
1	B	330	Total	C	N	O	S	61	0	0
			2571	1630	444	486	11			

- Molecule 2 is FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total	Fe	0	0
			2	2		
2	A	2	Total	Fe	0	0
			2	2		

- Molecule 3 is water.

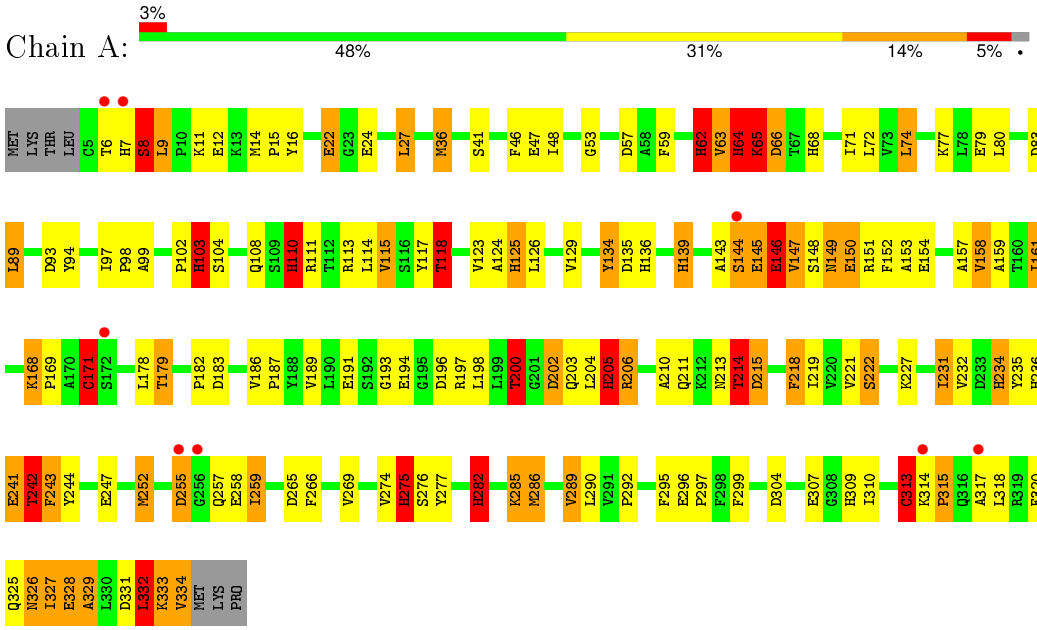
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	182	Total	O	0	0
			182	182		
3	B	181	Total	O	0	0
			181	181		

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.

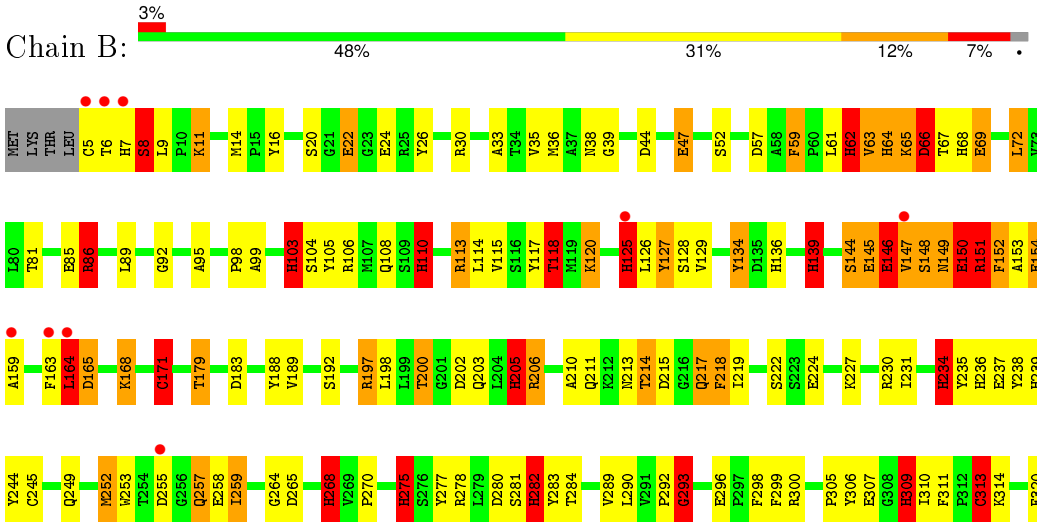
- Molecule 1: Hypothetical protein yxaG

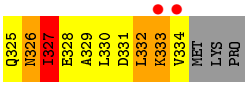
Chain A:



- Molecule 1: Hypothetical protein yxaG

Chain B:




Q325
N326
I327
E328
A329
L330
D331
L332
K333
V334
MET
LYS
PRO

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	128.42Å 128.43Å 51.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	91.29 – 2.40 19.77 – 2.40	Depositor EDS
% Data completeness (in resolution range)	97.5 (91.29-2.40) 97.8 (19.77-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	2.32 (at 2.41Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.217 , 0.277 0.221 , 0.278	Depositor DCC
R_{free} test set	1695 reflections (5.38%)	DCC
Wilson B-factor (Å^2)	41.0	Xtriage
Anisotropy	0.592	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 51.3	EDS
Estimated twinning fraction	0.011 for k,h,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Outliers	1 of 33243 reflections (0.003%)	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	5508	wwPDB-VP
Average B, all atoms (Å^2)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.22% of the height of the origin peak. No significant pseudotranslation is detected.*

[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: FE

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	2.32	103/2635 (3.9%)	1.70	58/3576 (1.6%)
1	B	2.47	107/2636 (4.1%)	1.70	72/3578 (2.0%)
All	All	2.39	210/5271 (4.0%)	1.70	130/7154 (1.8%)

