Full wwPDB X-ray Structure Validation Report (i)

Mar 9, 2026 – 11:25 AM UTC

PDB ID	:	5GHS / pdb_00005ghs
Title	:	DNA replication protein
Authors	:	Oyama, T.
Deposited on	:	2016-06-20
Resolution	:	2.59 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 (i) 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 (i)) were used in the production of this report:

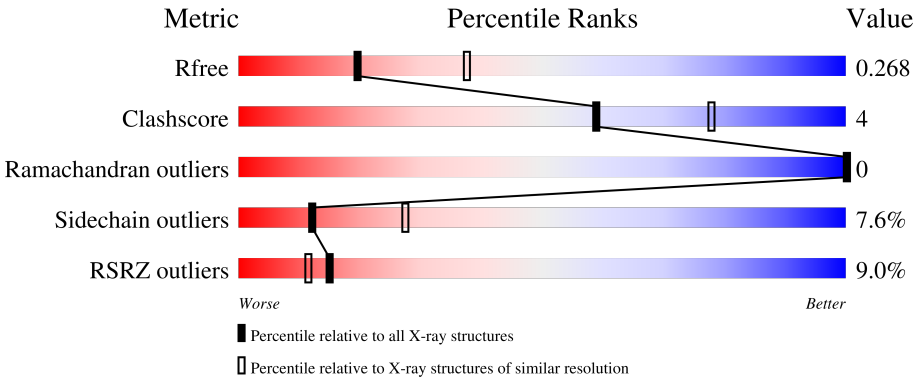
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.59 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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 <=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	477	12% 79% 13% · 6%
1	B	477	3% 62% 9% · 28%
2	C	80	2% 58% 12% 30%
2	D	80	9% 75% 14% 11%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 7252 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 SsDNA-specific exonuclease.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	450	Total	C	N	O	S	0	0	0
			3498	2207	612	667	12			
1	B	345	Total	C	N	O	S	0	0	0
			2708	1708	477	513	10			

- Molecule 2 is a protein called Putative uncharacterized protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	56	Total	C	N	O	S	0	0	0
			437	284	74	76	3			
2	D	71	Total	C	N	O	S	0	0	0
			540	344	95	97	4			

There are 44 discrepancies between the modelled and reference sequences:

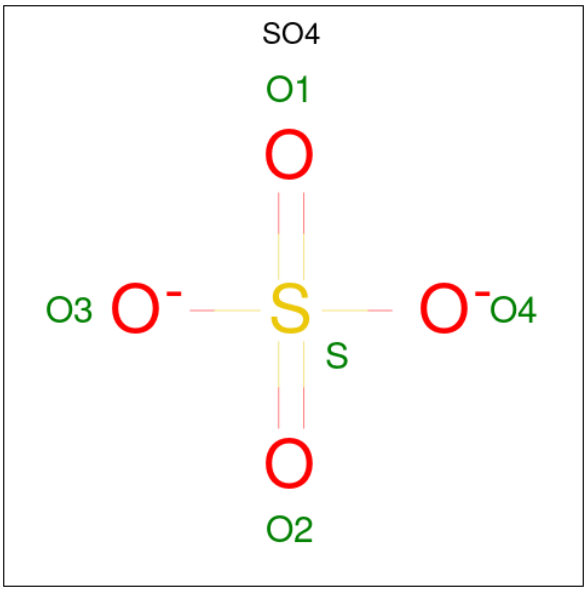
Chain	Residue	Modelled	Actual	Comment	Reference
C	109	MET	-	expression tag	UNP Q5JF31
C	110	GLY	-	expression tag	UNP Q5JF31
C	111	SER	-	expression tag	UNP Q5JF31
C	112	SER	-	expression tag	UNP Q5JF31
C	113	HIS	-	expression tag	UNP Q5JF31
C	114	HIS	-	expression tag	UNP Q5JF31
C	115	HIS	-	expression tag	UNP Q5JF31
C	116	HIS	-	expression tag	UNP Q5JF31
C	117	HIS	-	expression tag	UNP Q5JF31
C	118	HIS	-	expression tag	UNP Q5JF31
C	119	SER	-	expression tag	UNP Q5JF31
C	120	SER	-	expression tag	UNP Q5JF31
C	121	GLY	-	expression tag	UNP Q5JF31
C	122	GLU	-	expression tag	UNP Q5JF31
C	123	ASN	-	expression tag	UNP Q5JF31
C	124	LEU	-	expression tag	UNP Q5JF31

