



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:48 PM UTC

PDB ID : 9YUP / pdb_00009yup
Title : Crystal structure of PprA S-F-S tetramer from *Deinococcus radiodurans*
Authors : Szabla, R.; Junop, M.S.
Deposited on : 2025-10-22
Resolution : 2.07 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

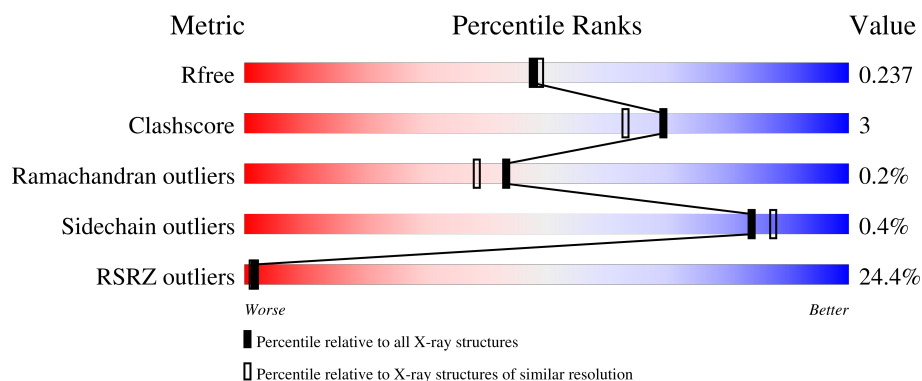
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.07 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	3774 (2.08-2.04)
Clashscore	190562	3883 (2.08-2.04)
Ramachandran outliers	187476	3860 (2.08-2.04)
Sidechain outliers	187428	3860 (2.08-2.04)
RSRZ outliers	180081	3775 (2.08-2.04)

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	307	5% 91% 5%
1	B	307	16% 85% 10%
1	C	307	9% 83% 6% 11%
1	D	307	55% 76% 11% 12%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 16960 atoms, of which 8305 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 DNA repair protein PprA.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	296	Total	C	H	N	O	Se	2220	0	0
			4472	1403	2216	414	435	4			
1	B	275	Total	C	H	N	O	Se	2125	0	0
			4120	1292	2040	384	400	4			
1	C	273	Total	C	H	N	O	Se	2036	0	0
			4104	1286	2034	383	397	4			
1	D	269	Total	C	H	N	O	Se	2154	0	0
			4039	1268	2000	376	391	4			

There are 132 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-31	MSE	-	initiating methionine	UNP O32504
A	-30	ARG	-	expression tag	UNP O32504
A	-29	SER	-	expression tag	UNP O32504
A	-28	GLY	-	expression tag	UNP O32504
A	-27	SER	-	expression tag	UNP O32504
A	-26	HIS	-	expression tag	UNP O32504
A	-25	HIS	-	expression tag	UNP O32504
A	-24	HIS	-	expression tag	UNP O32504
A	-23	HIS	-	expression tag	UNP O32504
A	-22	HIS	-	expression tag	UNP O32504
A	-21	HIS	-	expression tag	UNP O32504
A	-20	ARG	-	expression tag	UNP O32504
A	-19	SER	-	expression tag	UNP O32504
A	-18	ASP	-	expression tag	UNP O32504
A	-17	ILE	-	expression tag	UNP O32504
A	-16	THR	-	expression tag	UNP O32504
A	-15	SER	-	expression tag	UNP O32504
A	-14	LEU	-	expression tag	UNP O32504
A	-13	TYR	-	expression tag	UNP O32504
A	-12	LYS	-	expression tag	UNP O32504
A	-11	LYS	-	expression tag	UNP O32504

