Full wwPDB X-ray Structure Validation Report ⓘ

Mar 24, 2022 – 03:27 pm GMT

PDB ID	:	6QRQ
Title	:	Apo conformation of chemotaxis sensor ODP
Authors	:	Muok, A.R.; Crane, B.R.
Deposited on	:	2019-02-19
Resolution	:	2.56 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:

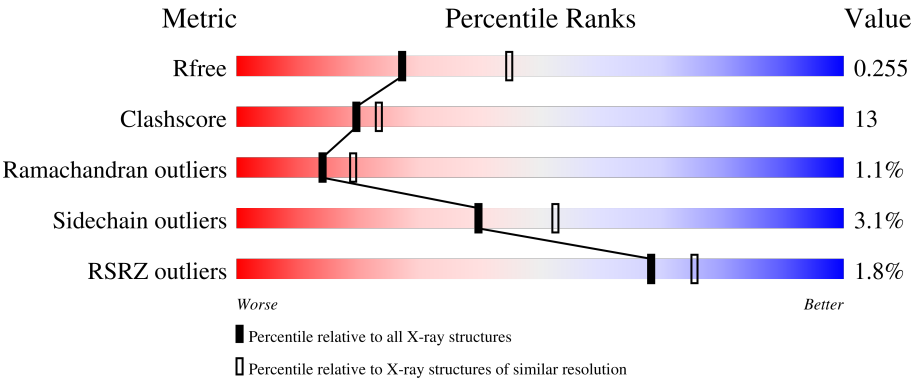
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.27
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.27

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 2.56 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}	130704	1279 (2.58-2.54)
Clashscore	141614	1327 (2.58-2.54)
Ramachandran outliers	138981	1312 (2.58-2.54)
Sidechain outliers	138945	1312 (2.58-2.54)
RSRZ outliers	127900	1269 (2.58-2.54)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	253	74% 19%
1	B	253	4% 77% 19%
1	C	253	% 66% 29%
1	D	253	2% 71% 23%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 8051 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 Oxygen-binding diiron protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	251	Total	C	N	O	S	0	0	0
			2011	1305	341	356	9			
1	A	244	Total	C	N	O	S	13	0	0
			1956	1269	333	345	9			
1	C	247	Total	C	N	O	S	6	0	0
			1990	1294	337	350	9			
1	D	250	Total	C	N	O	S	0	0	0
			2012	1306	340	357	9			

- Molecule 2 is water.

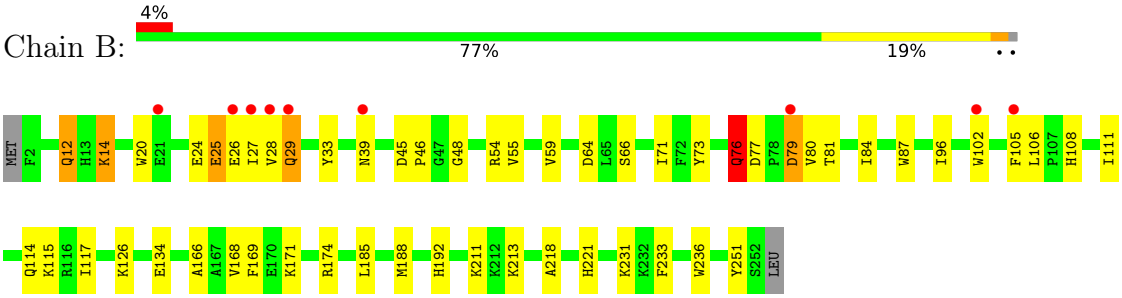
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	24	Total	O	0	0
			24	24		
2	A	14	Total	O	0	0
			14	14		
2	C	26	Total	O	0	0
			26	26		
2	D	18	Total	O	0	0
			18	18		

