



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 2, 2017 – 09:19 PM EDT

PDB ID : 1NMO
Title : Structural genomics, protein ybgI, unknown function
Authors : Ladner, J.E.; Obmolova, G.; Teplyakov, A.; Khil, P.P.; Camerini-Otero, R.D.;
Gilliland, G.L.; Structure 2 Function Project (S2F)
Deposited on : unknown
Resolution : 2.20 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 ⓘ symbol.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20030345
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	rb-20030345

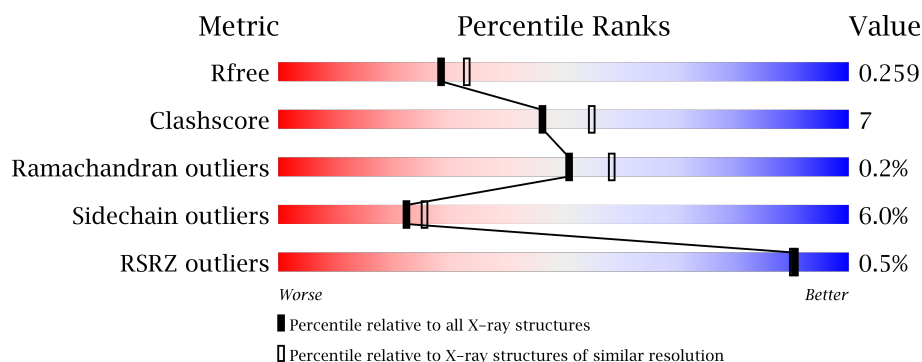
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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}	100719	4002 (2.20-2.20)
Clashscore	112137	4730 (2.20-2.20)
Ramachandran outliers	110173	4656 (2.20-2.20)
Sidechain outliers	110143	4657 (2.20-2.20)
RSRZ outliers	101464	4033 (2.20-2.20)

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 $\leq 5\%$. 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	247	<div> <div>80%</div> <div>18%</div> <div>.</div> </div>
1	B	247	<div> <div>77%</div> <div>19%</div> <div>.</div> </div>
1	C	247	<div> <div>80%</div> <div>18%</div> <div>.</div> </div>
1	D	247	<div> <div>80%</div> <div>17%</div> <div>.</div> </div>
1	E	247	<div> <div>76%</div> <div>20%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	247	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	FE	A	301	-	-	-	X
2	FE	B	301	-	-	-	X
2	FE	D	301	-	-	-	X
2	FE	E	301	-	-	-	X
2	FE	E	302	-	-	-	X
2	FE	F	301	-	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12031 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 ybgI.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	247	Total	C	N	O	S	Se	0	0	0
			1897	1200	332	359	2	4			
1	B	247	Total	C	N	O	S	Se	0	0	0
			1897	1200	332	359	2	4			
1	C	247	Total	C	N	O	S	Se	0	0	0
			1897	1200	332	359	2	4			
1	D	247	Total	C	N	O	S	Se	0	0	0
			1897	1200	332	359	2	4			
1	E	247	Total	C	N	O	S	Se	0	0	0
			1897	1200	332	359	2	4			
1	F	247	Total	C	N	O	S	Se	0	0	0
			1897	1200	332	359	2	4			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	MODIFIED RESIDUE	UNP P75743
A	78	MSE	MET	MODIFIED RESIDUE	UNP P75743
A	121	MSE	MET	MODIFIED RESIDUE	UNP P75743
A	135	MSE	MET	MODIFIED RESIDUE	UNP P75743
B	1	MSE	MET	MODIFIED RESIDUE	UNP P75743
B	78	MSE	MET	MODIFIED RESIDUE	UNP P75743
B	121	MSE	MET	MODIFIED RESIDUE	UNP P75743
B	135	MSE	MET	MODIFIED RESIDUE	UNP P75743
C	1	MSE	MET	MODIFIED RESIDUE	UNP P75743
C	78	MSE	MET	MODIFIED RESIDUE	UNP P75743
C	121	MSE	MET	MODIFIED RESIDUE	UNP P75743
C	135	MSE	MET	MODIFIED RESIDUE	UNP P75743
D	1	MSE	MET	MODIFIED RESIDUE	UNP P75743
D	78	MSE	MET	MODIFIED RESIDUE	UNP P75743
D	121	MSE	MET	MODIFIED RESIDUE	UNP P75743
D	135	MSE	MET	MODIFIED RESIDUE	UNP P75743
E	1	MSE	MET	MODIFIED RESIDUE	UNP P75743

