



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 02:52 AM UTC

PDB ID : 2FR4 / pdb_00002fr4
Title : Structure of Fab DNA-1 complexed with a stem-loop DNA ligand
Authors : Tanner, J.J.; Ou, Z.
Deposited on : 2006-01-18
Resolution : 1.95 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

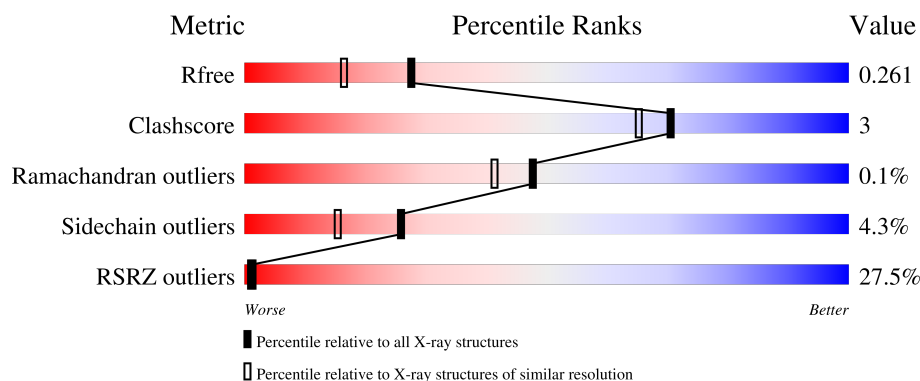
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

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	M	10	20% 90% 10%
1	N	10	40% 70% 30%
2	A	214	65% 89% 10% .
2	L	214	24% 88% 9% ..
3	B	230	11% 85% 8% 7%

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Mol	Chain	Length	Quality of chain
3	H	230	7% 83% 8% • 7%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7283 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 DNA chain called 5'-D(*CP*TP*GP*CP*CP*TP*TP*CP*AP*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	M	10	Total	C	N	O	P	0	0	0
			198	96	33	60	9			
1	N	10	Total	C	N	O	P	0	0	0
			198	96	33	60	9			

- Molecule 2 is a protein called antibody light chain FAB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	212	Total	C	N	O	S	0	0	0
			1628	1020	271	331	6			
2	A	213	Total	C	N	O	S	0	0	0
			1614	1011	268	329	6			

- Molecule 3 is a protein called antibody heavy chain FAB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	214	Total	C	N	O	S	0	0	0
			1622	1036	259	318	9			
3	B	214	Total	C	N	O	S	0	0	0
			1615	1033	257	316	9			

There are 20 discrepancies between the modelled and reference sequences:

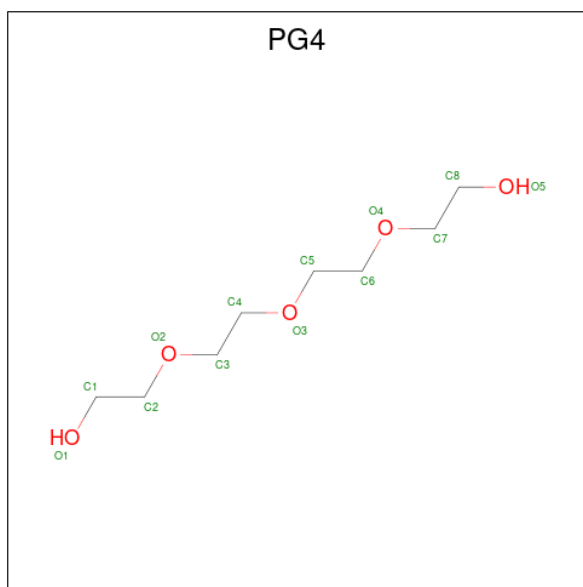
Chain	Residue	Modelled	Actual	Comment	Reference
H	1	GLN	-	cloning artifact	GB 3399661
H	2	VAL	-	cloning artifact	GB 3399661
H	3	LYS	-	cloning artifact	GB 3399661
H	4	LEU	-	cloning artifact	GB 3399661
H	218	HIS	-	expression tag	GB 3399661
H	219	HIS	-	expression tag	GB 3399661
H	220	HIS	-	expression tag	GB 3399661
H	221	HIS	-	expression tag	GB 3399661

