



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 07:05 AM UTC

PDB ID : 5FO7 / pdb_00005fo7
Title : Crystal Structure of Human Complement C3b at 2.8 Angstrom resolution
Authors : Forneris, F.; Wu, J.; Xue, X.; Gros, P.
Deposited on : 2015-11-18
Resolution : 2.80 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

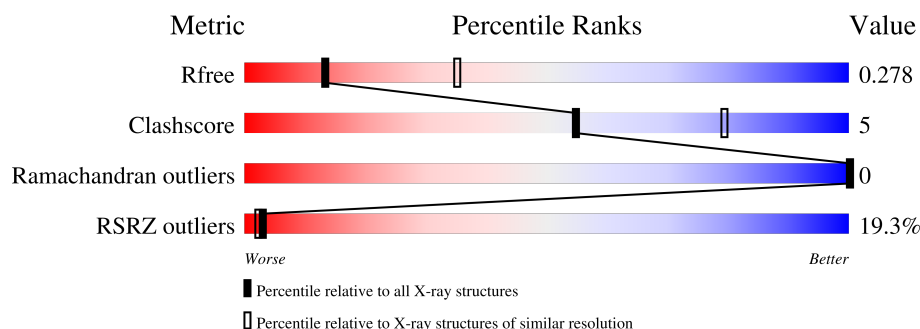
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	645	21% 87% 12% .
2	B	915	17% 86% 13% .

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 12150 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 COMPLEMENT C3 BETA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	637	Total	C	N	O	S	0	0	0
			4961	3158	841	947	15			

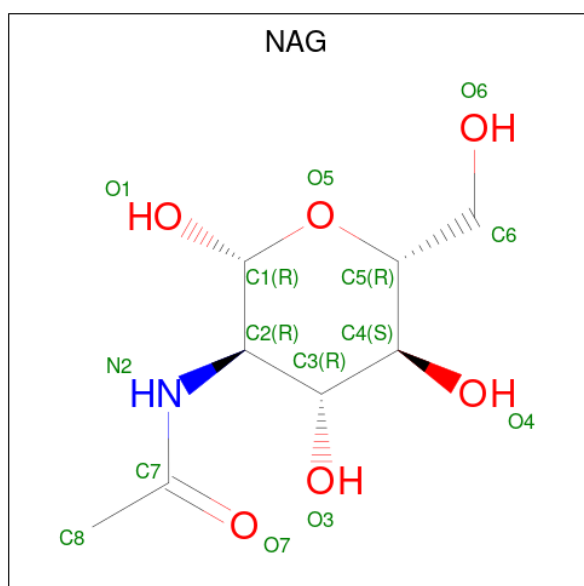
- Molecule 2 is a protein called COMPLEMENT C3B ALPHA' CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	900	Total	C	N	O	S	0	0	0
			7161	4540	1201	1382	38			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1013	GLU	GLN	SEE REMARK 999	UNP P01024

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).