3 Residue-property plots (i)

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

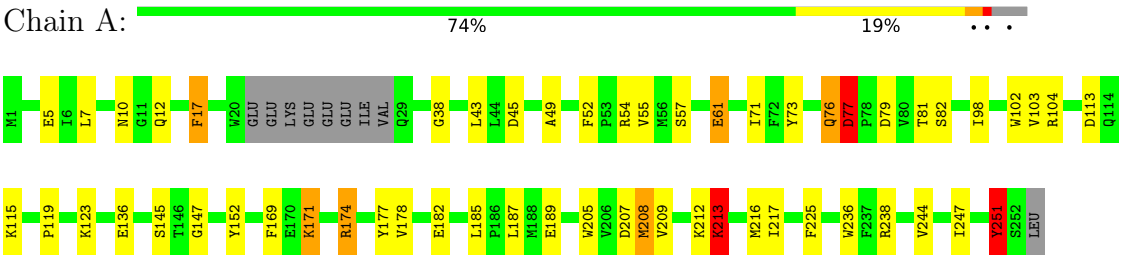
• Molecule 1: Oxygen-binding diiron protein

Chain B:



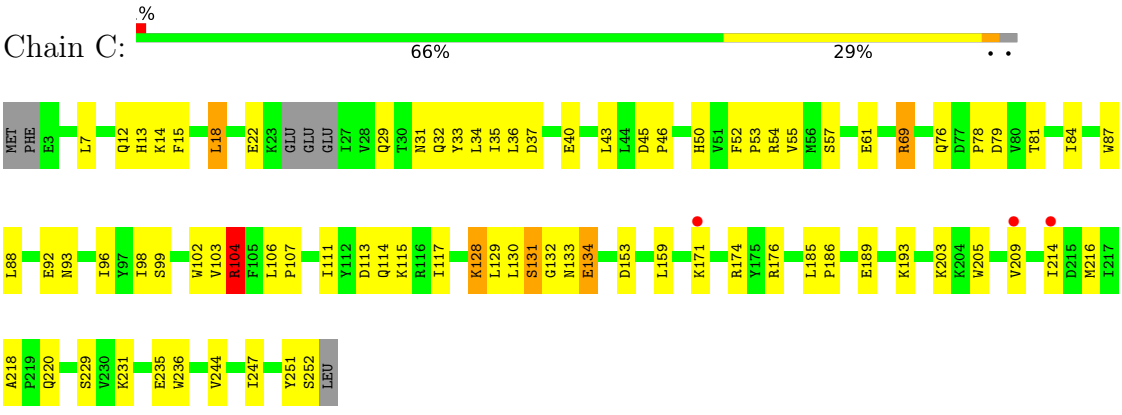
• Molecule 1: Oxygen-binding diiron protein

Chain A:



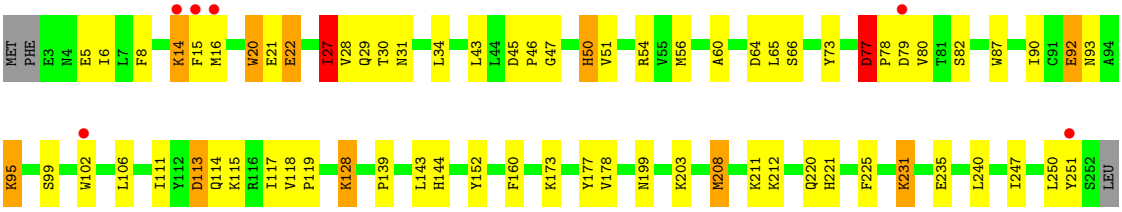
• Molecule 1: Oxygen-binding diiron protein

Chain C:



• Molecule 1: Oxygen-binding diiron protein

Chain D:


MET PHE E3 N4 E5 I6 L7 F8 K14 F15 M16 W20 E21 E22 I27 V28 Q29 T30 N31 L34 L43 L44 D45 P46 G47 H50 V51 R54 V55 M56 A60 D64 L65 S66 Y73 D77 P78 D79 V80 T81 S82 W87 I90 C91 E92 N93 A94
K95 S99 W102 L106 I111 Y112 D113 Q114 K115 R116 I117 V118 P119 K128 P139 L143 H144 Y152 F160 K173 Y177 V178 N199 K203 M208 K211 K212 Q220 H221 F225 K231 E235 L240 I247 L250 Y251 S252 LEU