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	17
1	B	0	19
All	All	0	36

All (210) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	164	LEU	C-N	-29.07	0.67	1.34
1	B	8	SER	CA-C	21.77	2.09	1.52
1	B	8	SER	CA-CB	-21.52	1.20	1.52
1	A	328	GLU	CD-OE1	19.70	1.47	1.25
1	A	164	LEU	C-N	-18.43	0.91	1.34
1	B	8	SER	C-N	-18.36	0.91	1.34
1	A	8	SER	C-N	-17.65	0.93	1.34
1	B	171	CYS	C-N	-17.27	0.94	1.34
1	B	147	VAL	CB-CG1	16.27	1.87	1.52
1	B	328	GLU	CD-OE1	14.58	1.41	1.25
1	B	149	ASN	C-N	-13.61	1.02	1.34
1	A	171	CYS	C-N	-13.17	1.03	1.34
1	B	154	GLU	CD-OE2	12.60	1.39	1.25
1	B	154	GLU	CD-OE1	11.09	1.37	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	158	VAL	CB-CG2	-10.96	1.29	1.52
1	A	154	GLU	CG-CD	10.95	1.68	1.51
1	A	110	HIS	CE1-NE2	10.88	1.57	1.32
1	A	8	SER	CA-C	10.49	1.80	1.52
1	B	328	GLU	CD-OE2	10.29	1.36	1.25
1	B	144	SER	CB-OG	10.26	1.55	1.42
1	A	276	SER	CB-OG	-9.90	1.29	1.42
1	B	47	GLU	CD-OE1	9.87	1.36	1.25
1	A	65	LYS	CD-CE	9.85	1.75	1.51
1	A	275	HIS	CA-CB	-9.75	1.32	1.53
1	B	309	HIS	CA-CB	9.71	1.75	1.53
1	B	154	GLU	CG-CD	9.55	1.66	1.51
1	B	146	GLU	CG-CD	9.39	1.66	1.51
1	A	247	GLU	CD-OE1	9.33	1.35	1.25
1	B	307	GLU	CD-OE2	9.18	1.35	1.25
1	B	52	SER	CB-OG	-9.13	1.30	1.42
1	A	147	VAL	CB-CG1	9.04	1.71	1.52
1	A	328	GLU	CG-CD	-9.03	1.38	1.51
1	B	127	TYR	CE1-CZ	-9.03	1.26	1.38
1	A	171	CYS	CA-CB	-8.92	1.34	1.53
1	B	63	VAL	CB-CG2	-8.92	1.34	1.52
1	B	281	SER	CB-OG	-8.63	1.31	1.42
1	A	152	PHE	C-N	-8.57	1.14	1.34
1	A	146	GLU	CG-CD	8.38	1.64	1.51
1	A	189	VAL	CB-CG2	8.38	1.70	1.52
1	A	123	VAL	CB-CG1	8.37	1.70	1.52
1	B	117	TYR	CE1-CZ	-8.12	1.27	1.38
1	B	16	TYR	CD2-CE2	8.07	1.51	1.39
1	A	222	SER	CB-OG	7.96	1.52	1.42
1	A	218	PHE	CE2-CZ	7.94	1.52	1.37
1	B	117	TYR	CG-CD2	-7.93	1.28	1.39
1	B	59	PHE	CE1-CZ	7.86	1.52	1.37
1	A	103	HIS	CA-CB	-7.84	1.36	1.53
1	A	118	THR	CB-CG2	-7.77	1.26	1.52
1	A	163	PHE	CG-CD1	7.71	1.50	1.38
1	A	258	GLU	CD-OE2	-7.71	1.17	1.25
1	B	241	GLU	CD-OE1	7.70	1.34	1.25
1	A	115	VAL	CB-CG1	-7.66	1.36	1.52
1	B	85	GLU	CD-OE2	7.52	1.33	1.25
1	B	327	ILE	N-CA	7.52	1.61	1.46
1	A	94	TYR	CD1-CE1	7.50	1.50	1.39
1	A	129	VAL	CB-CG2	7.46	1.68	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	153	ALA	CA-CB	7.45	1.68	1.52
1	B	62	HIS	CA-CB	-7.44	1.37	1.53
1	B	134	TYR	CD1-CE1	-7.36	1.28	1.39
1	B	33	ALA	CA-CB	7.31	1.67	1.52
1	B	313	CYS	CB-SG	-7.30	1.69	1.82
1	A	334	VAL	CB-CG1	7.21	1.68	1.52
1	A	65	LYS	CE-NZ	7.10	1.66	1.49
1	A	327	ILE	N-CA	7.10	1.60	1.46
1	A	313	CYS	CB-SG	-7.09	1.70	1.82
1	B	127	TYR	CG-CD1	-7.04	1.29	1.39
1	B	95	ALA	CA-CB	-7.00	1.37	1.52
1	A	24	GLU	CD-OE1	7.00	1.33	1.25
1	B	127	TYR	CE2-CZ	-6.95	1.29	1.38
1	A	274	VAL	CB-CG1	6.94	1.67	1.52
1	B	151	ARG	N-CA	6.92	1.60	1.46
1	B	129	VAL	CB-CG2	6.91	1.67	1.52
1	B	306	TYR	CE1-CZ	6.84	1.47	1.38
1	A	65	LYS	CG-CD	6.81	1.75	1.52
1	A	243	PHE	CG-CD2	-6.81	1.28	1.38
1	A	16	TYR	CE1-CZ	-6.77	1.29	1.38
1	B	118	THR	CB-CG2	-6.76	1.30	1.52
1	B	235	TYR	CD1-CE1	6.70	1.49	1.39
1	A	265	ASP	CG-OD2	6.65	1.40	1.25
1	A	161	ILE	CB-CG2	-6.64	1.32	1.52
1	A	299	PHE	CE2-CZ	-6.62	1.24	1.37
1	A	307	GLU	CD-OE2	6.62	1.32	1.25
1	A	205	HIS	CA-CB	6.62	1.68	1.53
1	B	189	VAL	CB-CG1	-6.58	1.39	1.52
1	A	143	ALA	CA-CB	-6.58	1.38	1.52
1	B	296	GLU	CD-OE2	6.58	1.32	1.25
1	A	63	VAL	CB-CG2	-6.54	1.39	1.52
1	B	237	GLU	CD-OE2	-6.53	1.18	1.25
1	B	158	VAL	CB-CG2	-6.47	1.39	1.52
1	A	24	GLU	C-O	6.44	1.35	1.23
1	A	150	GLU	CD-OE2	6.44	1.32	1.25
1	B	275	HIS	CB-CG	-6.43	1.38	1.50
1	B	268	HIS	CA-CB	-6.39	1.39	1.53
1	B	334	VAL	CA-CB	6.37	1.68	1.54
1	B	283	TYR	CD2-CE2	6.31	1.48	1.39
1	A	200	THR	CB-CG2	-6.29	1.31	1.52
1	B	26	TYR	CE2-CZ	-6.27	1.30	1.38
1	B	35	VAL	N-CA	-6.27	1.33	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	11	LYS	CD-CE	6.20	1.66	1.51
1	B	120	LYS	CD-CE	6.20	1.66	1.51
1	B	192	SER	CA-CB	6.18	1.62	1.52
1	B	108	GLN	CB-CG	6.15	1.69	1.52
1	B	79	GLU	CB-CG	-6.14	1.40	1.52
1	B	66	ASP	CG-OD2	6.14	1.39	1.25
1	B	244	TYR	CE2-CZ	-6.12	1.30	1.38
1	A	328	GLU	N-CA	-6.12	1.34	1.46
1	A	289	VAL	CA-CB	-6.10	1.42	1.54
1	B	65	LYS	CE-NZ	6.09	1.64	1.49
1	A	307	GLU	CG-CD	6.07	1.61	1.51
1	A	151	ARG	N-CA	6.06	1.58	1.46
1	A	232	VAL	C-O	6.06	1.34	1.23
1	A	327	ILE	CA-C	6.04	1.68	1.52
1	A	12	GLU	CD-OE2	6.03	1.32	1.25
1	A	241	GLU	CA-CB	-5.96	1.40	1.53
1	B	110	HIS	CA-CB	5.95	1.67	1.53
1	B	79	GLU	CD-OE1	5.95	1.32	1.25
1	B	234	HIS	CA-CB	-5.90	1.41	1.53
1	A	266	PHE	CG-CD2	5.88	1.47	1.38
1	B	69	GLU	CD-OE1	5.87	1.32	1.25
1	A	282	HIS	CA-CB	5.86	1.66	1.53
1	B	22	GLU	CD-OE2	5.83	1.32	1.25
1	B	79	GLU	CD-OE2	5.83	1.32	1.25
1	A	221	VAL	CB-CG1	-5.82	1.40	1.52
1	A	103	HIS	C-O	-5.80	1.12	1.23
1	B	230	ARG	C-O	-5.73	1.12	1.23
1	A	79	GLU	CA-CB	-5.73	1.41	1.53
1	A	108	GLN	CB-CG	5.72	1.68	1.52
1	A	193	GLY	C-O	-5.71	1.14	1.23
1	B	245	CYS	C-O	-5.71	1.12	1.23
1	B	6	THR	C-O	5.70	1.34	1.23
1	A	47	GLU	CD-OE1	5.68	1.31	1.25
1	A	41	SER	CB-OG	-5.67	1.34	1.42
1	A	235	TYR	CE1-CZ	5.67	1.46	1.38
1	A	162	VAL	CB-CG1	5.65	1.64	1.52
1	B	278	ARG	CZ-NH1	-5.63	1.25	1.33
1	A	191	GLU	CD-OE1	5.62	1.31	1.25
1	A	232	VAL	CB-CG1	5.60	1.64	1.52
1	B	151	ARG	C-O	-5.58	1.12	1.23
1	A	146	GLU	CB-CG	5.58	1.62	1.52
1	B	217	GLN	CD-OE1	-5.57	1.11	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	111	ARG	CZ-NH2	5.56	1.40	1.33
1	B	235	TYR	CZ-OH	5.56	1.47	1.37
1	A	320	PHE	CE1-CZ	5.55	1.48	1.37
1	B	39	GLY	C-O	-5.55	1.14	1.23
1	B	151	ARG	CG-CD	-5.54	1.38	1.51
1	B	75	ASP	CB-CG	-5.54	1.40	1.51
1	A	194	GLU	CD-OE1	-5.53	1.19	1.25
1	A	163	PHE	CE2-CZ	5.52	1.47	1.37
1	A	144	SER	CB-OG	5.51	1.49	1.42
1	A	218	PHE	CD2-CE2	-5.48	1.28	1.39
1	B	16	TYR	CG-CD1	5.47	1.46	1.39
1	B	150	GLU	CD-OE2	5.45	1.31	1.25
1	A	74	LEU	C-O	-5.43	1.13	1.23
1	A	110	HIS	CA-CB	-5.41	1.42	1.53
1	A	6	THR	C-O	5.40	1.33	1.23
1	B	151	ARG	CA-CB	-5.40	1.42	1.53
1	A	87	TYR	CD2-CE2	-5.39	1.31	1.39
1	A	285	LYS	CB-CG	-5.38	1.38	1.52
1	A	124	ALA	C-O	5.37	1.33	1.23
1	A	189	VAL	CB-CG1	-5.36	1.41	1.52
1	B	128	SER	CB-OG	-5.35	1.35	1.42
1	A	64	HIS	CA-CB	5.34	1.65	1.53
1	B	238	TYR	C-O	-5.34	1.13	1.23
1	A	12	GLU	CG-CD	5.33	1.59	1.51
1	A	154	GLU	CB-CG	5.33	1.62	1.52
1	A	134	TYR	CD1-CE1	-5.33	1.31	1.39
1	B	79	GLU	CA-C	-5.30	1.39	1.52
1	B	326	ASN	CG-ND2	5.29	1.46	1.32
1	A	46	PHE	CE1-CZ	-5.27	1.27	1.37
1	A	149	ASN	C-N	-5.26	1.22	1.34
1	A	202	ASP	C-O	-5.26	1.13	1.23
1	A	111	ARG	CZ-NH1	5.25	1.39	1.33
1	A	59	PHE	CG-CD1	-5.25	1.30	1.38
1	B	203	GLN	C-O	-5.22	1.13	1.23
1	A	182	PRO	CA-C	-5.21	1.42	1.52
1	B	277	TYR	C-O	-5.21	1.13	1.23
1	A	62	HIS	CB-CG	-5.21	1.40	1.50
1	B	326	ASN	C-O	5.20	1.33	1.23
1	A	231	ILE	CA-CB	5.19	1.66	1.54
1	B	243	PHE	C-O	-5.19	1.13	1.23
1	B	311	PHE	CE2-CZ	5.18	1.47	1.37
1	B	152	PHE	C-O	-5.18	1.13	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	202	ASP	C-O	-5.18	1.13	1.23
1	B	258	GLU	CD-OE1	-5.18	1.20	1.25
1	B	188	TYR	CB-CG	5.16	1.59	1.51
1	B	244	TYR	CD2-CE2	-5.16	1.31	1.39
1	A	247	GLU	CD-OE2	5.15	1.31	1.25
1	B	127	TYR	CD2-CE2	-5.14	1.31	1.39
1	B	146	GLU	CB-CG	5.14	1.61	1.52
1	A	154	GLU	CD-OE2	5.13	1.31	1.25
1	B	197	ARG	CZ-NH1	-5.11	1.26	1.33
1	B	63	VAL	CB-CG1	-5.10	1.42	1.52
1	B	159	ALA	CA-CB	5.10	1.63	1.52
1	A	326	ASN	C-O	5.09	1.33	1.23
1	B	241	GLU	CB-CG	-5.08	1.42	1.52
1	B	67	THR	C-O	-5.08	1.13	1.23
1	B	92	GLY	CA-C	5.07	1.59	1.51
1	B	320	PHE	CE1-CZ	5.07	1.47	1.37
1	B	151	ARG	CB-CG	5.07	1.66	1.52
1	A	244	TYR	CE2-CZ	-5.07	1.31	1.38
1	B	218	PHE	CE2-CZ	5.06	1.47	1.37
1	A	27	LEU	CG-CD2	5.06	1.70	1.51
1	B	298	PHE	CG-CD1	5.06	1.46	1.38
1	B	106	ARG	NE-CZ	5.05	1.39	1.33
1	A	110	HIS	ND1-CE1	5.04	1.47	1.34
1	B	306	TYR	CG-CD2	5.03	1.45	1.39
1	A	87	TYR	CE1-CZ	-5.02	1.32	1.38
1	B	300	ARG	CG-CD	5.02	1.64	1.51
1	B	147	VAL	CA-C	5.02	1.66	1.52
1	A	108	GLN	CG-CD	5.00	1.62	1.51

