



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 23, 2024 – 12:14 pm GMT

PDB ID : 8CNZ
Title : mmLarE-[4Fe-4S] phased by Fe-SAD
Authors : Pecqueur, L.; Zecchin, P.; Golinelli-Pimpaneau, B.
Deposited on : 2023-02-24
Resolution : 3.60 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 : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

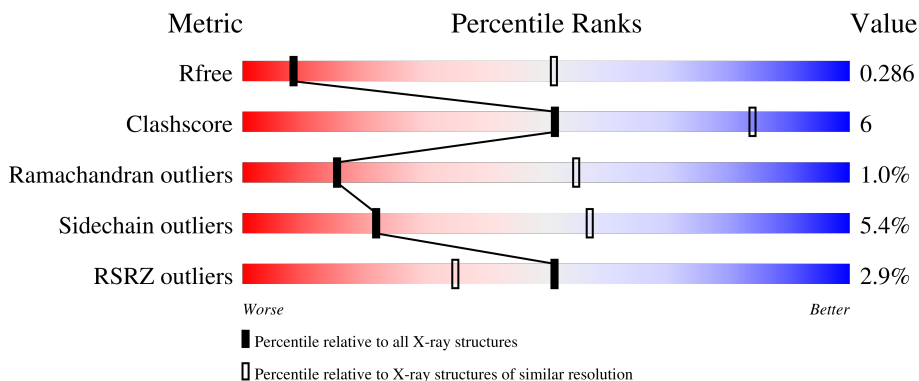
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.60 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	1257 (3.70-3.50)
Clashscore	141614	1353 (3.70-3.50)
Ramachandran outliers	138981	1307 (3.70-3.50)
Sidechain outliers	138945	1307 (3.70-3.50)
RSRZ outliers	127900	1161 (3.70-3.50)

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	271	
1	B	271	
1	C	271	
1	D	271	
1	E	271	

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Mol	Chain	Length	Quality of chain
1	F	271	<p>%</p> <p>75% 18% • 7%</p>
1	G	271	<p>8%</p> <p>77% 14% • 7%</p>

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	SF4	A	301	-	-	X	-
2	SF4	C	301	-	-	X	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 14443 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 NAD_synthase domain-containing protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	254	Total 2055	C 1312	N 341	O 397	S 5	0	0	0
1	B	254	Total 2050	C 1309	N 339	O 397	S 5	0	0	0
1	C	256	Total 2065	C 1318	N 343	O 399	S 5	0	0	0
1	D	261	Total 2103	C 1343	N 347	O 406	S 7	0	0	0
1	E	251	Total 2031	C 1294	N 336	O 396	S 5	0	0	0
1	F	253	Total 2040	C 1303	N 336	O 396	S 5	0	0	0
1	G	253	Total 2034	C 1300	N 333	O 396	S 5	0	0	0

There are 91 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-10	GLY	-	expression tag	UNP Q6LXV7
A	-9	PRO	-	expression tag	UNP Q6LXV7
A	-8	MET	-	expression tag	UNP Q6LXV7
A	-7	LEU	-	expression tag	UNP Q6LXV7
A	-6	GLU	-	expression tag	UNP Q6LXV7
A	-5	VAL	-	expression tag	UNP Q6LXV7
A	-4	LEU	-	expression tag	UNP Q6LXV7
A	-3	PHE	-	expression tag	UNP Q6LXV7
A	-2	GLN	-	expression tag	UNP Q6LXV7
A	-1	GLY	-	expression tag	UNP Q6LXV7
A	0	PRO	-	expression tag	UNP Q6LXV7
A	259	GLY	-	expression tag	UNP Q6LXV7
A	260	SER	-	expression tag	UNP Q6LXV7
B	-10	GLY	-	expression tag	UNP Q6LXV7
B	-9	PRO	-	expression tag	UNP Q6LXV7

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-8	MET	-	expression tag	UNP Q6LXV7
B	-7	LEU	-	expression tag	UNP Q6LXV7
B	-6	GLU	-	expression tag	UNP Q6LXV7
B	-5	VAL	-	expression tag	UNP Q6LXV7
B	-4	LEU	-	expression tag	UNP Q6LXV7
B	-3	PHE	-	expression tag	UNP Q6LXV7
B	-2	GLN	-	expression tag	UNP Q6LXV7
B	-1	GLY	-	expression tag	UNP Q6LXV7
B	0	PRO	-	expression tag	UNP Q6LXV7
B	259	GLY	-	expression tag	UNP Q6LXV7
B	260	SER	-	expression tag	UNP Q6LXV7
C	-10	GLY	-	expression tag	UNP Q6LXV7
C	-9	PRO	-	expression tag	UNP Q6LXV7
C	-8	MET	-	expression tag	UNP Q6LXV7
C	-7	LEU	-	expression tag	UNP Q6LXV7
C	-6	GLU	-	expression tag	UNP Q6LXV7
C	-5	VAL	-	expression tag	UNP Q6LXV7
C	-4	LEU	-	expression tag	UNP Q6LXV7
C	-3	PHE	-	expression tag	UNP Q6LXV7
C	-2	GLN	-	expression tag	UNP Q6LXV7
C	-1	GLY	-	expression tag	UNP Q6LXV7
C	0	PRO	-	expression tag	UNP Q6LXV7
C	259	GLY	-	expression tag	UNP Q6LXV7
C	260	SER	-	expression tag	UNP Q6LXV7
D	-10	GLY	-	expression tag	UNP Q6LXV7
D	-9	PRO	-	expression tag	UNP Q6LXV7
D	-8	MET	-	expression tag	UNP Q6LXV7
D	-7	LEU	-	expression tag	UNP Q6LXV7
D	-6	GLU	-	expression tag	UNP Q6LXV7
D	-5	VAL	-	expression tag	UNP Q6LXV7
D	-4	LEU	-	expression tag	UNP Q6LXV7
D	-3	PHE	-	expression tag	UNP Q6LXV7
D	-2	GLN	-	expression tag	UNP Q6LXV7
D	-1	GLY	-	expression tag	UNP Q6LXV7
D	0	PRO	-	expression tag	UNP Q6LXV7
D	259	GLY	-	expression tag	UNP Q6LXV7
D	260	SER	-	expression tag	UNP Q6LXV7
E	-10	GLY	-	expression tag	UNP Q6LXV7
E	-9	PRO	-	expression tag	UNP Q6LXV7
E	-8	MET	-	expression tag	UNP Q6LXV7
E	-7	LEU	-	expression tag	UNP Q6LXV7
E	-6	GLU	-	expression tag	UNP Q6LXV7