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-10	ALA	-	expression tag	UNP O32504
A	-9	GLY	-	expression tag	UNP O32504
A	-8	LEU	-	expression tag	UNP O32504
A	-7	GLU	-	expression tag	UNP O32504
A	-6	ASN	-	expression tag	UNP O32504
A	-5	LEU	-	expression tag	UNP O32504
A	-4	TYR	-	expression tag	UNP O32504
A	-3	PHE	-	expression tag	UNP O32504
A	-2	GLN	-	expression tag	UNP O32504
A	-1	GLY	-	expression tag	UNP O32504
A	180	LYS	ASP	engineered mutation	UNP O32504
A	184	LYS	ASP	engineered mutation	UNP O32504
B	-31	MSE	-	initiating methionine	UNP O32504
B	-30	ARG	-	expression tag	UNP O32504
B	-29	SER	-	expression tag	UNP O32504
B	-28	GLY	-	expression tag	UNP O32504
B	-27	SER	-	expression tag	UNP O32504
B	-26	HIS	-	expression tag	UNP O32504
B	-25	HIS	-	expression tag	UNP O32504
B	-24	HIS	-	expression tag	UNP O32504
B	-23	HIS	-	expression tag	UNP O32504
B	-22	HIS	-	expression tag	UNP O32504
B	-21	HIS	-	expression tag	UNP O32504
B	-20	ARG	-	expression tag	UNP O32504
B	-19	SER	-	expression tag	UNP O32504
B	-18	ASP	-	expression tag	UNP O32504
B	-17	ILE	-	expression tag	UNP O32504
B	-16	THR	-	expression tag	UNP O32504
B	-15	SER	-	expression tag	UNP O32504
B	-14	LEU	-	expression tag	UNP O32504
B	-13	TYR	-	expression tag	UNP O32504
B	-12	LYS	-	expression tag	UNP O32504
B	-11	LYS	-	expression tag	UNP O32504
B	-10	ALA	-	expression tag	UNP O32504
B	-9	GLY	-	expression tag	UNP O32504
B	-8	LEU	-	expression tag	UNP O32504
B	-7	GLU	-	expression tag	UNP O32504
B	-6	ASN	-	expression tag	UNP O32504
B	-5	LEU	-	expression tag	UNP O32504
B	-4	TYR	-	expression tag	UNP O32504
B	-3	PHE	-	expression tag	UNP O32504
B	-2	GLN	-	expression tag	UNP O32504

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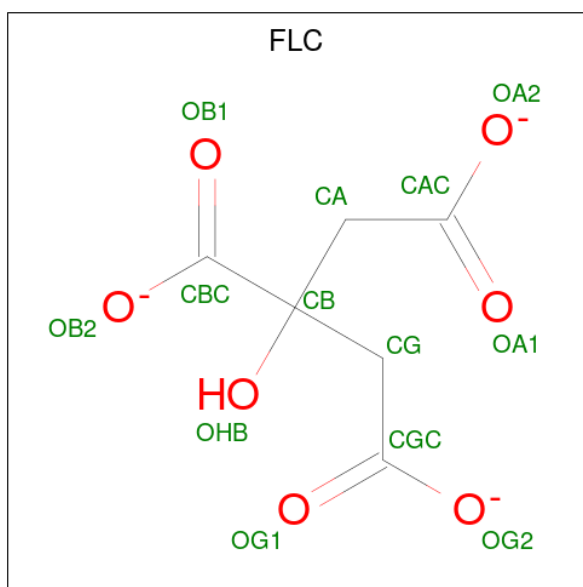
Chain	Residue	Modelled	Actual	Comment	Reference
B	-1	GLY	-	expression tag	UNP O32504
B	180	LYS	ASP	engineered mutation	UNP O32504
B	184	LYS	ASP	engineered mutation	UNP O32504
C	-22	MSE	-	initiating methionine	UNP O32504
C	-21	ARG	-	expression tag	UNP O32504
C	-20	SER	-	expression tag	UNP O32504
C	-19	GLY	-	expression tag	UNP O32504
C	-18	SER	-	expression tag	UNP O32504
C	-17	HIS	-	expression tag	UNP O32504
C	-16	HIS	-	expression tag	UNP O32504
C	-15	HIS	-	expression tag	UNP O32504
C	-14	HIS	-	expression tag	UNP O32504
C	-13	HIS	-	expression tag	UNP O32504
C	-12	HIS	-	expression tag	UNP O32504
C	-11	ARG	-	expression tag	UNP O32504
C	-10	SER	-	expression tag	UNP O32504
C	-9	ASP	-	expression tag	UNP O32504
C	-8	ILE	-	expression tag	UNP O32504
C	-7	THR	-	expression tag	UNP O32504
C	-6	SER	-	expression tag	UNP O32504
C	-5	LEU	-	expression tag	UNP O32504
C	-4	TYR	-	expression tag	UNP O32504
C	-3	LYS	-	expression tag	UNP O32504
C	-2	LYS	-	expression tag	UNP O32504
C	-1	ALA	-	expression tag	UNP O32504
C	0	GLY	-	expression tag	UNP O32504
C	1	LEU	-	expression tag	UNP O32504
C	2	GLU	-	expression tag	UNP O32504
C	3	ASN	-	expression tag	UNP O32504
C	4	LEU	-	expression tag	UNP O32504
C	5	TYR	-	expression tag	UNP O32504
C	6	PHE	-	expression tag	UNP O32504
C	7	GLN	-	expression tag	UNP O32504
C	8	GLY	-	expression tag	UNP O32504
C	180	LYS	ASP	engineered mutation	UNP O32504
C	184	LYS	ASP	engineered mutation	UNP O32504
D	-22	MSE	-	initiating methionine	UNP O32504
D	-21	ARG	-	expression tag	UNP O32504
D	-20	SER	-	expression tag	UNP O32504
D	-19	GLY	-	expression tag	UNP O32504
D	-18	SER	-	expression tag	UNP O32504
D	-17	HIS	-	expression tag	UNP O32504