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Chain	Residue	Modelled	Actual	Comment	Reference
E	78	MSE	MET	MODIFIED RESIDUE	UNP P75743
E	121	MSE	MET	MODIFIED RESIDUE	UNP P75743
E	135	MSE	MET	MODIFIED RESIDUE	UNP P75743
F	1	MSE	MET	MODIFIED RESIDUE	UNP P75743
F	78	MSE	MET	MODIFIED RESIDUE	UNP P75743
F	121	MSE	MET	MODIFIED RESIDUE	UNP P75743
F	135	MSE	MET	MODIFIED RESIDUE	UNP P75743

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	D	2	Total Fe 2 2	0	0
2	E	2	Total Fe 2 2	0	0
2	B	2	Total Fe 2 2	0	0
2	C	2	Total Fe 2 2	0	0
2	A	2	Total Fe 2 2	0	0
2	F	2	Total Fe 2 2	0	0

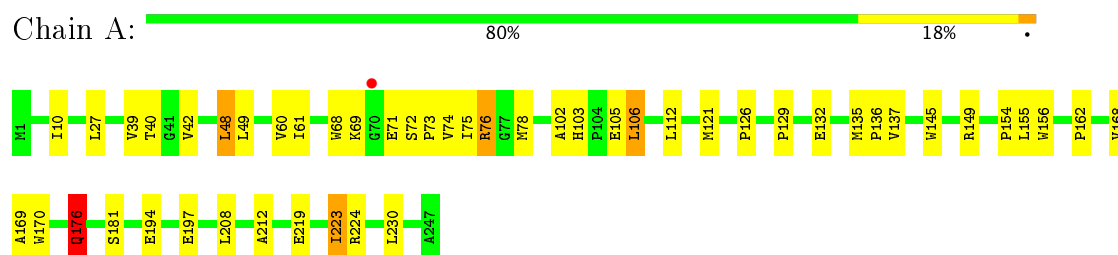
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	95	Total O 95 95	0	0
3	B	89	Total O 89 89	0	0
3	C	94	Total O 94 94	0	0
3	D	114	Total O 114 114	0	0
3	E	113	Total O 113 113	0	0
3	F	132	Total O 132 132	0	0

