



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 10:02 AM UTC

PDB ID : 9FE6 / pdb_00009fe6
Title : Short-chain dehydrogenase/reductase (SDR) from *Thermus caliditerrae*
Authors : Kapur, B.; Nar, H.
Deposited on : 2024-05-17
Resolution : 1.88 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
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

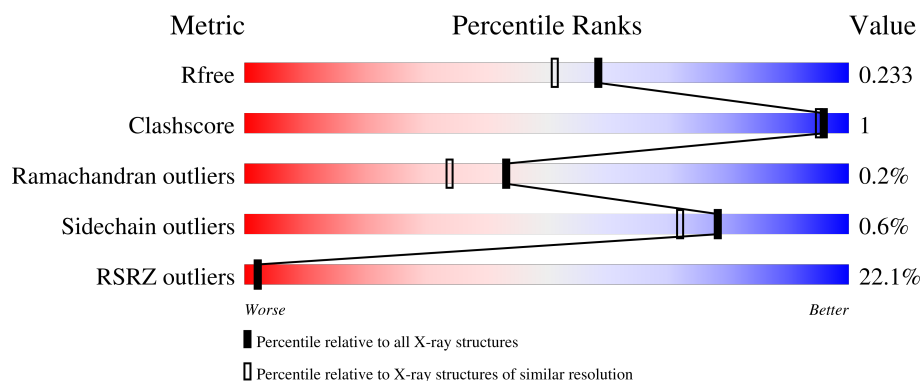
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.88 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	1220 (1.88-1.88)
Clashscore	190562	1234 (1.88-1.88)
Ramachandran outliers	187476	1222 (1.88-1.88)
Sidechain outliers	187428	1222 (1.88-1.88)
RSRZ outliers	180081	1220 (1.88-1.88)

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	282	24% 87% 5% 7%
1	B	282	13% 87% 5% 7%
1	C	282	20% 88% 5% 7%
1	D	282	24% 87% 5% 7%
1	E	282	% 99%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 16343 atoms, of which 8138 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 SDR family oxidoreductase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	261	Total	C	H	N	O	S	0	0	0
			3997	1248	2025	361	355	8			
1	B	261	Total	C	H	N	O	S	0	0	0
			3997	1248	2025	361	355	8			
1	C	261	Total	C	H	N	O	S	0	0	0
			3997	1248	2025	361	355	8			
1	D	261	Total	C	H	N	O	S	0	0	0
			3996	1248	2024	361	355	8			
1	E	4	Total	C	H	N	O		0	0	0
			72	22	39	7	4				

There are 105 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	MET	-	initiating methionine	UNP A0A7C5VFX3
A	-19	GLY	-	expression tag	UNP A0A7C5VFX3
A	-18	SER	-	expression tag	UNP A0A7C5VFX3
A	-17	SER	-	expression tag	UNP A0A7C5VFX3
A	-16	HIS	-	expression tag	UNP A0A7C5VFX3
A	-15	HIS	-	expression tag	UNP A0A7C5VFX3
A	-14	HIS	-	expression tag	UNP A0A7C5VFX3
A	-13	HIS	-	expression tag	UNP A0A7C5VFX3
A	-12	HIS	-	expression tag	UNP A0A7C5VFX3
A	-11	HIS	-	expression tag	UNP A0A7C5VFX3
A	-10	GLY	-	expression tag	UNP A0A7C5VFX3
A	-9	SER	-	expression tag	UNP A0A7C5VFX3
A	-8	GLY	-	expression tag	UNP A0A7C5VFX3
A	-7	LEU	-	expression tag	UNP A0A7C5VFX3
A	-6	VAL	-	expression tag	UNP A0A7C5VFX3
A	-5	PRO	-	expression tag	UNP A0A7C5VFX3
A	-4	ARG	-	expression tag	UNP A0A7C5VFX3
A	-3	GLY	-	expression tag	UNP A0A7C5VFX3
A	-2	SER	-	expression tag	UNP A0A7C5VFX3