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-5	VAL	-	expression tag	UNP Q6LXV7
E	-4	LEU	-	expression tag	UNP Q6LXV7
E	-3	PHE	-	expression tag	UNP Q6LXV7
E	-2	GLN	-	expression tag	UNP Q6LXV7
E	-1	GLY	-	expression tag	UNP Q6LXV7
E	0	PRO	-	expression tag	UNP Q6LXV7
E	259	GLY	-	expression tag	UNP Q6LXV7
E	260	SER	-	expression tag	UNP Q6LXV7
F	-10	GLY	-	expression tag	UNP Q6LXV7
F	-9	PRO	-	expression tag	UNP Q6LXV7
F	-8	MET	-	expression tag	UNP Q6LXV7
F	-7	LEU	-	expression tag	UNP Q6LXV7
F	-6	GLU	-	expression tag	UNP Q6LXV7
F	-5	VAL	-	expression tag	UNP Q6LXV7
F	-4	LEU	-	expression tag	UNP Q6LXV7
F	-3	PHE	-	expression tag	UNP Q6LXV7
F	-2	GLN	-	expression tag	UNP Q6LXV7
F	-1	GLY	-	expression tag	UNP Q6LXV7
F	0	PRO	-	expression tag	UNP Q6LXV7
F	259	GLY	-	expression tag	UNP Q6LXV7
F	260	SER	-	expression tag	UNP Q6LXV7
G	-10	GLY	-	expression tag	UNP Q6LXV7
G	-9	PRO	-	expression tag	UNP Q6LXV7
G	-8	MET	-	expression tag	UNP Q6LXV7
G	-7	LEU	-	expression tag	UNP Q6LXV7
G	-6	GLU	-	expression tag	UNP Q6LXV7
G	-5	VAL	-	expression tag	UNP Q6LXV7
G	-4	LEU	-	expression tag	UNP Q6LXV7
G	-3	PHE	-	expression tag	UNP Q6LXV7
G	-2	GLN	-	expression tag	UNP Q6LXV7
G	-1	GLY	-	expression tag	UNP Q6LXV7
G	0	PRO	-	expression tag	UNP Q6LXV7
G	259	GLY	-	expression tag	UNP Q6LXV7
G	260	SER	-	expression tag	UNP Q6LXV7

- Molecule 2 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Fe S	0	0
			8	4 4		
2	B	1	Total	Fe S	0	0
			8	4 4		
2	C	1	Total	Fe S	0	0
			8	4 4		
2	D	1	Total	Fe S	0	0
			8	4 4		
2	E	1	Total	Fe S	0	0
			8	4 4		
2	F	1	Total	Fe S	0	0
			8	4 4		
2	G	1	Total	Fe S	0	0
			8	4 4		

- Molecule 3 is IODIDE ION (three-letter code: IOD) (formula: I).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	I	0	0
			1	1		
3	B	1	Total	I	0	0
			1	1		
3	D	1	Total	I	0	0
			1	1		
3	G	1	Total	I	0	0
			1	1		

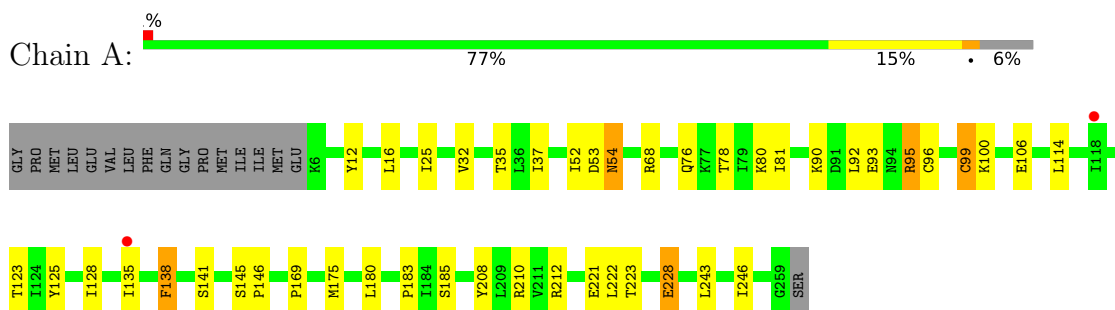
- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total 1	Cl 1	0	0
4	B	1	Total 1	Cl 1	0	0
4	C	1	Total 1	Cl 1	0	0
4	D	1	Total 1	Cl 1	0	0
4	E	1	Total 1	Cl 1	0	0