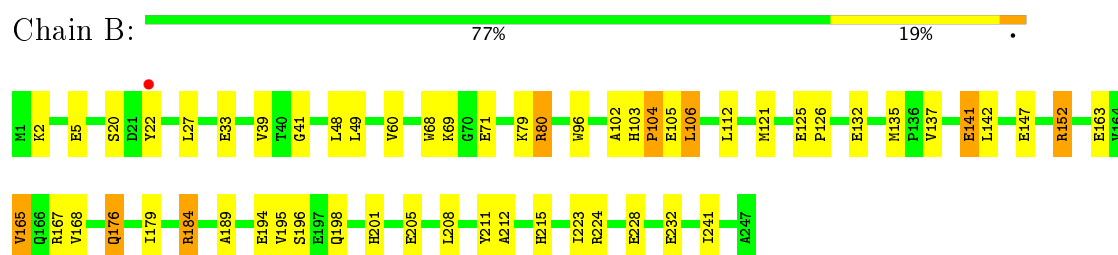
3 Residue-property plots

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

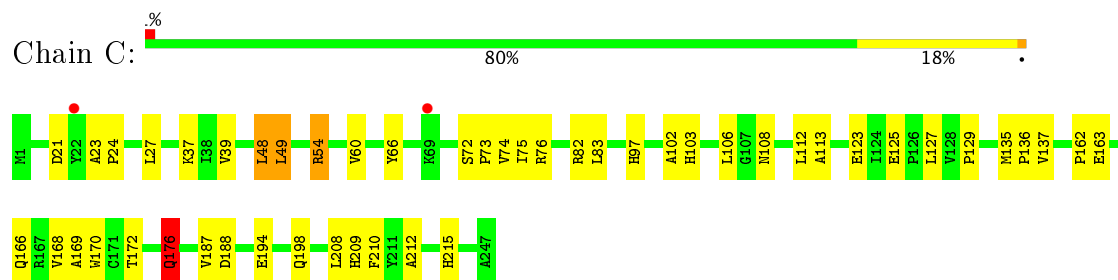
- Molecule 1: Hypothetical protein ybgl



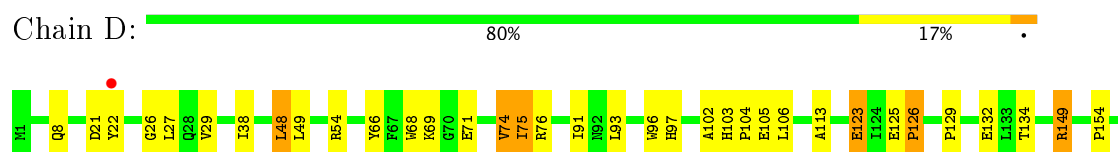
- Molecule 1: Hypothetical protein ybgl



- Molecule 1: Hypothetical protein ybgl



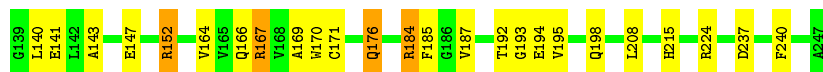
- Molecule 1: Hypothetical protein ybgl





- Molecule 1: Hypothetical protein ybgI

Chain E: 76% 20% •



- Molecule 1: Hypothetical protein ybgI

Chain F: 79% 18% •



4 Data and refinement statistics

Property	Value	Source
Space group	P 3	Depositor
Cell constants a, b, c, α , β , γ	154.66 Å 154.66 Å 57.52 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.60 – 2.20 19.60 – 2.20	Depositor EDS
% Data completeness (in resolution range)	94.2 (19.60-2.20) 95.2 (19.60-2.20)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.84 (at 2.19 Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.211 , 0.259 0.210 , 0.259	Depositor DCC
R_{free} test set	3655 reflections (4.92%)	DCC
Wilson B-factor (Å ²)	15.8	Xtriage
Anisotropy	0.228	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 44.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.017 for -h,-k,l 0.021 for h,-h-k,-l 0.015 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	12031	wwPDB-VP
Average B, all atoms (Å ²)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.55% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	1.13	0/1937	1.09	4/2632 (0.2%)
1	B	1.19	5/1937 (0.3%)	1.13	7/2632 (0.3%)
1	C	1.15	2/1937 (0.1%)	1.12	6/2632 (0.2%)
1	D	1.17	6/1937 (0.3%)	1.11	7/2632 (0.3%)
1	E	1.18	2/1937 (0.1%)	1.16	10/2632 (0.4%)
1	F	1.24	6/1937 (0.3%)	1.12	8/2632 (0.3%)
All	All	1.18	21/11622 (0.2%)	1.12	42/15792 (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	B	0	1
1	D	0	1
All	All	0	2

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	157	CYS	CB-SG	9.25	1.98	1.82
1	F	71	GLU	CG-CD	8.56	1.64	1.51
1	B	141	GLU	CD-OE2	7.30	1.33	1.25
1	E	62	VAL	CB-CG1	-7.08	1.38	1.52
1	B	165	VAL	CB-CG1	-6.66	1.38	1.52
1	B	141	GLU	CG-CD	6.58	1.61	1.51
1	C	125	GLU	CB-CG	-6.31	1.40	1.52
1	D	205	GLU	CB-CG	6.02	1.63	1.52
1	F	5	GLU	CD-OE2	5.57	1.31	1.25
1	E	147	GLU	CG-CD	5.53	1.60	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	228	GLU	CD-OE2	5.52	1.31	1.25
1	F	22	TYR	CE2-CZ	5.43	1.45	1.38
1	D	232	GLU	CD-OE1	5.29	1.31	1.25
1	F	128	VAL	CB-CG1	5.28	1.64	1.52
1	B	22	TYR	CD1-CE1	5.23	1.47	1.39
1	D	123	GLU	CG-CD	5.23	1.59	1.51
1	D	22	TYR	CD1-CE1	5.21	1.47	1.39
1	C	210	PHE	CE2-CZ	5.19	1.47	1.37
1	B	79	LYS	CD-CE	5.19	1.64	1.51
1	D	22	TYR	CD2-CE2	5.18	1.47	1.39
1	F	5	GLU	CG-CD	5.07	1.59	1.51

