



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:11 PM UTC

PDB ID : 3Q8F / pdb_00003q8f
Title : Crystal structure of 2-Fluorohistidine labeled Protective Antigen (pH 5.8)
Authors : Lovell, S.; Battaile, K.P.; Rajapaksha, M.; Janowiak, B.E.; Andra, K.K.;
Bann, J.G.
Deposited on : 2011-01-06
Resolution : 2.10 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

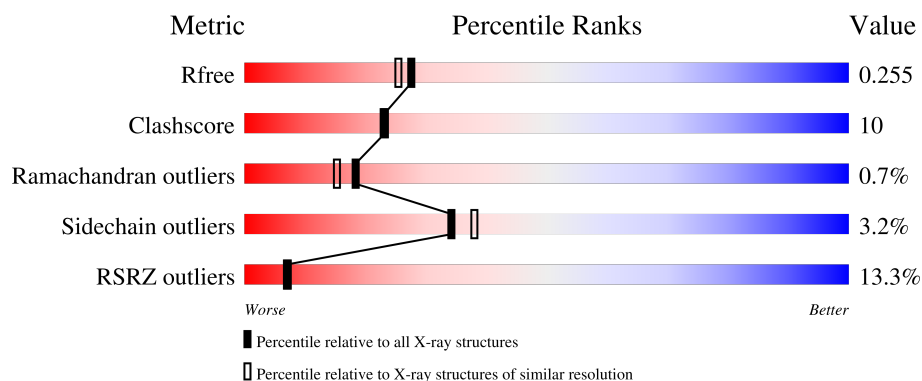
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	735	12% 69% 17% • 12%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 5204 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.

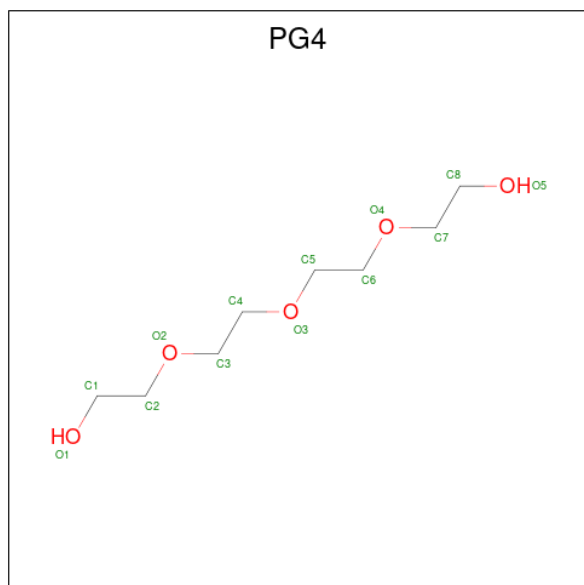
- Molecule 1 is a protein called Protective antigen.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	645	Total	C	F	N	O	S	0	0	0
			5052	3181	7	838	1018	8			

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Ca	0	0
			2	2		

- Molecule 3 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: C₈H₁₈O₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			13	8	5		
3	A	1	Total	C	O	0	0
			13	8	5		