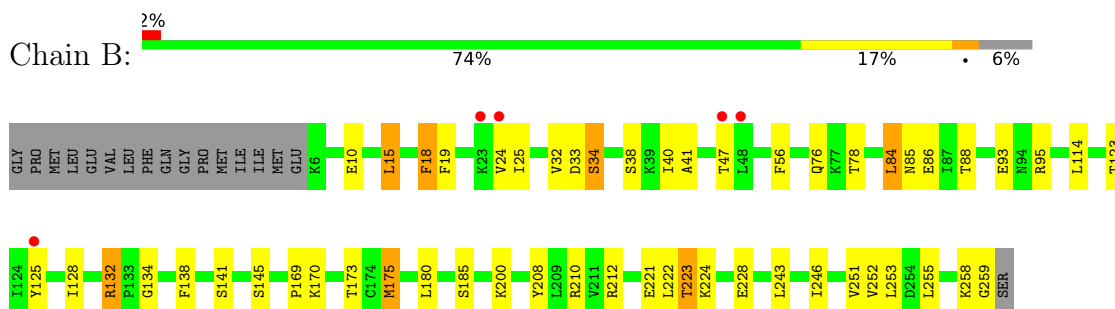
3 Residue-property plots [i](#)

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.

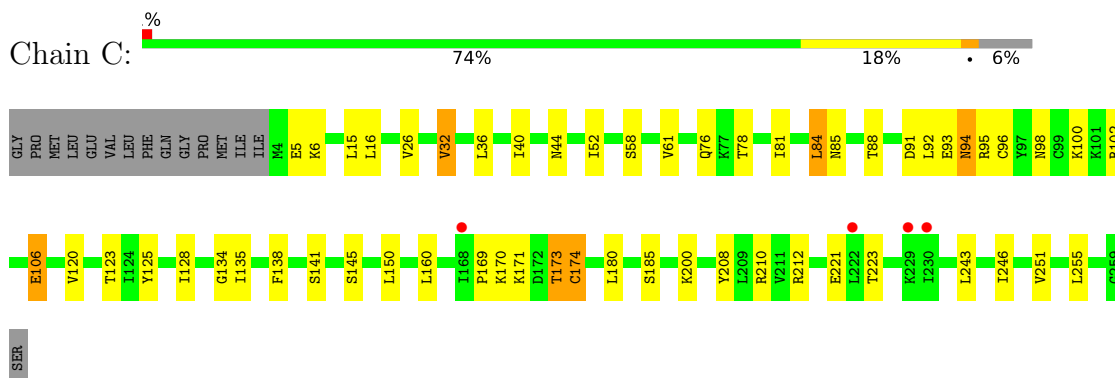
- Molecule 1: NAD_synthase domain-containing protein



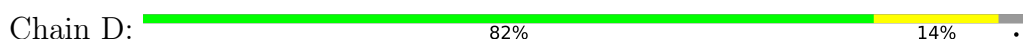
- Molecule 1: NAD_synthase domain-containing protein

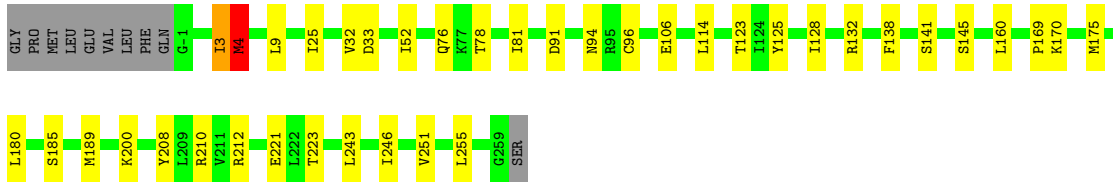


- Molecule 1: NAD_synthase domain-containing protein

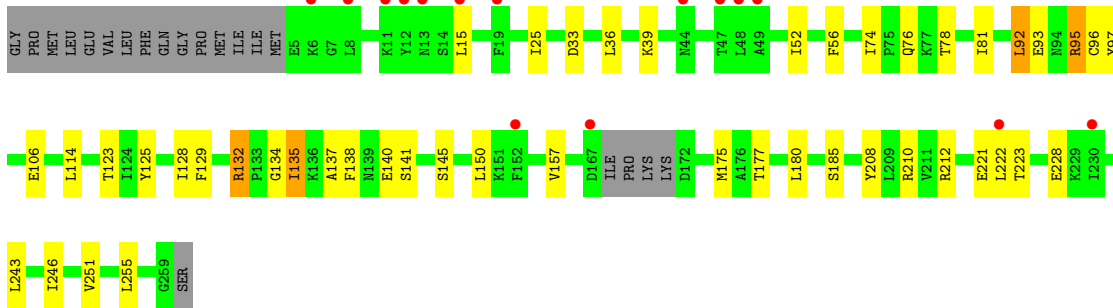
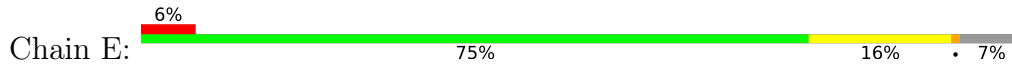