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Chain	Residue	Modelled	Actual	Comment	Reference
H	222	HIS	-	expression tag	GB 3399661
H	223	HIS	-	expression tag	GB 3399661
B	1	GLN	-	cloning artifact	GB 3399661
B	2	VAL	-	cloning artifact	GB 3399661
B	3	LYS	-	cloning artifact	GB 3399661
B	4	LEU	-	cloning artifact	GB 3399661
B	218	HIS	-	expression tag	GB 3399661
B	219	HIS	-	expression tag	GB 3399661
B	220	HIS	-	expression tag	GB 3399661
B	221	HIS	-	expression tag	GB 3399661
B	222	HIS	-	expression tag	GB 3399661
B	223	HIS	-	expression tag	GB 3399661

- Molecule 4 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	H	1	Total	C	O	0	0
			8	5	3		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	M	1	Total	O	0	0
			1	1		
5	N	3	Total	O	0	0
			3	3		

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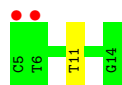
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	L	51	Total 51	O 51	0	0
5	H	146	Total 146	O 146	0	0
5	A	57	Total 57	O 57	0	0
5	B	142	Total 142	O 142	0	0

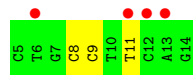
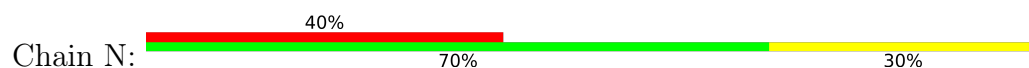
3 Residue-property plots [i](#)

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.

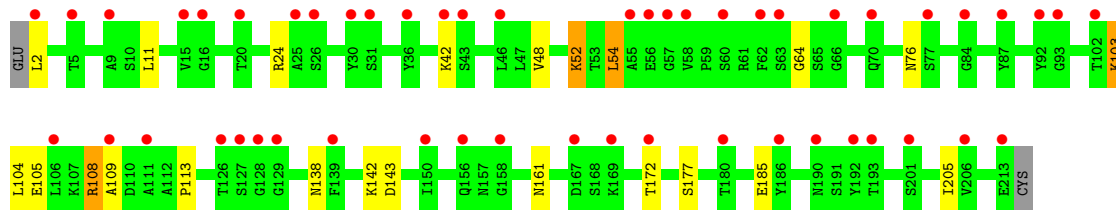
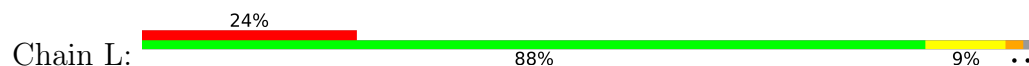
- Molecule 1: 5'-D(*CP*TP*GP*CP*CP*TP*TP*CP*AP*G)-3'



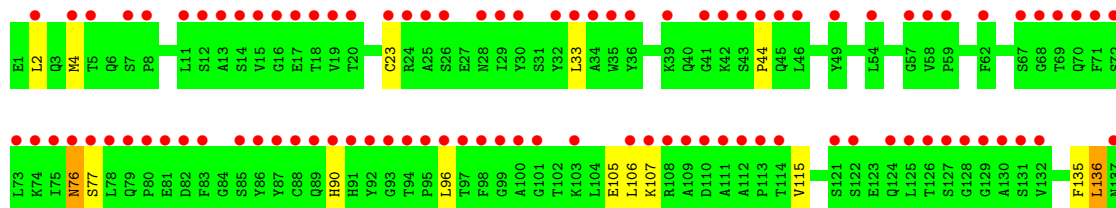
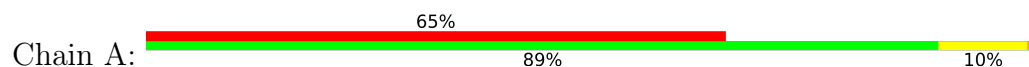
- Molecule 1: 5'-D(*CP*TP*GP*CP*CP*TP*TP*CP*AP*G)-3'