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	ALA	-	expression tag	UNP A0A7C5VFX3
A	0	GLY	-	expression tag	UNP A0A7C5VFX3
B	-20	MET	-	initiating methionine	UNP A0A7C5VFX3
B	-19	GLY	-	expression tag	UNP A0A7C5VFX3
B	-18	SER	-	expression tag	UNP A0A7C5VFX3
B	-17	SER	-	expression tag	UNP A0A7C5VFX3
B	-16	HIS	-	expression tag	UNP A0A7C5VFX3
B	-15	HIS	-	expression tag	UNP A0A7C5VFX3
B	-14	HIS	-	expression tag	UNP A0A7C5VFX3
B	-13	HIS	-	expression tag	UNP A0A7C5VFX3
B	-12	HIS	-	expression tag	UNP A0A7C5VFX3
B	-11	HIS	-	expression tag	UNP A0A7C5VFX3
B	-10	GLY	-	expression tag	UNP A0A7C5VFX3
B	-9	SER	-	expression tag	UNP A0A7C5VFX3
B	-8	GLY	-	expression tag	UNP A0A7C5VFX3
B	-7	LEU	-	expression tag	UNP A0A7C5VFX3
B	-6	VAL	-	expression tag	UNP A0A7C5VFX3
B	-5	PRO	-	expression tag	UNP A0A7C5VFX3
B	-4	ARG	-	expression tag	UNP A0A7C5VFX3
B	-3	GLY	-	expression tag	UNP A0A7C5VFX3
B	-2	SER	-	expression tag	UNP A0A7C5VFX3
B	-1	ALA	-	expression tag	UNP A0A7C5VFX3
B	0	GLY	-	expression tag	UNP A0A7C5VFX3
C	-20	MET	-	initiating methionine	UNP A0A7C5VFX3
C	-19	GLY	-	expression tag	UNP A0A7C5VFX3
C	-18	SER	-	expression tag	UNP A0A7C5VFX3
C	-17	SER	-	expression tag	UNP A0A7C5VFX3
C	-16	HIS	-	expression tag	UNP A0A7C5VFX3
C	-15	HIS	-	expression tag	UNP A0A7C5VFX3
C	-14	HIS	-	expression tag	UNP A0A7C5VFX3
C	-13	HIS	-	expression tag	UNP A0A7C5VFX3
C	-12	HIS	-	expression tag	UNP A0A7C5VFX3
C	-11	HIS	-	expression tag	UNP A0A7C5VFX3
C	-10	GLY	-	expression tag	UNP A0A7C5VFX3
C	-9	SER	-	expression tag	UNP A0A7C5VFX3
C	-8	GLY	-	expression tag	UNP A0A7C5VFX3
C	-7	LEU	-	expression tag	UNP A0A7C5VFX3
C	-6	VAL	-	expression tag	UNP A0A7C5VFX3
C	-5	PRO	-	expression tag	UNP A0A7C5VFX3
C	-4	ARG	-	expression tag	UNP A0A7C5VFX3
C	-3	GLY	-	expression tag	UNP A0A7C5VFX3
C	-2	SER	-	expression tag	UNP A0A7C5VFX3