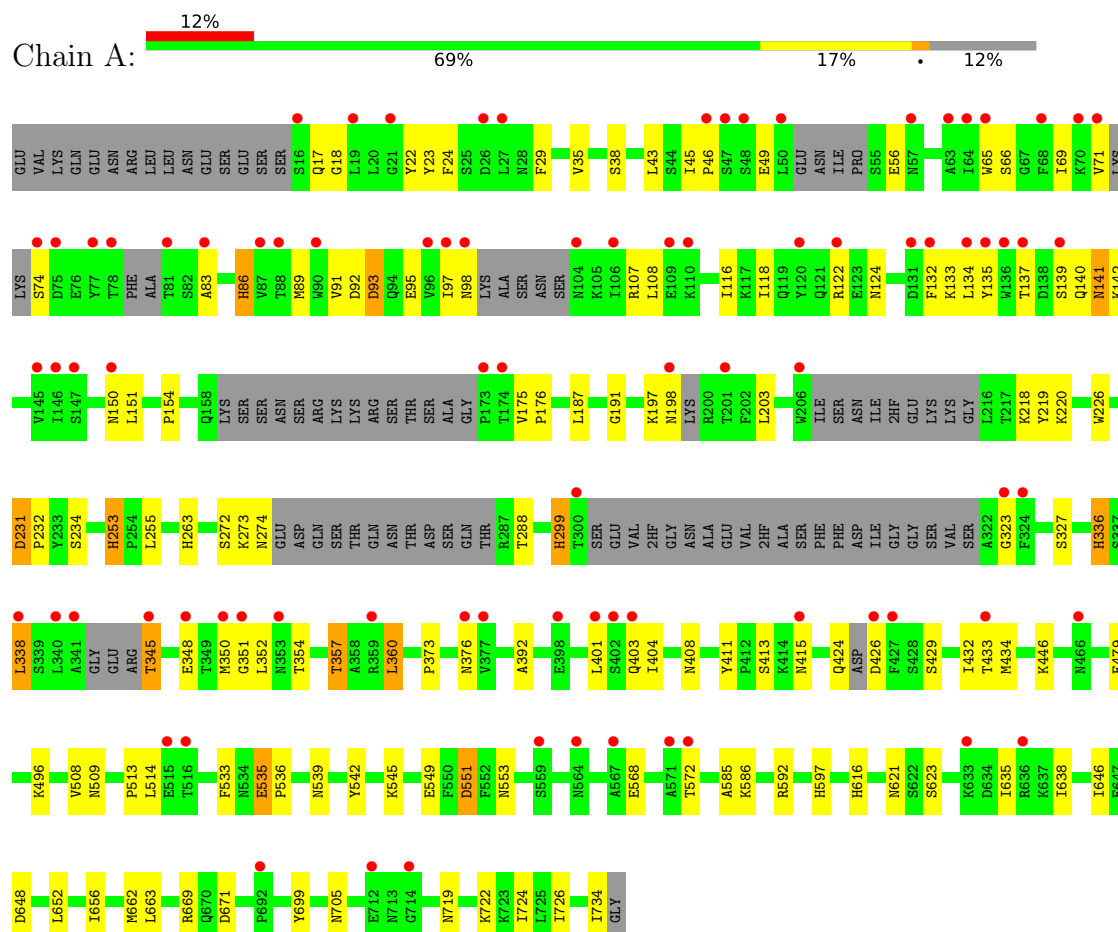
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	124	Total 124	O 124	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: Protective antigen



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	73.29Å 93.66Å 115.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.40 – 2.10 43.40 – 2.10	Depositor EDS
% Data completeness (in resolution range)	98.0 (43.40-2.10) 97.9 (43.40-2.10)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.79 (at 2.10Å)	Xtriage
Refinement program	PHENIX dev_601	Depositor
R, R_{free}	0.222 , 0.267 (Not available) , 0.255	Depositor DCC
R_{free} test set	2341 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	42.0	Xtriage
Anisotropy	0.462	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 42.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5204	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.97% 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: 2HF, CA, 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	A	0.64	0/5045	0.83	3/6839 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	56	GLU	N-CA-C	-5.57	106.44	113.18
1	A	231	ASP	CA-C-N	-5.08	115.11	121.00
1	A	231	ASP	C-N-CA	-5.08	115.11	121.00

There are no chirality outliers.

There are no planarity outliers.

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	5052	0	4852	103	0
2	A	2	0	0	0	0
3	A	26	0	36	3	0
4	A	124	0	0	5	0
All	All	5204	0	4888	103	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 10.