- Molecule 1: NAD_synthase domain-containing protein

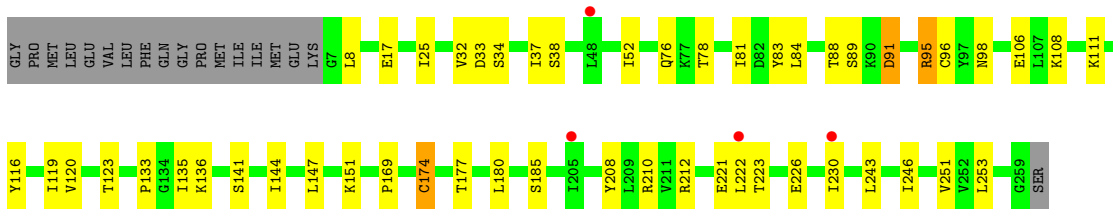
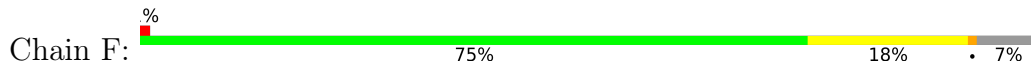




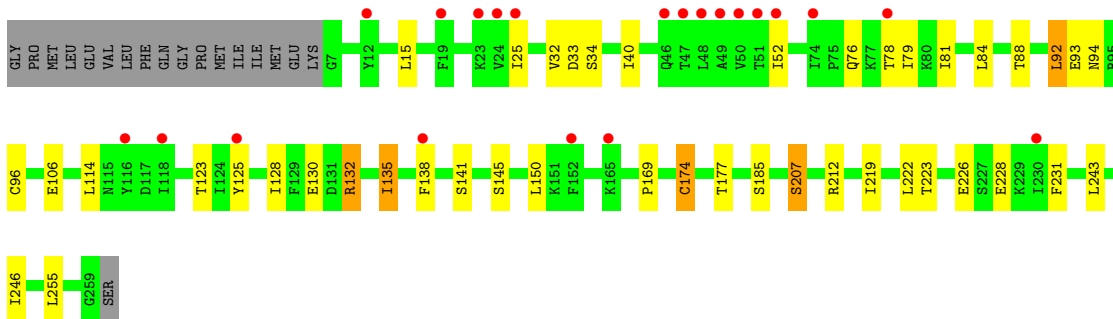
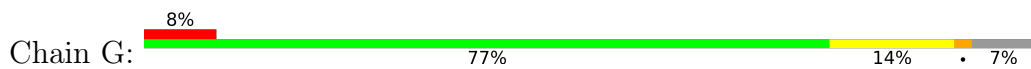
- Molecule 1: NAD_synthase domain-containing protein



- Molecule 1: NAD_synthase domain-containing protein



- Molecule 1: NAD_synthase domain-containing protein



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	187.52Å 209.22Å 195.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	55.37 – 3.60 55.37 – 3.60	Depositor EDS
% Data completeness (in resolution range)	89.7 (55.37-3.60) 89.7 (55.37-3.60)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.52 (at 3.57Å)	Xtrriage
Refinement program	BUSTER 2.10.4	Depositor
R, R_{free}	0.253 , 0.280 0.256 , 0.286	Depositor DCC
R_{free} test set	2006 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	101.5	Xtrriage
Anisotropy	0.066	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 72.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	14443	wwPDB-VP
Average B, all atoms (Å ²)	118.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.49% 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: SF4, CL, IOD

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	0.34	0/2083	0.55	0/2798
1	B	0.35	0/2078	0.55	0/2792
1	C	0.34	0/2093	0.55	0/2812
1	D	0.33	0/2132	0.54	0/2865
1	E	0.31	0/2057	0.53	0/2762
1	F	0.34	0/2068	0.57	0/2780
1	G	0.30	0/2062	0.53	0/2773
All	All	0.33	0/14573	0.54	0/19582

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	2055	0	2101	22	0
1	B	2050	0	2088	27	0
1	C	2065	0	2105	30	0
1	D	2103	0	2149	19	0
1	E	2031	0	2062	28	0
1	F	2040	0	2077	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	2034	0	2066	20	0
2	A	8	0	0	2	0
2	B	8	0	0	0	0
2	C	8	0	0	2	0
2	D	8	0	0	1	0
2	E	8	0	0	0	0
2	F	8	0	0	0	0
2	G	8	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	D	1	0	0	0	0
3	G	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
All	All	14443	0	14648	163	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 6.