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	-1	ALA	-	expression tag	UNP A0A7C5VFX3
C	0	GLY	-	expression tag	UNP A0A7C5VFX3
D	-20	MET	-	initiating methionine	UNP A0A7C5VFX3
D	-19	GLY	-	expression tag	UNP A0A7C5VFX3
D	-18	SER	-	expression tag	UNP A0A7C5VFX3
D	-17	SER	-	expression tag	UNP A0A7C5VFX3
D	-16	HIS	-	expression tag	UNP A0A7C5VFX3
D	-15	HIS	-	expression tag	UNP A0A7C5VFX3
D	-14	HIS	-	expression tag	UNP A0A7C5VFX3
D	-13	HIS	-	expression tag	UNP A0A7C5VFX3
D	-12	HIS	-	expression tag	UNP A0A7C5VFX3
D	-11	HIS	-	expression tag	UNP A0A7C5VFX3
D	-10	GLY	-	expression tag	UNP A0A7C5VFX3
D	-9	SER	-	expression tag	UNP A0A7C5VFX3
D	-8	GLY	-	expression tag	UNP A0A7C5VFX3
D	-7	LEU	-	expression tag	UNP A0A7C5VFX3
D	-6	VAL	-	expression tag	UNP A0A7C5VFX3
D	-5	PRO	-	expression tag	UNP A0A7C5VFX3
D	-4	ARG	-	expression tag	UNP A0A7C5VFX3
D	-3	GLY	-	expression tag	UNP A0A7C5VFX3
D	-2	SER	-	expression tag	UNP A0A7C5VFX3
D	-1	ALA	-	expression tag	UNP A0A7C5VFX3
D	0	GLY	-	expression tag	UNP A0A7C5VFX3
E	-12	MET	-	initiating methionine	UNP A0A7C5VFX3
E	-11	GLY	-	expression tag	UNP A0A7C5VFX3
E	-10	SER	-	expression tag	UNP A0A7C5VFX3
E	-9	SER	-	expression tag	UNP A0A7C5VFX3
E	-8	HIS	-	expression tag	UNP A0A7C5VFX3
E	-7	HIS	-	expression tag	UNP A0A7C5VFX3
E	-6	HIS	-	expression tag	UNP A0A7C5VFX3
E	-5	HIS	-	expression tag	UNP A0A7C5VFX3
E	-4	HIS	-	expression tag	UNP A0A7C5VFX3
E	-3	HIS	-	expression tag	UNP A0A7C5VFX3
E	-2	GLY	-	expression tag	UNP A0A7C5VFX3
E	-1	SER	-	expression tag	UNP A0A7C5VFX3
E	0	GLY	-	expression tag	UNP A0A7C5VFX3
E	1	LEU	-	expression tag	UNP A0A7C5VFX3
E	2	VAL	-	expression tag	UNP A0A7C5VFX3
E	3	PRO	-	expression tag	UNP A0A7C5VFX3
E	4	ARG	-	expression tag	UNP A0A7C5VFX3
E	5	GLY	-	expression tag	UNP A0A7C5VFX3
E	6	SER	-	expression tag	UNP A0A7C5VFX3

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
E	7	ALA	-	expression tag	UNP A0A7C5VFX3
E	8	GLY	-	expression tag	UNP A0A7C5VFX3

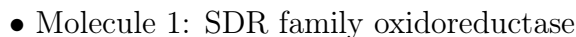
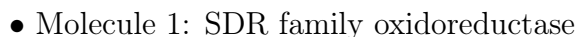
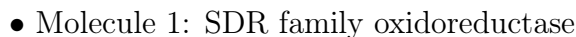
- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

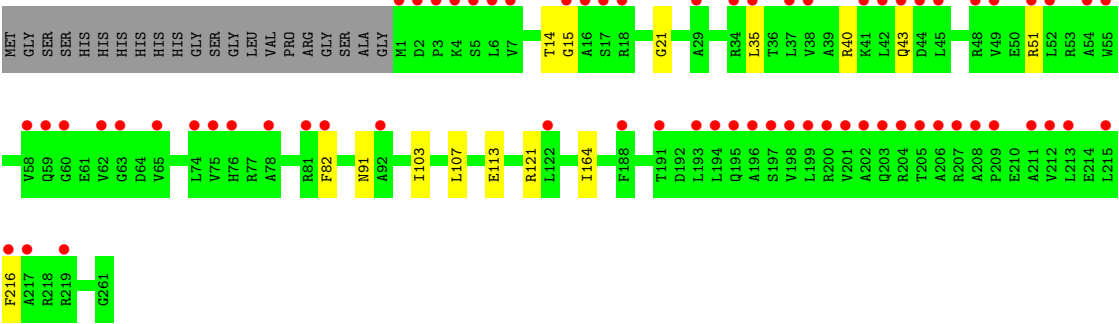
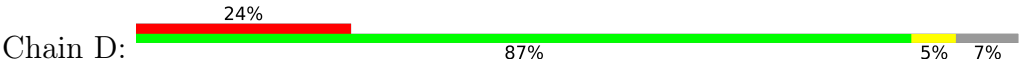
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Mg 1 1	0	0
2	B	1	Total Mg 1 1	0	0

- Molecule 3 is water.