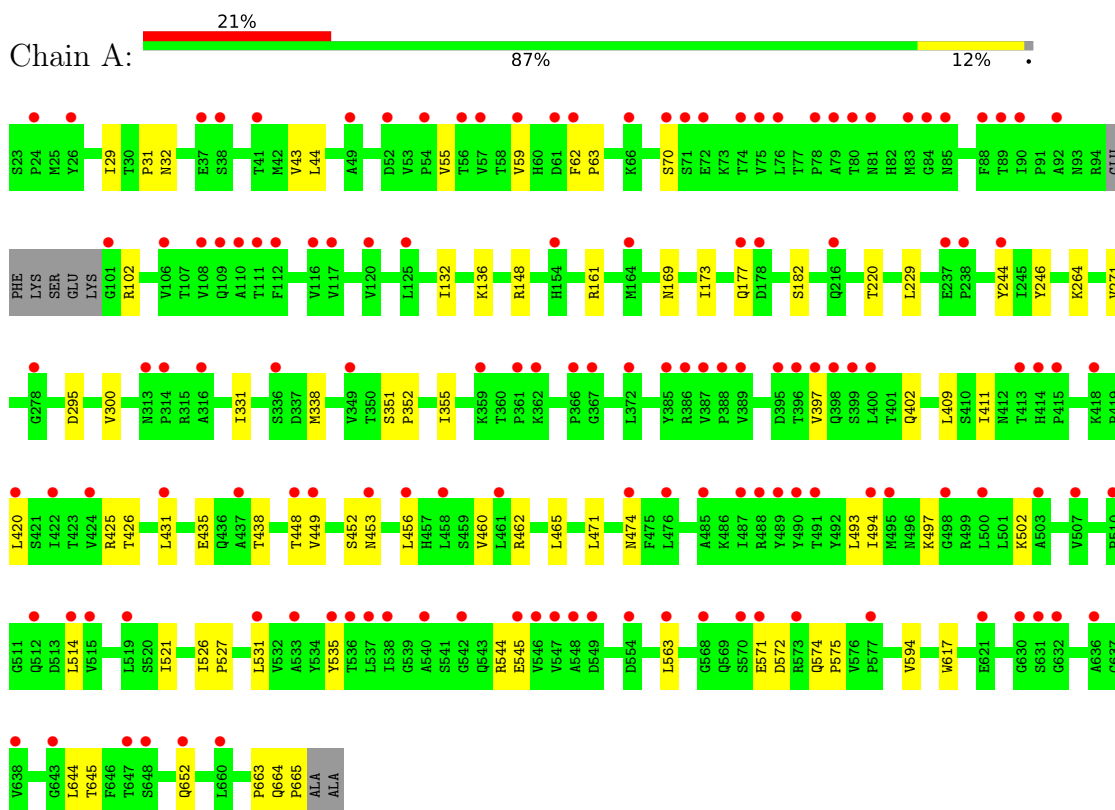


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		

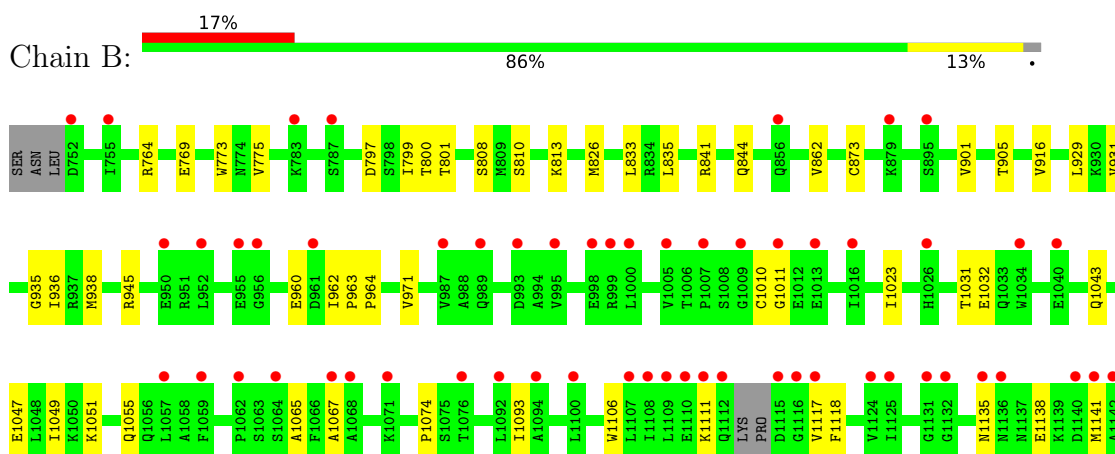
3 Residue-property plots [i](#)

