



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 03:27 PM UTC

PDB ID : 1NMO / pdb_00001nmo
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 : 2003-01-10
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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

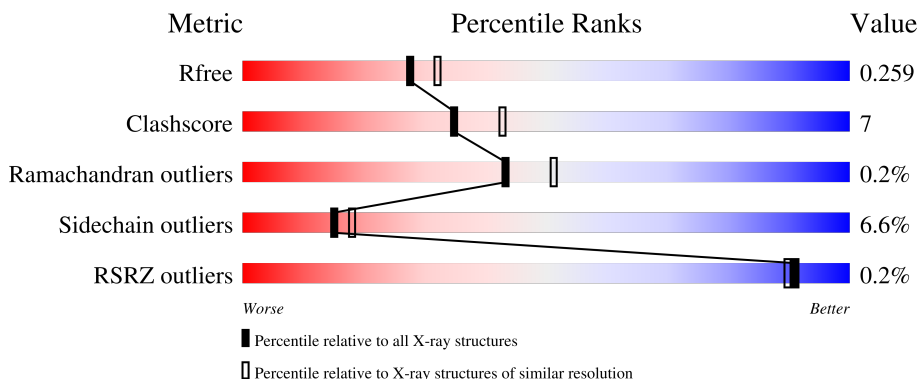
1 Overall quality at a glance

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}	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (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 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 $\leq 5\%$. 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	
1	B	247	
1	C	247	
1	D	247	
1	E	247	

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Mol	Chain	Length	Quality of chain
1	F	247	 75% 20% . .

2 Entry composition i

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
			Total	C	N	O	S	Se			
1	A	247	1897	1200	332	359	2	4	0	0	0
1	B	247	1897	1200	332	359	2	4	0	0	0
1	C	247	1897	1200	332	359	2	4	0	0	0
1	D	247	1897	1200	332	359	2	4	0	0	0
1	E	247	1897	1200	332	359	2	4	0	0	0
1	F	247	1897	1200	332	359	2	4	0	0	0

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 (CCD ID: FE) (formula: Fe).

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

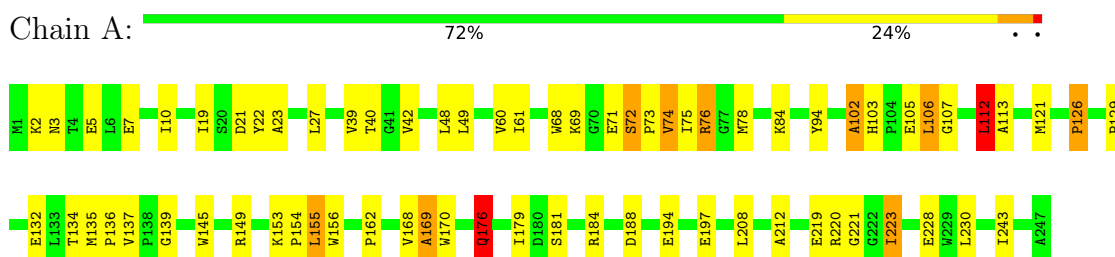
- Molecule 3 is water.

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

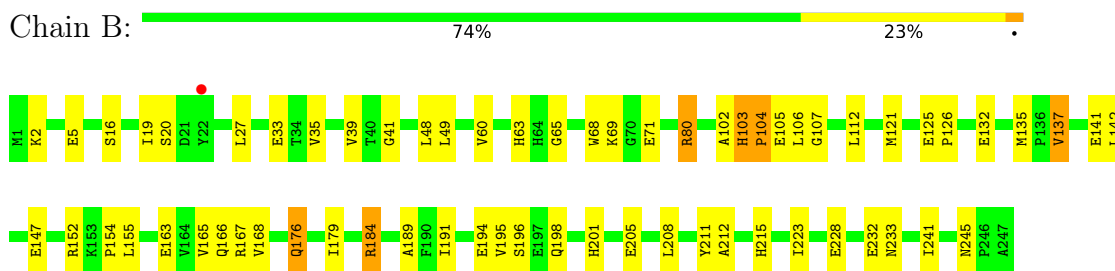
3 Residue-property plots

These plots are drawn for all protein, RNA, 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.