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	76	ARG	NE-CZ-NH2	-9.54	115.53	120.30
1	A	224	ARG	NE-CZ-NH2	-9.25	115.67	120.30
1	E	224	ARG	NE-CZ-NH2	-8.27	116.17	120.30
1	E	80	ARG	NE-CZ-NH2	-7.78	116.41	120.30
1	D	54	ARG	NE-CZ-NH2	-7.30	116.65	120.30
1	B	224	ARG	NE-CZ-NH2	-7.24	116.68	120.30
1	F	152	ARG	NE-CZ-NH1	-7.02	116.79	120.30
1	B	80	ARG	CG-CD-NE	6.83	126.15	111.80
1	F	149	ARG	NE-CZ-NH1	-6.74	116.93	120.30
1	E	167	ARG	NE-CZ-NH1	-6.30	117.15	120.30
1	E	55	LEU	CB-CG-CD1	-6.27	100.35	111.00
1	C	54	ARG	NE-CZ-NH1	6.21	123.41	120.30
1	A	212	ALA	N-CA-C	-6.06	94.63	111.00
1	B	152	ARG	NE-CZ-NH1	6.02	123.31	120.30
1	E	106	LEU	CA-CB-CG	5.94	128.97	115.30
1	F	224	ARG	NE-CZ-NH2	-5.92	117.34	120.30
1	B	106	LEU	CA-CB-CG	5.91	128.90	115.30
1	C	176	GLN	CB-CA-C	-5.88	98.64	110.40
1	C	82	ARG	NE-CZ-NH1	-5.85	117.38	120.30
1	F	39	VAL	CG1-CB-CG2	-5.81	101.60	110.90
1	B	212	ALA	N-CA-C	-5.76	95.46	111.00
1	D	224	ARG	NE-CZ-NH2	-5.68	117.46	120.30
1	D	224	ARG	NE-CZ-NH1	5.62	123.11	120.30
1	F	224	ARG	NE-CZ-NH1	5.60	123.10	120.30
1	C	48	LEU	CA-CB-CG	5.56	128.10	115.30
1	E	21	ASP	CB-CG-OD1	-5.51	113.34	118.30
1	D	48	LEU	CA-CB-CG	5.26	127.41	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	152	ARG	NE-CZ-NH1	5.23	122.92	120.30
1	F	48	LEU	CA-CB-CG	5.23	127.34	115.30
1	D	212	ALA	N-CA-C	-5.22	96.90	111.00
1	D	245	ASN	N-CA-C	-5.21	96.94	111.00
1	C	49	LEU	CB-CG-CD1	5.21	119.85	111.00
1	D	91	ILE	CG1-CB-CG2	-5.20	99.97	111.40
1	F	106	LEU	CA-CB-CG	5.19	127.24	115.30
1	A	176	GLN	CB-CA-C	-5.15	100.11	110.40
1	C	212	ALA	N-CA-C	-5.12	97.19	111.00
1	F	153	LYS	CD-CE-NZ	-5.06	100.06	111.70
1	B	184	ARG	CA-CB-CG	-5.05	102.29	113.40
1	B	102	ALA	N-CA-C	5.04	124.62	111.00
1	E	224	ARG	NE-CZ-NH1	5.03	122.82	120.30
1	A	48	LEU	CA-CB-CG	5.02	126.85	115.30
1	E	184	ARG	NE-CZ-NH2	-5.01	117.80	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	211	TYR	Sidechain
1	D	66	TYR	Sidechain

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	1897	0	1866	29	0
1	B	1897	0	1866	28	0
1	C	1897	0	1866	23	0
1	D	1897	0	1866	22	0
1	E	1897	0	1866	37	0
1	F	1897	0	1866	27	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	2	0	0	0	0
2	F	2	0	0	0	0
3	A	95	0	0	0	0
3	B	89	0	0	3	0
3	C	94	0	0	4	0
3	D	114	0	0	1	0
3	E	113	0	0	5	0
3	F	132	0	0	2	0
All	All	12031	0	11196	162	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 7.