All (130) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	164	LEU	O-C-N	-17.46	94.77	122.70
1	B	328	GLU	OE1-CD-OE2	-15.43	104.78	123.30
1	B	8	SER	C-N-CA	15.31	159.97	121.70
1	B	8	SER	O-C-N	-12.42	102.83	122.70
1	A	164	LEU	CA-C-N	12.12	143.88	117.20
1	A	151	ARG	CA-C-N	11.72	142.98	117.20
1	A	8	SER	C-N-CA	11.37	150.13	121.70
1	A	66	ASP	CB-CG-OD2	10.61	127.84	118.30
1	A	183	ASP	CB-CG-OD1	10.61	127.84	118.30
1	A	113	ARG	NE-CZ-NH1	10.57	125.59	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	151	ARG	O-C-N	-10.56	105.80	122.70
1	A	214	THR	OG1-CB-CG2	-10.12	86.72	110.00
1	A	331	ASP	CB-CG-OD2	9.77	127.10	118.30
1	A	36	MET	CG-SD-CE	-9.13	85.59	100.20
1	B	8	SER	CA-CB-OG	-8.51	88.23	111.20
1	B	8	SER	CB-CA-C	-8.37	94.19	110.10
1	B	332	LEU	CB-CG-CD2	-8.27	96.95	111.00
1	B	66	ASP	CB-CG-OD2	8.25	125.72	118.30
1	B	183	ASP	CB-CG-OD1	8.25	125.72	118.30
1	B	146	GLU	OE1-CD-OE2	-8.05	113.64	123.30
1	A	241	GLU	OE1-CD-OE2	8.01	132.91	123.30
1	B	214	THR	OG1-CB-CG2	-7.96	91.69	110.00
1	B	86	ARG	NE-CZ-NH2	7.94	124.27	120.30
1	B	147	VAL	O-C-N	7.79	135.16	122.70
1	B	63	VAL	CG1-CB-CG2	-7.78	98.45	110.90
1	B	110	HIS	CG-ND1-CE1	-7.64	95.77	105.70
1	A	111	ARG	NE-CZ-NH2	-7.59	116.50	120.30
1	B	86	ARG	NE-CZ-NH1	-7.37	116.62	120.30
1	A	110	HIS	ND1-CE1-NE2	-7.33	93.77	109.90
1	B	265	ASP	CB-CG-OD2	7.28	124.85	118.30
1	B	293	GLY	CA-C-O	-7.27	107.52	120.60
1	A	151	ARG	CA-CB-CG	-7.21	97.55	113.40
1	A	321	ASP	CB-CG-OD2	7.17	124.75	118.30
1	B	164	LEU	O-C-N	-7.16	111.25	122.70
1	B	106	ARG	NE-CZ-NH1	7.05	123.83	120.30
1	B	113	ARG	NE-CZ-NH1	7.04	123.82	120.30
1	B	331	ASP	CB-CG-OD1	6.78	124.40	118.30
1	A	8	SER	O-C-N	-6.78	111.85	122.70
1	B	259	ILE	CG1-CB-CG2	-6.76	96.52	111.40
1	B	198	LEU	CA-CB-CG	-6.74	99.81	115.30
1	B	147	VAL	C-N-CA	6.73	138.52	121.70
1	A	304	ASP	CB-CG-OD1	6.64	124.28	118.30
1	A	113	ARG	NE-CZ-NH2	-6.60	117.00	120.30
1	A	57	ASP	CB-CG-OD2	6.53	124.17	118.30
1	B	22	GLU	OE1-CD-OE2	-6.43	115.59	123.30
1	B	113	ARG	NE-CZ-NH2	-6.42	117.09	120.30
1	A	196	ASP	CB-CG-OD2	6.40	124.06	118.30
1	B	278	ARG	NE-CZ-NH1	-6.40	117.10	120.30
1	A	83	ASP	CB-CG-OD1	-6.39	112.55	118.30
1	B	151	ARG	CA-CB-CG	-6.39	99.33	113.40
1	A	304	ASP	CB-CG-OD2	-6.36	112.57	118.30
1	A	79	GLU	OE1-CD-OE2	6.35	130.92	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	8	SER	N-CA-C	-6.34	93.87	111.00
1	A	146	GLU	OE1-CD-OE2	-6.27	115.78	123.30
1	B	75	ASP	CB-CG-OD1	-6.26	112.67	118.30
1	B	309	HIS	CA-CB-CG	-6.25	102.98	113.60
1	B	293	GLY	O-C-N	-6.23	112.73	122.70
1	B	252	MET	CG-SD-CE	6.17	110.08	100.20
1	A	275	HIS	N-CA-CB	-6.12	99.58	110.60
1	B	103	HIS	CB-CA-C	6.09	122.58	110.40
1	B	44	ASP	CB-CG-OD1	6.06	123.76	118.30
1	B	321	ASP	CB-CG-OD2	5.99	123.69	118.30
1	A	259	ILE	CG1-CB-CG2	-5.98	98.25	111.40
1	B	241	GLU	OE1-CD-OE2	5.97	130.47	123.30
1	B	147	VAL	CA-CB-CG1	5.93	119.80	110.90
1	A	242	THR	N-CA-CB	-5.88	99.12	110.30
1	A	159	ALA	N-CA-CB	5.88	118.33	110.10
1	B	171	CYS	O-C-N	-5.83	113.36	122.70
1	B	328	GLU	CG-CD-OE2	5.83	129.95	118.30
1	A	328	GLU	N-CA-CB	-5.82	100.12	110.60
1	A	332	LEU	CB-CG-CD2	-5.78	101.17	111.00
1	A	135	ASP	CB-CG-OD1	-5.75	113.13	118.30
1	B	151	ARG	CB-CA-C	5.74	121.89	110.40
1	B	215	ASP	CB-CG-OD2	5.74	123.47	118.30
1	A	8	SER	CB-CA-C	-5.74	99.19	110.10
1	A	89	LEU	CB-CG-CD2	5.74	120.75	111.00
1	B	139	HIS	N-CA-C	-5.74	95.50	111.00
1	B	242	THR	N-CA-CB	-5.72	99.43	110.30
1	A	158	VAL	CB-CA-C	-5.72	100.54	111.40
1	B	309	HIS	N-CA-CB	5.71	120.87	110.60
1	B	150	GLU	N-CA-CB	5.70	120.86	110.60
1	A	215	ASP	CB-CG-OD2	5.69	123.42	118.30
1	A	66	ASP	CB-CG-OD1	-5.68	113.19	118.30
1	B	164	LEU	CA-C-N	5.67	129.68	117.20
1	B	103	HIS	CA-CB-CG	-5.67	103.96	113.60
1	A	252	MET	CG-SD-CE	5.67	109.27	100.20
1	A	215	ASP	CB-CG-OD1	5.64	123.38	118.30
1	A	63	VAL	CG1-CB-CG2	-5.62	101.90	110.90
1	B	75	ASP	CB-CG-OD2	5.61	123.35	118.30
1	B	300	ARG	NE-CZ-NH2	-5.61	117.50	120.30
1	A	151	ARG	CG-CD-NE	5.60	123.56	111.80
1	B	328	GLU	CB-CG-CD	-5.56	99.18	114.20
1	B	293	GLY	N-CA-C	-5.52	99.30	113.10
1	A	147	VAL	C-N-CA	5.51	135.49	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	147	VAL	O-C-N	5.51	131.52	122.70
1	A	277	TYR	CD1-CE1-CZ	5.48	124.73	119.80
1	A	332	LEU	CB-CG-CD1	-5.48	101.69	111.00
1	B	139	HIS	CB-CA-C	5.47	121.35	110.40
1	B	72	LEU	CB-CG-CD2	5.47	120.29	111.00
1	B	149	ASN	C-N-CA	5.45	135.32	121.70
1	A	255	ASP	CB-CG-OD2	-5.44	113.41	118.30
1	B	268	HIS	CA-CB-CG	5.42	122.81	113.60
1	B	306	TYR	CB-CG-CD1	-5.41	117.75	121.00
1	B	151	ARG	N-CA-C	5.36	125.47	111.00
1	A	215	ASP	OD1-CG-OD2	-5.34	113.15	123.30
1	B	305	PRO	N-CD-CG	-5.31	95.23	103.20
1	B	179	THR	N-CA-CB	-5.31	100.22	110.30
1	B	144	SER	N-CA-CB	-5.30	102.54	110.50
1	A	152	PHE	C-N-CA	5.29	134.94	121.70
1	B	165	ASP	CB-CG-OD2	5.29	123.06	118.30
1	A	22	GLU	OE1-CD-OE2	-5.28	116.97	123.30
1	A	150	GLU	OE1-CD-OE2	-5.27	116.98	123.30
1	B	330	LEU	CB-CG-CD2	5.25	119.93	111.00
1	A	9	LEU	CB-CG-CD2	5.24	119.91	111.00
1	A	158	VAL	CA-CB-CG1	5.24	118.76	110.90
1	A	111	ARG	NE-CZ-NH1	-5.22	117.69	120.30
1	B	151	ARG	CG-CD-NE	5.22	122.76	111.80
1	B	282	HIS	N-CA-CB	5.21	119.98	110.60
1	A	111	ARG	NH1-CZ-NH2	5.20	125.12	119.40
1	A	282	HIS	N-CA-CB	5.19	119.94	110.60
1	A	242	THR	CA-CB-CG2	5.15	119.61	112.40
1	B	36	MET	CG-SD-CE	-5.15	91.96	100.20
1	B	79	GLU	OE1-CD-OE2	5.15	129.48	123.30
1	B	148	SER	O-C-N	-5.15	114.46	122.70
1	A	198	LEU	CA-CB-CG	-5.14	103.47	115.30
1	A	165	ASP	CB-CG-OD2	5.13	122.92	118.30
1	B	327	ILE	N-CA-C	5.08	124.72	111.00
1	B	47	GLU	CG-CD-OE2	-5.03	108.24	118.30
1	B	57	ASP	CB-CG-OD2	5.03	122.83	118.30
1	B	146	GLU	CA-CB-CG	5.02	124.45	113.40