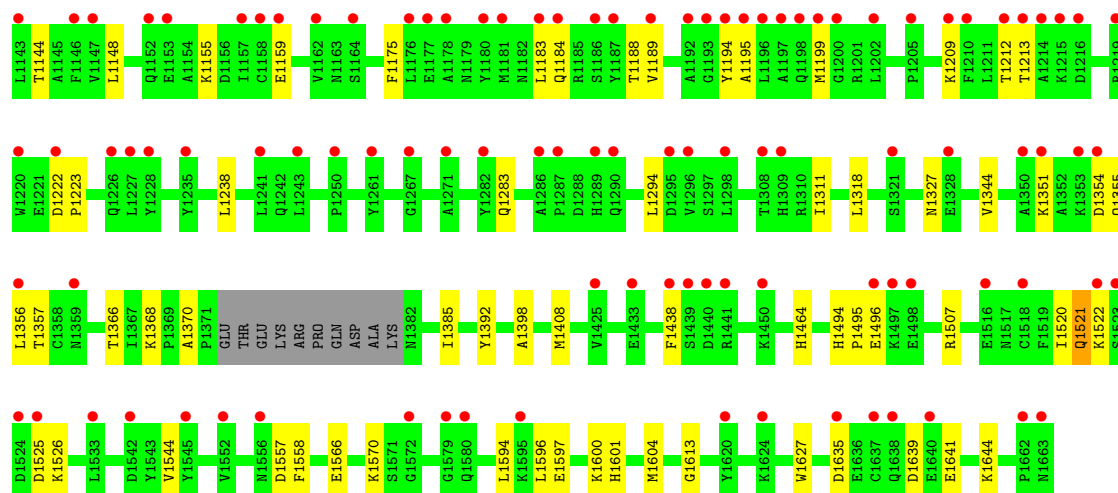
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: COMPLEMENT C3 BETA CHAIN



• Molecule 2: COMPLEMENT C3B ALPHA' CHAIN





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	57.58Å 136.51Å 140.93Å 90.00° 96.05° 90.00°	Depositor
Resolution (Å)	36.81 – 2.80 36.81 – 2.80	Depositor EDS
% Data completeness (in resolution range)	96.0 (36.81-2.80) 88.3 (36.81-2.80)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.35 (at 2.81Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.229 , 0.268 0.245 , 0.278	Depositor DCC
R_{free} test set	2608 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	62.5	Xtriage
Anisotropy	0.375	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 61.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	12150	wwPDB-VP
Average B, all atoms (Å ²)	106.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.34% 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: NAG

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	0/5061	0.71	0/6879
2	B	0.30	0/7302	0.73	2/9889 (0.0%)
All	All	0.29	0/12363	0.72	2/16768 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1521	GLN	CA-C-N	6.43	133.27	121.70
2	B	1521	GLN	C-N-CA	6.43	133.27	121.70

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	4961	0	5018	46	0
2	B	7161	0	7061	77	0
3	A	14	0	13	0	0
3	B	14	0	13	1	0
All	All	12150	0	12105	117	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 5.