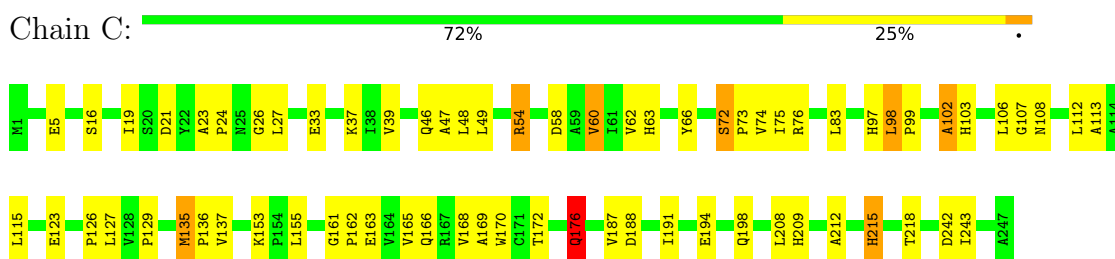
- Molecule 1: Hypothetical protein ybgI



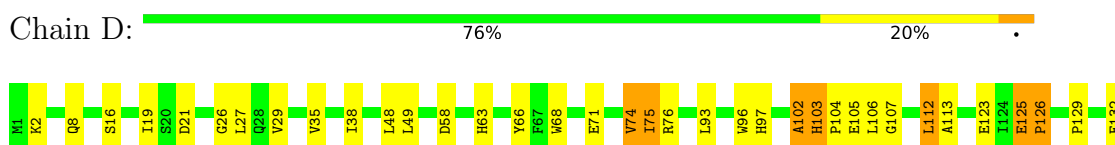
- Molecule 1: Hypothetical protein ybgI



- Molecule 1: Hypothetical protein ybgI

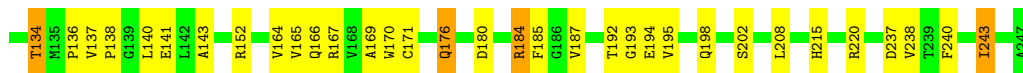


- Molecule 1: Hypothetical protein ybgI





- Molecule 1: Hypothetical protein ybgI



- Molecule 1: Hypothetical protein ybgI



4 Data and refinement statistics

Property	Value	Source
Space group	P 3	Depositor
Cell constants a, b, c, α , β , γ	154.66Å 154.66Å 57.52Å 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) 95.0 (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 2.19Å)	Xtrriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.211 , 0.259 0.210 , 0.259	Depositor DCC
R_{free} test set	6082 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	15.8	Xtrriage
Anisotropy	0.228	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 42.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.018 for -h,-k,l 0.021 for h,-h-k,-l 0.014 for -k,-h,-l	Xtrriage
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

Xtrriage'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.*

¹Intensities estimated from amplitudes.

²Theoretical 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 i

5.1 Standard geometry i

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	1.35	2/1937 (0.1%)	1.54	32/2632 (1.2%)
1	B	1.35	3/1937 (0.2%)	1.48	20/2632 (0.8%)
1	C	1.39	6/1937 (0.3%)	1.48	29/2632 (1.1%)
1	D	1.36	2/1937 (0.1%)	1.48	26/2632 (1.0%)
1	E	1.41	3/1937 (0.2%)	1.49	20/2632 (0.8%)
1	F	1.41	6/1937 (0.3%)	1.55	27/2632 (1.0%)
All	All	1.38	22/11622 (0.2%)	1.50	154/15792 (1.0%)