All (103) 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:327:SER:HA	4:A:862:HOH:O	1.87	0.75
1:A:376:ASN:HA	1:A:401:LEU:HD13	1.74	0.70
1:A:71:VAL:HG11	1:A:74:SER:N	2.08	0.68
1:A:69:ILE:HG23	1:A:116:ILE:HG13	1.77	0.67
1:A:253:2HF:HND1	1:A:255:LEU:H	1.47	0.62
1:A:513:PRO:HG2	1:A:514:LEU:HD12	1.81	0.62
1:A:17:GLN:HB2	4:A:747:HOH:O	1.98	0.62
1:A:18:GLY:HA3	1:A:38:SER:O	1.99	0.62
1:A:345:THR:HB	1:A:348:GLU:CB	2.32	0.59
1:A:69:ILE:HA	1:A:150:ASN:O	2.03	0.59
1:A:69:ILE:HG12	1:A:116:ILE:HD11	1.83	0.59
1:A:23:TYR:CD2	1:A:45:ILE:HD12	2.39	0.57
1:A:218:LYS:HE2	1:A:220:LYS:HE2	1.86	0.57
1:A:89:MET:HB3	1:A:97:ILE:HB	1.87	0.57
1:A:231:ASP:HB2	1:A:232:PRO:CD	2.35	0.57
1:A:726:ILE:C	1:A:726:ILE:HD12	2.30	0.57
1:A:69:ILE:HG22	1:A:151:LEU:HD23	1.86	0.57
1:A:403:GLN:HG2	1:A:411:TYR:HE2	1.69	0.56
1:A:403:GLN:HE22	1:A:413:SER:H	1.52	0.56
1:A:360:LEU:C	1:A:360:LEU:HD23	2.31	0.56
1:A:508:VAL:HG13	4:A:748:HOH:O	2.05	0.55
1:A:496:LYS:NZ	3:A:739:PG4:H71	2.20	0.55
1:A:272:SER:CB	1:A:288:THR:HG22	2.37	0.55
1:A:46:PRO:HD2	1:A:49:GLU:OE2	2.07	0.54
1:A:272:SER:HB3	1:A:288:THR:HG22	1.88	0.54
1:A:140:GLN:O	1:A:142:LYS:N	2.41	0.54
1:A:118:ILE:HD11	1:A:134:LEU:HD22	1.89	0.54
1:A:97:ILE:O	1:A:98:ASN:HB2	2.08	0.54
1:A:496:LYS:HE3	3:A:739:PG4:H71	1.90	0.53
1:A:350:MET:HB3	1:A:352:LEU:HD13	1.89	0.53
1:A:585:ALA:O	1:A:586:LYS:HB2	2.08	0.53
1:A:392:ALA:HB2	1:A:432:ILE:HG12	1.90	0.52
1:A:648:ASP:OD2	1:A:652:LEU:HB2	2.10	0.52
1:A:274:ASN:CB	1:A:357:THR:HG22	2.39	0.52
1:A:137:THR:HG23	1:A:142:LYS:C	2.35	0.52
1:A:142:LYS:HG3	1:A:142:LYS:O	2.10	0.52
1:A:496:LYS:CE	3:A:739:PG4:H71	2.41	0.51
1:A:273:LYS:HE2	1:A:351:GLY:C	2.35	0.51
1:A:403:GLN:CG	1:A:411:TYR:CE2	2.94	0.51
1:A:403:GLN:HG2	1:A:411:TYR:CE2	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:413:SER:HB3	1:A:415:ASN:OD1	2.11	0.51
1:A:479:GLU:OE2	4:A:852:HOH:O	2.17	0.50
1:A:97:ILE:CG2	1:A:98:ASN:N	2.73	0.50
1:A:545:LYS:HE3	1:A:549:GLU:OE1	2.10	0.50
1:A:345:THR:HB	1:A:348:GLU:H	1.77	0.49
1:A:231:ASP:HB2	1:A:232:PRO:HD2	1.94	0.49
1:A:23:TYR:CE1	1:A:45:ILE:HD11	2.47	0.49
1:A:357:THR:HG23	1:A:433:THR:HG23	1.94	0.49
1:A:663:LEU:HD23	1:A:663:LEU:N	2.27	0.49
1:A:403:GLN:HG3	1:A:411:TYR:CD2	2.48	0.48
1:A:646:ILE:HD12	1:A:656:ILE:HD11	1.94	0.48
1:A:24:PHE:CD2	1:A:29:PHE:HA	2.49	0.47