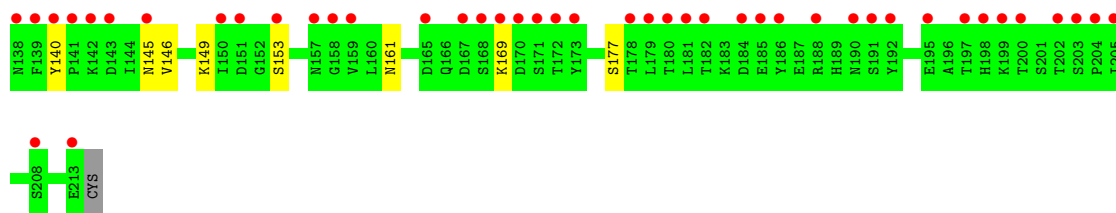


- Molecule 2: antibody light chain FAB

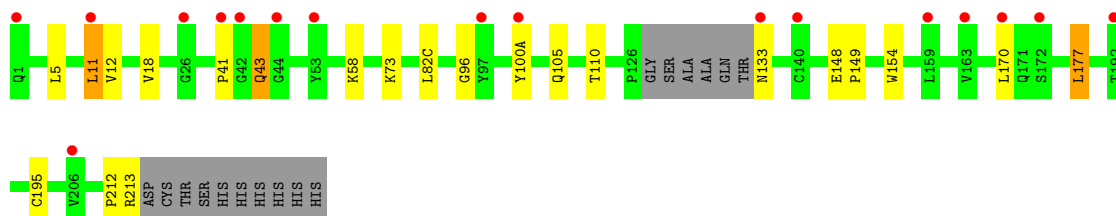
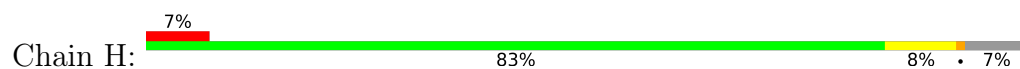


- Molecule 2: antibody light chain FAB

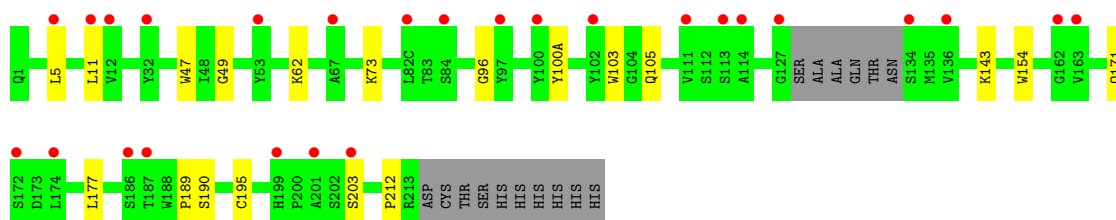
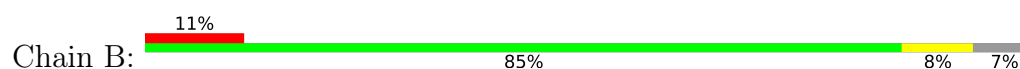




• Molecule 3: antibody heavy chain FAB



• Molecule 3: antibody heavy chain FAB



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	84.76Å 90.45Å 128.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	22.30 – 1.95 22.30 – 1.95	Depositor EDS
% Data completeness (in resolution range)	100.0 (22.30-1.95) 97.4 (22.30-1.95)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.73 (at 1.95Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.207 , 0.256 0.215 , 0.261	Depositor DCC
R_{free} test set	3596 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	30.8	Xtriage
Anisotropy	0.370	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 49.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	7283	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.11% 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: PG4

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	M	0.45	0/220	1.21	1/337 (0.3%)
1	N	0.50	0/220	1.41	4/337 (1.2%)
2	A	0.68	0/1652	0.78	0/2251
2	L	0.70	0/1666	0.79	0/2265
3	B	0.84	0/1661	0.87	0/2269
3	H	0.84	0/1668	0.93	1/2279 (0.0%)
All	All	0.75	0/7087	0.89	6/9738 (0.1%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	11	DT	O3'-P-O5'	-6.75	93.87	104.00
1	N	8	DC	O5'-C5'-C4'	-6.48	101.08	110.80
1	N	11	DT	C5'-C4'-C3'	-6.03	105.86	114.90
1	N	9	DC	C2'-C3'-O3'	5.88	120.31	111.50
1	N	8	DC	O3'-P-O5'	-5.29	96.06	104.00
3	H	177	LEU	CA-CB-CG	5.22	134.56	116.30