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 (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	243	ILE	CA-CB	-8.77	1.44	1.53
1	C	62	VAL	CA-C	-5.96	1.46	1.52
1	B	154	PRO	CA-C	-5.93	1.46	1.52
1	C	126	PRO	CA-C	5.89	1.60	1.52
1	F	126	PRO	C-O	5.83	1.31	1.24
1	C	26	GLY	C-O	5.82	1.27	1.24
1	F	165	VAL	C-O	5.81	1.30	1.24
1	C	47	ALA	CA-CB	5.76	1.62	1.53
1	E	113	ALA	CA-CB	-5.66	1.44	1.53
1	D	237	ASP	CA-C	5.56	1.59	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	166	GLN	CA-C	-5.52	1.47	1.52
1	F	47	ALA	CA-CB	5.41	1.61	1.53
1	F	203	ALA	CA-CB	5.37	1.61	1.53
1	D	164	VAL	CA-CB	-5.32	1.47	1.54
1	A	74	VAL	CA-CB	5.30	1.59	1.54
1	E	75	ILE	CA-CB	5.26	1.60	1.53
1	C	115	LEU	C-O	-5.20	1.18	1.24
1	C	54	ARG	CD-NE	5.16	1.53	1.46
1	B	184	ARG	CA-C	-5.11	1.45	1.52
1	F	71	GLU	CG-CD	5.10	1.64	1.52
1	E	243	ILE	N-CA	5.08	1.50	1.46
1	F	157	CYS	CB-SG	5.07	1.98	1.81