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Chain	Residue	Modelled	Actual	Comment	Reference
C	125	TYR	-	expression tag	UNP Q5JF31
C	126	PHE	-	expression tag	UNP Q5JF31
C	127	GLN	-	expression tag	UNP Q5JF31
C	128	GLY	-	expression tag	UNP Q5JF31
C	129	HIS	-	expression tag	UNP Q5JF31
C	130	MET	-	expression tag	UNP Q5JF31
D	109	MET	-	expression tag	UNP Q5JF31
D	110	GLY	-	expression tag	UNP Q5JF31
D	111	SER	-	expression tag	UNP Q5JF31
D	112	SER	-	expression tag	UNP Q5JF31
D	113	HIS	-	expression tag	UNP Q5JF31
D	114	HIS	-	expression tag	UNP Q5JF31
D	115	HIS	-	expression tag	UNP Q5JF31
D	116	HIS	-	expression tag	UNP Q5JF31
D	117	HIS	-	expression tag	UNP Q5JF31
D	118	HIS	-	expression tag	UNP Q5JF31
D	119	SER	-	expression tag	UNP Q5JF31
D	120	SER	-	expression tag	UNP Q5JF31
D	121	GLY	-	expression tag	UNP Q5JF31
D	122	GLU	-	expression tag	UNP Q5JF31
D	123	ASN	-	expression tag	UNP Q5JF31
D	124	LEU	-	expression tag	UNP Q5JF31
D	125	TYR	-	expression tag	UNP Q5JF31
D	126	PHE	-	expression tag	UNP Q5JF31
D	127	GLN	-	expression tag	UNP Q5JF31
D	128	GLY	-	expression tag	UNP Q5JF31
D	129	HIS	-	expression tag	UNP Q5JF31
D	130	MET	-	expression tag	UNP Q5JF31

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0

- Molecule 4 is water.

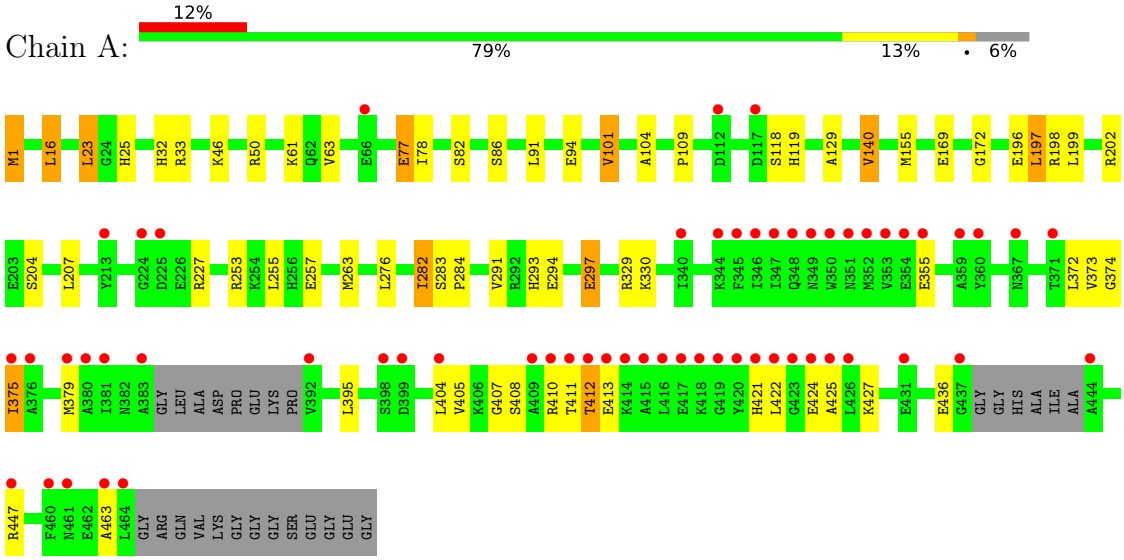
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	24	Total O 24 24	0	0
4	B	14	Total O 14 14	0	0
4	C	2	Total O 2 2	0	0
4	D	4	Total O 4 4	0	0

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.