All (163) 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:B:170:LYS:HZ1	1:B:200:LYS:NZ	1.59	0.99
1:B:170:LYS:NZ	1:B:200:LYS:HZ3	1.64	0.95
1:B:41:ALA:HB1	1:B:47:THR:HG21	1.58	0.84
1:B:170:LYS:NZ	1:B:200:LYS:NZ	2.23	0.83
1:B:170:LYS:HZ1	1:B:200:LYS:HZ3	0.82	0.81
1:D:96:CYS:HB3	2:D:301:SF4:S4	2.30	0.72
1:E:97:TYR:HD1	1:E:137:ALA:HB2	1.55	0.70
1:F:174:CYS:SG	1:F:177:THR:HG23	2.32	0.70
1:G:32:VAL:HG22	1:G:169:PRO:HD2	1.74	0.69
1:C:32:VAL:HG13	1:C:169:PRO:HD2	1.74	0.69
1:C:91:ASP:OD2	1:C:98:ASN:ND2	2.26	0.68
1:B:24:VAL:HB	1:B:47:THR:HG22	1.78	0.64
1:C:81:ILE:HD11	1:C:106:GLU:HG2	1.79	0.64
1:C:100:LYS:HE3	2:C:301:SF4:S4	2.38	0.64
1:E:132:ARG:HH21	1:E:134:GLY:HA3	1.64	0.62
1:E:97:TYR:CD1	1:E:137:ALA:HB2	2.35	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:132:ARG:HG3	1:E:135:ILE:HG13	1.82	0.61
1:B:15:LEU:HA	1:B:18:PHE:HB2	1.82	0.60
1:C:36:LEU:HD21	1:C:160:LEU:HD23	1.82	0.60
1:C:15:LEU:HD23	1:C:40:ILE:HD13	1.83	0.60
1:B:56:PHE:O	1:B:175:MET:HB2	2.02	0.59
1:C:100:LYS:NZ	1:C:134:GLY:HA3	2.18	0.59
1:A:210:ARG:HB2	1:A:221:GLU:HB2	1.85	0.59
1:C:58:SER:HB3	1:C:61:VAL:HG23	1.85	0.59
1:C:16:LEU:HD22	1:C:44:ASN:HD21	1.69	0.58
1:B:132:ARG:HD2	1:B:134:GLY:H	1.69	0.58
1:C:173:THR:O	1:C:174:CYS:HB3	2.04	0.58
1:B:224:LYS:HD2	1:B:259:GLY:HA2	1.86	0.57
1:A:32:VAL:HG22	1:A:169:PRO:HD2	1.87	0.57
1:F:230:ILE:HG22	1:F:230:ILE:O	2.04	0.57
1:D:32:VAL:HG22	1:D:169:PRO:HD2	1.85	0.57
1:B:32:VAL:HG22	1:B:169:PRO:HD2	1.87	0.57
1:A:90:LYS:HG2	1:A:183:PRO:HB3	1.87	0.56
1:F:91:ASP:OD2	1:F:98:ASN:ND2	2.38	0.56
1:F:32:VAL:HG22	1:F:169:PRO:HD2	1.87	0.56
1:D:4:MET:HG2	1:D:9:LEU:HB2	1.88	0.56
1:D:25:ILE:HD11	1:D:114:LEU:HD12	1.87	0.55
1:F:83:TYR:O	1:F:88:THR:OG1	2.25	0.55
1:B:15:LEU:HD13	1:B:40:ILE:HG21	1.87	0.55
1:F:25:ILE:HG13	1:F:116:TYR:CD2	2.43	0.54
1:E:132:ARG:HE	1:E:134:GLY:HA3	1.71	0.54
1:B:84:LEU:O	1:B:88:THR:OG1	2.25	0.54
1:E:39:LYS:HB2	1:E:74:ILE:HD11	1.88	0.54
1:E:36:LEU:HD13	1:E:157:VAL:HG13	1.90	0.54
1:A:95:ARG:NH2	1:A:96:CYS:SG	2.83	0.52
1:G:212:ARG:HB2	1:G:219:ILE:HB	1.90	0.52
1:C:52:ILE:HG23	1:C:81:ILE:HD12	1.91	0.52
1:C:98:ASN:O	1:C:102:ARG:HG2	2.11	0.51
1:F:222:LEU:HD11	1:F:230:ILE:HD12	1.92	0.51
1:G:15:LEU:HD23	1:G:40:ILE:HD13	1.93	0.51
1:A:54:ASN:ND2	1:A:99:CYS:SG	2.84	0.51
1:B:251:VAL:HG12	1:D:255:LEU:HD12	1.92	0.50
1:C:32:VAL:HG13	1:C:169:PRO:CD	2.41	0.50
1:A:76:GLN:NE2	1:A:78:THR:OG1	2.44	0.50
1:G:84:LEU:O	1:G:88:THR:OG1	2.28	0.50
1:G:25:ILE:HD11	1:G:114:LEU:HD12	1.94	0.50
1:F:95:ARG:NH2	1:F:96:CYS:SG	2.85	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:52:ILE:HG23	1:F:81:ILE:HD12	1.93	0.49
1:E:52:ILE:HG23	1:E:81:ILE:HD12	1.94	0.49
1:C:255:LEU:HD12	1:E:251:VAL:HG12	1.95	0.49
1:C:15:LEU:HD13	1:C:150:LEU:HD12	1.95	0.49
1:E:25:ILE:HD11	1:E:114:LEU:HD12	1.95	0.49
1:D:210:ARG:HB2	1:D:221:GLU:HB2	1.96	0.48
1:F:222:LEU:HD12	1:F:253:LEU:HD11	1.95	0.48
1:B:222:LEU:HD12	1:B:253:LEU:HD11	1.94	0.48
1:E:132:ARG:HE	1:E:134:GLY:CA	2.26	0.48
1:C:84:LEU:O	1:C:88:THR:OG1	2.30	0.48
1:D:170:LYS:NZ	1:D:200:LYS:NZ	2.61	0.48
1:E:210:ARG:HB2	1:E:221:GLU:HB2	1.96	0.47
1:E:56:PHE:O	1:E:175:MET:HB2	2.14	0.47
1:E:92:LEU:HD23	1:E:95:ARG:HG2	1.96	0.47
1:B:170:LYS:NZ	1:B:200:LYS:HZ2	2.11	0.47
1:C:170:LYS:HE2	1:C:200:LYS:HZ3	1.79	0.47
1:D:175:MET:HG3	1:D:189:MET:HB3	1.96	0.47
1:G:52:ILE:HG23	1:G:81:ILE:HD12	1.97	0.47
1:G:132:ARG:HB3	1:G:135:ILE:HG13	1.97	0.47
1:E:76:GLN:NE2	1:E:78:THR:OG1	2.45	0.47
1:A:25:ILE:HD11	1:A:114:LEU:HD12	1.96	0.47
1:C:251:VAL:HG12	1:E:255:LEU:HD12	1.97	0.47
1:D:52:ILE:HG23	1:D:81:ILE:HD12	1.96	0.47
1:E:129:PHE:HA	1:G:79:ILE:HG12	1.97	0.47
1:A:52:ILE:HG23	1:A:81:ILE:HD12	1.98	0.46