All (162) 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:F:135:MSE:CG	1:F:136:PRO:HD2	1.85	1.06
1:A:40:THR:HB	1:A:223:ILE:HD11	1.38	1.05
1:F:135:MSE:HG3	1:F:136:PRO:CD	1.91	1.00
1:E:75:ILE:HD12	1:E:80:ARG:HA	1.45	0.98
1:F:135:MSE:HG3	1:F:136:PRO:HD2	0.94	0.92
1:F:8:GLN:O	1:F:12:GLU:HG3	1.72	0.89
1:A:40:THR:CB	1:A:223:ILE:HD11	2.05	0.85
1:B:141:GLU:HB2	3:B:505:HOH:O	1.87	0.74
1:E:134:THR:HG22	3:E:930:HOH:O	1.88	0.73
1:A:176:GLN:HG3	1:A:194:GLU:O	1.89	0.72
1:E:75:ILE:O	1:E:75:ILE:HG13	1.89	0.71
1:A:10:ILE:HD11	1:A:230:LEU:HD21	1.74	0.70
1:E:60:VAL:C	1:E:61:ILE:HD12	2.13	0.68
1:F:113:ALA:HB2	1:F:170:TRP:CZ2	2.28	0.68
1:F:136:PRO:HB2	1:F:164:VAL:CG1	2.25	0.67
1:B:142:LEU:HD22	1:B:165:VAL:HG11	1.76	0.66
1:E:61:ILE:HD12	1:E:61:ILE:N	2.09	0.66
1:B:228:GLU:O	1:B:232:GLU:HG3	1.96	0.65
1:A:208:LEU:H	1:A:208:LEU:HD23	1.58	0.65
1:E:40:THR:OG1	1:E:240:PHE:HA	1.96	0.65
1:A:208:LEU:N	1:A:208:LEU:HD23	2.12	0.65
1:B:125:GLU:HB3	1:B:126:PRO:HD2	1.78	0.64
1:C:198:GLN:HG2	3:C:559:HOH:O	1.97	0.63
1:E:61:ILE:N	1:E:61:ILE:CD1	2.61	0.63
1:A:223:ILE:HD13	1:A:223:ILE:O	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:8:GLN:O	1:E:12:GLU:HG3	1.99	0.62
1:B:39:VAL:HG13	1:B:241:ILE:HD12	1.80	0.62
1:E:38:ILE:HG12	1:E:59:ALA:HB3	1.82	0.61
1:E:75:ILE:CD1	1:E:80:ARG:HA	2.28	0.61
1:C:215:HIS:CG	1:D:197:GLU:HB2	2.36	0.60
1:E:23:ALA:HB1	1:E:24:PRO:HD2	1.82	0.60
1:A:105:GLU:HG2	1:A:106:LEU:HD13	1.84	0.60
1:E:21:ASP:HB3	1:E:98:LEU:CD1	2.31	0.60
1:B:68:TRP:O	1:B:71:GLU:HG2	2.02	0.60
1:C:176:GLN:HG3	1:C:194:GLU:O	2.01	0.59
1:A:223:ILE:HD13	1:A:223:ILE:C	2.23	0.59
1:A:10:ILE:N	1:A:10:ILE:HD13	2.16	0.59
1:B:167:ARG:HD3	3:B:954:HOH:O	2.03	0.59
1:E:176:GLN:HG3	1:E:194:GLU:O	2.03	0.58
1:E:136:PRO:HG3	1:E:166:GLN:HG3	1.85	0.58
1:C:136:PRO:HG3	1:C:166:GLN:HG3	1.86	0.58
1:F:136:PRO:HB2	1:F:164:VAL:HG13	1.84	0.58
1:D:103:HIS:CE1	1:D:105:GLU:HB3	2.39	0.57
1:F:142:LEU:O	1:F:146:ILE:HG12	2.03	0.57
1:B:167:ARG:CD	3:B:954:HOH:O	2.53	0.57
1:E:13:LYS:HG3	1:E:13:LYS:O	2.05	0.57
1:F:208:LEU:HD23	1:F:208:LEU:H	1.70	0.57
1:B:125:GLU:HB3	1:B:126:PRO:CD	2.35	0.56
1:F:36:GLN:HA	1:F:36:GLN:NE2	2.19	0.56
1:E:208:LEU:C	1:E:208:LEU:HD12	2.27	0.55
1:E:21:ASP:HB3	1:E:98:LEU:HD12	1.88	0.55
1:F:208:LEU:HD23	1:F:208:LEU:N	2.22	0.54
1:A:155:LEU:HD12	1:A:156:TRP:N	2.23	0.54
1:E:198:GLN:HG2	3:E:715:HOH:O	2.05	0.54
1:E:176:GLN:HG2	1:E:195:VAL:HA	1.88	0.54
1:B:176:GLN:HG3	1:B:194:GLU:O	2.07	0.54