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-16	HIS	-	expression tag	UNP O32504
D	-15	HIS	-	expression tag	UNP O32504
D	-14	HIS	-	expression tag	UNP O32504
D	-13	HIS	-	expression tag	UNP O32504
D	-12	HIS	-	expression tag	UNP O32504
D	-11	ARG	-	expression tag	UNP O32504
D	-10	SER	-	expression tag	UNP O32504
D	-9	ASP	-	expression tag	UNP O32504
D	-8	ILE	-	expression tag	UNP O32504
D	-7	THR	-	expression tag	UNP O32504
D	-6	SER	-	expression tag	UNP O32504
D	-5	LEU	-	expression tag	UNP O32504
D	-4	TYR	-	expression tag	UNP O32504
D	-3	LYS	-	expression tag	UNP O32504
D	-2	LYS	-	expression tag	UNP O32504
D	-1	ALA	-	expression tag	UNP O32504
D	0	GLY	-	expression tag	UNP O32504
D	1	LEU	-	expression tag	UNP O32504
D	2	GLU	-	expression tag	UNP O32504
D	3	ASN	-	expression tag	UNP O32504
D	4	LEU	-	expression tag	UNP O32504
D	5	TYR	-	expression tag	UNP O32504
D	6	PHE	-	expression tag	UNP O32504
D	7	GLN	-	expression tag	UNP O32504
D	8	GLY	-	expression tag	UNP O32504
D	180	LYS	ASP	engineered mutation	UNP O32504
D	184	LYS	ASP	engineered mutation	UNP O32504

- Molecule 2 is CITRATE ANION (CCD ID: FLC) (formula: $C_6H_5O_7$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	H	O	5	0
			18	6	5	7		
2	C	1	Total	C	H	O	5	0
			18	6	5	7		
2	C	1	Total	C	H	O	5	0
			18	6	5	7		

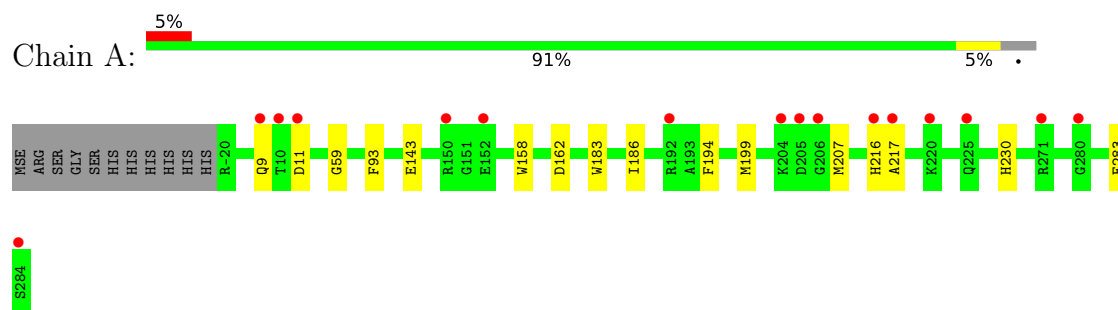
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	103	Total	O	0	0
			103	103		
3	B	38	Total	O	0	0
			38	38		
3	C	25	Total	O	0	0
			25	25		
3	D	5	Total	O	0	0
			5	5		