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	84.65Å 110.72Å 110.96Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.54 – 2.56 49.60 – 2.56	Depositor EDS
% Data completeness (in resolution range)	94.0 (49.54-2.56) 93.0 (49.60-2.56)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.75 (at 2.54Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.191 , 0.255 0.194 , 0.255	Depositor DCC
R_{free} test set	1998 reflections (5.97%)	wwPDB-VP
Wilson B-factor (Å^2)	44.6	Xtriage
Anisotropy	0.441	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.011 for -h,l,k	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	8051	wwPDB-VP
Average B, all atoms (Å^2)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.45% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	0.57	1/2006 (0.0%)	0.81	8/2706 (0.3%)
1	B	0.61	2/2064 (0.1%)	0.81	7/2787 (0.3%)
1	C	0.69	5/2042 (0.2%)	0.88	10/2757 (0.4%)
1	D	0.60	2/2065 (0.1%)	0.81	3/2789 (0.1%)
All	All	0.62	10/8177 (0.1%)	0.83	28/11039 (0.3%)

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	D	0	2
All	All	0	3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	235	GLU	CD-OE2	9.46	1.36	1.25
1	A	61	GLU	CD-OE2	7.57	1.33	1.25
1	C	229	SER	CB-OG	7.27	1.51	1.42
1	C	171	LYS	CE-NZ	7.14	1.67	1.49
1	B	76	GLN	CA-CB	-7.01	1.38	1.53
1	C	231	LYS	CE-NZ	6.87	1.66	1.49
1	C	134	GLU	CG-CD	6.13	1.61	1.51
1	B	14	LYS	CD-CE	5.92	1.66	1.51
1	D	92	GLU	CD-OE2	5.25	1.31	1.25
1	D	92	GLU	CB-CG	-5.10	1.42	1.52

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	213	LYS	CG-CD-CE	-10.60	80.10	111.90
1	C	128	LYS	CG-CD-CE	-8.98	84.97	111.90
1	C	104	ARG	NE-CZ-NH1	-8.68	115.96	120.30
1	C	69	ARG	NE-CZ-NH2	-8.14	116.23	120.30
1	C	92	GLU	CA-CB-CG	-7.99	95.82	113.40
1	A	251	TYR	CB-CG-CD2	-7.36	116.58	121.00
1	B	231	LYS	CD-CE-NZ	-7.26	95.01	111.70
1	B	14	LYS	CA-CB-CG	7.24	129.34	113.40
1	C	134	GLU	OE1-CD-OE2	-6.65	115.33	123.30
1	C	131	SER	CB-CA-C	-6.57	97.61	110.10
1	A	174	ARG	NE-CZ-NH2	-6.50	117.05	120.30
1	B	79	ASP	CB-CA-C	-6.39	97.61	110.40
1	C	229	SER	CB-CA-C	6.20	121.88	110.10
1	C	104	ARG	NE-CZ-NH2	6.08	123.34	120.30
1	A	76	GLN	C-N-CA	5.95	136.57	121.70
1	A	213	LYS	CD-CE-NZ	5.93	125.34	111.70
1	A	251	TYR	CB-CG-CD1	5.76	124.46	121.00
1	D	77	ASP	C-N-CD	-5.62	108.24	120.60
1	D	14	LYS	CB-CA-C	-5.62	99.17	110.40
1	D	95	LYS	CA-CB-CG	5.44	125.37	113.40
1	B	29	GLN	N-CA-CB	5.39	120.31	110.60
1	A	123	LYS	CB-CG-CD	-5.38	97.61	111.60
1	A	61	GLU	CB-CA-C	5.33	121.06	110.40
1	B	174	ARG	CB-CG-CD	-5.09	98.36	111.60
1	B	29	GLN	CB-CA-C	-5.06	100.28	110.40
1	C	231	LYS	CB-CA-C	-5.05	100.30	110.40
1	B	29	GLN	CA-CB-CG	5.01	124.42	113.40
1	C	128	LYS	CD-CE-NZ	5.01	123.22	111.70

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	77	ASP	Peptide
1	D	27	ILE	Peptide
1	D	28	VAL	Peptide

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	1956	0	1943	40	0
1	B	2011	0	1985	39	1
1	C	1990	0	1975	55	0
1	D	2012	0	1989	71	1
2	A	14	0	0	0	0
2	B	24	0	0	0	0
2	C	26	0	0	0	0
2	D	18	0	0	2	0
All	All	8051	0	7892	201	1

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 13.