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	M	198	0	115	0	0
1	N	198	0	115	0	0
2	A	1614	0	1501	16	0
2	L	1628	0	1534	10	0
3	B	1615	0	1572	7	0
3	H	1622	0	1579	13	0
4	H	8	0	9	2	0
5	A	57	0	0	1	0
5	B	142	0	0	1	0
5	H	146	0	0	0	0
5	L	51	0	0	0	0
5	M	1	0	0	0	0
5	N	3	0	0	0	0
All	All	7283	0	6425	45	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 (45) 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)
2:A:136:LEU:HD11	2:A:146:VAL:HG22	1.76	0.68
3:H:12:VAL:HG21	3:H:82(C):LEU:HD13	1.76	0.67
2:A:4:MET:HE3	2:A:23:CYS:SG	2.39	0.62
3:B:143:LYS:NZ	3:B:171:GLN:OE1	2.32	0.61
3:H:41:PRO:O	3:H:43:GLN:NE2	2.33	0.61
2:L:113:PRO:HG2	2:L:205:ILE:HD12	1.81	0.60
2:A:135:PHE:C	2:A:136:LEU:HD23	2.28	0.59
3:B:73:LYS:NZ	5:B:358:HOH:O	2.32	0.58
3:H:43:GLN:HE21	3:H:43:GLN:N	2.01	0.58
3:H:5:LEU:HD12	3:H:105:GLN:HE21	1.72	0.55
2:L:11:LEU:HD23	2:L:104:LEU:HD13	1.89	0.55
2:L:103:LYS:HD3	2:L:105:GLU:HG3	1.87	0.54
2:A:161:ASN:ND2	2:A:177:SER:OG	2.41	0.54
2:L:161:ASN:ND2	2:L:177:SER:OG	2.41	0.54
2:A:2:LEU:HD22	2:A:90:HIS:CE1	2.45	0.51
2:A:136:LEU:HD23	2:A:136:LEU:N	2.27	0.50
3:H:11:LEU:HD22	3:H:110:THR:HB	1.93	0.50
2:L:161:ASN:HD22	2:L:177:SER:HA	1.77	0.50
3:H:18:VAL:HG12	3:H:82(C):LEU:HD11	1.94	0.49
3:H:154:TRP:CZ3	3:H:195:CYS:HB3	2.49	0.48
2:A:136:LEU:HD11	2:A:146:VAL:CG2	2.43	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:52:LYS:HB2	2:L:64:GLY:O	2.15	0.46
2:A:161:ASN:HD22	2:A:177:SER:HA	1.80	0.46
3:B:189:PRO:HB3	3:B:212:PRO:HG3	1.98	0.45
2:A:115:VAL:HG13	2:A:136:LEU:HD22	1.99	0.45
3:H:96:GLY:HA3	3:H:100(A):TYR:HB2	2.00	0.44
2:L:103:LYS:CD	2:L:105:GLU:HG3	2.48	0.44
2:L:138:ASN:HA	2:L:172:THR:HB	1.99	0.44
3:H:5:LEU:HD12	3:H:105:GLN:NE2	2.33	0.44
2:A:4:MET:HE2	2:A:33:LEU:HD23	1.99	0.44
3:B:154:TRP:CZ3	3:B:195:CYS:HB3	2.53	0.43
3:H:12:VAL:HG21	3:H:82(C):LEU:CD1	2.47	0.43
3:H:149:PRO:HB3	4:H:501:PG4:H41	2.01	0.43
3:H:212:PRO:O	3:H:213:ARG:HB2	2.18	0.43
3:B:47:TRP:CZ2	3:B:49:GLY:HA2	2.55	0.42
2:A:76:ASN:O	2:A:76:ASN:ND2	2.54	0.41
3:H:148:GLU:HB3	4:H:501:PG4:H31	2.02	0.41
3:B:96:GLY:HA3	3:B:100(A):TYR:HB2	2.02	0.41
2:L:48:VAL:HG22	2:L:54:LEU:HD12	2.02	0.41
2:A:106:LEU:HD23	2:A:107:LYS:N	2.35	0.41
2:L:108:ARG:HD3	2:L:109:ALA:O	2.20	0.40
2:A:2:LEU:HD13	5:A:252:HOH:O	2.22	0.40
2:A:140:TYR:CD2	2:A:140:TYR:C	3.00	0.40
2:A:149:LYS:HA	2:A:153:SER:O	2.20	0.40
2:A:44:PRO:HD2	3:B:103:TRP:CE3	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
2	A	211/214 (99%)	205 (97%)	5 (2%)	1 (0%)	24 16