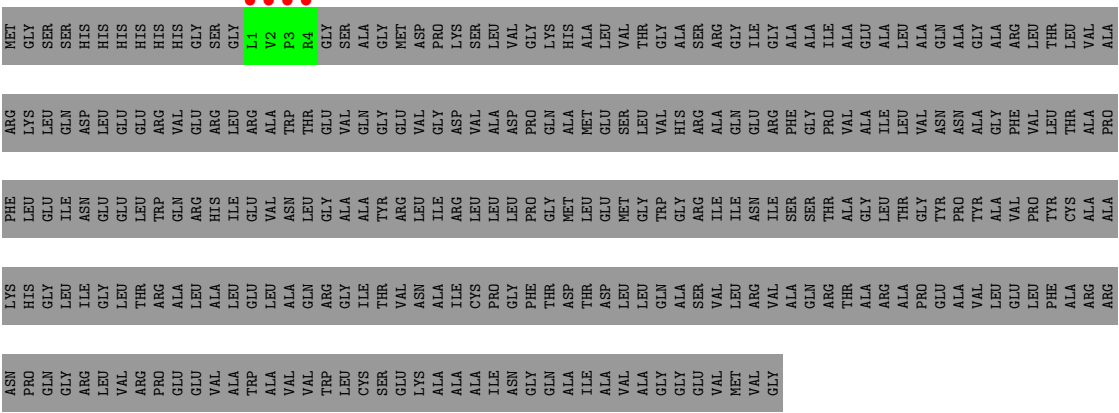
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	56	Total O 56 56	0	0
3	B	92	Total O 92 92	0	0
3	C	85	Total O 85 85	0	0
3	D	49	Total O 49 49	0	0

- Molecule 1: SDR family oxidoreductase





• Molecule 1: SDR family oxidoreductase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	56.67Å 122.99Å 163.35Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	98.25 – 1.88 98.25 – 1.88	Depositor EDS
% Data completeness (in resolution range)	52.6 (98.25-1.88) 52.6 (98.25-1.88)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.51 (at 1.87Å)	Xtriage
Refinement program	BUSTER 2.11.8	Depositor
R, R_{free}	0.217 , 0.245 0.208 , 0.233	Depositor DCC
R_{free} test set	2522 reflections (2.67%)	wwPDB-VP
Wilson B-factor (Å ²)	33.2	Xtriage
Anisotropy	0.059	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 42.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	16343	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.05% 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: MG

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	0.77	1/2005 (0.0%)	0.96	2/2724 (0.1%)
1	B	0.79	1/2005 (0.0%)	0.98	2/2724 (0.1%)
1	C	0.79	1/2005 (0.0%)	0.98	3/2724 (0.1%)
1	D	0.78	1/2005 (0.0%)	0.97	3/2724 (0.1%)
1	E	1.18	0/33	0.99	0/44
All	All	0.78	4/8053 (0.0%)	0.97	10/10940 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	164	ILE	CG1-CD1	-7.72	1.21	1.51
1	C	164	ILE	CG1-CD1	-6.83	1.25	1.51
1	A	164	ILE	CG1-CD1	-6.50	1.26	1.51
1	D	164	ILE	CG1-CD1	-5.86	1.28	1.51

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	35	LEU	N-CA-C	5.85	119.01	109.59
1	C	35	LEU	N-CA-C	5.83	118.98	109.59
1	B	82	PHE	CA-CB-CG	5.72	119.52	113.80
1	B	35	LEU	N-CA-C	5.70	118.77	109.59
1	D	35	LEU	N-CA-C	5.57	118.56	109.59
1	C	216	PHE	CA-CB-CG	5.29	119.09	113.80
1	D	82	PHE	CA-CB-CG	5.27	119.07	113.80
1	A	82	PHE	CA-CB-CG	5.26	119.06	113.80
1	C	82	PHE	CA-CB-CG	5.20	119.00	113.80
1	D	216	PHE	CA-CB-CG	5.16	118.96	113.80

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	1972	2025	2027	5	1
1	B	1972	2025	2027	5	1
1	C	1972	2025	2027	5	0
1	D	1972	2024	2027	4	0
1	E	33	39	42	0	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	56	0	0	0	0
3	B	92	0	0	0	0
3	C	85	0	0	0	0
3	D	49	0	0	0	0
All	All	8205	8138	8150	18	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 1.