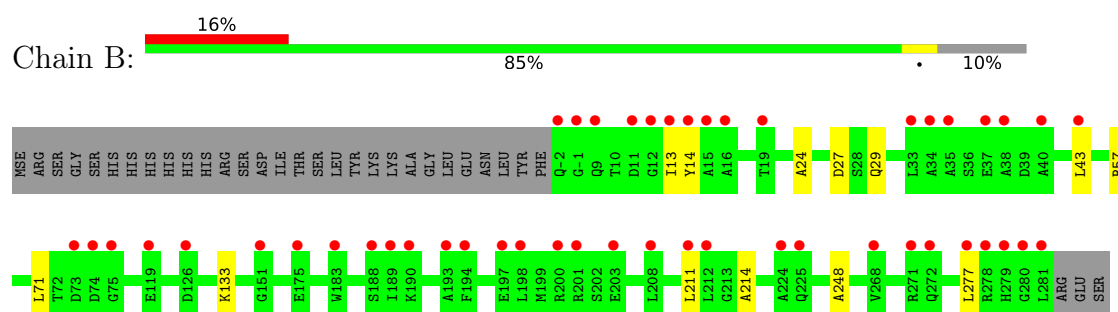
3 Residue-property plots [i](#)

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.

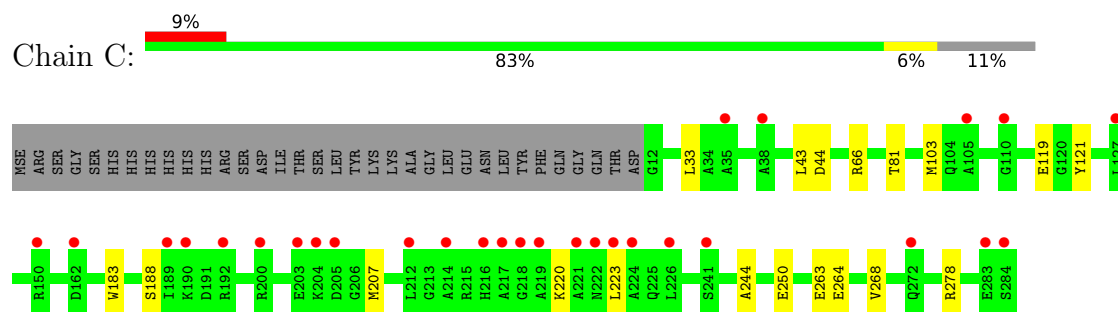
• Molecule 1: DNA repair protein PprA



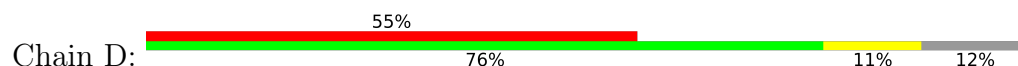
• Molecule 1: DNA repair protein PprA



• Molecule 1: DNA repair protein PprA



• Molecule 1: DNA repair protein PprA





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	49.68Å 123.22Å 139.29Å 90.00° 93.69° 90.00°	Depositor
Resolution (Å)	41.65 – 2.07 41.65 – 2.07	Depositor EDS
% Data completeness (in resolution range)	51.5 (41.65-2.07) 51.8 (41.65-2.07)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.92 (at 2.06Å)	Xtriage
Refinement program	PHENIX 2.0_5824	Depositor
R, R_{free}	0.211 , 0.236 0.212 , 0.237	Depositor DCC
R_{free} test set	2489 reflections (2.44%)	wwPDB-VP
Wilson B-factor (Å ²)	36.5	Xtriage
Anisotropy	0.076	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 53.9	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	0.93	EDS
Total number of atoms	16960	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.54% 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: FLC

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	0.29	0/2290	0.51	0/3087
1	B	0.29	0/2111	0.50	0/2849
1	C	0.22	0/2101	0.41	0/2833
1	D	0.37	0/2070	0.57	0/2794
All	All	0.30	0/8572	0.50	0/11563

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	D	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	196	ARG	Sidechain
1	D	70	ARG	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	2256	2216	2218	11	0
1	B	2080	2040	2043	10	0
1	C	2070	2034	2034	13	0
1	D	2039	2000	2000	24	0
2	A	13	5	5	1	0
2	C	26	10	10	0	0
3	A	103	0	0	1	0
3	B	38	0	0	0	0
3	C	25	0	0	2	0
3	D	5	0	0	0	0
All	All	8655	8305	8310	56	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 3.