All (154) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	135	MSE	CA-C-N	10.63	132.31	119.98
1	F	135	MSE	C-N-CA	10.63	132.31	119.98
1	D	16	SER	N-CA-C	9.55	122.89	111.33
1	A	220	ARG	N-CA-C	-9.21	102.17	113.41
1	B	102	ALA	N-CA-C	9.19	124.62	113.23
1	A	72	SER	CA-C-N	9.06	128.79	119.64
1	A	72	SER	C-N-CA	9.06	128.79	119.64
1	C	153	LYS	CA-C-N	-8.95	110.90	120.66
1	C	153	LYS	C-N-CA	-8.95	110.90	120.66
1	E	134	THR	N-CA-C	-8.74	102.05	112.89
1	E	98	LEU	CA-C-N	-8.32	110.12	119.28
1	E	98	LEU	C-N-CA	-8.32	110.12	119.28
1	A	107	GLY	N-CA-C	8.26	121.42	112.33
1	F	220	ARG	N-CA-C	-8.14	103.48	113.41
1	D	102	ALA	N-CA-C	8.12	123.29	113.23
1	A	243	ILE	CA-C-N	8.11	128.61	119.93
1	A	243	ILE	C-N-CA	8.11	128.61	119.93
1	D	19	ILE	N-CA-C	8.03	119.71	107.99
1	A	153	LYS	CA-C-N	-8.01	111.93	120.66
1	A	153	LYS	C-N-CA	-8.01	111.93	120.66
1	A	102	ALA	N-CA-C	7.83	120.90	111.82
1	C	46	GLN	N-CA-C	-7.81	102.77	111.28
1	F	179	ILE	N-CA-C	7.74	118.52	110.62
1	E	21	ASP	N-CA-C	7.74	118.75	108.07
1	A	112	LEU	N-CA-C	-7.58	102.96	111.14
1	E	117	GLY	CA-C-N	-7.55	113.83	123.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	117	GLY	C-N-CA	-7.55	113.83	123.19
1	A	84	LYS	N-CA-C	-7.43	103.26	111.36
1	E	238	VAL	N-CA-C	7.30	118.34	108.11
1	F	63	HIS	N-CA-C	-7.28	102.33	112.45
1	B	212	ALA	N-CA-C	-7.08	95.46	107.99
1	D	35	VAL	N-CA-C	7.08	118.32	107.99
1	D	63	HIS	N-CA-C	-7.04	103.67	112.90
1	C	155	LEU	N-CA-C	-6.98	98.66	109.76
1	E	102	ALA	N-CA-C	6.95	121.93	113.38
1	F	128	VAL	CA-C-N	6.94	126.90	120.03
1	F	128	VAL	C-N-CA	6.94	126.90	120.03
1	F	221	GLY	N-CA-C	6.88	120.96	112.64
1	D	112	LEU	N-CA-C	-6.83	103.83	111.28
1	D	134	THR	N-CA-C	-6.77	104.99	113.18
1	C	72	SER	CA-C-N	6.67	126.30	119.56
1	C	72	SER	C-N-CA	6.67	126.30	119.56
1	A	212	ALA	N-CA-C	-6.59	94.63	107.62
1	B	155	LEU	N-CA-C	-6.57	99.32	109.76
1	D	155	LEU	N-CA-C	-6.50	98.67	109.46
1	B	80	ARG	CG-CD-NE	6.43	126.15	112.00
1	E	184	ARG	N-CA-C	-6.43	103.96	110.97
1	F	243	ILE	CA-C-N	6.40	127.84	119.84
1	F	243	ILE	C-N-CA	6.40	127.84	119.84
1	B	103	HIS	CA-C-N	6.38	126.87	119.47
1	B	103	HIS	C-N-CA	6.38	126.87	119.47
1	A	23	ALA	CA-C-N	-6.36	113.21	119.76
1	A	23	ALA	C-N-CA	-6.36	113.21	119.76
1	F	33	GLU	N-CA-C	6.36	119.20	111.82
1	C	16	SER	N-CA-C	6.36	118.21	111.28
1	B	19	ILE	N-CA-C	6.35	117.26	107.99
1	A	188	ASP	N-CA-C	-6.34	105.67	113.41
1	A	74	VAL	CA-C-N	-6.33	114.49	123.10
1	A	74	VAL	C-N-CA	-6.33	114.49	123.10
1	F	16	SER	N-CA-C	6.24	118.08	111.28
1	D	220	ARG	N-CA-C	-6.23	104.74	112.90
1	C	243	ILE	N-CA-C	-6.18	101.43	107.55
1	A	179	ILE	N-CA-C	6.12	116.86	110.62
1	C	212	ALA	N-CA-C	-6.10	97.19	107.99
1	C	176	GLN	CB-CA-C	-6.09	98.64	110.46
1	A	126	PRO	CA-C-N	-6.01	113.57	122.83
1	A	126	PRO	C-N-CA	-6.01	113.57	122.83
1	C	60	VAL	N-CA-C	-6.01	99.51	108.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	133	LEU	N-CA-C	-5.98	102.07	110.50
1	E	16	SER	N-CA-C	5.97	117.79	111.28
1	E	243	ILE	N-CA-C	-5.96	101.65	107.55
1	B	16	SER	N-CA-C	5.94	117.55	111.14
1	B	184	ARG	CA-CB-CG	-5.91	102.29	114.10
1	F	67	PHE	N-CA-C	5.91	119.83	111.92
1	D	212	ALA	N-CA-C	-5.83	96.90	107.75