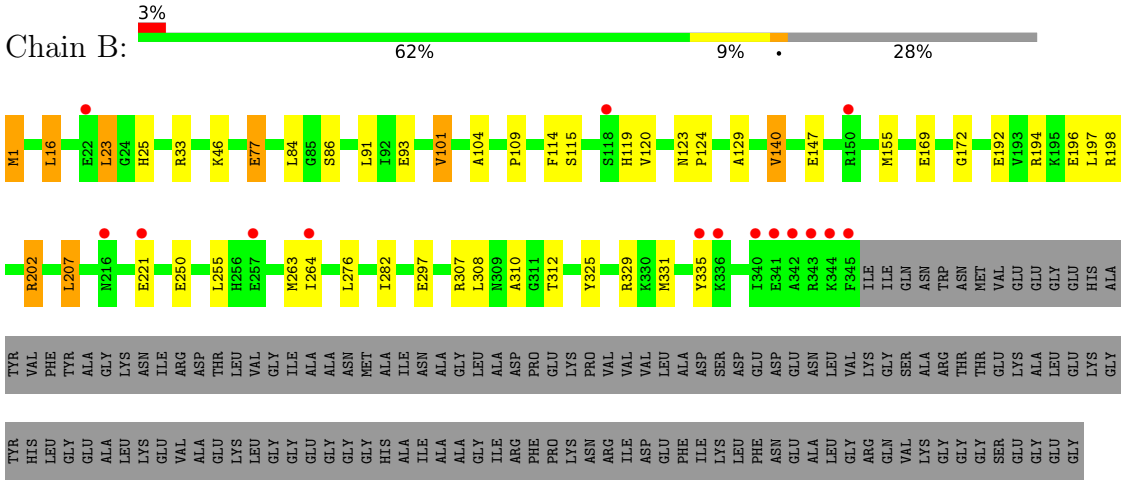
• Molecule 1: SsDNA-specific exonuclease

Chain A:



• Molecule 1: SsDNA-specific exonuclease

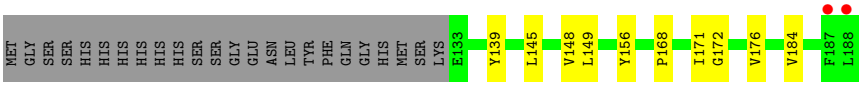
Chain B:



• Molecule 2: Putative uncharacterized protein

Chain C:

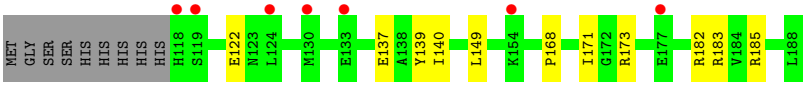




• Molecule 2: Putative uncharacterized protein

Chain D:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	48.04Å 116.28Å 235.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.48 – 2.59 44.48 – 2.59	Depositor EDS
% Data completeness (in resolution range)	99.6 (44.48-2.59) 99.6 (44.48-2.59)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.19 (at 2.58Å)	Xtriage
Refinement program	PHENIX 1.7.3_928	Depositor
R, R_{free}	0.237 , 0.273 0.233 , 0.268	Depositor DCC
R_{free} test set	2126 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	32.9	Xtriage
Anisotropy	0.745	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 35.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	7252	wwPDB-VP
Average B, all atoms (Å^2)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.58% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: SO4

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	0.28	0/3554	0.70	1/4793 (0.0%)
1	B	0.28	0/2754	0.71	0/3712
2	C	0.29	0/445	0.71	0/602
2	D	0.28	0/551	0.74	0/745
All	All	0.28	0/7304	0.71	1/9852 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	78	ILE	N-CA-C	5.17	115.36	108.27

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	3498	0	3452	34	0
1	B	2708	0	2697	20	0
2	C	437	0	458	4	0
2	D	540	0	533	5	0
3	A	15	0	0	0	0
3	B	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	5	0	0	0	0
4	A	24	0	0	1	0
4	B	14	0	0	0	0
4	C	2	0	0	0	0
4	D	4	0	0	0	0
All	All	7252	0	7140	63	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 4.