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	L	210/214 (98%)	202 (96%)	8 (4%)	0	100	100
3	B	210/230 (91%)	206 (98%)	4 (2%)	0	100	100
3	H	210/230 (91%)	206 (98%)	4 (2%)	0	100	100
All	All	841/888 (95%)	819 (97%)	21 (2%)	1 (0%)	48	41

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	77	SER

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	
2	A	175/188 (93%)	169 (97%)	6 (3%)	32	23
2	L	179/188 (95%)	168 (94%)	11 (6%)	17	7
3	B	182/200 (91%)	175 (96%)	7 (4%)	29	19
3	H	184/200 (92%)	177 (96%)	7 (4%)	29	19
All	All	720/776 (93%)	689 (96%)	31 (4%)	26	15

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	L	2	LEU
2	L	24	ARG
2	L	42	LYS
2	L	52	LYS
2	L	54	LEU
2	L	76	ASN
2	L	103	LYS
2	L	108	ARG
2	L	142	LYS
2	L	143	ASP

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Mol	Chain	Res	Type
2	L	185	GLU
3	H	11	LEU
3	H	43	GLN
3	H	58	LYS
3	H	73	LYS
3	H	133	ASN
3	H	170	LEU
3	H	177	LEU
2	A	76	ASN
2	A	96	LEU
2	A	105	GLU
2	A	136	LEU
2	A	145	ASN
2	A	169	LYS
3	B	5	LEU
3	B	11	LEU
3	B	62	LYS
3	B	105	GLN
3	B	177	LEU
3	B	190	SER
3	B	203	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
2	L	3	GLN
2	L	137	ASN
2	L	157	ASN
2	L	161	ASN
3	H	1	GLN
3	H	43	GLN
3	H	105	GLN
2	A	89	GLN
2	A	157	ASN
2	A	161	ASN
2	A	210	ASN

5.3.3 RNA ⓘ

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](#)

1 ligand is 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	$\# Z > 2$
4	PG4	H	501	-	7,7,12	0.55	0	6,6,11	0.71	0

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
4	PG4	H	501	-	-	2/5/5/10	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	H	501	PG4	C1-C2-O2-C3
4	H	501	PG4	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	H	501	PG4	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	M	10/10 (100%)	1.44	2 (20%) 3 3	28, 37, 42, 43	0
1	N	10/10 (100%)	1.82	4 (40%) 1 0	30, 37, 44, 44	0
2	A	213/214 (99%)	2.55	140 (65%) 0 0	35, 41, 46, 55	0
2	L	212/214 (99%)	1.52	51 (24%) 2 2	35, 40, 45, 49	0
3	B	214/230 (93%)	1.00	26 (12%) 8 10	34, 40, 45, 52	0
3	H	214/230 (93%)	1.04	17 (7%) 18 21	32, 40, 48, 55	0
All	All	873/908 (96%)	1.53	240 (27%) 1 1	28, 40, 46, 55	0

All (240) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	A	68	GLY	5.8
2	A	130	ALA	5.1
2	A	129	GLY	5.0
2	A	125	LEU	5.0
2	A	16	GLY	4.9
2	A	23	CYS	4.9
2	A	43	SER	4.8
2	A	111	ALA	4.7
2	A	140	TYR	4.6
2	A	203	SER	4.6
2	A	87	TYR	4.5
2	A	69	THR	4.5
2	A	30	TYR	4.4
2	A	184	ASP	4.4
2	A	67	SER	4.3
2	A	182	THR	4.2
2	A	188	ARG	4.2
2	L	172	THR	4.1
2	A	71	PHE	4.1