1:A:135:ILE:HA	1:A:138:PHE:HB2	1.96	0.46
1:B:25:ILE:HD11	1:B:114:LEU:HD12	1.98	0.46
1:C:180:LEU:HD21	1:C:212:ARG:HD2	1.97	0.46
1:E:125:TYR:O	1:E:128:ILE:HG12	2.15	0.46
1:A:12:TYR:O	1:A:16:LEU:HG	2.16	0.46
1:A:125:TYR:O	1:A:128:ILE:HG12	2.14	0.46
1:C:26:VAL:HG13	1:C:120:VAL:HG23	1.96	0.46
1:C:95:ARG:HG3	1:C:96:CYS:N	2.31	0.46
1:E:132:ARG:HE	1:E:134:GLY:H	1.63	0.46
1:G:125:TYR:O	1:G:128:ILE:HG12	2.16	0.46
1:C:171:LYS:HG2	1:C:173:THR:HG23	1.97	0.46
1:D:4:MET:HE1	1:D:160:LEU:HD13	1.97	0.46
1:D:125:TYR:O	1:D:128:ILE:HG12	2.16	0.46
1:F:180:LEU:HD21	1:F:212:ARG:HD2	1.98	0.46
1:B:180:LEU:HD21	1:B:212:ARG:HD2	1.98	0.46
1:B:210:ARG:HB2	1:B:221:GLU:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:210:ARG:HB2	1:F:221:GLU:HB2	1.98	0.45
1:B:125:TYR:O	1:B:128:ILE:HG12	2.16	0.45
1:C:243:LEU:HA	1:C:246:ILE:HD12	1.99	0.45
1:E:243:LEU:HA	1:E:246:ILE:HD12	1.98	0.45
1:C:125:TYR:O	1:C:128:ILE:HG12	2.16	0.45
1:E:180:LEU:HD21	1:E:212:ARG:HD2	1.98	0.45
1:F:133:PRO:HA	1:F:136:LYS:HB2	1.99	0.45
1:B:243:LEU:HA	1:B:246:ILE:HD12	1.99	0.45
1:F:111:LYS:HD3	1:F:119:ILE:HG13	1.98	0.45
1:A:243:LEU:HA	1:A:246:ILE:HD12	1.99	0.44
1:A:100:LYS:HG3	2:A:301:SF4:S4	2.58	0.44
1:D:123:THR:HB	1:D:145:SER:HB3	1.98	0.44
1:D:170:LYS:HE2	1:D:200:LYS:HZ3	1.82	0.44
1:E:137:ALA:O	1:E:140:GLU:HB2	2.17	0.44
1:B:123:THR:HB	1:B:145:SER:HB3	1.99	0.44
1:B:76:GLN:NE2	1:B:78:THR:OG1	2.49	0.44
1:A:81:ILE:HD11	1:A:106:GLU:HG3	1.99	0.44
1:G:123:THR:HB	1:G:145:SER:HB3	2.00	0.44
1:G:76:GLN:NE2	1:G:78:THR:OG1	2.47	0.44
1:E:15:LEU:HD13	1:E:150:LEU:HD12	2.00	0.44
1:A:35:THR:HG21	1:A:68:ARG:HH21	1.82	0.43
1:D:76:GLN:NE2	1:D:78:THR:OG1	2.47	0.43
1:E:81:ILE:CD1	1:E:106:GLU:HG3	2.48	0.43
1:A:123:THR:HB	1:A:145:SER:HB3	1.99	0.43
1:A:180:LEU:HD21	1:A:212:ARG:HD2	2.01	0.43
1:G:130:GLU:HB2	1:G:132:ARG:HD2	2.00	0.43
1:F:251:VAL:HG12	1:G:255:LEU:HD12	2.01	0.43
1:G:223:THR:HB	1:G:226:GLU:CG	2.48	0.43
1:E:123:THR:HB	1:E:145:SER:HB3	2.00	0.43
1:D:243:LEU:HA	1:D:246:ILE:HD12	1.99	0.43
1:F:243:LEU:HA	1:F:246:ILE:HD12	2.00	0.43
1:G:177:THR:HG22	1:G:212:ARG:HH12	1.83	0.43
1:B:34:SER:O	1:B:38:SER:OG	2.28	0.43
1:B:255:LEU:HD12	1:D:251:VAL:HG12	2.00	0.43
1:C:100:LYS:HG3	2:C:301:SF4:S4	2.59	0.43
1:G:243:LEU:HA	1:G:246:ILE:HD12	2.01	0.43
1:C:123:THR:HB	1:C:145:SER:HB3	1.99	0.43
1:F:76:GLN:NE2	1:F:78:THR:OG1	2.47	0.43
1:E:81:ILE:HD11	1:E:106:GLU:HG3	2.01	0.42
1:B:223:THR:HG23	1:B:258:LYS:HD3	2.00	0.42
1:C:93:GLU:O	1:C:94:ASN:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:123:THR:O	1:F:147:LEU:HB2	2.20	0.42
1:F:223:THR:HB	1:F:226:GLU:CG	2.49	0.42
1:A:81:ILE:CD1	1:A:106:GLU:HG3	2.49	0.42
1:E:177:THR:HG22	1:E:212:ARG:HH12	1.85	0.42
1:C:170:LYS:NZ	1:C:200:LYS:NZ	2.68	0.42
1:G:174:CYS:SG	1:G:177:THR:OG1	2.78	0.42
1:G:81:ILE:CD1	1:G:106:GLU:HG3	2.50	0.42
1:B:19:PHE:CD1	1:B:24:VAL:HG21	2.55	0.41
1:C:210:ARG:HB2	1:C:221:GLU:HB2	2.01	0.41
1:F:223:THR:HB	1:F:226:GLU:HB2	2.02	0.41
1:G:15:LEU:HD13	1:G:150:LEU:HD12	2.01	0.41
1:D:81:ILE:CD1	1:D:106:GLU:HG3	2.51	0.41
1:D:180:LEU:HD21	1:D:212:ARG:HD2	2.01	0.41
1:F:34:SER:O	1:F:38:SER:OG	2.29	0.41
1:D:91:ASP:OD2	1:D:94:ASN:HB2	2.20	0.41
1:E:132:ARG:HE	1:E:134:GLY:N	2.18	0.41
1:F:81:ILE:HD11	1:F:106:GLU:HG3	2.03	0.40
1:G:228:GLU:HA	1:G:231:PHE:CD2	2.56	0.40
1:A:37:ILE:HD11	1:A:146:PRO:HG2	2.03	0.40
1:A:100:LYS:CG	2:A:301:SF4:S4	3.09	0.40
1:C:76:GLN:NE2	1:C:78:THR:OG1	2.47	0.40
1:A:53:ASP:HB3	1:A:80:LYS:HA	2.03	0.40
1:A:228:GLU:H	1:A:228:GLU:HG3	1.47	0.40
1:F:120:VAL:HA	1:F:144:ILE: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	252/271 (93%)	239 (95%)	12 (5%)	1 (0%)	34 71