All (18) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:113:GLU:OE2	1:D:121:ARG:NH2	2.34	0.60
1:A:75:VAL:O	1:A:79:GLN:HG2	2.05	0.57
1:C:113:GLU:OE2	1:C:121:ARG:NH2	2.42	0.52
1:C:15:GLY:O	1:C:21:GLY:HA3	2.13	0.48
1:C:14:THR:O	1:C:91:ASN:HB3	2.15	0.47
1:B:100:PHE:HA	1:B:103:ILE:HD12	1.97	0.46
1:B:14:THR:O	1:B:91:ASN:HB3	2.15	0.46
1:A:14:THR:O	1:A:91:ASN:HB3	2.16	0.46
1:D:14:THR:O	1:D:91:ASN:HB3	2.17	0.45
1:D:103:ILE:HD13	1:D:107:LEU:HD23	1.98	0.45
1:A:15:GLY:O	1:A:21:GLY:HA3	2.17	0.45
1:D:15:GLY:O	1:D:21:GLY:HA3	2.18	0.44
1:A:100:PHE:HA	1:A:103:ILE:HD12	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:100:PHE:HA	1:C:103:ILE:HD12	1.99	0.43
1:B:201:VAL:CG1	1:B:212:VAL:HG11	2.48	0.43
1:A:205:THR:HG22	1:A:205:THR:O	2.20	0.41
1:B:233:TRP:NE1	1:C:237:TRP:CD1	2.89	0.41
1:B:15:GLY:O	1:B:21:GLY:HA3	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:203:GLN:O	1:B:97:THR:HG1[1_655]	1.47	0.13

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	259/282 (92%)	251 (97%)	7 (3%)	1 (0%)	30	18
1	B	259/282 (92%)	250 (96%)	9 (4%)	0	100	100
1	C	259/282 (92%)	249 (96%)	10 (4%)	0	100	100
1	D	259/282 (92%)	250 (96%)	8 (3%)	1 (0%)	30	18
1	E	2/282 (1%)	2 (100%)	0	0	100	100
All	All	1038/1410 (74%)	1002 (96%)	34 (3%)	2 (0%)	43	34

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	43	GLN
1	D	43	GLN

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	196/211 (93%)	195 (100%)	1 (0%)	81	76
1	B	196/211 (93%)	194 (99%)	2 (1%)	68	60
1	C	196/211 (93%)	196 (100%)	0	100	100
1	D	196/211 (93%)	194 (99%)	2 (1%)	68	60
1	E	4/211 (2%)	4 (100%)	0	100	100
All	All	788/1055 (75%)	783 (99%)	5 (1%)	78	72

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	204	ARG
1	B	59	GLN
1	B	215	LEU
1	D	40	ARG
1	D	51	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	140	ASN
1	C	91	ASN
1	D	222	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 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

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	261/282 (92%)	1.28	69 (26%) 1 1	26, 56, 100, 110	0
1	B	261/282 (92%)	0.71	36 (13%) 6 7	22, 43, 77, 96	0
1	C	261/282 (92%)	0.85	56 (21%) 2 2	20, 42, 81, 102	0
1	D	261/282 (92%)	1.25	67 (25%) 1 1	23, 51, 108, 124	0
1	E	4/282 (1%)	6.18	4 (100%) 0 0	84, 85, 86, 89	0
All	All	1048/1410 (74%)	1.04	232 (22%) 2 2	20, 48, 97, 124	0