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Mol	Chain	Res	Type	RSRZ
2	A	75	ILE	4.1
2	A	159	VAL	4.1
2	A	93	GLY	4.1
2	A	24	ARG	4.0
2	A	41	GLY	4.0
3	H	41	PRO	4.0
2	A	13	ALA	4.0
2	A	25	ALA	4.0
2	A	7	SER	4.0
2	L	25	ALA	3.9
2	A	200	THR	3.9
2	A	141	PRO	3.9
2	A	106	LEU	3.8
2	A	205	ILE	3.8
2	A	126	THR	3.7
2	L	126	THR	3.7
2	A	74	LYS	3.7
2	A	186	TYR	3.7
2	A	150	ILE	3.7
2	A	2	LEU	3.6
2	A	124	GLN	3.6
2	A	58	VAL	3.6
2	A	95	PRO	3.5
2	A	100	ALA	3.5
3	H	97	TYR	3.5
2	A	109	ALA	3.5
2	L	16	GLY	3.5
2	A	28	ASN	3.4
2	L	43	SER	3.4
2	A	98	PHE	3.4
2	A	80	PRO	3.4
2	A	92	TYR	3.4
2	A	180	THR	3.4
2	A	198	HIS	3.3
2	A	199	LYS	3.3
2	L	84	GLY	3.3
2	A	33	LEU	3.3
2	L	213	GLU	3.3
2	L	58	VAL	3.3
2	A	62	PHE	3.3
2	L	128	GLY	3.3
2	A	108	ARG	3.3

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Mol	Chain	Res	Type	RSRZ
2	A	32	TYR	3.3
2	A	97	THR	3.3
2	A	197	THR	3.3
2	A	8	PRO	3.3
2	A	88	CYS	3.3
2	A	78	LEU	3.2
3	H	172	SER	3.2
2	A	46	LEU	3.2
2	A	94	THR	3.2
2	A	167	ASP	3.2
2	A	5	THR	3.1
2	A	44	PRO	3.1
2	A	192	TYR	3.1
2	L	31	SER	3.1
2	L	77	SER	3.1
2	A	72	SER	3.1
2	A	171	SER	3.1
2	A	114	THR	3.1
2	A	158	GLY	3.1
2	A	96	LEU	3.1
2	A	153	SER	3.1
3	B	186	SER	3.1
2	A	14	SER	3.1
2	A	18	THR	3.1
3	H	159	LEU	3.0
3	B	136	VAL	3.0
3	H	133	ASN	3.0
2	A	17	GLU	3.0
2	A	168	SER	3.0
3	B	113	SER	3.0
2	L	129	GLY	3.0
2	A	15	VAL	3.0
2	A	191	SER	3.0
2	A	11	LEU	2.9
2	A	20	THR	2.9
2	L	2	LEU	2.9
2	A	26	SER	2.9
2	A	142	LYS	2.9
2	L	109	ALA	2.9
2	A	79	GLN	2.9
3	B	172	SER	2.9
2	A	73	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
2	A	91	HIS	2.9
2	A	34	ALA	2.9
2	A	165	ASP	2.9
2	A	213	GLU	2.9
2	A	112	ALA	2.8
2	A	121	SER	2.8
2	A	4	MET	2.8
2	A	42	LYS	2.8
2	A	36	TYR	2.8
3	B	102	TYR	2.8
3	B	114	ALA	2.8
2	A	29	ILE	2.8
2	L	30	TYR	2.8
2	A	12	SER	2.8
2	A	77	SER	2.8
2	A	122	SER	2.8
2	L	111	ALA	2.8
1	M	5	DC	2.8
2	A	35	TRP	2.8
2	A	90	HIS	2.7
2	A	82	ASP	2.7
2	A	181	LEU	2.7
2	A	85	SER	2.7
1	N	6	DT	2.7
2	A	190	ASN	2.7
3	B	32	TYR	2.7
2	L	60	SER	2.7
2	L	63	SER	2.7
2	L	36	TYR	2.6
2	A	70	GLN	2.6
2	A	81	GLU	2.6
2	L	201	SER	2.6
2	A	107	LYS	2.6
2	A	57	GLY	2.6
2	A	143	ASP	2.6
2	A	131	SER	2.6
2	A	76	ASN	2.6
2	A	137	ASN	2.6
2	A	173	TYR	2.6
2	A	83	PHE	2.6
2	L	26	SER	2.6
2	L	193	THR	2.5

