



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 05:28 AM UTC

PDB ID : 8CNZ / pdb_00008cnz
Title : mmLarE-[4Fe-4S] phased by Fe-SAD
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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	:	4-5-2 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

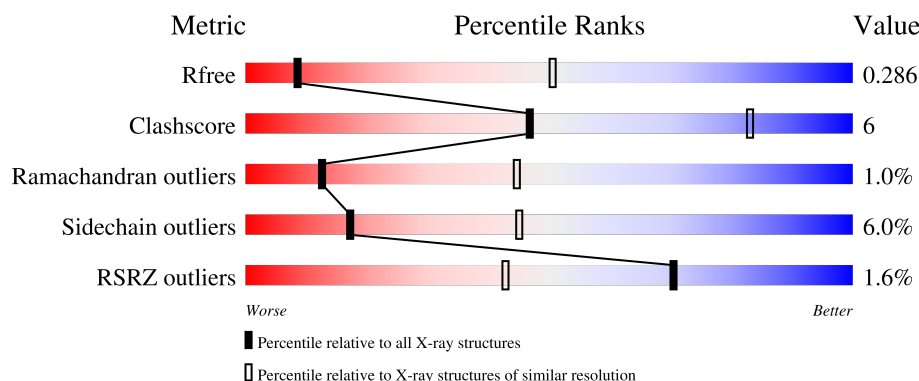
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	1747 (3.70-3.50)
Clashscore	190562	1827 (3.70-3.50)
Ramachandran outliers	187476	1773 (3.70-3.50)
Sidechain outliers	187428	1772 (3.70-3.50)
RSRZ outliers	180081	1745 (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	76% 16% • 6%
1	B	271	73% 17% • 6%
1	C	271	72% 20% • 6%
1	D	271	80% 14% • •
1	E	271	3% 73% 17% • 7%

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Mol	Chain	Length	Quality of chain
1	F	271	% 73% 18% • 7%
1	G	271	3% 76% 15% • 7%

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

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

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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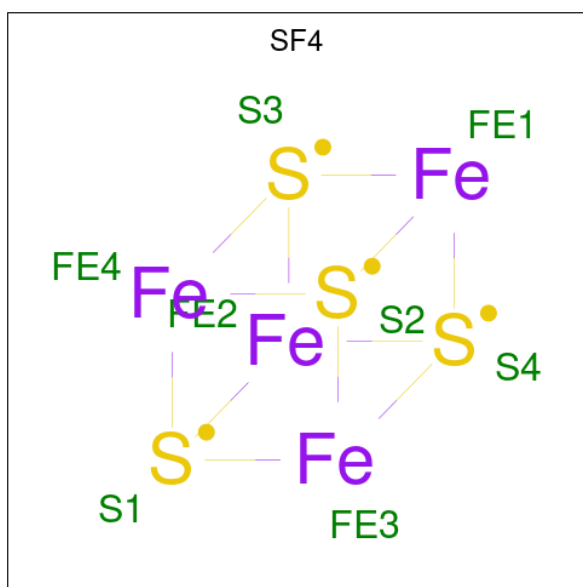
Chain	Residue	Modelled	Actual	Comment	Reference
B	-8	MET	-	expression tag	UNP Q6LXV7
B	-7	LEU	-	expression tag	UNP Q6LXV7
B	-6	GLU	-	expression tag	UNP Q6LXV7
B	-5	VAL	-	expression tag	UNP Q6LXV7
B	-4	LEU	-	expression tag	UNP Q6LXV7
B	-3	PHE	-	expression tag	UNP Q6LXV7
B	-2	GLN	-	expression tag	UNP Q6LXV7
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 (CCD ID: 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 (CCD ID: 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 (CCD ID: 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

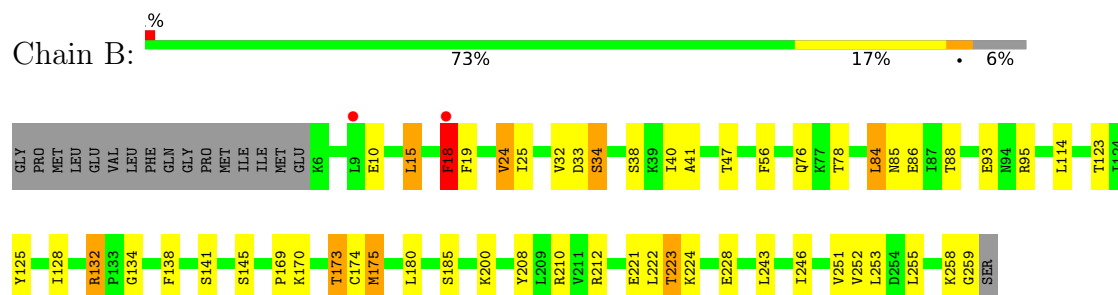
3 Residue-property plots

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.