1:A:24:PHE:N	1:A:24:PHE:CD1	2.82	0.47
1:A:122:ARG:HG3	1:A:122:ARG:HH11	1.79	0.47
1:A:273:LYS:HE2	1:A:351:GLY:O	2.14	0.47
1:A:338:LEU:HD11	1:A:662:MET:HG2	1.97	0.47
1:A:273:LYS:CE	1:A:351:GLY:O	2.62	0.47
1:A:408:ASN:HD21	1:A:496:LYS:NZ	2.13	0.47
1:A:22:TYR:HD2	1:A:35:VAL:HG22	1.80	0.46
1:A:43:LEU:HD13	1:A:65:TRP:CE2	2.49	0.46
1:A:89:MET:O	1:A:95:GLU:HA	2.15	0.46
1:A:299:2HF:HE2	1:A:323:GLY:H	1.63	0.46
1:A:533:PHE:CE2	1:A:542:TYR:HB2	2.51	0.46
1:A:336:2HF:HB	1:A:446:LYS:HD2	1.98	0.46
1:A:274:ASN:HB2	1:A:357:THR:HG22	1.98	0.46
1:A:107:ARG:O	1:A:108:LEU:HD23	2.16	0.45
1:A:514:LEU:HD12	1:A:514:LEU:N	2.32	0.45
1:A:135:TYR:CD1	1:A:135:TYR:N	2.83	0.45
1:A:226:TRP:CZ2	1:A:234:SER:HB3	2.51	0.45
1:A:648:ASP:C	1:A:648:ASP:OD1	2.60	0.44
1:A:403:GLN:CG	1:A:411:TYR:CD2	3.00	0.44
1:A:92:ASP:O	1:A:93:ASP:C	2.59	0.44
1:A:175:VAL:HG22	1:A:176:PRO:HD2	1.99	0.44
1:A:197:LYS:O	1:A:198:ASN:CB	2.66	0.44
1:A:623:SER:HA	1:A:734:ILE:CG2	2.47	0.44
1:A:408:ASN:HD21	1:A:496:LYS:HZ1	1.64	0.43
1:A:433:THR:HG22	1:A:434:MET:N	2.32	0.43
1:A:17:GLN:HB3	1:A:18:GLY:H	1.68	0.43
1:A:23:TYR:CE2	1:A:45:ILE:HD12	2.54	0.43
1:A:662:MET:C	1:A:663:LEU:HD23	2.44	0.43
1:A:66:SER:HB3	1:A:154:PRO:HG3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:274:ASN:HD22	1:A:357:THR:HG22	1.84	0.42
1:A:705:ASN:ND2	1:A:722:LYS:HD2	2.35	0.42
1:A:43:LEU:HD13	1:A:65:TRP:CD2	2.53	0.42
1:A:139:SER:C	1:A:141:ASN:H	2.28	0.42
1:A:509:ASN:OD1	1:A:509:ASN:C	2.63	0.42
1:A:91:VAL:O	1:A:92:ASP:HB2	2.19	0.42
1:A:373:PRO:HB3	1:A:404:ILE:HD11	2.02	0.41
1:A:191:GLY:HA2	1:A:219:TYR:O	2.19	0.41
1:A:553:ASN:ND2	1:A:592:ARG:HH21	2.18	0.41
1:A:35:VAL:HB	1:A:203:LEU:HB3	2.02	0.41
1:A:513:PRO:HG2	1:A:514:LEU:CD1	2.49	0.41
1:A:535:GLU:HA	1:A:536:PRO:HD2	1.91	0.41
1:A:551:ASP:OD2	4:A:744:HOH:O	2.22	0.41
1:A:231:ASP:CB	1:A:232:PRO:CD	2.99	0.41
1:A:83:ALA:O	1:A:86:2HF:N	2.54	0.41
1:A:132:PHE:C	1:A:133:LYS:HG3	2.46	0.40
1:A:413:SER:CB	1:A:415:ASN:OD1	2.69	0.40
1:A:187:LEU:HD23	1:A:187:LEU:HA	1.84	0.40
1:A:635:ILE:O	1:A:638:ILE:HG13	2.22	0.40
1:A:699:TYR:HA	1:A:724:ILE:O	2.22	0.40
1:A:669:ARG:NH2	1:A:671:ASP:OD2	2.54	0.40
1:A:424:GLN:O	1:A:426:ASP:N	2.55	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	614/735 (84%)	581 (95%)	29 (5%)	4 (1%)	18 15