All (117) 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:664:GLN:HB2	1:A:665:PRO:HD2	1.72	0.72
2:B:862:VAL:HG22	2:B:916:VAL:HG12	1.74	0.68
2:B:1525:ASP:N	2:B:1525:ASP:OD1	2.25	0.67
2:B:764:ARG:HB3	2:B:797:ASP:HB3	1.77	0.66
1:A:44:LEU:HD13	1:A:55:VAL:HG11	1.77	0.66
2:B:1521:GLN:HA	2:B:1522:LYS:HB3	1.76	0.66
1:A:544:ARG:O	1:A:652:GLN:NE2	2.30	0.64
1:A:474:ASN:HB3	1:A:514:LEU:HD11	1.79	0.64
2:B:1438:PHE:HZ	2:B:1464:HIS:HB2	1.66	0.61
2:B:1294:LEU:HB2	2:B:1311:ILE:HB	1.82	0.61
1:A:456:LEU:HB2	1:A:535:TYR:HE1	1.65	0.60
1:A:465:LEU:HD21	1:A:521:ILE:HG13	1.82	0.59
2:B:1049:ILE:HG22	2:B:1093:ILE:HD13	1.84	0.59
1:A:331:ILE:HG12	1:A:338:MET:HG3	1.85	0.58
2:B:1494:HIS:NE2	2:B:1496:GLU:HB3	2.19	0.58
2:B:1521:GLN:HA	2:B:1522:LYS:CB	2.33	0.57
1:A:161:ARG:H	1:A:182:SER:HB3	1.68	0.57
2:B:1354:ASP:OD1	2:B:1354:ASP:N	2.37	0.57
2:B:1118:PHE:CD1	2:B:1144:THR:HA	2.39	0.57
2:B:835:LEU:HG	2:B:929:LEU:HD23	1.88	0.55
2:B:1141:MET:HE2	2:B:1183:LEU:HD11	1.90	0.54
1:A:229:LEU:HD11	2:B:769:GLU:HG2	1.90	0.54
2:B:1566:GLU:OE2	2:B:1601:HIS:NE2	2.41	0.54
2:B:1355:GLN:HG3	2:B:1357:THR:H	1.72	0.54
1:A:402:GLN:NE2	1:A:462:ARG:O	2.38	0.54
1:A:460:VAL:HG13	1:A:471:LEU:HD11	1.92	0.52
1:A:169:ASN:HD21	1:A:173:ILE:HB	1.74	0.52
2:B:810:SER:HB3	2:B:813:LYS:HB2	1.91	0.52
2:B:1135:ASN:N	2:B:1135:ASN:OD1	2.44	0.51
2:B:1148:LEU:HD23	2:B:1195:ALA:HB1	1.93	0.50
2:B:1141:MET:HG3	2:B:1183:LEU:HD21	1.92	0.50
2:B:1209:LYS:HA	2:B:1212:THR:HG22	1.94	0.50
2:B:1117:VAL:HG21	2:B:1175:PHE:CG	2.47	0.49
2:B:1043:GLN:NE2	2:B:1047:GLU:OE2	2.46	0.49
2:B:873:CYS:HB3	2:B:901:VAL:HB	1.94	0.48
2:B:1392:TYR:CG	2:B:1398:ALA:HB2	2.47	0.48
2:B:799:ILE:HG23	2:B:826:MET:HA	1.96	0.48
2:B:1594:LEU:HB3	2:B:1596:LEU:HG	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:411:ILE:HD11	1:A:420:LEU:HD21	1.96	0.48
1:A:148:ARG:HG3	2:B:773:TRP:CZ2	2.49	0.48
1:A:663:PRO:HA	1:A:664:GLN:HA	1.54	0.48
2:B:1051:LYS:NZ	2:B:1055:GLN:OE1	2.42	0.48
2:B:945:ARG:NH1	2:B:960:GLU:OE1	2.46	0.47
2:B:1635:ASP:OD1	2:B:1635:ASP:N	2.46	0.47
1:A:132:ILE:HB	1:A:220:THR:OG1	2.14	0.47
2:B:962:ILE:HA	2:B:963:PRO:HD3	1.74	0.47
1:A:397:VAL:HG12	1:A:409:LEU:HD22	1.95	0.47
1:A:425:ARG:HG2	1:A:438:THR:HB	1.96	0.47
2:B:800:THR:OG1	2:B:801:THR:N	2.47	0.47
2:B:964:PRO:HB2	2:B:1327:ASN:HD21	1.80	0.46
1:A:271:VAL:HG21	1:A:300:VAL:HG11	1.98	0.46
2:B:1148:LEU:HD21	2:B:1199:MET:HE3	1.96	0.46
1:A:448:THR:HG21	1:A:453:ASN:H	1.80	0.46
1:A:494:ILE:HD12	1:A:502:LYS:HB3	1.97	0.46
2:B:1074:PRO:HB2	2:B:1106:TRP:CZ2	2.51	0.46
1:A:43:VAL:HG11	1:A:493:LEU:HD21	1.98	0.45
2:B:905:THR:HA	2:B:931:VAL:HB	1.97	0.45
2:B:1520:ILE:O	2:B:1522:LYS:NZ	2.49	0.45
1:A:177:GLN:HG3	2:B:1318:LEU:HD13	1.99	0.45
2:B:1370:ALA:HB2	2:B:1385:ILE:HG13	1.98	0.45