All (56) 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:27:ASP:OD1	1:D:29:GLN:HG2	1.80	0.81
1:A:186:ILE:HD12	1:A:207:MSE:HE3	1.74	0.69
1:D:13:ILE:HG12	1:D:76:ASP:HA	1.77	0.66
1:A:183:TRP:HA	1:A:207:MSE:HE2	1.78	0.65
1:D:21:MSE:SE	1:D:54:ALA:HB2	2.47	0.65
1:A:162:ASP:O	1:A:162:ASP:OD1	2.16	0.62
1:C:81:THR:OG1	1:C:103:MSE:HE1	2.02	0.60
1:A:143:GLU:HG3	1:A:158:TRP:HB3	1.86	0.58
1:B:27:ASP:OD1	1:B:29:GLN:NE2	2.35	0.58
1:B:27:ASP:OD1	1:B:29:GLN:HG2	2.03	0.58
1:D:268:VAL:HG22	1:D:271:ARG:HH21	1.68	0.57
1:D:82:ASP:O	1:D:82:ASP:OD1	2.23	0.57
1:D:124:PRO:HG2	1:D:127:LEU:CD1	2.35	0.56
1:C:264:GLU:O	1:C:268:VAL:HG23	2.06	0.55
1:B:211:LEU:HD22	1:B:277:LEU:HD13	1.89	0.54
1:C:33:LEU:HD23	1:C:43:LEU:HD23	1.87	0.54
1:D:183:TRP:CD1	1:D:183:TRP:C	2.88	0.52
1:B:27:ASP:CG	1:B:29:GLN:HE21	2.17	0.52
1:D:93:PHE:CE2	1:D:227:PRO:HD3	2.44	0.52
1:D:252:ARG:HG3	1:D:252:ARG:HH11	1.75	0.51
1:D:152:GLU:HA	1:D:152:GLU:OE1	2.11	0.50
1:D:150:ARG:O	1:D:153:THR:HG23	2.12	0.50
1:A:59:GLY:HA2	3:A:459:HOH:O	2.11	0.49
1:A:194:PHE:HB2	1:A:283:GLU:HG3	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:244:ALA:HB1	1:C:250:GLU:HG2	1.95	0.48
1:D:165:PHE:CD1	1:D:239:THR:HG22	2.49	0.47
1:B:43:LEU:HD13	1:B:71:LEU:HD11	1.97	0.47
1:D:186:ILE:HD12	1:D:207:MSE:SE	2.65	0.47
1:C:44:ASP:HB3	3:C:408:HOH:O	2.14	0.47
1:D:27:ASP:OD1	1:D:27:ASP:C	2.57	0.46
1:A:186:ILE:HD12	1:A:207:MSE:CE	2.44	0.46
1:D:152:GLU:OE1	1:D:152:GLU:CA	2.63	0.45
1:C:119:GLU:HA	1:C:119:GLU:OE1	2.17	0.45
1:B:27:ASP:OD1	1:B:27:ASP:C	2.60	0.44
1:C:263:GLU:HA	1:C:263:GLU:OE1	2.17	0.44
1:D:183:TRP:O	1:D:183:TRP:HD1	2.01	0.44
1:C:220:LYS:HA	1:C:223:LEU:HD21	2.00	0.44
1:B:13:ILE:HG23	1:B:14:TYR:CD1	2.53	0.44
1:B:133:LYS:HG3	1:B:248:ALA:HB2	2.00	0.43
1:B:211:LEU:CD2	1:B:277:LEU:HD13	2.48	0.43
1:C:66:ARG:HH11	1:C:66:ARG:HB2	1.82	0.43
1:A:207:MSE:HG2	3:C:407:HOH:O	2.19	0.43
1:A:93:PHE:HB2	1:A:230:HIS:ND1	2.33	0.43
1:D:279:HIS:O	1:D:279:HIS:ND1	2.52	0.42
1:C:188:SER:OG	1:C:278:ARG:NH1	2.52	0.42
1:D:114:TRP:HA	1:D:114:TRP:CE3	2.54	0.42
1:D:21:MSE:HG3	1:D:28:SER:HB3	2.01	0.42
1:D:189:ILE:HG22	1:D:191:ASP:H	1.83	0.41
1:D:132:LEU:HD21	1:D:136:ILE:HD11	2.02	0.41
1:B:24:ALA:O	1:B:57:ARG:HD2	2.21	0.41
1:D:183:TRP:C	1:D:183:TRP:HD1	2.29	0.41
1:A:199:MSE:HE2	1:C:183:TRP:HH2	1.85	0.41
2:A:301:FLC:HG1	1:C:207:MSE:HE2	2.03	0.41
1:A:216:HIS:O	1:A:217:ALA:HB3	2.20	0.41
1:C:121:TYR:CE2	1:D:138:HIS:HA	2.56	0.40
1:D:185:VAL:O	1:D:188:SER:OG	2.37	0.40

There are no symmetry-related clashes.