All (201) 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:D:29:GLN:HG3	1:D:30:THR:H	1.35	0.90
1:D:251:TYR:OH	2:D:301:HOH:O	1.89	0.90
1:D:6:ILE:HG23	1:D:14:LYS:HD2	1.55	0.89
1:B:77:ASP:HB3	1:B:79:ASP:OD1	1.74	0.85
1:D:14:LYS:CE	1:D:16:MET:HG2	2.07	0.84
1:D:14:LYS:HZ1	1:D:16:MET:HG2	1.42	0.84
1:C:37:ASP:OD1	1:C:131:SER:OG	1.96	0.83
1:C:209:VAL:HG12	1:C:214:ILE:CD1	2.09	0.82
1:B:76:GLN:HE22	1:B:102:TRP:HB2	1.45	0.81
1:A:49:ALA:H	1:A:82:SER:HB2	1.45	0.81
1:D:14:LYS:NZ	1:D:16:MET:HG2	1.96	0.81
1:D:113:ASP:HB3	1:D:115:LYS:HD3	1.66	0.77
1:D:139:PRO:HG2	1:D:208:MET:HE1	1.68	0.76
1:A:77:ASP:H	1:A:81:THR:HG23	1.51	0.75
1:B:28:VAL:HG11	1:B:168:VAL:HA	1.69	0.74
1:C:128:LYS:NZ	1:C:132:GLY:O	2.18	0.74
1:B:28:VAL:HG21	1:B:169:PHE:H	1.53	0.74
1:C:29:GLN:HE21	1:C:174:ARG:HH11	1.35	0.74
1:B:76:GLN:NE2	1:B:102:TRP:HB2	2.04	0.73
1:D:92:GLU:OE2	1:D:93:ASN:ND2	2.23	0.72
1:B:39:ASN:ND2	1:C:117:ILE:O	2.22	0.72
1:D:6:ILE:HG12	1:D:14:LYS:NZ	2.06	0.70
1:D:8:PHE:O	1:D:14:LYS:HG3	1.92	0.70
1:A:113:ASP:OD1	1:A:115:LYS:HG3	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:34:LEU:HD23	1:D:43:LEU:HD23	1.74	0.69
1:C:29:GLN:HE21	1:C:174:ARG:NH1	1.92	0.68
1:C:76:GLN:NE2	1:C:102:TRP:HB3	2.09	0.68
1:D:14:LYS:HG2	1:D:15:PHE:N	2.08	0.68
1:D:247:ILE:HD12	1:D:250:LEU:HD12	1.74	0.68
1:C:209:VAL:CG1	1:C:214:ILE:CD1	2.72	0.68
1:D:199:ASN:OD1	1:D:203:LYS:HE2	1.94	0.68
1:C:34:LEU:HD13	1:C:43:LEU:HD23	1.77	0.66
1:D:78:PRO:HB2	1:D:79:ASP:HA	1.77	0.66
1:A:5:GLU:OE2	1:A:177:TYR:OH	2.11	0.65
1:B:20:TRP:CD2	1:B:29:GLN:NE2	2.63	0.64
1:D:113:ASP:CB	1:D:115:LYS:HD3	2.27	0.64
1:A:247:ILE:HG12	1:A:251:TYR:CE2	2.33	0.63
1:C:128:LYS:HE3	1:C:134:GLU:HG3	1.81	0.63
1:D:14:LYS:HZ1	1:D:16:MET:CG	2.09	0.63
1:A:103:VAL:HG11	1:A:119:PRO:HB3	1.80	0.63
1:D:6:ILE:HG12	1:D:14:LYS:HZ3	1.62	0.63
1:B:114:GLN:HG2	1:B:117:ILE:HG13	1.80	0.62
1:D:139:PRO:HG2	1:D:208:MET:CE	2.30	0.60
1:D:45:ASP:OD1	1:D:73:TYR:HA	2.01	0.60
1:D:113:ASP:CG	1:D:115:LYS:HD3	2.23	0.59
1:D:20:TRP:HZ3	1:D:31:ASN:OD1	1.85	0.59
1:D:128:LYS:NZ	2:D:302:HOH:O	2.34	0.59
1:D:14:LYS:HE2	1:D:16:MET:HE2	1.85	0.59
1:D:77:ASP:HB3	1:D:78:PRO:C	2.24	0.58