2:B:1065:ALA:HB2	2:B:1106:TRP:CE2	2.52	0.45
2:B:1194:TYR:CE1	2:B:1238:LEU:HB3	2.52	0.45
1:A:62:PHE:HA	1:A:63:PRO:HA	1.79	0.45
2:B:1138:GLU:OE1	2:B:1188:THR:OG1	2.28	0.45
1:A:431:LEU:HD12	1:A:435:GLU:HB2	1.98	0.44
2:B:1604:MET:HA	2:B:1627:TRP:O	2.17	0.44
1:A:527:PRO:HG3	1:A:617:TRP:CE3	2.52	0.44
1:A:574:GLN:HA	1:A:575:PRO:HD3	1.87	0.44
2:B:833:LEU:HG	2:B:835:LEU:HD13	2.00	0.43
2:B:841:ARG:HE	2:B:905:THR:HG23	1.83	0.43
2:B:1023:ILE:HD12	2:B:1023:ILE:HA	1.92	0.43
1:A:594:VAL:HG12	2:B:775:VAL:HG22	2.01	0.43
2:B:1118:PHE:HD1	2:B:1144:THR:HA	1.83	0.43
2:B:962:ILE:HG21	2:B:1344:VAL:HG21	2.01	0.43
2:B:1111:LYS:O	2:B:1118:PHE:HA	2.19	0.43
2:B:938:MET:HE3	3:B:1917:NAG:H81	2.01	0.43
1:A:136:LYS:HB2	1:A:136:LYS:HE3	1.87	0.42
1:A:449:VAL:HB	1:A:545:GLU:HG3	2.01	0.42
2:B:1507:ARG:NH2	2:B:1613:GLY:HA3	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1031:THR:HG22	2:B:1283:GLN:HG3	2.00	0.42
2:B:844:GLN:HA	2:B:901:VAL:HG22	2.02	0.42
1:A:271:VAL:HG11	1:A:300:VAL:HG11	2.02	0.42
2:B:1067:ALA:HB2	2:B:1074:PRO:HA	2.01	0.42
2:B:1597:GLU:O	2:B:1600:LYS:HB2	2.19	0.42
2:B:1183:LEU:O	2:B:1184:GLN:HB3	2.19	0.42
2:B:1641:GLU:OE1	2:B:1641:GLU:N	2.52	0.42
1:A:59:VAL:HB	1:A:70:SER:HB2	2.02	0.41
1:A:32:ASN:HA	1:A:645:THR:HG23	2.02	0.41
1:A:244:TYR:CE2	1:A:246:TYR:HB2	2.55	0.41
1:A:494:ILE:HG12	1:A:531:LEU:HD13	2.02	0.41
2:B:1544:VAL:HG23	2:B:1570:LYS:HE2	2.01	0.41
1:A:31:PRO:HA	1:A:644:LEU:HD23	2.00	0.41
1:A:102:ARG:NH1	2:B:1032:GLU:O	2.53	0.41
2:B:1639:ASP:HB3	2:B:1641:GLU:CD	2.45	0.41
2:B:1010:CYS:HB3	2:B:1011:GLY:H	1.69	0.41
2:B:1117:VAL:HG21	2:B:1175:PHE:CD2	2.56	0.41
2:B:1644:LYS:HE3	2:B:1644:LYS:HB2	1.95	0.41
1:A:264:LYS:HD3	1:A:295:ASP:O	2.21	0.41
1:A:571:GLU:HB3	1:A:572:ASP:HA	2.01	0.41
2:B:1494:HIS:ND1	2:B:1495:PRO:HD2	2.36	0.41
1:A:563:LEU:HD22	2:B:808:SER:HB3	2.03	0.41
1:A:148:ARG:CZ	1:A:594:VAL:HB	2.51	0.41
2:B:1189:VAL:HG11	2:B:1213:THR:HG21	2.03	0.41
2:B:1366:THR:HG21	2:B:1368:LYS:HE3	2.02	0.41
2:B:1557:ASP:OD1	2:B:1558:PHE:N	2.51	0.41
2:B:1222:ASP:HA	2:B:1223:PRO:HD2	1.91	0.40
2:B:1525:ASP:HB2	2:B:1526:LYS:H	1.63	0.40
2:B:971:VAL:HG22	2:B:1351:LYS:HG2	2.02	0.40
1:A:29:ILE:HB	1:A:43:VAL:CG1	2.52	0.40
1:A:351:SER:HA	1:A:352:PRO:HD3	1.82	0.40
2:B:935:GLY:HA3	2:B:971:VAL:HG21	2.03	0.40
2:B:1155:LYS:O	2:B:1159:GLU:HB2	2.21	0.40
2:B:1408:MET:SD	2:B:1495:PRO:HD3	2.62	0.40
1:A:355:ILE:HD11	1:A:426:THR:HG23	2.03	0.40
1:A:497:LYS:NZ	1:A:526:ILE:O	2.55	0.40
1:A:452:SER:OG	1:A:545:GLU:OE2	2.38	0.40
2:B:936:ILE:HB	2:B:1356:LEU:HD21	2.02	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	440/645 (68%)	426 (97%)	14 (3%)	0	100	100
2	B	894/915 (98%)	854 (96%)	40 (4%)	0	100	100
All	All	1334/1560 (86%)	1280 (96%)	54 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