1	D	245	ASN	N-CA-C	-5.82	96.94	109.81
1	D	224	ARG	N-CA-C	-5.79	104.88	111.14
1	C	63	HIS	N-CA-C	-5.79	104.93	112.23
1	A	7	GLU	N-CA-C	-5.78	104.90	111.14
1	A	169	ALA	N-CA-C	-5.77	100.54	109.14
1	D	164	VAL	N-CA-C	5.77	116.42	108.12
1	B	245	ASN	CA-C-N	5.70	125.32	119.56
1	B	245	ASN	C-N-CA	5.70	125.32	119.56
1	B	137	VAL	N-CA-C	5.66	115.41	109.01
1	F	155	LEU	N-CA-C	-5.66	100.76	109.76
1	C	33	GLU	N-CA-C	5.65	117.52	111.36
1	B	65	GLY	CA-C-N	-5.65	114.71	122.16
1	B	65	GLY	C-N-CA	-5.65	114.71	122.16
1	F	125	GLU	CA-C-N	5.63	126.88	119.84
1	F	125	GLU	C-N-CA	5.63	126.88	119.84
1	D	207	GLY	N-CA-C	5.62	123.80	114.48
1	B	107	GLY	N-CA-C	5.61	119.72	112.54
1	B	63	HIS	N-CA-C	-5.60	105.56	112.90
1	F	241	ILE	CB-CA-C	-5.58	102.85	110.77
1	D	103	HIS	CA-C-N	5.57	126.80	119.84
1	D	103	HIS	C-N-CA	5.57	126.80	119.84
1	C	191	ILE	N-CA-C	5.55	115.88	108.11
1	B	35	VAL	N-CA-C	5.53	116.26	108.36
1	A	19	ILE	N-CA-C	5.49	116.63	108.23
1	F	122	GLY	CA-C-O	5.47	127.21	121.08
1	B	233	ASN	N-CA-C	5.45	119.62	112.92
1	D	176	GLN	CB-CA-C	-5.44	100.57	110.63
1	C	161	GLY	CA-C-N	5.44	125.74	119.92
1	C	161	GLY	C-N-CA	5.44	125.74	119.92
1	E	19	ILE	N-CA-C	5.41	115.89	107.99
1	A	94	TYR	N-CA-C	-5.40	101.08	109.72
1	C	242	ASP	CA-C-N	-5.39	116.70	122.85
1	C	242	ASP	C-N-CA	-5.39	116.70	122.85
1	C	5	GLU	N-CA-C	-5.37	105.50	111.36
1	D	107	GLY	N-CA-C	5.35	118.08	111.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	176	GLN	CB-CA-C	-5.34	100.11	110.46
1	F	102	ALA	N-CA-C	5.33	120.06	113.50
1	C	58	ASP	N-CA-C	-5.31	107.35	113.88
1	F	126	PRO	N-CA-C	5.30	123.39	112.47
1	A	21	ASP	N-CA-C	5.28	117.89	109.81
1	D	233	ASN	N-CA-C	5.27	119.81	113.17
1	E	35	VAL	CB-CA-C	-5.27	103.76	110.98
1	E	58	ASP	N-CA-C	-5.26	106.91	113.38
1	C	19	ILE	CB-CA-C	-5.25	103.79	110.98
1	A	228	GLU	N-CA-C	-5.25	105.64	111.36
1	D	221	GLY	N-CA-C	5.25	118.99	112.64
1	D	58	ASP	N-CA-C	-5.24	107.02	113.41
1	B	191	ILE	CB-CA-C	-5.24	103.03	110.83
1	E	220	ARG	N-CA-C	-5.24	106.73	113.23
1	C	98	LEU	CA-C-N	-5.22	113.25	119.05
1	C	98	LEU	C-N-CA	-5.22	113.25	119.05
1	D	159	ASP	N-CA-C	5.22	117.65	111.33
1	D	234	THR	N-CA-C	-5.22	101.54	108.74
1	C	165	VAL	CB-CA-C	-5.20	104.46	110.91
1	A	5	GLU	N-CA-C	-5.19	105.06	111.40
1	C	215	HIS	N-CA-C	-5.19	105.31	110.97
1	A	221	GLY	N-CA-C	5.18	118.91	112.64
1	E	18	ALA	N-CA-C	5.17	118.69	112.38
1	C	102	ALA	N-CA-C	5.13	119.59	113.23
1	E	137	VAL	CA-C-N	5.12	125.12	120.21
1	E	137	VAL	C-N-CA	5.12	125.12	120.21
1	E	86	LEU	N-CA-C	5.11	116.53	111.07
1	F	176	GLN	CB-CA-C	-5.11	102.00	110.68
1	C	218	THR	CA-C-N	-5.10	114.48	122.49
1	C	218	THR	C-N-CA	-5.10	114.48	122.49
1	D	125	GLU	CA-C-N	5.10	126.22	119.84
1	D	125	GLU	C-N-CA	5.10	126.22	119.84
1	F	238	VAL	N-CA-C	5.09	115.30	108.17
1	A	22	TYR	N-CA-C	-5.08	107.06	113.20
1	F	106	LEU	N-CA-C	5.07	119.74	113.50
1	A	139	GLY	N-CA-C	5.06	118.80	112.73
1	E	112	LEU	N-CA-C	-5.05	105.85	111.36
1	B	245	ASN	N-CA-C	-5.03	98.69	109.81
1	D	213	ALA	N-CA-C	5.03	119.06	113.02
1	F	205	GLU	CA-C-N	-5.02	114.77	122.60
1	F	205	GLU	C-N-CA	-5.02	114.77	122.60
1	C	107	GLY	N-CA-C	5.01	118.61	112.14