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	252/271 (93%)	241 (96%)	9 (4%)	2 (1%)	19	59
1	C	254/271 (94%)	238 (94%)	11 (4%)	5 (2%)	7	41
1	D	259/271 (96%)	245 (95%)	11 (4%)	3 (1%)	13	51
1	E	247/271 (91%)	234 (95%)	12 (5%)	1 (0%)	34	71
1	F	251/271 (93%)	235 (94%)	13 (5%)	3 (1%)	13	51
1	G	251/271 (93%)	236 (94%)	12 (5%)	3 (1%)	13	51
All	All	1766/1897 (93%)	1668 (94%)	80 (4%)	18 (1%)	15	55

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	94	ASN
1	D	3	ILE
1	D	4	MET
1	F	151	LYS
1	G	92	LEU
1	G	207	SER
1	C	5	GLU
1	C	6	LYS
1	G	94	ASN
1	A	208	TYR
1	B	208	TYR
1	B	85	ASN
1	C	208	TYR
1	D	208	TYR
1	E	208	TYR
1	F	84	LEU
1	F	208	TYR
1	C	85	ASN

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	232/248 (94%)	220 (95%)	12 (5%)	23	58
1	B	231/248 (93%)	213 (92%)	18 (8%)	12	44
1	C	232/248 (94%)	221 (95%)	11 (5%)	26	61
1	D	237/248 (96%)	229 (97%)	8 (3%)	37	69
1	E	229/248 (92%)	216 (94%)	13 (6%)	20	55
1	F	230/248 (93%)	218 (95%)	12 (5%)	23	58
1	G	229/248 (92%)	216 (94%)	13 (6%)	20	55
All	All	1620/1736 (93%)	1533 (95%)	87 (5%)	22	57

All (87) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	54	ASN
1	A	92	LEU
1	A	93	GLU
1	A	95	ARG
1	A	99	CYS
1	A	138	PHE
1	A	141	SER
1	A	175	MET
1	A	185	SER
1	A	222	LEU
1	A	223	THR
1	A	228	GLU
1	B	10	GLU
1	B	15	LEU
1	B	18	PHE
1	B	33	ASP
1	B	34	SER
1	B	84	LEU
1	B	86	GLU
1	B	93	GLU
1	B	95	ARG
1	B	132	ARG
1	B	138	PHE
1	B	141	SER
1	B	173	THR
1	B	175	MET
1	B	185	SER
1	B	223	THR
1	B	228	GLU

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Mol	Chain	Res	Type
1	B	252	VAL
1	C	32	VAL
1	C	84	LEU
1	C	92	LEU
1	C	106	GLU
1	C	135	ILE
1	C	138	PHE
1	C	141	SER
1	C	173	THR
1	C	174	CYS
1	C	185	SER
1	C	223	THR
1	D	3	ILE
1	D	4	MET
1	D	33	ASP
1	D	132	ARG
1	D	138	PHE
1	D	141	SER
1	D	185	SER
1	D	223	THR
1	E	33	ASP
1	E	92	LEU
1	E	93	GLU
1	E	95	ARG
1	E	96	CYS
1	E	132	ARG
1	E	135	ILE
1	E	138	PHE
1	E	141	SER
1	E	185	SER
1	E	222	LEU
1	E	223	THR
1	E	228	GLU
1	F	8	LEU
1	F	17	GLU
1	F	33	ASP
1	F	37	ILE
1	F	89	SER
1	F	91	ASP
1	F	95	ARG
1	F	108	LYS
1	F	135	ILE

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Mol	Chain	Res	Type
1	F	141	SER
1	F	174	CYS
1	F	185	SER
1	G	33	ASP
1	G	34	SER
1	G	92	LEU
1	G	93	GLU
1	G	96	CYS
1	G	132	ARG
1	G	135	ILE
1	G	138	PHE
1	G	141	SER
1	G	174	CYS
1	G	185	SER
1	G	207	SER
1	G	222	LEU

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

Mol	Chain	Res	Type
1	A	256	ASN
1	C	44	ASN
1	C	139	ASN
1	D	256	ASN
1	E	256	ASN
1	F	85	ASN
1	G	139	ASN
1	G	256	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 monosaccharides in this entry.