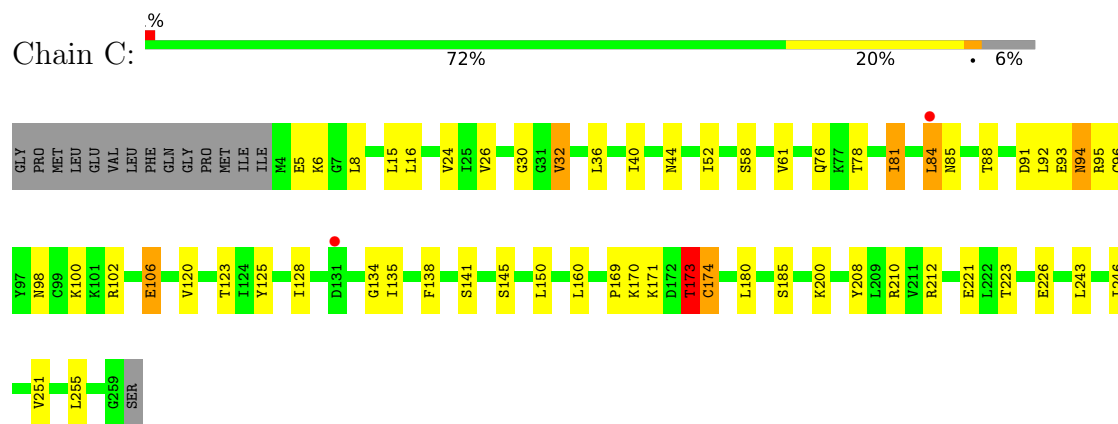
- Molecule 1: NAD_synthase domain-containing protein



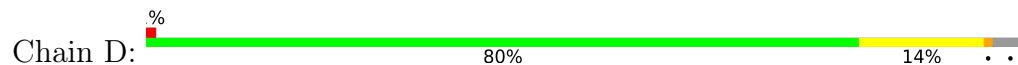
- Molecule 1: NAD_synthase domain-containing protein



- Molecule 1: NAD_synthase domain-containing protein



- Molecule 1: NAD_synthase domain-containing protein





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) 89.6 (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)	Xtriage
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	Xtriage
Anisotropy	0.066	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 110.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	14443	wwPDB-VP
Average B, all atoms (Å ²)	118.0	wwPDB-VP

Xtriage'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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: CL, SF4, 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	0.64	1/2083 (0.0%)	1.10	3/2798 (0.1%)
1	B	0.64	0/2078	1.08	6/2792 (0.2%)
1	C	0.64	0/2093	1.10	6/2812 (0.2%)
1	D	0.62	0/2132	1.09	4/2865 (0.1%)
1	E	0.60	0/2057	1.07	8/2762 (0.3%)
1	F	0.66	0/2068	1.14	8/2780 (0.3%)
1	G	0.60	0/2062	1.07	8/2773 (0.3%)
All	All	0.63	1/14573 (0.0%)	1.09	43/19582 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	175	MET	SD-CE	5.63	1.93	1.79