All (63) 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:A:425:ALA:HB1	1:A:463:ALA:HB1	1.67	0.75
1:B:263:MET:HE2	1:B:276:LEU:HD22	1.74	0.70
1:A:1:MET:HE3	1:A:129:ALA:HB2	1.80	0.61
1:A:196:GLU:OE1	1:A:202:ARG:NH1	2.33	0.61
1:A:202:ARG:HD3	1:A:294:GLU:HG3	1.85	0.58
1:B:25:HIS:CE1	1:B:77:GLU:HG2	2.40	0.56
1:A:263:MET:HE2	1:A:276:LEU:HD22	1.88	0.55
1:B:93:GLU:HG3	1:B:114:PHE:HD1	1.72	0.54
1:A:412:THR:OG1	1:A:413:GLU:N	2.39	0.54
1:A:373:VAL:HG12	1:A:408:SER:HB2	1.89	0.53
1:B:310:ALA:HB3	1:B:331:MET:HE1	1.90	0.53
2:C:168:PRO:HG2	2:C:171:ILE:HD12	1.92	0.52
1:A:25:HIS:CE1	1:A:77:GLU:HG2	2.46	0.51
1:A:282:ILE:HG13	1:A:293:HIS:CE1	2.46	0.50
1:B:101:VAL:HG13	1:B:119:HIS:CD2	2.47	0.50
1:A:101:VAL:HG13	1:A:119:HIS:CD2	2.47	0.49
1:B:23:LEU:HD23	1:B:25:HIS:CE1	2.47	0.49
1:A:33:ARG:HH21	1:A:61:LYS:HB2	1.77	0.49
1:A:204:SER:OG	1:A:297:GLU:OE2	2.19	0.49
1:A:197:LEU:HD22	1:A:199:LEU:HG	1.95	0.49
1:B:308:LEU:HD21	1:B:335:TYR:CD1	2.48	0.49
2:D:137:GLU:OE1	2:D:183:ARG:NH1	2.46	0.48
1:A:436:GLU:HG3	1:A:447:ARG:HH11	1.77	0.48
1:A:395:LEU:HD23	1:A:407:GLY:HA3	1.96	0.48
1:B:192:GLU:OE1	1:B:194:ARG:NH2	2.46	0.48
1:A:104:ALA:HB1	1:A:140:VAL:HG22	1.95	0.47
1:B:1:MET:HE3	1:B:129:ALA:HB2	1.97	0.47
2:D:168:PRO:HG2	2:D:171:ILE:HD12	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:291:VAL:HA	1:A:297:GLU:HG2	1.97	0.46
1:B:325:TYR:CZ	1:B:329:ARG:HD2	2.50	0.46
1:A:172:GLY:HA2	1:A:198:ARG:HD2	1.98	0.45
1:A:411:THR:HB	1:A:422:LEU:HD11	1.97	0.45
1:A:23:LEU:HD12	1:A:23:LEU:HA	1.86	0.45
1:A:46:LYS:HD3	1:A:155:MET:SD	2.57	0.45
2:D:173:ARG:NH2	2:D:183:ARG:HG3	2.32	0.44
1:B:172:GLY:HA2	1:B:198:ARG:HD2	1.99	0.44
2:D:139:TYR:CE2	2:D:183:ARG:HG2	2.53	0.43
1:A:375:ILE:HD12	1:A:379:MET:HE2	2.01	0.43
1:B:46:LYS:HD3	1:B:155:MET:SD	2.58	0.43
2:C:139:TYR:CZ	2:C:172:GLY:HA3	2.53	0.43
1:A:421:HIS:CG	1:A:424:GLU:HB2	2.54	0.43
1:B:16:LEU:HD12	1:B:16:LEU:HA	1.85	0.43
1:B:104:ALA:HB1	1:B:140:VAL:HG22	2.00	0.43
1:A:297:GLU:HG3	4:A:618:HOH:O	2.19	0.42
1:B:86:SER:HB3	1:B:109:PRO:HA	2.00	0.42
1:B:123:ASN:HA	1:B:124:PRO:HD3	1.87	0.42
2:C:172:GLY:O	2:C:176:VAL:HG23	2.20	0.42
1:A:32:HIS:CG	1:A:33:ARG:H	2.38	0.41
1:A:253:ARG:NH1	1:A:257:GLU:OE2	2.53	0.41
1:A:374:GLY:HA3	1:A:410:ARG:HH21	1.84	0.41
1:B:196:GLU:OE1	1:B:202:ARG:NH1	2.50	0.41
1:A:283:SER:HA	1:A:284:PRO:HD3	1.91	0.41
1:A:33:ARG:CZ	1:A:61:LYS:HD3	2.50	0.41
1:A:46:LYS:HE2	1:A:50:ARG:NH2	2.35	0.41
1:A:16:LEU:HD12	1:A:16:LEU:HA	1.94	0.41
1:A:86:SER:HB3	1:A:109:PRO:HA	2.03	0.41
1:A:32:HIS:CG	1:A:33:ARG:N	2.90	0.41
2:D:140:ILE:HB	2:D:182:ARG:HG2	2.01	0.41
1:B:93:GLU:OE2	1:B:115:SER:N	2.41	0.40
1:A:404:LEU:HD21	1:A:447:ARG:HE	1.86	0.40
1:B:23:LEU:HD12	1:B:23:LEU:HA	1.89	0.40
1:B:207:LEU:HD13	1:B:207:LEU:HA	1.86	0.40
2:C:156:TYR:CZ	2:C:168:PRO:HD3	2.57	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	444/477 (93%)	427 (96%)	17 (4%)	0	100	100
1	B	343/477 (72%)	332 (97%)	11 (3%)	0	100	100
2	C	54/80 (68%)	54 (100%)	0	0	100	100
2	D	69/80 (86%)	64 (93%)	5 (7%)	0	100	100
All	All	910/1114 (82%)	877 (96%)	33 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	357/383 (93%)	331 (93%)	26 (7%)	13	29
1	B	281/383 (73%)	258 (92%)	23 (8%)	10	24
2	C	45/66 (68%)	41 (91%)	4 (9%)	9	20
2	D	54/66 (82%)	51 (94%)	3 (6%)	19	40
All	All	737/898 (82%)	681 (92%)	56 (8%)	12	27