1:D:176:GLN:HG3	1:D:194:GLU:O	2.08	0.54
1:B:137:VAL:O	1:B:165:VAL:HG12	2.08	0.54
1:E:152:ARG:CZ	3:E:744:HOH:O	2.56	0.53
1:E:37:LYS:HD2	1:E:237:ASP:OD2	2.08	0.53
1:A:129:PRO:HG2	1:A:170:TRP:CE2	2.43	0.53
1:C:39:VAL:O	1:C:60:VAL:HA	2.09	0.53
1:D:21:ASP:OD2	1:D:97:HIS:HB3	2.09	0.52
1:D:125:GLU:HB3	1:D:126:PRO:HD2	1.92	0.52
1:C:23:ALA:HB1	1:C:24:PRO:HD2	1.92	0.52
1:C:37:LYS:HE3	3:C:578:HOH:O	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:197:GLU:HB2	1:B:215:HIS:CG	2.46	0.51
1:C:113:ALA:HB2	1:C:170:TRP:CZ2	2.46	0.51
1:D:134:THR:HG22	3:D:663:HOH:O	2.11	0.51
1:F:121:MSE:SE	1:F:132:GLU:HG3	2.61	0.51
1:D:26:GLY:HA2	1:D:96:TRP:CZ2	2.47	0.50
1:D:38:ILE:HD11	1:D:236:LEU:HD13	1.93	0.50
1:D:68:TRP:O	1:D:71:GLU:HG2	2.13	0.49
1:C:135:MSE:O	1:C:137:VAL:HG13	2.11	0.49
1:C:21:ASP:OD2	1:C:97:HIS:HB3	2.12	0.49
1:A:135:MSE:O	1:A:137:VAL:HG13	2.12	0.49
1:F:80:ARG:HG3	1:F:81:ASN:N	2.27	0.49
1:E:192:THR:HG23	1:E:193:GLY:N	2.28	0.48
1:A:68:TRP:O	1:A:71:GLU:HG2	2.13	0.48
1:C:74:VAL:HG11	1:C:76:ARG:HD3	1.95	0.48
1:F:125:GLU:HB3	1:F:126:PRO:HD2	1.96	0.48
1:F:136:PRO:HB3	1:F:166:GLN:HB2	1.95	0.48
1:D:29:VAL:HB	1:D:93:LEU:HB3	1.94	0.48
1:D:149:ARG:HE	1:D:149:ARG:HA	1.78	0.48
1:A:145:TRP:O	1:A:149:ARG:HG2	2.14	0.48
1:A:39:VAL:O	1:A:60:VAL:HA	2.13	0.48
1:C:168:VAL:HG12	1:C:169:ALA:N	2.28	0.48
1:A:78:MSE:HG2	1:B:205:GLU:HB3	1.96	0.48
1:D:102:ALA:O	1:D:103:HIS:C	2.51	0.47
1:E:136:PRO:CG	1:E:166:GLN:HG3	2.44	0.47
1:B:121:MSE:SE	1:B:132:GLU:HG3	2.64	0.47
1:C:127:LEU:N	3:C:594:HOH:O	2.06	0.47
1:C:75:ILE:O	1:C:75:ILE:HG23	2.14	0.47
1:E:169:ALA:HB2	1:E:187:VAL:HG11	1.96	0.47
1:A:103:HIS:CE1	1:A:105:GLU:HB3	2.49	0.47
1:B:176:GLN:HG2	1:B:195:VAL:HA	1.97	0.47
1:E:98:LEU:O	1:E:99:PRO:C	2.52	0.47
1:E:167:ARG:NH1	3:E:880:HOH:O	2.34	0.46
1:F:52:ALA:HB1	1:F:57:ALA:HB3	1.98	0.46
1:A:74:VAL:HG12	1:A:76:ARG:HG2	1.96	0.46
1:D:113:ALA:HB2	1:D:170:TRP:CZ2	2.50	0.46
1:E:87:LEU:HD23	3:E:916:HOH:O	2.15	0.46
1:C:123:GLU:HA	1:C:129:PRO:HA	1.98	0.46
1:C:169:ALA:HB2	1:C:187:VAL:HG11	1.98	0.46
1:E:140:LEU:O	1:E:143:ALA:HB3	2.15	0.46
1:C:102:ALA:O	1:C:103:HIS:C	2.53	0.45
1:E:138:PRO:HB2	1:E:141:GLU:OE1	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:103:HIS:CE1	1:B:105:GLU:HB3	2.52	0.45
1:E:75:ILE:HD12	1:E:80:ARG:CA	2.32	0.45
1:F:13:LYS:HE2	1:F:229:TRP:NE1	2.31	0.45
1:D:75:ILE:HG12	1:D:75:ILE:O	2.14	0.45
1:F:136:PRO:HB2	1:F:164:VAL:HG11	1.96	0.45
1:A:42:VAL:HG22	1:A:219:GLU:O	2.16	0.45