All (232) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	1	LEU	10.4
1	A	206	ALA	7.7
1	D	206	ALA	7.5
1	E	2	VAL	6.8
1	A	202	ALA	6.7
1	D	211	ALA	6.7
1	C	3	PRO	6.5
1	C	42	LEU	6.5
1	B	1	MET	5.7
1	D	42	LEU	5.7
1	D	201	VAL	5.6
1	D	202	ALA	5.6
1	D	196	ALA	5.5
1	D	212	VAL	5.3
1	D	208	ALA	5.3
1	B	65	VAL	5.0
1	D	209	PRO	5.0
1	D	215	LEU	5.0
1	D	1	MET	4.9
1	A	1	MET	4.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	1	MET	4.9
1	A	201	VAL	4.9
1	D	199	LEU	4.7
1	A	212	VAL	4.7
1	A	199	LEU	4.7
1	A	198	VAL	4.6
1	A	3	PRO	4.5
1	D	198	VAL	4.5
1	C	193	LEU	4.5
1	D	205	THR	4.5
1	C	194	LEU	4.4
1	B	3	PRO	4.4
1	B	60	GLY	4.4
1	A	197	SER	4.4
1	D	3	PRO	4.3
1	D	216	PHE	4.2
1	E	3	PRO	4.2
1	A	42	LEU	4.2
1	C	197	SER	4.1
1	C	201	VAL	4.1
1	C	200	ARG	4.1
1	A	209	PRO	4.1
1	A	208	ALA	4.0
1	A	35	LEU	4.0
1	A	55	TRP	4.0
1	D	217	ALA	3.9
1	D	195	GLN	3.9
1	C	198	VAL	3.9
1	D	200	ARG	3.9
1	C	43	GLN	3.8
1	B	74	LEU	3.8
1	B	71	MET	3.8
1	C	203	GLN	3.8
1	C	204	ARG	3.7
1	A	122	LEU	3.7
1	B	75	VAL	3.6
1	A	66	ALA	3.6
1	B	66	ALA	3.6
1	C	206	ALA	3.6
1	A	207	ARG	3.6
1	D	55	TRP	3.5
1	A	205	THR	3.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	204	ARG	3.5
1	D	4	LYS	3.5
1	C	45	LEU	3.5
1	C	196	ALA	3.5
1	D	43	GLN	3.5
1	A	196	ALA	3.5
1	B	122	LEU	3.5
1	C	199	LEU	3.5
1	D	213	LEU	3.5
1	A	213	LEU	3.4
1	C	202	ALA	3.4
1	C	6	LEU	3.4
1	A	68	PRO	3.4
1	A	204	ARG	3.4
1	D	41	LYS	3.4
1	A	203	GLN	3.4
1	A	193	LEU	3.4
1	B	2	ASP	3.3
1	D	38	VAL	3.3
1	D	75	VAL	3.3
1	A	74	LEU	3.3
1	D	193	LEU	3.3
1	A	194	LEU	3.3
1	A	58	VAL	3.2
1	E	4	ARG	3.2
1	A	65	VAL	3.2
1	C	216	PHE	3.2
1	B	70	ALA	3.1
1	C	213	LEU	3.1
1	C	16	ALA	3.1
1	D	197	SER	3.1
1	A	251	ILE	3.0
1	A	233	TRP	3.0
1	D	6	LEU	3.0
1	A	38	VAL	3.0
1	A	5	SER	3.0
1	C	2	ASP	3.0
1	D	58	VAL	3.0
1	A	56	THR	3.0
1	A	45	LEU	2.9
1	A	75	VAL	2.9
1	A	2	ASP	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	4	LYS	2.9
1	C	55	TRP	2.9
1	B	54	ALA	2.9
1	D	194	LEU	2.9
1	C	65	VAL	2.9
1	C	191	THR	2.9
1	B	78	ALA	2.9
1	C	66	ALA	2.9
1	B	4	LYS	2.9
1	A	71	MET	2.9
1	B	215	LEU	2.9
1	D	45	LEU	2.9
1	A	62	VAL	2.8
1	C	49	VAL	2.8
1	A	54	ALA	2.8
1	A	211	ALA	2.8