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	16	LEU

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Mol	Chain	Res	Type
1	A	23	LEU
1	A	63	VAL
1	A	77	GLU
1	A	82	SER
1	A	91	LEU
1	A	94	GLU
1	A	101	VAL
1	A	118	SER
1	A	140	VAL
1	A	169	GLU
1	A	197	LEU
1	A	207	LEU
1	A	227	ARG
1	A	255	LEU
1	A	282	ILE
1	A	297	GLU
1	A	329	ARG
1	A	330	LYS
1	A	355	GLU
1	A	372	LEU
1	A	375	ILE
1	A	405	VAL
1	A	412	THR
1	A	427	LYS
1	B	1	MET
1	B	16	LEU
1	B	23	LEU
1	B	33	ARG
1	B	77	GLU
1	B	84	LEU
1	B	91	LEU
1	B	101	VAL
1	B	120	VAL
1	B	140	VAL
1	B	147	GLU
1	B	169	GLU
1	B	197	LEU
1	B	202	ARG
1	B	207	LEU
1	B	221	GLU
1	B	250	GLU
1	B	255	LEU

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Mol	Chain	Res	Type
1	B	264	ILE
1	B	282	ILE
1	B	297	GLU
1	B	307	ARG
1	B	312	THR
2	C	145	LEU
2	C	148	VAL
2	C	149	LEU
2	C	184	VAL
2	D	122	GLU
2	D	149	LEU
2	D	185	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	B	303	ASN
2	C	142	GLN
2	D	142	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)