There are no chirality outliers.

All (36) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	103	HIS	Sidechain

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Mol	Chain	Res	Type	Group
1	A	110	HIS	Sidechain
1	A	145	GLU	Peptide
1	A	146	GLU	Peptide
1	A	150	GLU	Mainchain,Peptide
1	A	164	LEU	Mainchain
1	A	169	PRO	Peptide
1	A	171	CYS	Peptide
1	A	205	HIS	Sidechain
1	A	234	HIS	Sidechain
1	A	239	HIS	Sidechain
1	A	275	HIS	Sidechain
1	A	282	HIS	Sidechain
1	A	327	ILE	Peptide
1	A	62	HIS	Sidechain
1	A	64	HIS	Sidechain
1	B	103	HIS	Sidechain
1	B	110	HIS	Sidechain
1	B	125	HIS	Sidechain
1	B	139	HIS	Sidechain
1	B	145	GLU	Peptide
1	B	146	GLU	Peptide
1	B	150	GLU	Mainchain,Peptide
1	B	151	ARG	Peptide
1	B	164	LEU	Mainchain
1	B	171	CYS	Peptide
1	B	205	HIS	Sidechain
1	B	268	HIS	Sidechain
1	B	275	HIS	Sidechain
1	B	293	GLY	Mainchain
1	B	309	HIS	Sidechain
1	B	327	ILE	Peptide
1	B	62	HIS	Sidechain
1	B	8	SER	Mainchain

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	2570	0	2478	162	0
1	B	2571	0	2480	150	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	182	0	0	30	0
3	B	181	0	0	31	0
All	All	5508	0	4958	291	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 29.