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	141	ASN
1	A	354	THR
1	A	93	ASP
1	A	124	ASN

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	374/651 (58%)	362 (97%)	12 (3%)	34	38

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	338	LEU
1	A	345	THR
1	A	357	THR
1	A	360	LEU
1	A	429	SER
1	A	535	GLU
1	A	539	ASN
1	A	551	ASP
1	A	568	GLU
1	A	572	THR
1	A	621	ASN
1	A	719	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	274	ASN
1	A	389	GLN
1	A	403	GLN
1	A	408	ASN
1	A	422	ASN
1	A	437	ASN

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Mol	Chain	Res	Type
1	A	499	ASN
1	A	539	ASN
1	A	541	GLN
1	A	553	ASN
1	A	560	GLN
1	A	584	ASN
1	A	601	ASN
1	A	697	ASN
1	A	705	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

7 non-standard protein/DNA/RNA residues 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
1	2HF	A	616	1	9,11,12	1.49	2 (22%)	7,14,16	1.91	2 (28%)
1	2HF	A	86	1	9,11,12	1.21	1 (11%)	7,14,16	2.42	2 (28%)
1	2HF	A	597	1	9,11,12	1.23	1 (11%)	7,14,16	2.10	2 (28%)
1	2HF	A	336	1	9,11,12	1.43	3 (33%)	7,14,16	2.05	3 (42%)
1	2HF	A	299	1	9,11,12	1.15	2 (22%)	7,14,16	2.50	3 (42%)
1	2HF	A	253	1	9,11,12	1.42	2 (22%)	7,14,16	2.43	3 (42%)
1	2HF	A	263	1	9,11,12	1.43	2 (22%)	7,14,16	2.25	2 (28%)

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
1	2HF	A	616	1	-	1/5/6/8	0/1/1/1
1	2HF	A	86	1	-	0/5/6/8	0/1/1/1
1	2HF	A	597	1	-	3/5/6/8	0/1/1/1
1	2HF	A	336	1	-	0/5/6/8	0/1/1/1
1	2HF	A	299	1	-	0/5/6/8	0/1/1/1
1	2HF	A	253	1	-	0/5/6/8	0/1/1/1
1	2HF	A	263	1	-	0/5/6/8	0/1/1/1

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	253	2HF	CE1-NE2	-2.91	1.32	1.35
1	A	336	2HF	CE1-NE2	-2.52	1.32	1.35
1	A	616	2HF	CG-ND1	-2.37	1.34	1.38
1	A	597	2HF	CD2-CG	2.36	1.41	1.36
1	A	263	2HF	CE1-NE2	-2.33	1.32	1.35
1	A	336	2HF	CG-ND1	-2.26	1.34	1.38
1	A	263	2HF	CD2-CG	2.24	1.41	1.36
1	A	86	2HF	CD2-CG	2.22	1.40	1.36
1	A	336	2HF	CD2-CG	2.21	1.40	1.36
1	A	299	2HF	CD2-CG	2.14	1.40	1.36
1	A	299	2HF	CG-ND1	-2.09	1.34	1.38
1	A	253	2HF	CG-ND1	-2.08	1.34	1.38
1	A	616	2HF	CE1-ND1	2.00	1.34	1.32

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	86	2HF	NE2-CE1-ND1	5.33	116.01	111.17
1	A	597	2HF	NE2-CE1-ND1	4.80	115.52	111.17
1	A	253	2HF	NE2-CE1-ND1	4.80	115.52	111.17
1	A	263	2HF	NE2-CE1-ND1	4.71	115.44	111.17
1	A	299	2HF	CA-CB-CG	-4.32	103.12	113.77
1	A	299	2HF	NE2-CE1-ND1	4.27	115.04	111.17
1	A	336	2HF	NE2-CE1-ND1	4.25	115.02	111.17
1	A	616	2HF	NE2-CE1-ND1	4.00	114.80	111.17
1	A	253	2HF	CE1-ND1-CG	-2.89	103.08	109.80
1	A	86	2HF	CE1-ND1-CG	-2.74	103.42	109.80
1	A	263	2HF	CE1-ND1-CG	-2.66	103.61	109.80
1	A	597	2HF	CE1-ND1-CG	-2.34	104.36	109.80
1	A	253	2HF	CB-CG-CD2	-2.22	124.80	129.33
1	A	336	2HF	CE1-ND1-CG	-2.21	104.65	109.80
1	A	336	2HF	CA-CB-CG	-2.21	108.33	113.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	299	2HF	CE1-ND1-CG	-2.18	104.73	109.80
1	A	616	2HF	CE1-ND1-CG	-2.12	104.87	109.80

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	597	2HF	O-C-CA-CB
1	A	616	2HF	O-C-CA-CB
1	A	597	2HF	CA-CB-CG-CD2
1	A	597	2HF	CA-CB-CG-ND1