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Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	134	THR	N-CA-C	-5.00	107.24	113.19
1	F	60	VAL	N-CA-C	-5.00	100.92	108.12

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 [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	1897	0	1866	32	0
1	B	1897	0	1866	28	0
1	C	1897	0	1866	24	0
1	D	1897	0	1866	22	0
1	E	1897	0	1866	38	0
1	F	1897	0	1866	29	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
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	169	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 (169) 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:E:60:VAL:C	1:E:61:ILE:HD12	2.13	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: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:HD23	1:A:208:LEU:N	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:A:223:ILE:C	1:A:223:ILE:HD13	2.23	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
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:E:208:LEU:C	1:E:208:LEU:HD12	2.27	0.60
1:C:176:GLN:HG3	1:C:194:GLU:O	2.01	0.59
1:A:10:ILE:HD13	1:A:10:ILE:N	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:O	1:E:13:LYS:HG3	2.05	0.57
1:F:208:LEU:H	1:F:208:LEU:HD23	1.70	0.57
1:B:125:GLU:HB3	1:B:126:PRO:CD	2.35	0.56
1:F:36:GLN:NE2	1:F:36:GLN:HA	2.19	0.56
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:D:102:ALA:O	1:D:103:HIS:C	2.51	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
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:C:102:ALA:O	1:C:103:HIS:C	2.53	0.49
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:98:LEU:O	1:E:99:PRO:C	2.52	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HA	1:D:149:ARG:HE	1.78	0.48
1:F:102:ALA:O	1:F:103:HIS:C	2.57	0.48
1:A:39:VAL:O	1:A:60:VAL:HA	2.13	0.48
1:A:145:TRP:O	1:A:149:ARG:HG2	2.14	0.48
1:A:78:MSE:HG2	1:B:205:GLU:HB3	1.96	0.48
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:75:ILE:O	1:C:75:ILE:HG23	2.14	0.47
1:C:127:LEU:N	3:C:594:HOH:O	2.06	0.47
1:E:169:ALA:HB2	1:E:187:VAL:HG11	1.96	0.47
1:C:168:VAL:HG12	1:C:169:ALA:N	2.28	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:167:ARG:NH1	3:E:880:HOH:O	2.34	0.46
1:E:184:ARG:O	1:E:185:PHE:C	2.58	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:D:237:ASP:C	1:D:237:ASP:OD1	2.58	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:E:138:PRO:HB2	1:E:141:GLU:OE1	2.15	0.45
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:O	1:D:75:ILE:HG12	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:136:PRO:C	1:A:137:VAL:HG13	2.42	0.45
1:A:40:THR:OG1	1:A:223:ILE:HD11	2.17	0.44
1:A:102:ALA:O	1:A:103:HIS:C	2.59	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:112:LEU:O	1:A:113:ALA:C	2.58	0.43
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: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:180:ASP:OD1	1:E:202:SER:OG	2.36	0.42
1:E:215:HIS:CG	1:F:197:GLU:HB2	2.54	0.42
1:A:2:LYS:O	1:A:3:ASN:C	2.61	0.42
1:E:21:ASP:N	1:E:21:ASP:OD1	2.52	0.42
1:E:171:CYS:O	1:E:192:THR:HA	2.19	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: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:HD23	1:F:133:LEU:HA	1.84	0.41
1:C:98:LEU:O	1:C:99:PRO:C	2.63	0.41
1:C:66:TYR:HB3	3:C:997:HOH:O	2.19	0.41
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: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:F:237:ASP:OD1	1:F:237:ASP:C	2.64	0.40
1:A:155:LEU:HD12	1:A:155:LEU:C	2.45	0.40
1:A:168:VAL:HG12	1:A:169:ALA:N	2.35	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:129:PRO:HD2	1:E:170:TRP:O	2.22	0.40
1:F:133:LEU:O	1:F:134:THR:C	2.63	0.40
1:D:74:VAL:CG1	1:D:76:ARG:HG3	2.52	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%)	30	34
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%)	16	16
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%)	43	51