5 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	$\#\|Z\| > 2$
3	SO4	A	502	-	4,4,4	0.23	0	6,6,6	0.11	0
3	SO4	D	201	-	4,4,4	0.24	0	6,6,6	0.15	0
3	SO4	A	503	-	4,4,4	0.24	0	6,6,6	0.08	0
3	SO4	A	501	-	4,4,4	0.23	0	6,6,6	0.09	0
3	SO4	B	501	-	4,4,4	0.22	0	6,6,6	0.13	0

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

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, 95^{th} 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	450/477 (94%)	0.57	59 (13%) 7 5	11, 32, 77, 112	0
1	B	345/477 (72%)	0.23	15 (4%) 40 34	13, 28, 58, 85	0
2	C	56/80 (70%)	0.16	2 (3%) 46 40	16, 30, 49, 73	0
2	D	71/80 (88%)	0.58	7 (9%) 13 10	17, 37, 72, 83	0
All	All	922/1114 (82%)	0.42	83 (9%) 15 11	11, 30, 72, 112	0

All (83) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	419	GLY	7.4
1	A	412	THR	6.1
1	A	411	THR	5.5
1	A	360	TYR	5.4
1	A	420	TYR	4.5
1	A	409	ALA	4.5
1	A	464	LEU	4.4
1	A	416	LEU	4.3
2	D	119	SER	4.2
1	A	347	ILE	4.1
1	A	417	GLU	4.0
1	A	418	LYS	4.0
1	A	345	PHE	4.0
1	A	213	TYR	4.0
1	B	343	ARG	4.0
1	A	381	ILE	3.9
1	A	415	ALA	3.9
1	A	392	VAL	3.8
1	B	345	PHE	3.6
1	A	379	MET	3.5
1	A	444	ALA	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	414	LYS	3.5
1	B	340	ILE	3.4
1	A	423	GLY	3.4
1	B	336	LYS	3.3
1	A	351	ASN	3.3
1	A	375	ILE	3.3
1	A	355	GLU	3.2
1	B	341	GLU	3.2
1	A	383	ALA	3.2
1	A	460	PHE	3.2
1	A	353	VAL	3.2
1	A	350	TRP	3.2
1	A	447	ARG	3.1
1	B	342	ALA	3.1
1	A	399	ASP	3.1
1	A	422	LEU	3.1
1	A	425	ALA	3.0
1	A	437	GLY	3.0
2	D	133	GLU	2.9
1	A	421	HIS	2.8
1	A	112	ASP	2.7
1	A	461	ASN	2.7
1	B	216	ASN	2.7
1	A	431	GLU	2.6
1	A	380	ALA	2.6
1	A	348	GLN	2.6
2	D	130	MET	2.5
1	A	352	MET	2.5
1	A	359	ALA	2.5
1	B	150	ARG	2.5
1	A	426	LEU	2.5
2	D	124	LEU	2.5
2	D	177	GLU	2.4
2	C	187	PHE	2.4
1	A	371	THR	2.4
1	B	221	GLU	2.4
1	A	410	ARG	2.4
1	A	367	ASN	2.4
1	A	413	GLU	2.4
2	D	154	LYS	2.4
1	A	463	ALA	2.4
1	A	66	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	224	GLY	2.4
1	B	335	TYR	2.4
1	B	264	ILE	2.3
1	A	404	LEU	2.3
1	A	344	LYS	2.3
1	B	257	GLU	2.3
1	B	118	SER	2.3
2	C	188	LEU	2.3
1	A	349	ASN	2.2
1	A	117	ASP	2.2
1	A	424	GLU	2.2
1	A	340	ILE	2.1
1	A	354	GLU	2.1
1	B	22	GLU	2.1
1	A	225	ASP	2.1
1	A	376	ALA	2.1
1	A	346	ILE	2.0
1	B	344	LYS	2.0
1	A	398	SER	2.0
2	D	118	HIS	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, 95^{th} 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	SO4	A	502	5/5	0.83	0.11	63,65,73,90	0
3	SO4	A	503	5/5	0.87	0.18	59,66,69,89	0
3	SO4	D	201	5/5	0.87	0.15	54,65,72,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	SO4	A	501	5/5	0.91	0.15	37,42,49,53	0
3	SO4	B	501	5/5	0.93	0.14	32,38,48,52	0

6.5 Other polymers (i)

There are no such residues in this entry.