All (291) 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:71:ILE:CD1	1:A:71:ILE:CG1	1.75	1.61
1:B:309:HIS:CB	1:B:309:HIS:CA	1.75	1.59
1:A:65:LYS:CD	1:A:65:LYS:CE	1.75	1.59
1:A:65:LYS:CD	1:A:65:LYS:CG	1.75	1.58
1:B:147:VAL:CG1	1:B:147:VAL:CB	1.87	1.50
1:A:286:MET:CE	1:A:286:MET:SD	2.05	1.44
1:B:145:GLU:O	1:B:146:GLU:CG	1.65	1.43
1:A:310:ILE:HG21	1:B:139:HIS:CE1	1.54	1.43
1:B:197:ARG:CZ	1:B:309:HIS:HE1	1.32	1.41
1:A:110:HIS:CE1	1:B:309:HIS:CG	2.11	1.39
1:B:329:ALA:HB1	3:B:575:HOH:O	1.28	1.33
1:B:146:GLU:HB3	3:B:435:HOH:O	1.33	1.29
1:B:197:ARG:CZ	1:B:309:HIS:CE1	2.22	1.22
1:A:310:ILE:CG2	1:B:139:HIS:HE1	1.51	1.21
1:B:5:CYS:SG	3:B:553:HOH:O	2.01	1.18
1:B:156:ALA:HB3	3:B:486:HOH:O	1.42	1.15
1:B:146:GLU:CB	3:B:435:HOH:O	1.90	1.13
1:B:146:GLU:OE2	3:B:425:HOH:O	1.62	1.12
1:A:147:VAL:C	3:A:515:HOH:O	1.88	1.11
1:A:227:LYS:HE3	1:A:282:HIS:CE1	1.84	1.10
1:B:150:GLU:OE2	3:B:510:HOH:O	1.69	1.10
1:A:313:CYS:HB2	3:A:414:HOH:O	1.52	1.09
1:A:125:HIS:HE1	1:A:157:ALA:HB2	1.07	1.09
1:B:145:GLU:C	1:B:146:GLU:HG2	1.74	1.08
1:A:110:HIS:HE1	1:B:309:HIS:ND1	1.51	1.07
1:A:329:ALA:HB1	3:A:583:HOH:O	0.92	1.07
1:A:97:ILE:HG21	1:A:103:HIS:ND1	1.70	1.06
1:A:239:HIS:CE1	1:A:295:PHE:HB2	1.90	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:110:HIS:CE1	1:B:309:HIS:ND1	2.23	1.05
1:A:269:VAL:HG11	1:A:275:HIS:ND1	1.73	1.02
1:B:146:GLU:O	3:B:461:HOH:O	1.78	1.02
1:A:62:HIS:CE1	1:A:64:HIS:HE1	1.78	1.01
1:A:97:ILE:HG21	1:A:103:HIS:CE1	1.94	1.01
1:B:241:GLU:OE1	3:B:572:HOH:O	1.79	1.01
1:A:125:HIS:CE1	1:A:157:ALA:HB2	1.96	1.00
1:A:146:GLU:CB	3:A:549:HOH:O	2.09	0.99
1:B:146:GLU:OE1	3:B:425:HOH:O	1.80	0.99
1:A:214:THR:HG21	1:A:218:PHE:O	1.63	0.98
1:A:210:ALA:H	1:A:213:ASN:HD22	1.05	0.97
1:A:146:GLU:HB3	3:A:549:HOH:O	1.65	0.97
1:A:68:HIS:HD2	1:A:99:ALA:H	1.14	0.95
1:A:146:GLU:OE1	3:A:480:HOH:O	1.86	0.94
1:A:62:HIS:NE2	1:A:64:HIS:CE1	2.35	0.94
1:A:333:LYS:HD2	1:A:333:LYS:C	1.87	0.94
1:B:309:HIS:CG	1:B:309:HIS:CA	2.51	0.94
1:A:227:LYS:CE	1:A:282:HIS:CE1	2.51	0.93
1:B:146:GLU:CD	3:B:425:HOH:O	2.03	0.93
1:B:197:ARG:NH2	1:B:309:HIS:CE1	2.37	0.91
1:A:234:HIS:HE1	1:A:275:HIS:CD2	1.89	0.91
1:A:227:LYS:CE	1:A:282:HIS:HE1	1.83	0.90
1:A:242:THR:HG22	1:A:289:VAL:H	1.37	0.90
1:B:145:GLU:O	1:B:146:GLU:HG2	0.72	0.89
1:A:269:VAL:HG11	1:A:275:HIS:CE1	2.08	0.88
1:A:227:LYS:HE3	1:A:282:HIS:HE1	1.35	0.88
1:A:146:GLU:CD	3:A:480:HOH:O	2.11	0.87
1:B:197:ARG:NE	1:B:309:HIS:CE1	2.42	0.87
1:A:269:VAL:HG11	1:A:275:HIS:HD1	1.41	0.85
1:B:327:ILE:HA	3:B:577:HOH:O	1.76	0.85
1:B:197:ARG:NH2	1:B:309:HIS:HE1	1.72	0.84
1:A:326:ASN:O	3:A:424:HOH:O	1.95	0.84
1:B:333:LYS:HD2	1:B:333:LYS:C	1.98	0.83
1:A:97:ILE:HG21	1:A:103:HIS:HD1	1.38	0.82
1:A:8:SER:CA	1:A:9:LEU:N	2.42	0.82
1:B:327:ILE:CG1	3:B:577:HOH:O	2.27	0.82
1:B:59:PHE:CE2	1:B:62:HIS:CE1	2.67	0.82
1:A:146:GLU:HB2	3:A:549:HOH:O	1.75	0.82
1:B:147:VAL:O	3:B:569:HOH:O	1.97	0.81
1:A:62:HIS:CE1	1:A:64:HIS:CE1	2.68	0.80
1:A:62:HIS:NE2	1:A:64:HIS:HE1	1.78	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:234:HIS:CD2	1:B:275:HIS:HE1	2.00	0.80
1:A:328:GLU:OE1	3:A:571:HOH:O	2.00	0.80
1:A:97:ILE:HD13	1:A:103:HIS:CE1	2.17	0.79
1:B:68:HIS:HD2	1:B:99:ALA:H	1.30	0.79
1:A:110:HIS:CE1	1:B:309:HIS:CB	2.65	0.78
1:A:227:LYS:NZ	1:A:282:HIS:HE1	1.82	0.78
1:B:309:HIS:CB	1:B:309:HIS:HA	2.10	0.78
1:B:65:LYS:H	1:B:158:VAL:HG12	1.48	0.78
1:B:214:THR:HG21	1:B:218:PHE:O	1.84	0.78
1:B:68:HIS:CD2	1:B:99:ALA:H	2.03	0.77
1:A:313:CYS:SG	1:B:136:HIS:CD2	2.78	0.76
1:B:242:THR:HG22	1:B:289:VAL:H	1.48	0.76
1:B:321:ASP:O	1:B:325:GLN:HG3	1.86	0.76
1:B:125:HIS:CD2	3:B:456:HOH:O	2.39	0.76
1:A:200:THR:HB	1:A:205:HIS:NE2	2.01	0.75
1:B:200:THR:HG22	1:B:200:THR:O	1.86	0.75
1:B:59:PHE:HE2	1:B:62:HIS:CE1	2.03	0.75
1:A:239:HIS:CE1	1:A:295:PHE:CB	2.69	0.75
1:A:333:LYS:HB2	3:A:403:HOH:O	1.85	0.75
1:B:234:HIS:NE2	1:B:236:HIS:CE1	2.55	0.75
1:A:147:VAL:O	3:A:430:HOH:O	2.02	0.75
1:B:59:PHE:CE2	1:B:62:HIS:HE1	2.04	0.74
1:A:241:GLU:OE1	3:A:512:HOH:O	2.03	0.74
1:A:252:MET:HB2	1:A:259:ILE:HD11	1.68	0.74
1:A:139:HIS:CD2	1:A:139:HIS:C	2.62	0.73
1:B:252:MET:HB2	1:B:259:ILE:HD11	1.68	0.73
1:A:200:THR:HG22	1:A:200:THR:O	1.89	0.73
1:A:310:ILE:CG2	1:B:139:HIS:CE1	2.42	0.72
1:B:24:GLU:OE2	3:B:503:HOH:O	2.07	0.71