5.6 Ligand geometry

Of 16 ligands modelled in this entry, 9 are monoatomic - leaving 7 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	SF4	B	301	1	0,12,12	-	-	-		
2	SF4	D	301	1	0,12,12	-	-	-		
2	SF4	E	301	1	0,12,12	-	-	-		
2	SF4	F	301	1	0,12,12	-	-	-		
2	SF4	C	301	1	0,12,12	-	-	-		
2	SF4	G	301	1	0,12,12	-	-	-		
2	SF4	A	301	1	0,12,12	-	-	-		

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SF4	B	301	1	-	-	0/6/5/5
2	SF4	D	301	1	-	-	0/6/5/5
2	SF4	E	301	1	-	-	0/6/5/5
2	SF4	F	301	1	-	-	0/6/5/5
2	SF4	C	301	1	-	-	0/6/5/5
2	SF4	G	301	1	-	-	0/6/5/5
2	SF4	A	301	1	-	-	0/6/5/5

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.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	301	SF4	1	0
2	C	301	SF4	2	0
2	A	301	SF4	2	0

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, 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	254/271 (93%)	0.28	2 (0%) 86 75	75, 109, 128, 138	0
1	B	254/271 (93%)	0.16	5 (1%) 65 49	67, 104, 129, 144	0
1	C	256/271 (94%)	0.31	4 (1%) 72 57	90, 108, 128, 141	0
1	D	261/271 (96%)	0.15	0 100 100	79, 113, 130, 138	0
1	E	251/271 (92%)	0.53	15 (5%) 21 12	81, 127, 194, 206	0
1	F	253/271 (93%)	0.31	4 (1%) 72 57	108, 126, 147, 156	0
1	G	253/271 (93%)	0.53	21 (8%) 11 7	109, 139, 166, 174	0
All	All	1782/1897 (93%)	0.32	51 (2%) 51 35	67, 117, 154, 206	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	47	THR	4.5
1	E	48	LEU	4.5
1	G	24	VAL	3.9
1	E	152	PHE	3.7
1	E	15	LEU	3.5
1	E	6	LYS	3.3
1	E	11	LYS	3.2
1	F	205	ILE	3.1
1	E	19	PHE	3.1
1	F	230	ILE	3.1
1	E	230	ILE	3.0
1	G	25	ILE	3.0
1	E	44	ASN	3.0
1	F	222	LEU	2.9
1	E	49	ALA	2.9
1	B	23	LYS	2.9
1	E	8	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	230	ILE	2.8
1	G	78	THR	2.8
1	G	12	TYR	2.8
1	B	24	VAL	2.8
1	G	230	ILE	2.7
1	G	48	LEU	2.6
1	G	118	ILE	2.5
1	G	116	TYR	2.5
1	G	46	GLN	2.4
1	G	23	LYS	2.4
1	A	118	ILE	2.3
1	E	47	THR	2.3
1	G	152	PHE	2.3
1	A	135	ILE	2.3
1	G	125	TYR	2.3
1	E	167	ASP	2.3
1	E	13	ASN	2.3
1	C	222	LEU	2.3
1	B	125	TYR	2.2
1	G	49	ALA	2.2
1	G	19	PHE	2.2
1	G	74	ILE	2.2
1	G	138	PHE	2.2
1	B	48	LEU	2.1
1	G	52	ILE	2.1
1	C	229	LYS	2.1
1	F	48	LEU	2.1
1	G	51	THR	2.1
1	C	168	ILE	2.1
1	E	222	LEU	2.1
1	G	50	VAL	2.1
1	E	12	TYR	2.1
1	B	47	THR	2.0
1	G	165	LYS	2.0

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

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](#)

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
3	IOD	A	302	1/1	0.88	0.12	82,82,82,82	1
4	CL	C	302	1/1	0.89	0.36	82,82,82,82	0
4	CL	D	303	1/1	0.90	0.39	73,73,73,73	0
2	SF4	G	301	8/8	0.96	0.26	94,94,94,94	0
4	CL	E	302	1/1	0.96	0.23	76,76,76,76	1
4	CL	B	303	1/1	0.97	0.27	79,79,79,79	0
3	IOD	B	302	1/1	0.97	0.20	97,97,97,97	1
3	IOD	D	302	1/1	0.97	0.21	108,108,108,108	1
4	CL	A	303	1/1	0.97	0.23	100,100,100,100	0
3	IOD	G	302	1/1	0.98	0.23	72,72,72,72	1
2	SF4	F	301	8/8	0.98	0.24	87,88,88,88	0
2	SF4	B	301	8/8	0.99	0.24	76,76,76,76	0
2	SF4	C	301	8/8	0.99	0.24	83,84,84,84	0
2	SF4	D	301	8/8	0.99	0.26	82,83,83,83	0
2	SF4	E	301	8/8	0.99	0.21	86,86,86,86	0
2	SF4	A	301	8/8	0.99	0.21	80,80,80,80	0

6.5 Other polymers [i](#)

There are no such residues in this entry.