1:A:40:THR:OG1	1:A:223:ILE:HD11	2.17	0.44
1:B:195:VAL:HG22	1:B:196:SER:N	2.32	0.44
1:B:41:GLY:O	1:B:223:ILE:HG12	2.18	0.44
1:F:176:GLN:HG3	1:F:194:GLU:O	2.16	0.44
1:D:129:PRO:HG2	1:D:170:TRP:CE2	2.52	0.44
1:F:221:GLY:HA3	3:F:782:HOH:O	2.17	0.44
1:B:2:LYS:HB2	1:B:5:GLU:HG3	1.98	0.44
1:C:108:ASN:HB3	1:C:172:THR:HG21	2.00	0.43
1:D:103:HIS:HA	1:D:104:PRO:HD3	1.84	0.43
1:F:102:ALA:O	1:F:103:HIS:C	2.57	0.43
1:C:162:PRO:HD2	1:C:209:HIS:CD2	2.54	0.43
1:D:103:HIS:HE1	1:D:105:GLU:HB3	1.82	0.43
1:A:40:THR:HG22	1:A:61:ILE:HB	2.01	0.43
1:C:72:SER:HA	1:C:73:PRO:HD3	1.80	0.43
1:F:136:PRO:HA	1:F:165:VAL:O	2.19	0.43
1:D:123:GLU:HA	1:D:129:PRO:HA	2.01	0.42
1:A:121:MSE:SE	1:A:132:GLU:HG3	2.70	0.42
1:B:147:GLU:HA	1:B:152:ARG:O	2.19	0.42
1:B:198:GLN:HA	1:B:201:HIS:HD2	1.84	0.42
1:C:75:ILE:HD12	1:C:83:LEU:HD12	2.01	0.42
1:B:168:VAL:HG22	1:B:189:ALA:HB3	2.02	0.42
1:E:215:HIS:CG	1:F:197:GLU:HB2	2.54	0.42
1:E:171:CYS:O	1:E:192:THR:HA	2.19	0.42
1:E:21:ASP:OD1	1:E:21:ASP:N	2.52	0.42
1:F:79:LYS:HE2	3:F:981:HOH:O	2.19	0.42
1:A:72:SER:HA	1:A:73:PRO:HD3	1.78	0.41
1:B:176:GLN:O	1:B:179:ILE:HG22	2.20	0.41
1:D:237:ASP:C	1:D:237:ASP:OD1	2.58	0.41
1:E:184:ARG:O	1:E:185:PHE:C	2.58	0.41
1:F:162:PRO:HD2	1:F:209:HIS:CD2	2.55	0.41
1:B:103:HIS:HA	1:B:104:PRO:HD3	1.87	0.41
1:D:38:ILE:CD1	1:D:236:LEU:HD13	2.49	0.41
1:E:176:GLN:HG2	1:E:195:VAL:CA	2.50	0.41
1:F:133:LEU:HA	1:F:133:LEU:HD23	1.84	0.41
1:C:66:TYR:HB3	3:C:997:HOH:O	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:29:VAL:HB	1:E:93:LEU:HB3	2.02	0.41
1:A:40:THR:HA	1:A:61:ILE:O	2.20	0.41
1:B:39:VAL:O	1:B:60:VAL:HA	2.21	0.41
1:C:162:PRO:HG3	1:C:188:ASP:HB3	2.03	0.41
1:A:102:ALA:O	1:A:103:HIS:C	2.59	0.40
1:F:23:ALA:HB2	1:F:68:TRP:CE3	2.56	0.40
1:B:103:HIS:HE1	1:B:105:GLU:HB3	1.87	0.40
1:B:184:ARG:HH11	1:B:184:ARG:HD2	1.67	0.40
1:A:168:VAL:HG12	1:A:169:ALA:N	2.35	0.40
1:E:129:PRO:HD2	1:E:170:TRP:O	2.22	0.40
1:D:74:VAL:CG1	1:D:76:ARG:HG3	2.52	0.40
1:A:136:PRO:C	1:A:137:VAL:HG13	2.42	0.40
1:B:2:LYS:HD2	1:B:33:GLU:OE2	2.21	0.40
1:D:132:GLU:HA	1:D:166:GLN:O	2.22	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	245/247 (99%)	237 (97%)	7 (3%)	1 (0%)	38	41
1	B	245/247 (99%)	234 (96%)	11 (4%)	0	100	100
1	C	245/247 (99%)	236 (96%)	9 (4%)	0	100	100
1	D	245/247 (99%)	235 (96%)	8 (3%)	2 (1%)	22	21
1	E	245/247 (99%)	233 (95%)	12 (5%)	0	100	100
1	F	245/247 (99%)	234 (96%)	11 (4%)	0	100	100
All	All	1470/1482 (99%)	1409 (96%)	58 (4%)	3 (0%)	51	58