1:A:52:PHE:HA	1:A:55:VAL:HG22	1.85	0.58
1:A:185:LEU:HD21	1:A:236:TRP:CE2	2.38	0.58
1:D:29:GLN:CG	1:D:30:THR:H	2.14	0.58
1:C:209:VAL:HG12	1:C:214:ILE:HD13	1.85	0.57
1:A:169:PHE:CD2	1:A:174:ARG:HB3	2.39	0.57
1:C:98:ILE:HD11	1:C:103:VAL:HG12	1.84	0.57
1:C:209:VAL:CG1	1:C:214:ILE:HD11	2.34	0.57
1:B:20:TRP:CG	1:B:29:GLN:NE2	2.73	0.56
1:A:169:PHE:HA	1:A:187:LEU:HD23	1.88	0.56
1:D:231:LYS:HE3	1:D:235:GLU:OE1	2.05	0.56
1:C:76:GLN:HE21	1:C:102:TRP:HB3	1.70	0.55
1:B:81:THR:HA	1:B:84:ILE:HG13	1.88	0.55
1:B:71:ILE:HB	1:B:96:ILE:HG22	1.88	0.55
1:A:247:ILE:HG12	1:A:251:TYR:HE2	1.72	0.54
1:B:45:ASP:OD1	1:B:73:TYR:HA	2.07	0.54
1:D:14:LYS:HG2	1:D:15:PHE:H	1.71	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:50:HIS:CE1	1:C:79:ASP:HB2	2.43	0.54
1:D:77:ASP:HB3	1:D:78:PRO:CA	2.38	0.54
1:C:209:VAL:CG1	1:C:214:ILE:HD13	2.37	0.54
1:D:99:SER:HB3	1:D:102:TRP:CD1	2.42	0.54
1:D:56:MET:HG3	1:D:90:ILE:HD13	1.89	0.54
1:B:79:ASP:OD1	1:B:80:VAL:N	2.41	0.54
1:C:189:GLU:O	1:C:193:LYS:HG3	2.06	0.54
1:D:60:ALA:HB2	1:D:65:LEU:HD21	1.89	0.53
1:A:76:GLN:HG2	1:A:102:TRP:CD2	2.43	0.53
1:A:102:TRP:HH2	1:A:145:SER:HB3	1.73	0.53
1:D:27:ILE:HD12	1:D:29:GLN:OE1	2.09	0.53
1:C:76:GLN:HG3	1:C:102:TRP:CG	2.44	0.53
1:C:104:ARG:O	1:C:107:PRO:HD2	2.09	0.53
1:D:34:LEU:HD23	1:D:43:LEU:CD2	2.39	0.53
1:B:28:VAL:HG21	1:B:169:PHE:N	2.21	0.52
1:C:185:LEU:HD11	1:C:236:TRP:CE2	2.45	0.52
1:B:126:LYS:HE3	1:B:134:GLU:OE2	2.09	0.52
1:C:12:GLN:O	1:C:37:ASP:HA	2.09	0.52
1:D:6:ILE:HA	1:D:14:LYS:HZ2	1.74	0.52
1:B:55:VAL:O	1:B:59:VAL:HG23	2.10	0.52
1:A:76:GLN:HG2	1:A:102:TRP:CE2	2.44	0.52
1:C:185:LEU:HD11	1:C:236:TRP:CZ2	2.44	0.52
1:D:21:GLU:O	1:D:54:ARG:HD2	2.10	0.52
1:D:29:GLN:HG3	1:D:30:THR:N	2.17	0.52
1:B:12:GLN:OE1	1:B:12:GLN:O	2.28	0.52
1:B:64:ASP:OD2	1:B:66:SER:OG	2.23	0.51
1:C:18:LEU:O	1:C:176:ARG:NH2	2.31	0.50
1:C:113:ASP:OD1	1:C:115:LYS:HG2	2.12	0.49
1:C:31:ASN:O	1:C:32:GLN:NE2	2.45	0.49
1:A:104:ARG:HH11	1:A:104:ARG:HG2	1.76	0.49
1:A:136:GLU:OE2	1:A:212:LYS:NZ	2.35	0.49
1:B:76:GLN:OE1	1:B:102:TRP:CG	2.66	0.49
1:D:14:LYS:HE3	1:D:16:MET:HG2	1.92	0.48
1:C:15:PHE:CE2	1:C:35:ILE:HD11	2.49	0.48
1:D:114:GLN:HG2	1:D:117:ILE:HG13	1.96	0.48