1:A:74:LEU:HD11	1:A:115:VAL:HG23	1.72	0.71
1:B:146:GLU:CB	1:B:147:VAL:HG23	2.21	0.70
1:A:139:HIS:O	1:A:139:HIS:HD2	1.74	0.70
1:B:210:ALA:H	1:B:213:ASN:HD22	1.38	0.70
1:A:146:GLU:OE2	3:A:480:HOH:O	2.08	0.69
1:A:234:HIS:CE1	1:A:275:HIS:CD2	2.75	0.69
1:A:97:ILE:CG2	1:A:103:HIS:HD1	2.05	0.69
1:A:242:THR:HG22	1:A:289:VAL:N	2.07	0.69
1:B:147:VAL:CG1	1:B:147:VAL:CG2	2.70	0.68
1:A:162:VAL:O	3:A:412:HOH:O	2.11	0.67
1:A:310:ILE:HG21	1:B:139:HIS:HE1	0.62	0.67
1:B:200:THR:CG2	1:B:200:THR:O	2.41	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:139:HIS:CD2	1:B:310:ILE:HG21	2.30	0.66
1:A:329:ALA:CB	3:A:583:HOH:O	1.76	0.66
1:A:269:VAL:CG1	1:A:275:HIS:HD1	2.08	0.66
1:B:327:ILE:HG12	3:B:577:HOH:O	1.94	0.66
1:B:30:ARG:HG2	1:B:139:HIS:HD2	1.60	0.65
1:B:7:HIS:CD2	1:B:22:GLU:OE2	2.50	0.65
1:A:318:LEU:HD12	3:A:543:HOH:O	1.96	0.64
1:A:231:ILE:HG23	3:A:503:HOH:O	1.97	0.64
1:B:86:ARG:HD3	3:B:472:HOH:O	1.96	0.64
1:A:242:THR:CG2	1:A:289:VAL:H	2.09	0.63
1:A:118:THR:HG23	3:A:417:HOH:O	1.97	0.63
1:B:206:ARG:NH1	1:B:222:SER:O	2.31	0.63
1:B:205:HIS:CE1	1:B:299:PHE:CE2	2.86	0.63
1:B:20:SER:HB2	1:B:264:GLY:HA3	1.78	0.63
1:B:145:GLU:C	1:B:146:GLU:CG	2.45	0.63
1:B:65:LYS:H	1:B:158:VAL:CG1	2.11	0.63
1:A:252:MET:HB2	1:A:259:ILE:CD1	2.29	0.62
1:A:219:ILE:HD11	1:A:290:LEU:HD12	1.81	0.62
1:B:146:GLU:HB2	3:B:435:HOH:O	1.76	0.62
1:B:62:HIS:CD2	1:B:103:HIS:HE1	2.18	0.62
1:A:146:GLU:CB	1:A:147:VAL:HG23	2.29	0.62
1:B:327:ILE:HG13	3:B:577:HOH:O	1.93	0.62
1:B:68:HIS:HD2	1:B:98:PRO:HA	1.65	0.62
1:B:252:MET:HB2	1:B:259:ILE:CD1	2.29	0.62
1:B:333:LYS:HB2	3:B:419:HOH:O	1.99	0.61
1:A:118:THR:CG2	3:A:417:HOH:O	2.48	0.61
1:B:234:HIS:CD2	1:B:275:HIS:CE1	2.86	0.61
1:B:242:THR:HG23	3:B:438:HOH:O	1.99	0.61
1:B:282:HIS:HD2	3:B:417:HOH:O	1.84	0.60
1:A:110:HIS:CE1	1:B:309:HIS:HB3	2.37	0.60
1:A:110:HIS:CG	1:B:309:HIS:HB3	2.37	0.60
1:B:74:LEU:HD11	1:B:115:VAL:HG23	1.84	0.60
1:B:219:ILE:HD11	1:B:290:LEU:HD12	1.83	0.60
1:B:206:ARG:HD3	1:B:206:ARG:N	2.17	0.60
1:A:65:LYS:H	1:A:158:VAL:HG12	1.67	0.59
1:A:242:THR:HG21	1:A:289:VAL:HB	1.83	0.59
1:A:110:HIS:ND1	1:B:309:HIS:HB3	2.18	0.59
1:B:66:ASP:H	1:B:158:VAL:HG11	1.68	0.59
1:A:36:MET:CE	3:A:454:HOH:O	2.50	0.59
1:A:227:LYS:NZ	1:A:282:HIS:CE1	2.67	0.59
1:A:309:HIS:ND1	1:B:110:HIS:CD2	2.70	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:103:HIS:HD1	1:B:103:HIS:N	2.00	0.59
1:A:234:HIS:HE2	1:A:236:HIS:CE1	2.19	0.58
1:B:103:HIS:N	1:B:103:HIS:ND1	2.48	0.58
1:A:259:ILE:O	1:A:259:ILE:HD12	2.03	0.58
1:B:146:GLU:HB2	1:B:147:VAL:CG2	2.33	0.58
1:B:118:THR:HB	3:B:468:HOH:O	2.02	0.58
1:A:65:LYS:CG	1:A:65:LYS:CE	2.81	0.58
1:B:146:GLU:HB2	1:B:147:VAL:HG23	1.84	0.58
1:B:68:HIS:CD2	1:B:98:PRO:HA	2.38	0.58
1:A:286:MET:CG	1:A:286:MET:CE	2.81	0.58
1:B:125:HIS:HB3	3:B:502:HOH:O	2.03	0.58
1:A:321:ASP:O	1:A:325:GLN:HG3	2.02	0.58
1:A:66:ASP:H	1:A:158:VAL:HG11	1.69	0.58
1:B:66:ASP:O	1:B:120:LYS:NZ	2.32	0.58
1:A:110:HIS:NE2	1:B:309:HIS:CG	2.72	0.57
1:A:333:LYS:C	1:A:333:LYS:CD	2.69	0.57
1:B:236:HIS:CG	1:B:239:HIS:CE1	2.91	0.57
1:A:333:LYS:HD2	1:A:333:LYS:O	2.04	0.57
1:A:146:GLU:HB2	1:A:147:VAL:HG23	1.86	0.56
1:B:64:HIS:NE2	1:B:69:GLU:OE1	2.33	0.56
1:A:62:HIS:CE1	1:A:103:HIS:CD2	2.92	0.56
1:A:14:MET:HB2	1:A:15:PRO:HD2	1.85	0.56
1:B:146:GLU:CA	1:B:147:VAL:HG23	2.36	0.56
1:B:68:HIS:HD2	1:B:99:ALA:N	2.02	0.56
1:B:309:HIS:CB	1:B:309:HIS:C	2.67	0.56
1:A:68:HIS:HE1	1:A:215:ASP:OD2	1.89	0.56
1:B:259:ILE:O	1:B:259:ILE:HD12	2.06	0.56
1:A:309:HIS:CE1	1:B:110:HIS:NE2	2.74	0.55
1:A:313:CYS:CB	3:A:414:HOH:O	2.31	0.55
1:A:68:HIS:CD2	1:A:99:ALA:H	2.07	0.55
1:B:81:THR:O	1:B:103:HIS:HA	2.05	0.55
1:A:210:ALA:H	1:A:213:ASN:ND2	1.89	0.55
1:B:205:HIS:CE1	1:B:299:PHE:HE2	2.23	0.55
1:B:38:ASN:HA	1:B:47:GLU:HG2	1.89	0.55
1:B:211:GLN:NE2	1:B:293:GLY:O	2.40	0.55
1:B:333:LYS:C	1:B:333:LYS:CD	2.73	0.55
1:A:64:HIS:N	1:A:64:HIS:ND1	2.50	0.55
1:A:139:HIS:HD2	1:A:139:HIS:C	2.04	0.55
1:A:200:THR:CG2	1:A:200:THR:O	2.54	0.55
1:B:126:LEU:HD12	1:B:126:LEU:C	2.27	0.55
1:B:65:LYS:N	1:B:158:VAL:HG12	2.21	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:102:PRO:O	1:A:103:HIS:HB3	2.06	0.54
1:B:205:HIS:CE1	1:B:299:PHE:CD2	2.96	0.54
1:B:86:ARG:CD	3:B:472:HOH:O	2.54	0.54
1:A:206:ARG:NH1	1:A:222:SER:O	2.41	0.54