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](#)

2 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	NAG	A	1063	-	14,14,15	0.37	0	17,19,21	0.61	0
3	NAG	B	1917	-	14,14,15	0.41	0	17,19,21	0.48	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	NAG	A	1063	-	-	2/6/23/26	0/1/1/1
3	NAG	B	1917	-	-	0/6/23/26	0/1/1/1

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
3	A	1063	NAG	O5-C5-C6-O6
3	A	1063	NAG	C4-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1917	NAG	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	637/645 (98%)	1.26	138 (21%) 2 2	42, 107, 185, 241	0
2	B	900/915 (98%)	1.16	159 (17%) 4 3	41, 99, 176, 279	0
All	All	1537/1560 (98%)	1.20	297 (19%) 3 2	41, 102, 181, 279	0

All (297) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	1116	GLY	6.5
2	B	1112	GLN	5.3
2	B	1109	LEU	4.8
1	A	630	GLY	4.7
1	A	542	GLY	4.6
2	B	1176	LEU	4.4
2	B	1184	GLN	4.4
2	B	1637	CYS	4.2
2	B	752	ASP	4.1
2	B	1524	ASP	4.1
2	B	1497	LYS	4.1
2	B	1290	GLN	4.1
2	B	1108	ILE	4.0
2	B	1220	TRP	4.0
1	A	117	VAL	3.9
1	A	92	ALA	3.9
2	B	1199	MET	3.8
2	B	1287	PRO	3.8
2	B	1196	LEU	3.8
2	B	955	GLU	3.7
2	B	1579	GLY	3.7
1	A	80	THR	3.7
2	B	1142	ALA	3.6
2	B	1356	LEU	3.6