1:A:45:ASP:OD1	1:A:73:TYR:HA	2.14	0.48
1:A:43:LEU:HB2	1:A:71:ILE:HG23	1.96	0.47
1:C:99:SER:HB3	1:C:102:TRP:CD1	2.50	0.47
1:C:159:LEU:HD22	1:C:209:VAL:CG1	2.44	0.47
1:A:7:LEU:HD11	1:A:17:PHE:HB2	1.95	0.47
1:A:247:ILE:HG12	1:A:251:TYR:CD2	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:247:ILE:O	1:A:251:TYR:HD2	1.96	0.47
1:D:65:LEU:HD22	1:D:65:LEU:N	2.29	0.47
1:A:182:GLU:OE2	1:D:173:LYS:NZ	2.24	0.47
1:D:247:ILE:O	1:D:247:ILE:HG13	2.15	0.47
1:C:205:TRP:CZ2	1:C:209:VAL:HG21	2.50	0.47
1:A:208:MET:HG3	1:A:209:VAL:N	2.29	0.47
1:D:8:PHE:O	1:D:14:LYS:CG	2.62	0.47
1:D:247:ILE:HD12	1:D:250:LEU:CD1	2.44	0.46
1:A:217:ILE:HB	1:A:225:PHE:HB2	1.97	0.46
1:A:152:TYR:OH	1:A:213:LYS:O	2.20	0.46
1:D:95:LYS:HD3	1:D:118:VAL:HG21	1.96	0.46
1:B:26:GLU:O	1:B:26:GLU:HG3	2.16	0.46
1:B:185:LEU:HD11	1:B:236:TRP:CE2	2.50	0.46
1:D:79:ASP:O	1:D:80:VAL:C	2.52	0.46
1:A:7:LEU:HD22	1:A:216:MET:HE2	1.98	0.46
1:A:207:ASP:OD1	1:A:238:ARG:NH1	2.49	0.46
1:A:244:VAL:HG13	1:A:247:ILE:HD12	1.97	0.46
1:D:78:PRO:CB	1:D:79:ASP:HA	2.46	0.46
1:C:84:ILE:HG22	1:C:88:LEU:HD12	1.97	0.45
1:D:79:ASP:O	1:D:82:SER:N	2.46	0.45
1:C:40:GLU:OE2	1:C:130:LEU:N	2.48	0.45
1:C:244:VAL:HA	1:C:247:ILE:HB	1.98	0.45
1:B:27:ILE:HD12	1:B:28:VAL:HG23	1.99	0.45
1:B:39:ASN:ND2	1:C:114:GLN:O	2.40	0.45
1:A:77:ASP:N	1:A:81:THR:HG23	2.25	0.45
1:B:28:VAL:HG22	1:B:29:GLN:H	1.81	0.45
1:D:64:ASP:OD2	1:D:66:SER:HB2	2.16	0.45
1:A:57:SER:O	1:A:61:GLU:HB2	2.17	0.45
1:A:205:TRP:CE2	1:A:209:VAL:HG21	2.52	0.45
1:C:209:VAL:HG13	1:C:214:ILE:HD11	1.98	0.45
1:D:160:PHE:CE1	1:D:220:GLN:HG2	2.52	0.45
1:D:160:PHE:CZ	1:D:220:GLN:HG2	2.51	0.45
1:D:20:TRP:CZ3	1:D:31:ASN:OD1	2.69	0.44
1:A:73:TYR:HB2	1:A:98:ILE:HG22	1.98	0.44
1:A:178:VAL:HG11	1:A:225:PHE:CD2	2.52	0.44
1:D:47:GLY:HA3	1:D:51:VAL:CG2	2.48	0.44
1:A:77:ASP:HA	1:A:81:THR:HG23	2.00	0.44
1:C:205:TRP:O	1:C:209:VAL:HG23	2.18	0.44
1:C:69:ARG:HD3	1:C:93:ASN:HB3	2.00	0.44
1:D:46:PRO:HB2	1:D:87:TRP:CE2	2.53	0.44
1:C:13:HIS:HA	1:C:36:LEU:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:96:ILE:HB	1:C:117:ILE:HD13	1.99	0.44
1:B:25:GLU:N	1:B:26:GLU:HB2	2.33	0.43
1:A:104:ARG:HG2	1:A:104:ARG:NH1	2.32	0.43