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	294/307 (96%)	288 (98%)	5 (2%)	1 (0%)	36	30
1	B	273/307 (89%)	266 (97%)	6 (2%)	1 (0%)	30	23
1	C	271/307 (88%)	264 (97%)	7 (3%)	0	100	100
1	D	267/307 (87%)	260 (97%)	7 (3%)	0	100	100
All	All	1105/1228 (90%)	1078 (98%)	25 (2%)	2 (0%)	43	38

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	214	ALA
1	A	11	ASP

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	217/222 (98%)	216 (100%)	1 (0%)	81	85
1	B	198/222 (89%)	198 (100%)	0	100	100
1	C	197/222 (89%)	197 (100%)	0	100	100
1	D	194/222 (87%)	192 (99%)	2 (1%)	68	71
All	All	806/888 (91%)	803 (100%)	3 (0%)	84	87

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	GLN
1	D	43	LEU
1	D	76	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	9	GLN

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](#)

3 ligands are modelled in this entry.

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	FLC	C	301	-	12,12,12	1.45	1 (8%)	17,17,17	1.67	6 (35%)
2	FLC	A	301	-	12,12,12	1.45	1 (8%)	17,17,17	1.81	5 (29%)
2	FLC	C	302	-	12,12,12	1.34	1 (8%)	17,17,17	1.51	3 (17%)

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	FLC	C	301	-	-	5/16/16/16	-
2	FLC	A	301	-	-	3/16/16/16	-
2	FLC	C	302	-	-	0/16/16/16	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	302	FLC	CB-CBC	2.77	1.56	1.53
2	A	301	FLC	CB-CBC	2.65	1.56	1.53
2	C	301	FLC	CB-CBC	2.40	1.56	1.53

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	301	FLC	OB1-CBC-CB	-3.53	115.25	122.09
2	C	302	FLC	OB1-CBC-CB	-3.24	115.83	122.09
2	A	301	FLC	CA-CB-CBC	-3.15	103.06	110.03
2	A	301	FLC	OB1-CBC-CB	-3.14	116.01	122.09
2	A	301	FLC	CB-CG-CGC	2.92	121.90	113.92
2	C	301	FLC	CB-CA-CAC	2.89	121.83	113.92
2	A	301	FLC	OHB-CB-CBC	2.82	112.95	108.96
2	C	302	FLC	OB2-CBC-CB	2.69	118.31	113.14
2	A	301	FLC	OB2-CBC-CB	2.66	118.24	113.14
2	C	301	FLC	CG-CB-CA	2.61	116.01	109.31
2	C	301	FLC	OB2-CBC-CB	2.59	118.11	113.14
2	C	302	FLC	OHB-CB-CBC	2.32	112.25	108.96
2	C	301	FLC	OHB-CB-CA	-2.08	104.62	109.38
2	C	301	FLC	CB-CG-CGC	2.01	119.40	113.92

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301	FLC	CAC-CA-CB-OHB
2	C	301	FLC	CA-CB-CBC-OB1
2	C	301	FLC	CA-CB-CBC-OB2
2	C	301	FLC	OHB-CB-CBC-OB1
2	C	301	FLC	OHB-CB-CBC-OB2
2	A	301	FLC	CAC-CA-CB-CBC
2	A	301	FLC	CAC-CA-CB-CG
2	C	301	FLC	CAC-CA-CB-OHB

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	FLC	1	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	292/307 (95%)	0.12	16 (5%)	30 30	7, 16, 39, 55	1 (0%)
1	B	259/307 (84%)	0.90	48 (18%)	3 3	9, 25, 56, 76	1 (0%)
1	C	269/307 (87%)	0.83	29 (10%)	11 11	13, 25, 44, 63	1 (0%)
1	D	252/307 (82%)	2.65	169 (67%)	0 0	18, 51, 75, 110	18 (7%)
All	All	1072/1228 (87%)	1.08	262 (24%)	2 1	7, 26, 64, 110	21 (1%)

All (262) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	233	VAL	6.2
1	B	212	LEU	6.2
1	D	194	PHE	5.4
1	D	211	LEU	5.4
1	D	226	LEU	5.3
1	D	189	ILE	5.2
1	B	-1	GLY	5.1
1	D	183	TRP	5.1
1	B	281	LEU	4.9
1	B	190	LYS	4.9
1	D	76	ASP	4.9
1	D	231	PHE	4.8
1	D	59	GLY	4.8
1	C	217	ALA	4.7
1	D	60	LEU	4.6
1	D	31	ALA	4.6
1	D	35	ALA	4.5
1	D	95	ALA	4.5
1	C	284	SER	4.5
1	D	80	LEU	4.4
1	D	56	GLY	4.4