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	87	ILE	CA-C-N	8.38	132.19	120.29
1	D	87	ILE	C-N-CA	8.38	132.19	120.29
1	B	18	PHE	CA-CB-CG	7.48	121.28	113.80
1	F	24	VAL	N-CA-C	6.17	116.81	108.17
1	F	139	ASN	CA-C-N	6.16	133.31	121.54
1	F	139	ASN	C-N-CA	6.16	133.31	121.54
1	B	174	CYS	CA-C-N	5.80	128.86	120.38
1	B	174	CYS	C-N-CA	5.80	128.86	120.38
1	C	24	VAL	N-CA-C	5.72	116.18	108.17
1	G	176	ALA	CA-C-N	5.64	128.10	120.38
1	G	176	ALA	C-N-CA	5.64	128.10	120.38
1	G	226	GLU	CA-C-N	5.63	128.15	120.54
1	G	226	GLU	C-N-CA	5.63	128.15	120.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	24	VAL	N-CA-C	5.56	115.95	108.17
1	E	33	ASP	CA-CB-CG	5.55	118.15	112.60
1	G	30	GLY	CA-C-N	5.54	125.36	120.10
1	G	30	GLY	C-N-CA	5.54	125.36	120.10
1	E	24	VAL	N-CA-C	5.54	115.92	108.17
1	B	173	THR	CA-C-N	5.53	132.11	121.54
1	B	173	THR	C-N-CA	5.53	132.11	121.54
1	A	136	LYS	N-CA-C	-5.51	104.14	111.24
1	C	173	THR	N-CA-C	5.49	119.61	111.87
1	A	33	ASP	CA-CB-CG	5.47	118.07	112.60
1	F	33	ASP	CA-CB-CG	5.47	118.07	112.60
1	D	24	VAL	N-CA-C	5.41	115.74	108.17
1	F	226	GLU	CA-C-N	5.36	128.86	120.82
1	F	226	GLU	C-N-CA	5.36	128.86	120.82
1	G	24	VAL	N-CA-C	5.36	115.68	108.17
1	C	30	GLY	CA-C-N	5.34	125.05	119.92
1	C	30	GLY	C-N-CA	5.34	125.05	119.92
1	B	24	VAL	N-CA-C	5.30	115.60	108.17
1	D	33	ASP	CA-CB-CG	5.23	117.83	112.60
1	C	226	GLU	CA-C-N	5.22	128.64	120.82
1	C	226	GLU	C-N-CA	5.22	128.64	120.82
1	E	226	GLU	CA-C-N	5.21	128.64	120.82
1	E	226	GLU	C-N-CA	5.21	128.64	120.82
1	E	30	GLY	CA-C-N	5.20	125.04	120.10
1	E	30	GLY	C-N-CA	5.20	125.04	120.10
1	E	157	VAL	CA-C-N	5.17	127.46	120.38
1	E	157	VAL	C-N-CA	5.17	127.46	120.38
1	F	30	GLY	CA-C-N	5.04	124.89	120.10
1	F	30	GLY	C-N-CA	5.04	124.89	120.10
1	G	33	ASP	CA-CB-CG	5.01	117.61	112.60

There are no chirality outliers.

There are no planarity outliers.

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	2055	0	2101	22	0
1	B	2050	0	2088	27	0
1	C	2065	0	2105	30	0
1	D	2103	0	2149	20	0
1	E	2031	0	2062	29	0
1	F	2040	0	2077	24	0
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	166	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 (166) 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	1.57	1.00
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	0.81	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:84:LEU:O	1:C:88:THR:OG1	2.30	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: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:C:95:ARG:HG3	1:C:96:CYS:N	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:D:170:LYS:HZ1	1:D:200:LYS:NZ	2.16	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:123:THR:HB	1:C:145:SER:HB3	1.99	0.43
1:E:84:LEU:O	1:E:88:THR:OG1	2.29	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
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:F:175:MET:HE2	1:F:189:MET:O	2.21	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:D:-1:GLY:HA3	1:D:0:PRO:C	2.46	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%)	30	61
1	B	252/271 (93%)	241 (96%)	9 (4%)	2 (1%)	16	49
1	C	254/271 (94%)	238 (94%)	11 (4%)	5 (2%)	6	32
1	D	259/271 (96%)	245 (95%)	11 (4%)	3 (1%)	10	41
1	E	247/271 (91%)	234 (95%)	12 (5%)	1 (0%)	30	61
1	F	251/271 (93%)	235 (94%)	13 (5%)	3 (1%)	10	41
1	G	251/271 (93%)	236 (94%)	12 (5%)	3 (1%)	10	41
All	All	1766/1897 (93%)	1668 (94%)	80 (4%)	18 (1%)	12	45

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 ⓘ

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%)	221 (95%)	11 (5%)	23	50
1	B	231/248 (93%)	213 (92%)	18 (8%)	11	38
1	C	232/248 (94%)	219 (94%)	13 (6%)	19	47
1	D	237/248 (96%)	225 (95%)	12 (5%)	21	49
1	E	229/248 (92%)	214 (93%)	15 (7%)	15	43
1	F	230/248 (93%)	215 (94%)	15 (6%)	15	43
1	G	229/248 (92%)	215 (94%)	14 (6%)	17	45
All	All	1620/1736 (93%)	1522 (94%)	98 (6%)	17	45

All (98) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	81	ILE
1	A	92	LEU
1	A	93	GLU
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

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Mol	Chain	Res	Type
1	B	223	THR
1	B	228	GLU
1	B	252	VAL
1	C	8	LEU
1	C	32	VAL
1	C	81	ILE
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	25	ILE
1	D	33	ASP
1	D	81	ILE
1	D	132	ARG
1	D	138	PHE
1	D	141	SER
1	D	185	SER
1	D	215	GLU
1	D	223	THR
1	D	230	ILE
1	E	33	ASP
1	E	81	ILE
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	215	GLU
1	E	222	LEU
1	E	223	THR