1:D:50:HIS:ND1	1:D:50:HIS:N	2.65	0.43
1:B:27:ILE:HA	1:B:28:VAL:HA	1.36	0.43
1:B:33:TYR:CZ	1:B:218:ALA:HB1	2.53	0.43
1:D:30:THR:HG22	1:D:221:HIS:ND1	2.32	0.43
1:D:106:LEU:HD23	1:D:106:LEU:HA	1.81	0.43
1:C:46:PRO:HB2	1:C:87:TRP:NE1	2.34	0.43
1:D:20:TRP:O	1:D:20:TRP:HD1	2.02	0.43
1:C:69:ARG:HD2	1:C:69:ARG:HA	1.58	0.43
1:C:185:LEU:HB3	1:C:186:PRO:HD3	2.01	0.43
1:C:220:GLN:HA	1:C:220:GLN:OE1	2.19	0.43
1:D:16:MET:HB2	1:D:34:LEU:HB3	2.00	0.43
1:A:102:TRP:CZ3	1:A:147:GLY:O	2.72	0.43
1:B:54:ARG:CZ	1:B:54:ARG:HB3	2.48	0.43
1:B:166:ALA:HA	1:B:221:HIS:O	2.18	0.43
1:C:78:PRO:O	1:C:81:THR:HG22	2.19	0.43
1:D:5:GLU:OE1	1:D:177:TYR:OH	2.24	0.42
1:D:21:GLU:H	1:D:22:GLU:C	2.18	0.42
1:A:77:ASP:H	1:A:81:THR:CG2	2.26	0.42
1:C:13:HIS:NE2	1:C:153:ASP:OD2	2.37	0.42
1:B:106:LEU:HD22	1:B:111:ILE:HD12	2.01	0.42
1:D:106:LEU:HB3	1:D:111:ILE:HB	2.01	0.42
1:C:106:LEU:HB3	1:C:111:ILE:HB	2.01	0.42
1:D:178:VAL:HB	1:D:225:PHE:HA	2.01	0.42
1:B:46:PRO:HB2	1:B:87:TRP:CE2	2.55	0.42
1:A:216:MET:HA	1:A:225:PHE:O	2.20	0.42
1:C:52:PHE:HA	1:C:55:VAL:HG22	2.02	0.42
1:D:247:ILE:HD11	1:D:251:TYR:CZ	2.55	0.42
1:B:166:ALA:O	1:B:192:HIS:HE1	2.03	0.41
1:B:48:GLY:HA3	1:B:79:ASP:O	2.20	0.41
1:C:7:LEU:HD22	1:C:216:MET:HE1	2.03	0.41
1:B:105:PHE:CD1	1:B:105:PHE:N	2.89	0.41
1:C:203:LYS:HB2	1:C:203:LYS:HE3	1.96	0.41
1:D:30:THR:HG22	1:D:221:HIS:CE1	2.56	0.41
1:C:45:ASP:HB3	1:C:220:GLN:NE2	2.36	0.41
1:C:57:SER:O	1:C:61:GLU:HB2	2.21	0.41
1:B:188:MET:HE1	1:B:233:PHE:CE1	2.55	0.41
1:B:251:TYR:N	1:B:251:TYR:CD1	2.88	0.41
1:C:40:GLU:OE2	1:C:129:LEU:HB3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:211:LYS:NZ	1:A:38:GLY:O	2.50	0.41
1:C:159:LEU:CD2	1:C:209:VAL:HG11	2.50	0.41
1:D:152:TYR:CZ	1:D:212:LYS:HB3	2.56	0.41
1:D:115:LYS:H	1:D:115:LYS:HG2	1.42	0.40
1:D:143:LEU:HA	1:D:144:HIS:HA	1.93	0.40
1:A:52:PHE:HA	1:A:55:VAL:CG2	2.50	0.40
1:D:117:ILE:O	1:D:119:PRO:HD3	2.21	0.40
1:D:199:ASN:ND2	1:D:240:LEU:O	2.53	0.40
1:B:251:TYR:N	1:B:251:TYR:HD1	2.19	0.40
1:C:14:LYS:HB2	1:C:36:LEU:HD23	2.04	0.40
1:C:128:LYS:HE2	1:C:133:ASN:C	2.42	0.40
1:C:33:TYR:CZ	1:C:218:ALA:HB1	2.56	0.40
1:B:213:LYS:HA	1:B:213:LYS:HD3	1.76	0.40