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Mol	Chain	Res	Type	RSRZ
2	B	1125	ILE	3.5
1	A	54	PRO	3.4
1	A	70	SER	3.4
1	A	56	THR	3.4
1	A	366	PRO	3.3
1	A	487	ILE	3.3
2	B	1213	THR	3.3
2	B	1298	LEU	3.3
2	B	1132	GLY	3.3
2	B	1040	GLU	3.3
1	A	456	LEU	3.2
1	A	507	VAL	3.2
1	A	515	VAL	3.2
2	B	1180	TYR	3.2
1	A	24	PRO	3.2
1	A	26	TYR	3.1
1	A	514	LEU	3.1
2	B	1107	LEU	3.1
2	B	1177	GLU	3.1
2	B	1068	ALA	3.1
2	B	987	VAL	3.1
2	B	1498	GLU	3.1
1	A	461	LEU	3.1
2	B	1286	ALA	3.1
2	B	1289	HIS	3.1
2	B	1189	VAL	3.1
1	A	108	VAL	3.1
1	A	237	GLU	3.1
1	A	489	TYR	3.0
2	B	1200	GLY	3.0
2	B	1000	LEU	3.0
1	A	546	VAL	3.0
2	B	1227	LEU	3.0
2	B	1425	VAL	3.0
2	B	956	GLY	3.0
1	A	75	VAL	3.0
1	A	573	ARG	3.0
1	A	400	LEU	3.0
1	A	396	THR	3.0
2	B	1197	ALA	3.0
1	A	112	PHE	3.0
2	B	1143	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
2	B	1187	TYR	2.9
1	A	570	SER	2.9
2	B	1640	GLU	2.9
1	A	621	GLU	2.9
2	B	1067	ALA	2.9
1	A	362	LYS	2.9
2	B	879	LYS	2.9
2	B	1157	ILE	2.9
2	B	856	GLN	2.9
2	B	1178	ALA	2.9
1	A	488	ARG	2.9
1	A	164	MET	2.9
2	B	1135	ASN	2.9
1	A	537	LEU	2.9
1	A	37	GLU	2.8
2	B	1556	ASN	2.8
1	A	336	SER	2.8
1	A	631	SER	2.8
2	B	1181	MET	2.8
2	B	1159	GLU	2.8
1	A	418	LYS	2.8
2	B	1351	LYS	2.8
2	B	1076	THR	2.8
2	B	1572	GLY	2.8
1	A	216	GLN	2.8
1	A	388	PRO	2.8
1	A	397	VAL	2.7
1	A	420	LEU	2.7
1	A	314	PRO	2.7
2	B	1580	GLN	2.7
1	A	531	LEU	2.7
2	B	1243	LEU	2.7
2	B	1271	ALA	2.7
2	B	1438	PHE	2.7
1	A	361	PRO	2.7
1	A	116	VAL	2.7
1	A	125	LEU	2.7
2	B	1210	PHE	2.7
2	B	1215	LYS	2.7
1	A	385	TYR	2.7
2	B	1321	SER	2.7
2	B	1162	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
2	B	1016	ILE	2.7
2	B	1009	GLY	2.7
2	B	1158	CYS	2.6
1	A	84	GLY	2.6
1	A	387	VAL	2.6
2	B	989	GLN	2.6
2	B	1496	GLU	2.6
1	A	83	MET	2.6
2	B	1164	SER	2.6
2	B	1111	LYS	2.6
1	A	76	LEU	2.6
1	A	72	GLU	2.6
1	A	538	ILE	2.6
1	A	636	ALA	2.6
1	A	359	LYS	2.6
1	A	88	PHE	2.6
2	B	1214	ALA	2.6
1	A	399	SER	2.6
1	A	643	GLY	2.6
2	B	1124	VAL	2.6
2	B	1153	GLU	2.6
1	A	110	ALA	2.6
2	B	1663	ASN	2.6
2	B	1440	ASP	2.6
2	B	1183	LEU	2.5
2	B	1117	VAL	2.5
1	A	660	LEU	2.5
1	A	485	ALA	2.5
2	B	1115	ASP	2.5
2	B	1523	SER	2.5
1	A	632	GLY	2.5
2	B	1141	MET	2.5
1	A	449	VAL	2.5
1	A	638	VAL	2.5
1	A	571	GLU	2.5
2	B	1195	ALA	2.5
2	B	1198	GLN	2.5
2	B	1026	HIS	2.5
1	A	57	VAL	2.5
2	B	1624	LYS	2.5
1	A	38	SER	2.4
2	B	1186	SER	2.4