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Mol	Chain	Res	Type	RSRZ
1	D	106	LEU	4.4
1	D	19	THR	4.3
1	D	61	GLY	4.3
1	D	33	LEU	4.3
1	D	12	GLY	4.3
1	D	47	LEU	4.3
1	D	185	VAL	4.3
1	D	114	TRP	4.2
1	D	277	LEU	4.2
1	D	77	ILE	4.2
1	D	79	ILE	4.2
1	C	218	GLY	4.2
1	D	13	ILE	4.2
1	D	181	ALA	4.2
1	B	9	GLN	4.2
1	D	258	ALA	4.2
1	D	229	ALA	4.1
1	D	172	ALA	4.1
1	D	87	ALA	4.0
1	D	100	TYR	4.0
1	D	272	GLN	4.0
1	B	211	LEU	4.0
1	D	78	GLU	4.0
1	D	208	LEU	4.0
1	D	90	SER	4.0
1	D	273	LEU	4.0
1	D	30	ILE	3.9
1	D	70	ARG	3.9
1	D	186	ILE	3.9
1	D	269	THR	3.9
1	A	217	ALA	3.9
1	D	105	ALA	3.9
1	B	12	GLY	3.8
1	D	93	PHE	3.8
1	D	43	LEU	3.7
1	A	10	THR	3.7
1	D	14	TYR	3.7
1	D	68	GLU	3.7
1	D	115	ALA	3.7
1	B	11	ASP	3.7
1	D	58	TRP	3.6
1	D	230	HIS	3.6

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Mol	Chain	Res	Type	RSRZ
1	D	232	THR	3.6
1	D	15	ALA	3.6
1	D	51	LEU	3.6
1	D	274	SER	3.6
1	D	72	THR	3.6
1	D	224	ALA	3.6
1	C	204	LYS	3.6
1	B	40	ALA	3.5
1	A	280	GLY	3.5
1	D	74	ASP	3.5
1	B	279	HIS	3.5
1	B	183	TRP	3.5
1	D	177	ALA	3.5
1	D	94	GLY	3.5
1	D	178	LEU	3.5
1	D	34	ALA	3.4
1	D	40	ALA	3.4
1	D	235	ALA	3.4
1	D	11	ASP	3.4
1	D	91	GLU	3.4
1	B	280	GLY	3.4
1	D	62	LEU	3.4
1	B	225	GLN	3.4
1	D	99	ALA	3.4
1	C	190	LYS	3.4
1	A	11	ASP	3.4
1	D	180	LYS	3.3
1	A	206	GLY	3.3
1	D	86	SER	3.3
1	B	224	ALA	3.3
1	D	24	ALA	3.3
1	D	210	ALA	3.3
1	D	201	ARG	3.3
1	D	102	PRO	3.3
1	D	84	ARG	3.3
1	D	23	THR	3.3
1	D	42	THR	3.3
1	D	89	VAL	3.3
1	D	71	LEU	3.3
1	A	284	SER	3.2
1	D	67	HIS	3.2
1	D	276	VAL	3.2