All (1) 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)
1:B:108:HIS:ND1	1:D:79:ASP:OD2[3_644]	2.18	0.02

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	240/253 (95%)	228 (95%)	9 (4%)	3 (1%)	12	15
1	B	249/253 (98%)	235 (94%)	11 (4%)	3 (1%)	13	17
1	C	243/253 (96%)	228 (94%)	13 (5%)	2 (1%)	19	27
1	D	248/253 (98%)	236 (95%)	9 (4%)	3 (1%)	13	17
All	All	980/1012 (97%)	927 (95%)	42 (4%)	11 (1%)	14	19

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	24	GLU
1	B	25	GLU
1	C	22	GLU
1	D	77	ASP
1	B	171	LYS
1	A	77	ASP
1	A	251	TYR
1	A	171	LYS
1	C	18	LEU
1	D	27	ILE
1	D	22	GLU

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	211/224 (94%)	201 (95%)	10 (5%)	26	35
1	B	216/224 (96%)	212 (98%)	4 (2%)	57	71
1	C	215/224 (96%)	210 (98%)	5 (2%)	50	64
1	D	217/224 (97%)	209 (96%)	8 (4%)	34	45
All	All	859/896 (96%)	832 (97%)	27 (3%)	40	52

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	12	GLN
1	B	14	LYS
1	B	76	GLN
1	B	115	LYS
1	A	10	ASN
1	A	12	GLN
1	A	17	PHE
1	A	54	ARG
1	A	77	ASP
1	A	79	ASP
1	A	171	LYS

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Mol	Chain	Res	Type
1	A	189	GLU
1	A	208	MET
1	A	213	LYS
1	C	53	PRO
1	C	54	ARG
1	C	104	ARG
1	C	251	TYR
1	C	252	SER
1	D	20	TRP
1	D	50	HIS
1	D	77	ASP
1	D	113	ASP
1	D	128	LYS
1	D	208	MET
1	D	211	LYS
1	D	231	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	76	GLN
1	C	29	GLN
1	C	32	GLN
1	C	108	HIS
1	D	76	GLN
1	D	114	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	244/253 (96%)	0.01	0 100 100	30, 45, 66, 82	3 (1%)
1	B	251/253 (99%)	0.11	9 (3%) 42 51	26, 44, 72, 100	0
1	C	247/253 (97%)	0.16	3 (1%) 79 84	32, 50, 68, 85	1 (0%)
1	D	250/253 (98%)	0.23	6 (2%) 59 67	33, 48, 75, 92	0
All	All	992/1012 (98%)	0.13	18 (1%) 68 75	26, 47, 71, 100	4 (0%)

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	102	TRP	5.2
1	D	251	TYR	4.5
1	B	27	ILE	4.1
1	B	21	GLU	3.9
1	D	14	LYS	3.6
1	B	29	GLN	3.4
1	D	79	ASP	3.1
1	D	15	PHE	2.9
1	B	28	VAL	2.8
1	B	79	ASP	2.8
1	B	26	GLU	2.5
1	D	16	MET	2.5
1	C	209	VAL	2.5
1	C	171	LYS	2.4
1	B	39	ASN	2.3
1	C	214	ILE	2.2
1	D	102	TRP	2.2
1	B	105	PHE	2.1

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 monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.