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Mol	Chain	Res	Type	RSRZ
2	A	151	ASP	2.5
3	B	5	LEU	2.5
2	L	55	ALA	2.5
2	A	89	GLN	2.5
2	L	42	LYS	2.5
2	L	192	TYR	2.5
2	A	49	TYR	2.5
2	L	46	LEU	2.5
2	A	208	SER	2.5
2	A	172	THR	2.5
3	B	187	THR	2.5
2	L	206	VAL	2.5
2	A	170	ASP	2.5
3	H	26	GLY	2.4
3	H	42	GLY	2.4
3	B	67	ALA	2.4
2	A	204	PRO	2.4
2	A	45	GLN	2.4
2	A	185	GLU	2.4
3	B	53	TYR	2.4
2	L	56	GLU	2.4
2	L	190	ASN	2.4
3	H	44	GLY	2.4
2	A	54	LEU	2.4
3	B	11	LEU	2.4
2	L	186	TYR	2.4
2	L	139	PHE	2.4
2	A	132	VAL	2.4
2	A	169	LYS	2.4
3	H	53	TYR	2.3
2	A	139	PHE	2.3
2	A	128	GLY	2.3
2	L	70	GLN	2.3
3	H	170	LEU	2.3
2	A	113	PRO	2.3
3	B	111	VAL	2.3
2	L	106	LEU	2.3
2	A	179	LEU	2.3
2	A	202	THR	2.3
2	L	66	GLY	2.3
2	A	157	ASN	2.3
2	A	127	SER	2.2

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Mol	Chain	Res	Type	RSRZ
2	L	150	ILE	2.2
2	L	156	GLN	2.2
2	A	103	LYS	2.2
3	B	174	LEU	2.2
2	A	59	PRO	2.2
2	L	92	TYR	2.2
2	A	145	ASN	2.2
2	L	15	VAL	2.2
2	L	180	THR	2.2
3	B	162	GLY	2.2
1	N	12	DC	2.2
2	A	138	ASN	2.2
1	N	11	DT	2.2
3	H	206	VAL	2.2
2	L	5	THR	2.2
2	L	20	THR	2.2
2	L	127	SER	2.2
3	B	134	SER	2.2
3	B	203	SER	2.2
2	A	101	GLY	2.2
1	N	13	DA	2.2
3	B	97	TYR	2.1
1	M	6	DT	2.1
2	A	110	ASP	2.1
2	A	19	VAL	2.1
3	H	163	VAL	2.1
3	B	12	VAL	2.1
3	B	82(C)	LEU	2.1
3	H	1	GLN	2.1
2	A	86	TYR	2.1
3	B	100	TYR	2.1
2	L	93	GLY	2.1
2	A	39	LYS	2.1
3	H	140	CYS	2.1
3	B	201	ALA	2.1
2	L	62	PHE	2.1
2	L	169	LYS	2.1
3	H	11	LEU	2.1
3	B	84	SER	2.0
2	A	178	THR	2.0
3	H	192	THR	2.0
2	L	57	GLY	2.0

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Mol	Chain	Res	Type	RSRZ
3	B	127	GLY	2.0
3	B	199	HIS	2.0
2	L	9	ALA	2.0
2	L	167	ASP	2.0
2	A	195	GLU	2.0
2	L	102	THR	2.0
2	L	158	GLY	2.0
2	A	99	GLY	2.0
2	L	87	TYR	2.0
3	H	100(A)	TYR	2.0
3	B	163	VAL	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
4	PG4	H	501	8/13	0.64	0.17	56,57,58,58	0

6.5 Other polymers [i](#)

There are no such residues in this entry.