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Mol	Chain	Res	Type	RSRZ
2	B	1441	ARG	2.4
1	A	536	THR	2.4
1	A	414	HIS	2.4
2	B	1309	HIS	2.4
1	A	238	PRO	2.4
2	B	1595	LYS	2.4
1	A	500	LEU	2.4
1	A	101	GLY	2.4
2	B	1209	LYS	2.4
1	A	316	ALA	2.4
1	A	519	LEU	2.4
2	B	1533	LEU	2.4
2	B	1662	PRO	2.4
2	B	1011	GLY	2.4
1	A	74	THR	2.4
1	A	647	THR	2.4
1	A	81	ASN	2.3
2	B	1525	ASP	2.3
1	A	503	ALA	2.3
2	B	787	SER	2.3
2	B	1205	PRO	2.3
2	B	1250	PRO	2.3
2	B	1147	VAL	2.3
2	B	1131	GLY	2.3
2	B	1136	ASN	2.3
2	B	1140	ASP	2.3
2	B	1516	GLU	2.3
2	B	1202	LEU	2.3
2	B	1439	SER	2.3
1	A	41	THR	2.3
1	A	494	ILE	2.3
2	B	1228	TYR	2.3
2	B	1620	TYR	2.3
2	B	1522	LYS	2.3
1	A	78	PRO	2.3
1	A	120	VAL	2.3
1	A	453	ASN	2.3
1	A	62	PHE	2.3
1	A	49	ALA	2.3
1	A	90	ILE	2.3
1	A	413	THR	2.3
2	B	1261	TYR	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	389	VAL	2.3
1	A	278	GLY	2.3
1	A	313	ASN	2.3
2	B	1359	ASN	2.3
1	A	545	GLU	2.3
2	B	1350	ALA	2.3
1	A	395	ASP	2.3
1	A	431	LEU	2.3
2	B	1353	LYS	2.3
2	B	1282	TYR	2.3
1	A	548	ALA	2.2
2	B	1328	GLU	2.2
2	B	1057	LEU	2.2
1	A	154	HIS	2.2
1	A	349	VAL	2.2
1	A	577	PRO	2.2
2	B	1267	GLY	2.2
2	B	1059	PHE	2.2
2	B	950	GLU	2.2
2	B	1110	GLU	2.2
2	B	1450	LYS	2.2
1	A	61	ASP	2.2
2	B	1219	ARG	2.2
1	A	415	PRO	2.2
1	A	491	THR	2.2
2	B	1552	VAL	2.2
1	A	490	TYR	2.2
2	B	1094	ALA	2.2
1	A	52	ASP	2.2
2	B	961	ASP	2.2
2	B	995	VAL	2.2
1	A	89	THR	2.2
2	B	1194	TYR	2.2
2	B	1545	TYR	2.2
1	A	372	LEU	2.2
2	B	1092	LEU	2.2
1	A	398	GLN	2.2
2	B	1007	PRO	2.2
2	B	1216	ASP	2.2
2	B	1542	ASP	2.2
2	B	1635	ASP	2.2
1	A	448	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	568	GLY	2.2
2	B	1518	CYS	2.2
2	B	999	ARG	2.1
1	A	512	GLN	2.1
1	A	652	GLN	2.1
2	B	1638	GLN	2.1
1	A	547	VAL	2.1
1	A	178	ASP	2.1
1	A	111	THR	2.1
1	A	367	GLY	2.1
2	B	952	LEU	2.1
2	B	1146	PHE	2.1
2	B	1241	LEU	2.1
1	A	648	SER	2.1
1	A	177	GLN	2.1
2	B	1152	GLN	2.1
1	A	85	ASN	2.1
1	A	474	ASN	2.1
1	A	106	VAL	2.1
2	B	783	LYS	2.1
1	A	554	ASP	2.1
2	B	1222	ASP	2.1
2	B	1193	GLY	2.1
1	A	533	ALA	2.1
2	B	1013	GLU	2.1
2	B	1064	SER	2.1
1	A	510	PRO	2.1
1	A	498	GLY	2.1
1	A	563	LEU	2.1
2	B	1100	LEU	2.1
2	B	1212	THR	2.1
2	B	1354	ASP	2.1
2	B	1034	TRP	2.1
2	B	1235	TYR	2.1
2	B	1226	GLN	2.1
1	A	66	LYS	2.1
1	A	458	LEU	2.1
1	A	476	LEU	2.1
1	A	386	ARG	2.1
1	A	79	ALA	2.1
2	B	1192	ALA	2.1
2	B	998	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	244	TYR	2.1
1	A	71	SER	2.0
2	B	1071	LYS	2.0
1	A	422	ILE	2.0
1	A	540	ALA	2.0
1	A	549	ASP	2.0
2	B	993	ASP	2.0
2	B	1433	GLU	2.0
1	A	535	TYR	2.0
1	A	59	VAL	2.0
1	A	109	GLN	2.0
2	B	895	SER	2.0
2	B	1005	VAL	2.0
2	B	1062	PRO	2.0
2	B	755	ILE	2.0
1	A	437	ALA	2.0
2	B	1308	THR	2.0
2	B	1295	ASP	2.0
1	A	495	MET	2.0
1	A	424	VAL	2.0
2	B	1296	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
3	NAG	A	1063	14/15	0.40	0.15	151,155,159,160	0
3	NAG	B	1917	14/15	0.40	0.18	134,139,150,151	0

6.5 Other polymers [i](#)

There are no such residues in this entry.