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Mol	Chain	Res	Type	RSRZ
1	D	20	LEU	3.2
1	D	110	GLY	3.2
1	D	227	PRO	3.2
1	B	35	ALA	3.2
1	B	272	GLN	3.2
1	D	32	ALA	3.1
1	D	17	PHE	3.1
1	D	97	ALA	3.1
1	D	279	HIS	3.1
1	D	154	PHE	3.1
1	D	165	PHE	3.1
1	D	82	ASP	3.1
1	D	182	ALA	3.1
1	D	268	VAL	3.1
1	B	38	ALA	3.1
1	D	261	ALA	3.1
1	D	265	TYR	3.0
1	A	271	ARG	3.0
1	D	73	ASP	3.0
1	D	16	ALA	3.0
1	D	96	LEU	3.0
1	D	36	SER	3.0
1	D	104	GLN	3.0
1	A	225	GLN	3.0
1	D	38	ALA	3.0
1	B	208	LEU	3.0
1	D	200	ARG	3.0
1	D	190	LYS	3.0
1	D	85	PRO	3.0
1	D	66	ARG	2.9
1	D	188	SER	2.9
1	D	65	LEU	2.9
1	D	151	GLY	2.9
1	C	162	ASP	2.9
1	A	205	ASP	2.9
1	D	171	PRO	2.9
1	A	216	HIS	2.9
1	D	83	GLY	2.9
1	D	158	TRP	2.9
1	C	205	ASP	2.8
1	D	278	ARG	2.8
1	C	219	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	45	ALA	2.8
1	D	259	ALA	2.8
1	C	150	ARG	2.8
1	B	201	ARG	2.7
1	B	188	SER	2.7
1	B	151	GLY	2.7
1	D	118	GLY	2.7
1	B	34	ALA	2.7
1	C	226	LEU	2.7
1	B	203	GLU	2.7
1	B	13	ILE	2.7
1	B	16	ALA	2.7
1	D	191	ASP	2.6
1	D	202	SER	2.6
1	D	196	ARG	2.6
1	B	75	GLY	2.6
1	D	275	GLU	2.6
1	B	193	ALA	2.6
1	D	174	ALA	2.6
1	B	19	THR	2.6
1	B	189	ILE	2.6
1	B	175	GLU	2.6
1	D	126	ASP	2.6
1	D	146	TRP	2.6
1	D	75	GLY	2.5
1	A	204	LYS	2.5
1	D	271	ARG	2.5
1	D	270	THR	2.5
1	D	108	GLU	2.5
1	D	260	ALA	2.5
1	D	236	PHE	2.5
1	D	37	GLU	2.5
1	C	212	LEU	2.5
1	C	223	LEU	2.5
1	B	278	ARG	2.5
1	D	88	ARG	2.5
1	B	-2	GLN	2.4
1	D	234	GLN	2.4
1	C	105	ALA	2.4
1	A	192	ARG	2.4
1	D	57	ARG	2.4
1	C	224	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	126	ASP	2.4
1	D	26	VAL	2.4
1	D	101	ALA	2.3
1	D	264	GLU	2.3
1	B	198	LEU	2.3
1	B	277	LEU	2.3
1	D	98	GLN	2.3
1	D	198	LEU	2.3
1	D	92	GLY	2.3
1	B	73	ASP	2.3
1	B	37	GLU	2.3
1	B	271	ARG	2.3
1	C	200	ARG	2.3
1	D	184	LYS	2.3
1	D	166	VAL	2.3
1	A	9	GLN	2.3
1	D	46	ALA	2.3
1	C	127	LEU	2.3
1	D	192	ARG	2.3
1	D	256	LYS	2.3
1	D	48	THR	2.3
1	D	81	THR	2.3
1	A	150	ARG	2.3
1	C	192	ARG	2.3
1	D	170	ARG	2.3
1	C	35	ALA	2.3
1	D	39	ASP	2.3
1	D	206	GLY	2.3
1	B	33	LEU	2.3
1	C	203	GLU	2.2
1	D	119	GLU	2.2
1	C	221	ALA	2.2
1	D	193	ALA	2.2
1	D	243	ALA	2.2
1	C	216	HIS	2.2
1	D	241	SER	2.2
1	B	268	VAL	2.2
1	D	168	VAL	2.2
1	D	169	ALA	2.2
1	D	197	GLU	2.2
1	D	28	SER	2.2
1	C	222	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	142	PHE	2.2
1	D	205	ASP	2.2
1	C	189	ILE	2.1
1	C	272	GLN	2.1
1	D	255	LEU	2.1
1	B	74	ASP	2.1
1	D	225	GLN	2.1
1	B	200	ARG	2.1
1	D	176	ALA	2.1
1	D	117	LEU	2.1
1	D	132	LEU	2.1
1	D	173	SER	2.1
1	C	110	GLY	2.1
1	D	209	GLY	2.1
1	B	15	ALA	2.1
1	C	38	ALA	2.1
1	B	43	LEU	2.1
1	B	119	GLU	2.1
1	A	152	GLU	2.0
1	C	214	ALA	2.1
1	C	241	SER	2.1
1	D	112	SER	2.1
1	D	187	ALA	2.1
1	B	194	PHE	2.0
1	B	197	GLU	2.0
1	C	283	GLU	2.0
1	D	111	LEU	2.0
1	A	220	LYS	2.0
1	D	257	THR	2.0
1	D	25	GLY	2.0
1	B	14	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($\text{\AA}^2$)	Q<0.9
2	FLC	A	301	13/13	0.84	0.18	15,81,114,125	5
2	FLC	C	301	13/13	0.84	0.22	15,86,116,124	5
2	FLC	C	302	13/13	0.88	0.19	15,90,115,122	5

6.5 Other polymers [i](#)

There are no such residues in this entry.