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 [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	197/193 (102%)	182 (92%)	15 (8%)	12	14
1	B	197/193 (102%)	184 (93%)	13 (7%)	15	18
1	C	197/193 (102%)	187 (95%)	10 (5%)	21	27
1	D	197/193 (102%)	184 (93%)	13 (7%)	15	18
1	E	197/193 (102%)	183 (93%)	14 (7%)	13	16
1	F	197/193 (102%)	184 (93%)	13 (7%)	15	18
All	All	1182/1158 (102%)	1104 (93%)	78 (7%)	15	18

All (78) 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	155	LEU
1	A	176	GLN
1	A	181	SER
1	A	184	ARG
1	A	223	ILE
1	B	20	SER
1	B	27	LEU
1	B	48	LEU
1	B	49	LEU
1	B	69	LYS
1	B	80	ARG
1	B	104	PRO

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Mol	Chain	Res	Type
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	135	MSE
1	C	163	GLU
1	C	176	GLN
1	C	208	LEU
1	D	2	LYS
1	D	8	GLN
1	D	27	LEU
1	D	48	LEU
1	D	49	LEU
1	D	75	ILE
1	D	106	LEU
1	D	112	LEU
1	D	135	MSE
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	39	VAL
1	E	48	LEU
1	E	49	LEU
1	E	61	ILE
1	E	75	ILE
1	E	106	LEU
1	E	112	LEU
1	E	126	PRO
1	E	164	VAL
1	E	165	VAL
1	E	176	GLN

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Mol	Chain	Res	Type
1	E	243	ILE
1	F	27	LEU
1	F	39	VAL
1	F	48	LEU
1	F	49	LEU
1	F	80	ARG
1	F	106	LEU
1	F	112	LEU
1	F	134	THR
1	F	135	MSE
1	F	164	VAL
1	F	165	VAL
1	F	176	GLN
1	F	246	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	166	GLN
1	A	206	GLN
1	B	36	GLN
1	C	15	ASN
1	C	36	GLN
1	C	46	GLN
1	C	81	ASN
1	C	166	GLN
1	C	206	GLN
1	D	36	GLN
1	D	46	GLN
1	E	36	GLN
1	E	46	GLN
1	F	36	GLN
1	F	46	GLN
1	F	81	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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 [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 [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%)	-0.35	0 100 100	9, 16, 26, 31	0
1	B	243/247 (98%)	-0.32	1 (0%) 88 87	8, 17, 28, 30	0
1	C	243/247 (98%)	-0.40	0 100 100	8, 15, 25, 30	0
1	D	243/247 (98%)	-0.38	1 (0%) 88 87	9, 15, 27, 31	0
1	E	243/247 (98%)	-0.41	1 (0%) 88 87	6, 15, 25, 32	0
1	F	243/247 (98%)	-0.46	0 100 100	5, 14, 22, 29	0
All	All	1458/1482 (98%)	-0.39	3 (0%) 91 90	5, 15, 26, 32	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	22	TYR	2.3
1	D	232	GLU	2.0
1	E	22	TYR	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 oligosaccharides 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. 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	B-factors(Å ²)	Q<0.9
2	FE	F	301	1/1	0.94	0.13	30,30,30,30	0
2	FE	B	301	1/1	0.96	0.19	27,27,27,27	0
2	FE	C	302	1/1	0.96	0.11	26,26,26,26	0
2	FE	D	302	1/1	0.96	0.14	18,18,18,18	0
2	FE	A	301	1/1	0.96	0.17	30,30,30,30	0
2	FE	C	301	1/1	0.97	0.13	27,27,27,27	0
2	FE	E	301	1/1	0.97	0.14	22,22,22,22	0
2	FE	E	302	1/1	0.97	0.16	17,17,17,17	0
2	FE	B	302	1/1	0.97	0.12	22,22,22,22	0
2	FE	F	302	1/1	0.98	0.14	21,21,21,21	0
2	FE	D	301	1/1	0.99	0.17	27,27,27,27	0
2	FE	A	302	1/1	0.99	0.09	25,25,25,25	0

6.5 Other polymers [i](#)

There are no such residues in this entry.