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Mol	Chain	Res	Type
1	E	228	GLU
1	F	8	LEU
1	F	33	ASP
1	F	37	ILE
1	F	81	ILE
1	F	84	LEU
1	F	89	SER
1	F	91	ASP
1	F	95	ARG
1	F	108	LYS
1	F	120	VAL
1	F	135	ILE
1	F	141	SER
1	F	174	CYS
1	F	185	SER
1	F	215	GLU
1	G	33	ASP
1	G	34	SER
1	G	81	ILE
1	G	86	GLU
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	185	SER
1	G	207	SER
1	G	222	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	162	ASN
1	A	256	ASN
1	B	162	ASN
1	B	233	ASN
1	C	44	ASN
1	C	115	ASN
1	C	139	ASN
1	C	162	ASN

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Mol	Chain	Res	Type
1	C	233	ASN
1	D	233	ASN
1	D	256	ASN
1	E	44	ASN
1	E	233	ASN
1	E	256	ASN
1	F	162	ASN
1	G	139	ASN
1	G	162	ASN
1	G	233	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	G	301	1	0,12,12	-	-	-		
2	SF4	D	301	1	0,12,12	-	-	-		
2	SF4	C	301	1	0,12,12	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SF4	E	301	1	0,12,12	-	-	-		
2	SF4	F	301	1	0,12,12	-	-	-		
2	SF4	A	301	1	0,12,12	-	-	-		
2	SF4	B	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	G	301	1	-	-	0/6/5/5
2	SF4	D	301	1	-	-	0/6/5/5
2	SF4	C	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	A	301	1	-	-	0/6/5/5
2	SF4	B	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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	0.12	2 (0%) 82 58	75, 109, 128, 138	0
1	B	254/271 (93%)	0.08	2 (0%) 82 58	67, 104, 129, 144	0
1	C	256/271 (94%)	0.17	2 (0%) 82 58	90, 108, 128, 141	0
1	D	261/271 (96%)	0.19	3 (1%) 78 52	79, 113, 130, 138	0
1	E	251/271 (92%)	0.33	9 (3%) 46 26	81, 127, 194, 206	0
1	F	253/271 (93%)	0.44	4 (1%) 70 43	108, 126, 147, 156	0
1	G	253/271 (93%)	0.54	7 (2%) 55 31	109, 139, 166, 174	0
All	All	1782/1897 (93%)	0.27	29 (1%) 70 43	67, 117, 154, 206	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	135	ILE	3.7
1	G	92	LEU	3.6
1	G	230	ILE	3.2
1	F	133	PRO	3.1
1	E	13	ASN	3.0
1	G	125	TYR	3.0
1	E	48	LEU	3.0
1	A	134	GLY	2.9
1	E	12	TYR	2.7
1	C	131	ASP	2.7
1	G	259	GLY	2.7
1	F	135	ILE	2.5
1	D	-1	GLY	2.5
1	B	18	PHE	2.4
1	G	47	THR	2.3
1	G	100	LYS	2.3
1	E	150	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	G	121	ASP	2.2
1	E	9	LEU	2.2
1	F	177	THR	2.1
1	B	9	LEU	2.1
1	C	84	LEU	2.1
1	E	29	SER	2.1
1	D	32	VAL	2.1
1	D	6	LYS	2.0
1	E	113	GLU	2.0
1	E	6	LYS	2.0
1	E	259	GLY	2.0
1	F	134	GLY	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
4	CL	A	303	1/1	0.90	0.06	100,100,100,100	0
4	CL	C	302	1/1	0.91	0.07	82,82,82,82	0
4	CL	D	303	1/1	0.92	0.09	73,73,73,73	0
4	CL	E	302	1/1	0.94	0.05	76,76,76,76	1
2	SF4	G	301	8/8	0.96	0.07	94,94,94,94	0
3	IOD	G	302	1/1	0.96	0.10	72,72,72,72	1
3	IOD	A	302	1/1	0.97	0.07	82,82,82,82	1
2	SF4	F	301	8/8	0.97	0.06	87,88,88,88	0
2	SF4	D	301	8/8	0.98	0.05	82,83,83,83	0
3	IOD	D	302	1/1	0.98	0.06	108,108,108,108	1
4	CL	B	303	1/1	0.98	0.02	79,79,79,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SF4	C	301	8/8	0.99	0.05	83,84,84,84	0
2	SF4	A	301	8/8	0.99	0.04	80,80,80,80	0
3	IOD	B	302	1/1	0.99	0.03	97,97,97,97	1
2	SF4	E	301	8/8	0.99	0.04	86,86,86,86	0
2	SF4	B	301	8/8	0.99	0.04	76,76,76,76	0

6.5 Other polymers [i](#)

There are no such residues in this entry.