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	86	2HF	1	0
1	A	336	2HF	1	0
1	A	299	2HF	1	0
1	A	253	2HF	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	PG4	A	739	-	12,12,12	0.46	0	11,11,11	0.91	0
3	PG4	A	738	-	12,12,12	0.69	0	11,11,11	0.67	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
3	PG4	A	739	-	-	5/10/10/10	-
3	PG4	A	738	-	-	2/10/10/10	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	739	PG4	O3-C5-C6-O4
3	A	738	PG4	O4-C7-C8-O5
3	A	739	PG4	O2-C3-C4-O3
3	A	739	PG4	C5-C6-O4-C7
3	A	738	PG4	C5-C6-O4-C7
3	A	739	PG4	C1-C2-O2-C3
3	A	739	PG4	C3-C4-O3-C5

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	739	PG4	3	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	638/735 (86%)	0.80	85 (13%) 7 7	30, 50, 80, 90	0

All (85) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	135	TYR	5.3
1	A	87	VAL	5.0
1	A	78	THR	4.8
1	A	104	ASN	4.6
1	A	74	SER	4.4
1	A	377	VAL	4.3
1	A	137	THR	4.2
1	A	173	PRO	4.1
1	A	402	SER	4.0
1	A	146	ILE	3.9
1	A	340	LEU	3.8
1	A	63	ALA	3.7
1	A	145	VAL	3.7
1	A	110	LYS	3.7
1	A	136	TRP	3.5
1	A	90	TRP	3.5
1	A	341	ALA	3.5
1	A	88	THR	3.5
1	A	83	ALA	3.4
1	A	46	PRO	3.4
1	A	466	ASN	3.4
1	A	71	VAL	3.4
1	A	712	GLU	3.3
1	A	198	ASN	3.2
1	A	353	ASN	3.2
1	A	174	THR	3.2
1	A	348	GLU	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	515	GLU	3.0
1	A	564	ASN	3.0
1	A	345	THR	3.0
1	A	401	LEU	2.9
1	A	47	SER	2.9
1	A	109	GLU	2.9
1	A	567	ALA	2.9
1	A	323	GLY	2.9
1	A	81	THR	2.8
1	A	426	ASP	2.8
1	A	106	ILE	2.8
1	A	16	SER	2.7
1	A	48	SER	2.7
1	A	68	PHE	2.7
1	A	120	TYR	2.7
1	A	571	ALA	2.7
1	A	300	THR	2.6
1	A	427	PHE	2.6
1	A	636	ARG	2.6
1	A	516	THR	2.6
1	A	415	ASN	2.5
1	A	147	SER	2.5
1	A	324	PHE	2.5
1	A	57	ASN	2.5
1	A	398	GLU	2.4
1	A	96	VAL	2.4
1	A	77	TYR	2.3
1	A	131	ASP	2.3
1	A	70	LYS	2.3
1	A	139	SER	2.3
1	A	403	GLN	2.3
1	A	98	ASN	2.3
1	A	150	ASN	2.3
1	A	714	GLY	2.3
1	A	122	ARG	2.2
1	A	376	ASN	2.2
1	A	27	LEU	2.2
1	A	201	THR	2.2
1	A	433	THR	2.2
1	A	50	LEU	2.2
1	A	65	TRP	2.2
1	A	19	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	26	ASP	2.1
1	A	75	ASP	2.1
1	A	206	TRP	2.1
1	A	97	ILE	2.1
1	A	633	LYS	2.1
1	A	359	ARG	2.1
1	A	132	PHE	2.1
1	A	350	MET	2.0
1	A	134	LEU	2.0
1	A	572	THR	2.0
1	A	351	GLY	2.0
1	A	64	ILE	2.0
1	A	559	SER	2.0
1	A	338	LEU	2.0
1	A	692	PRO	2.0
1	A	21	GLY	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	2HF	A	86	11/12	0.74	0.16	76,81,85,86	0
1	2HF	A	299	11/12	0.94	0.09	36,44,52,57	0
1	2HF	A	336	11/12	0.94	0.08	38,41,46,60	0
1	2HF	A	597	11/12	0.95	0.07	33,40,48,50	0
1	2HF	A	253	11/12	0.96	0.06	31,37,41,41	0
1	2HF	A	616	11/12	0.96	0.08	35,37,43,44	0
1	2HF	A	263	11/12	0.97	0.06	28,31,34,35	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	PG4	A	739	13/13	0.87	0.12	50,59,65,75	0
3	PG4	A	738	13/13	0.94	0.09	43,45,53,53	0
2	CA	A	736	1/1	0.99	0.02	33,33,33,33	0
2	CA	A	737	1/1	0.99	0.02	38,38,38,38	0

6.5 Other polymers [i](#)

There are no such residues in this entry.