1:B:146:GLU:C	1:B:147:VAL:HG23	2.28	0.54
1:B:333:LYS:HD2	1:B:333:LYS:O	2.07	0.53
1:B:8:SER:CA	1:B:9:LEU:N	2.72	0.53
1:A:68:HIS:CD2	1:A:98:PRO:HA	2.45	0.52
1:B:326:ASN:O	3:B:577:HOH:O	2.18	0.52
1:A:239:HIS:NE2	1:A:295:PHE:HB2	2.23	0.52
1:B:146:GLU:C	1:B:147:VAL:CG2	2.78	0.52
1:A:27:LEU:HD22	1:A:134:TYR:CE1	2.45	0.52
1:A:97:ILE:CD1	1:A:103:HIS:CE1	2.91	0.51
1:A:110:HIS:HD2	3:A:488:HOH:O	1.93	0.51
1:A:292:PRO:O	3:A:423:HOH:O	2.19	0.51
1:A:36:MET:HE1	3:A:454:HOH:O	2.09	0.51
1:B:61:LEU:O	1:B:62:HIS:HB3	2.10	0.51
1:A:333:LYS:HD2	1:A:334:VAL:N	2.25	0.51
1:A:68:HIS:HD2	1:A:99:ALA:N	1.97	0.50
1:A:242:THR:HG22	1:A:289:VAL:O	2.11	0.50
1:A:7:HIS:CD2	1:A:22:GLU:OE2	2.64	0.50
1:A:65:LYS:CD	1:A:65:LYS:CB	2.82	0.50
1:A:239:HIS:HE1	1:A:295:PHE:CB	2.20	0.50
1:B:211:GLN:HA	1:B:214:THR:HG22	1.93	0.50
1:B:234:HIS:C	1:B:234:HIS:CD2	2.85	0.50
1:B:227:LYS:NZ	3:B:539:HOH:O	2.30	0.49
1:A:227:LYS:HE3	1:A:282:HIS:ND1	2.22	0.49
1:B:65:LYS:N	1:B:158:VAL:CG1	2.75	0.49
1:A:74:LEU:HD11	1:A:115:VAL:CG2	2.42	0.49
1:A:77:LYS:HB3	1:A:88:LEU:HD11	1.93	0.49
1:A:62:HIS:C	1:A:62:HIS:ND1	2.63	0.49
1:B:14:MET:O	1:B:268:HIS:CD2	2.66	0.49
1:B:309:HIS:CG	1:B:309:HIS:HA	2.41	0.49
1:B:118:THR:HG23	3:B:566:HOH:O	2.12	0.48
1:A:71:ILE:CB	1:A:71:ILE:CD1	2.81	0.48
1:B:253:TRP:HA	1:B:257:GLN:O	2.13	0.48
1:B:253:TRP:O	1:B:275:HIS:HA	2.13	0.48
1:A:285:LYS:NZ	3:A:558:HOH:O	2.45	0.48
1:A:197:ARG:HB3	1:A:204:LEU:HD11	1.95	0.48
1:A:146:GLU:CA	1:A:147:VAL:HG23	2.44	0.47
1:A:146:GLU:HB2	1:A:147:VAL:CG2	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:242:THR:HG22	1:B:289:VAL:N	2.22	0.47
1:A:65:LYS:N	1:A:158:VAL:HG12	2.29	0.47
1:B:268:HIS:CD2	1:B:270:PRO:HD3	2.50	0.47
1:A:332:LEU:HD13	1:A:333:LYS:N	2.29	0.47
1:B:110:HIS:ND1	1:B:110:HIS:N	2.63	0.46
1:A:296:GLU:N	1:A:297:PRO:HD2	2.31	0.46
1:A:48:ILE:HG12	1:A:117:TYR:HD2	1.81	0.46
1:B:139:HIS:CE1	1:B:139:HIS:O	2.69	0.46
1:A:7:HIS:HD2	1:A:22:GLU:OE2	1.99	0.46
1:A:161:ILE:HG21	3:A:576:HOH:O	2.15	0.46
1:A:310:ILE:HD13	1:B:139:HIS:ND1	2.31	0.45
1:B:59:PHE:HB2	1:B:105:TYR:CZ	2.51	0.45
1:A:211:GLN:HA	1:A:214:THR:HG22	1.98	0.45
1:A:227:LYS:HD2	1:A:282:HIS:ND1	2.31	0.45
1:A:234:HIS:ND1	1:A:234:HIS:C	2.70	0.45
1:A:210:ALA:O	1:A:214:THR:HG22	2.15	0.45
1:A:53:GLY:HA2	1:A:139:HIS:ND1	2.32	0.45
1:A:234:HIS:NE2	1:A:236:HIS:CE1	2.85	0.45
1:B:200:THR:HB	1:B:205:HIS:NE2	2.31	0.45
1:B:20:SER:HB2	1:B:264:GLY:CA	2.47	0.45
1:A:282:HIS:HB3	3:A:562:HOH:O	2.16	0.44
1:B:329:ALA:CB	3:B:575:HOH:O	2.15	0.44
1:A:36:MET:HE3	3:A:406:HOH:O	2.18	0.44
1:B:275:HIS:N	1:B:275:HIS:ND1	2.63	0.44
1:B:62:HIS:CD2	1:B:103:HIS:CE1	3.03	0.43
1:B:151:ARG:HA	1:B:153:ALA:H	1.82	0.43
1:A:126:LEU:HD12	1:A:126:LEU:C	2.39	0.43
1:A:74:LEU:CD1	1:A:115:VAL:HG23	2.44	0.43
1:A:186:VAL:HB	1:A:187:PRO:HD2	2.00	0.43
1:A:234:HIS:HE1	1:A:275:HIS:NE2	2.15	0.43
1:A:66:ASP:H	1:A:158:VAL:CG1	2.32	0.43
1:B:217:GLN:O	1:B:292:PRO:HA	2.19	0.43
1:B:75:ASP:OD2	1:B:113:ARG:HD3	2.19	0.42
1:A:89:LEU:HB3	1:A:93:ASP:HB2	2.00	0.42
1:B:275:HIS:HD1	1:B:275:HIS:N	2.17	0.42
1:B:126:LEU:HD12	1:B:127:TYR:N	2.34	0.42
1:A:80:LEU:HD12	1:A:104:SER:O	2.20	0.42
1:A:202:ASP:HB3	1:A:315:PRO:HB3	2.01	0.42
1:B:234:HIS:NE2	1:B:236:HIS:HE1	2.13	0.42
1:A:62:HIS:HE1	1:A:103:HIS:CD2	2.36	0.42
1:A:243:PHE:CE1	1:A:252:MET:HE1	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:110:HIS:CD2	1:B:309:HIS:CB	3.03	0.42
1:B:134:TYR:CE2	1:B:136:HIS:HB2	2.54	0.42
1:B:61:LEU:HA	1:B:104:SER:HB3	2.01	0.41
1:A:309:HIS:CE1	1:B:110:HIS:HE2	2.38	0.41
1:B:242:THR:HG21	1:B:289:VAL:HB	2.01	0.41
1:A:178:LEU:HG	1:A:179:THR:N	2.35	0.41
1:B:64:HIS:HB3	1:B:158:VAL:O	2.20	0.41
1:A:97:ILE:CG2	1:A:103:HIS:ND1	2.58	0.41
1:B:158:VAL:HG22	3:B:409:HOH:O	2.20	0.41
1:A:136:HIS:CD2	1:B:313:CYS:SG	3.14	0.41
1:A:242:THR:CG2	1:A:289:VAL:HB	2.47	0.41
1:B:224:GLU:HA	1:B:284:THR:O	2.21	0.41
1:A:110:HIS:CG	1:B:309:HIS:CB	3.03	0.41
1:B:249:GLN:O	1:B:280:ASP:HB2	2.21	0.41
1:A:317:ALA:HA	3:A:543:HOH:O	2.22	0.40
1:A:200:THR:CB	1:A:205:HIS:NE2	2.79	0.40
1:A:203:GLN:HB3	1:A:205:HIS:HE1	1.86	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	328/337 (97%)	299 (91%)	19 (6%)	10 (3%)	5	4
1	B	328/337 (97%)	304 (93%)	15 (5%)	9 (3%)	6	6
All	All	656/674 (97%)	603 (92%)	34 (5%)	19 (3%)	6	5