1	C	205	THR	2.8
1	D	81	ARG	2.8
1	D	188	PHE	2.8
1	A	52	LEU	2.8
1	D	207	ARG	2.8
1	B	100	PHE	2.8
1	C	188	PHE	2.8
1	A	200	ARG	2.8
1	D	51	ARG	2.8
1	A	60	GLY	2.8
1	B	6	LEU	2.8
1	A	123	ILE	2.8
1	C	192	ASP	2.8
1	D	54	ALA	2.7
1	D	49	VAL	2.7
1	B	43	GLN	2.7
1	D	65	VAL	2.7
1	C	60	GLY	2.7
1	C	207	ARG	2.7
1	A	6	LEU	2.7
1	D	37	LEU	2.7
1	C	50	GLU	2.7
1	A	49	VAL	2.7
1	C	7	VAL	2.7
1	B	63	GLY	2.6
1	B	261	GLY	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	29	ALA	2.6
1	D	219	ARG	2.6
1	C	4	LYS	2.6
1	A	37	LEU	2.6
1	A	59	GLN	2.6
1	C	5	SER	2.6
1	C	215	LEU	2.6
1	D	52	LEU	2.6
1	D	2	ASP	2.6
1	C	54	ALA	2.5
1	B	68	PRO	2.5
1	A	67	ASP	2.5
1	C	208	ALA	2.5
1	A	79	GLN	2.5
1	D	62	VAL	2.5
1	D	60	GLY	2.5
1	A	69	GLN	2.5
1	B	69	GLN	2.5
1	A	85	VAL	2.5
1	D	122	LEU	2.4
1	B	5	SER	2.4
1	D	44	ASP	2.4
1	C	58	VAL	2.4
1	D	63	GLY	2.4
1	D	203	GLN	2.4
1	A	238	LEU	2.4
1	B	73	SER	2.4
1	C	52	LEU	2.4
1	B	41	LYS	2.4
1	A	39	ALA	2.4
1	D	18	ARG	2.4
1	B	7	VAL	2.4
1	B	55	TRP	2.4
1	C	62	VAL	2.4
1	C	63	GLY	2.4
1	D	15	GLY	2.4
1	D	35	LEU	2.4
1	C	76	HIS	2.4
1	B	67	ASP	2.3
1	A	216	PHE	2.3
1	C	56	THR	2.3
1	D	92	ALA	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	76	HIS	2.3
1	D	16	ALA	2.3
1	D	59	GLN	2.3
1	C	211	ALA	2.3
1	B	38	VAL	2.3
1	C	48	ARG	2.2
1	A	61	GLU	2.2
1	A	100	PHE	2.2
1	B	94	PHE	2.2
1	D	17	SER	2.2
1	C	59	GLN	2.2
1	A	7	VAL	2.2
1	A	40	ARG	2.2
1	D	74	LEU	2.2
1	C	17	SER	2.2
1	A	210	GLU	2.2
1	D	5	SER	2.2
1	C	209	PRO	2.2
1	B	218	ARG	2.2
1	D	78	ALA	2.2
1	C	51	ARG	2.2
1	A	82	PHE	2.1
1	D	82	PHE	2.1
1	C	237	TRP	2.1
1	A	64	ASP	2.1
1	B	201	VAL	2.1
1	A	53	ARG	2.1
1	A	108	TRP	2.1
1	A	237	TRP	2.1
1	A	18	ARG	2.1
1	D	48	ARG	2.1
1	A	41	LYS	2.1
1	B	76	HIS	2.1
1	C	8	GLY	2.1
1	B	37	LEU	2.1
1	B	42	LEU	2.1
1	C	190	ASP	2.1
1	D	34	ARG	2.1
1	C	47	GLU	2.0
1	A	261	GLY	2.0
1	D	7	VAL	2.0
1	B	81	ARG	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	70	ALA	2.0
1	D	191	THR	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($\text{\AA}^2$)	Q<0.9
2	MG	A	301	1/1	0.86	0.22	54,54,54,54	0
2	MG	B	301	1/1	0.95	0.17	50,50,50,50	0

6.5 Other polymers [i](#)

There are no such residues in this entry.