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	74	VAL
1	D	126	PRO
1	A	162	PRO

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	197/193 (102%)	184 (93%)	13 (7%)	19	21
1	B	197/193 (102%)	183 (93%)	14 (7%)	17	18
1	C	197/193 (102%)	188 (95%)	9 (5%)	31	39
1	D	197/193 (102%)	186 (94%)	11 (6%)	25	29
1	E	197/193 (102%)	184 (93%)	13 (7%)	19	21
1	F	197/193 (102%)	186 (94%)	11 (6%)	25	29
All	All	1182/1158 (102%)	1111 (94%)	71 (6%)	22	25

All (71) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	LEU
1	A	48	LEU
1	A	49	LEU
1	A	69	LYS
1	A	75	ILE
1	A	76	ARG
1	A	106	LEU
1	A	112	LEU
1	A	126	PRO
1	A	154	PRO
1	A	176	GLN
1	A	181	SER
1	A	223	ILE
1	B	20	SER
1	B	27	LEU
1	B	48	LEU

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Mol	Chain	Res	Type
1	B	49	LEU
1	B	69	LYS
1	B	80	ARG
1	B	96	TRP
1	B	104	PRO
1	B	106	LEU
1	B	112	LEU
1	B	135	MSE
1	B	163	GLU
1	B	176	GLN
1	B	208	LEU
1	C	27	LEU
1	C	48	LEU
1	C	49	LEU
1	C	54	ARG
1	C	106	LEU
1	C	112	LEU
1	C	163	GLU
1	C	176	GLN
1	C	208	LEU
1	D	8	GLN
1	D	27	LEU
1	D	48	LEU
1	D	49	LEU
1	D	69	LYS
1	D	75	ILE
1	D	106	LEU
1	D	149	ARG
1	D	154	PRO
1	D	176	GLN
1	D	208	LEU
1	E	21	ASP
1	E	27	LEU
1	E	48	LEU
1	E	49	LEU
1	E	61	ILE
1	E	69	LYS
1	E	75	ILE
1	E	96	TRP
1	E	106	LEU
1	E	112	LEU
1	E	126	PRO

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Mol	Chain	Res	Type
1	E	164	VAL
1	E	176	GLN
1	F	27	LEU
1	F	48	LEU
1	F	49	LEU
1	F	80	ARG
1	F	106	LEU
1	F	112	LEU
1	F	135	MSE
1	F	164	VAL
1	F	165	VAL
1	F	176	GLN
1	F	246	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	36	GLN
1	A	233	ASN
1	B	36	GLN
1	B	166	GLN
1	B	233	ASN
1	C	36	GLN
1	C	166	GLN
1	D	36	GLN
1	D	233	ASN
1	E	36	GLN
1	F	36	GLN

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 12 ligands modelled in this entry, 12 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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	243/247 (98%)	-0.43	1 (0%) 92 91	9, 16, 26, 31	0
1	B	243/247 (98%)	-0.35	1 (0%) 92 91	8, 17, 28, 30	0
1	C	243/247 (98%)	-0.43	2 (0%) 86 85	8, 15, 25, 30	0
1	D	243/247 (98%)	-0.43	1 (0%) 92 91	9, 15, 27, 31	0
1	E	243/247 (98%)	-0.41	1 (0%) 92 91	6, 15, 25, 32	0
1	F	243/247 (98%)	-0.50	1 (0%) 92 91	5, 14, 22, 29	0
All	All	1458/1482 (98%)	-0.42	7 (0%) 90 90	5, 15, 26, 32	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	22	TYR	3.7
1	B	22	TYR	3.5
1	A	70	GLY	3.5
1	F	22	TYR	3.3
1	D	22	TYR	2.8
1	C	22	TYR	2.8
1	C	69	LYS	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 carbohydrates in this entry.

6.4 Ligands

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	FE	A	301	1/1	0.98	0.18	7.92	30,30,30,30	0
2	FE	B	301	1/1	0.97	0.18	5.20	27,27,27,27	0
2	FE	E	301	1/1	0.98	0.14	4.07	22,22,22,22	0
2	FE	F	301	1/1	0.96	0.15	3.10	30,30,30,30	0
2	FE	D	301	1/1	0.98	0.14	2.46	27,27,27,27	0
2	FE	E	302	1/1	0.98	0.15	2.17	17,17,17,17	0
2	FE	F	302	1/1	0.99	0.12	0.51	21,21,21,21	0
2	FE	C	301	1/1	0.97	0.10	-0.28	27,27,27,27	0
2	FE	B	302	1/1	0.98	0.09	-0.83	22,22,22,22	0
2	FE	D	302	1/1	0.97	0.09	-0.89	18,18,18,18	0
2	FE	A	302	1/1	0.99	0.08	-1.43	25,25,25,25	0
2	FE	C	302	1/1	0.98	0.08	-2.19	26,26,26,26	0

6.5 Other polymers

There are no such residues in this entry.