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	8	SER

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Mol	Chain	Res	Type
1	A	146	GLU
1	A	148	SER
1	A	149	ASN
1	A	168	LYS
1	A	171	CYS
1	B	146	GLU
1	B	148	SER
1	B	149	ASN
1	B	165	ASP
1	B	168	LYS
1	B	171	CYS
1	B	152	PHE
1	B	255	ASP
1	A	165	ASP
1	A	329	ALA
1	A	145	GLU
1	A	255	ASP
1	B	164	LEU

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	273/285 (96%)	239 (88%)	34 (12%)	6 7
1	B	273/285 (96%)	237 (87%)	36 (13%)	5 6
All	All	546/570 (96%)	476 (87%)	70 (13%)	5 6

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	SER
1	A	11	LYS
1	A	62	HIS
1	A	63	VAL
1	A	64	HIS

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Mol	Chain	Res	Type
1	A	65	LYS
1	A	72	LEU
1	A	86	ARG
1	A	103	HIS
1	A	114	LEU
1	A	118	THR
1	A	125	HIS
1	A	139	HIS
1	A	144	SER
1	A	146	GLU
1	A	163	PHE
1	A	168	LYS
1	A	179	THR
1	A	200	THR
1	A	206	ARG
1	A	214	THR
1	A	239	HIS
1	A	242	THR
1	A	257	GLN
1	A	275	HIS
1	A	282	HIS
1	A	286	MET
1	A	313	CYS
1	A	314	LYS
1	A	315	PRO
1	A	322	ARG
1	A	324	LEU
1	A	332	LEU
1	A	333	LYS
1	B	8	SER
1	B	11	LYS
1	B	62	HIS
1	B	63	VAL
1	B	64	HIS
1	B	66	ASP
1	B	72	LEU
1	B	86	ARG
1	B	89	LEU
1	B	114	LEU
1	B	118	THR
1	B	125	HIS
1	B	139	HIS

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Mol	Chain	Res	Type
1	B	144	SER
1	B	146	GLU
1	B	151	ARG
1	B	154	GLU
1	B	163	PHE
1	B	164	LEU
1	B	168	LYS
1	B	179	THR
1	B	200	THR
1	B	205	HIS
1	B	206	ARG
1	B	231	ILE
1	B	234	HIS
1	B	242	THR
1	B	257	GLN
1	B	268	HIS
1	B	282	HIS
1	B	313	CYS
1	B	314	LYS
1	B	322	ARG
1	B	324	LEU
1	B	332	LEU
1	B	333	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	7	HIS
1	A	64	HIS
1	A	68	HIS
1	A	110	HIS
1	A	122	ASN
1	A	125	HIS
1	A	136	HIS
1	A	211	GLN
1	A	213	ASN
1	A	268	HIS
1	A	282	HIS
1	B	7	HIS
1	B	62	HIS
1	B	68	HIS
1	B	136	HIS

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Mol	Chain	Res	Type
1	B	139	HIS
1	B	211	GLN
1	B	213	ASN
1	B	268	HIS
1	B	282	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 4 ligands modelled in this entry, 4 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	320/337 (94%)	-0.23	11 (3%) 49 49	28, 39, 64, 88	1 (0%)
1	B	321/337 (95%)	-0.17	11 (3%) 49 49	28, 38, 64, 89	1 (0%)
All	All	641/674 (95%)	-0.20	22 (3%) 49 49	28, 38, 64, 89	2 (0%)

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	7	HIS	5.3
1	A	163	PHE	5.0
1	A	7	HIS	4.1
1	B	5	CYS	3.3
1	B	147	VAL	3.3
1	B	6	THR	3.2
1	A	164	LEU	3.1
1	A	6	THR	2.8
1	B	333	LYS	2.8
1	B	159	ALA	2.7
1	A	256	GLY	2.7
1	A	172	SER	2.7
1	A	255	ASP	2.6
1	A	317	ALA	2.6
1	B	163	PHE	2.6
1	B	125	HIS	2.4
1	A	144	SER	2.3
1	B	255	ASP	2.3
1	A	238	TYR	2.3
1	B	334	VAL	2.3
1	A	314	LYS	2.1
1	B	164	LEU	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	FE	B	401	1/1	0.99	0.12	-	50,50,50,50	0
2	FE	A	402	1/1	0.99	0.16	-	43,43,43,43	0
2	FE	B	402	1/1	0.97	0.13	-	43,43,43,43	0
2	FE	A	401	1/1	0.98	0.12	-	51,51,51,51	0

6.5 Other polymers (i)

There are no such residues in this entry.