



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2020 – 02:20 AM BST

PDB ID : 5JTW
Title : Crystal structure of complement C4b re-refined using iMDFF
Authors : Croll, T.I.; Andersen, G.R.
Deposited on : 2016-05-09
Resolution : 3.50 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

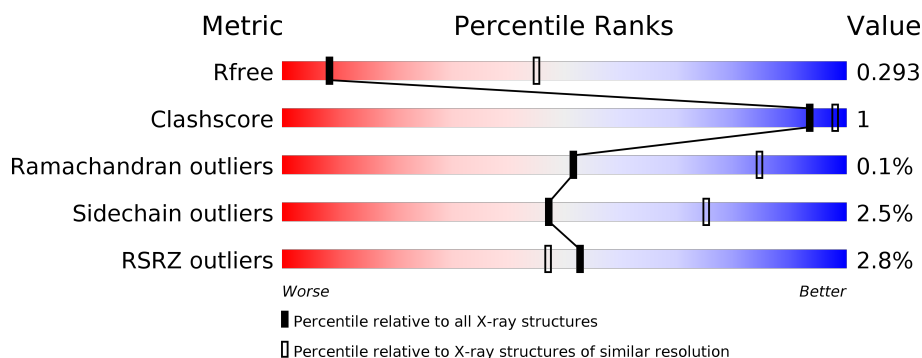
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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}	130704	1659 (3.60-3.40)
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (3.60-3.40)

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 on 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	656	<div> <div style="width: 92%;"></div> <div style="width: 7%;"></div> <div style="width: 1%;"></div> </div> <div>92% 7% ..</div>
1	D	656	<div> <div style="width: 94%;"></div> <div style="width: 5%;"></div> <div style="width: 1%;"></div> </div> <div>94% 5% .</div>
2	B	690	<div> <div style="width: 7%;"></div> <div style="width: 86%;"></div> <div style="width: 5%;"></div> <div style="width: 8%;"></div> </div> <div>7% 86% 5% 8%</div>
2	E	690	<div> <div style="width: 2%;"></div> <div style="width: 87%;"></div> <div style="width: 5%;"></div> <div style="width: 8%;"></div> </div> <div>2% 87% 5% 8%</div>
3	C	291	<div> <div style="width: 3%;"></div> <div style="width: 93%;"></div> <div style="width: 5%;"></div> <div style="width: 1%;"></div> </div> <div>3% 93% 5% .</div>
3	F	291	<div> <div style="width: 2%;"></div> <div style="width: 90%;"></div> <div style="width: 7%;"></div> <div style="width: 1%;"></div> </div> <div>2% 90% 7% .</div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	NAG	A	1801	-	-	-	X

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 24312 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 C4-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	651	Total	C	N	O	S	0	0	0
			5012	3185	872	939	16			
1	D	651	Total	C	N	O	S	0	0	0
			5012	3185	872	939	16			

- Molecule 2 is a protein called Complement C4-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	632	Total	C	N	O	S	0	0	0
			4876	3085	844	932	15			
2	E	632	Total	C	N	O	S	0	0	0
			4876	3085	844	932	15			

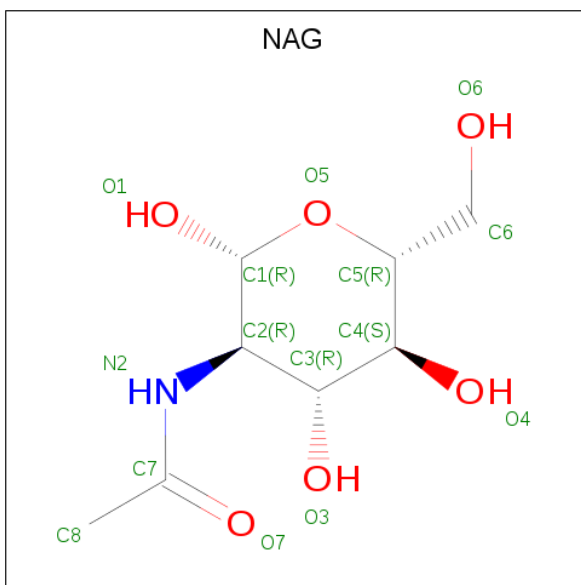
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1201	SER	THR	conflict	UNP P0C0L4
E	1201	SER	THR	conflict	UNP P0C0L4

- Molecule 3 is a protein called Complement C4-A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	281	Total	C	N	O	S	0	0	0
			2240	1407	400	416	17			
3	F	281	Total	C	N	O	S	0	0	0
			2240	1407	400	416	17			

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).

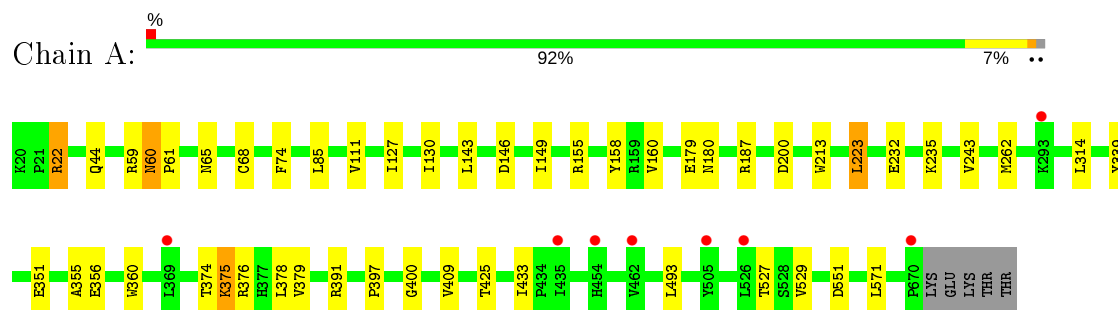


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	D	1	Total	C	N	O	0	0
			14	8	1	5		
4	E	1	Total	C	N	O	0	0
			14	8	1	5		

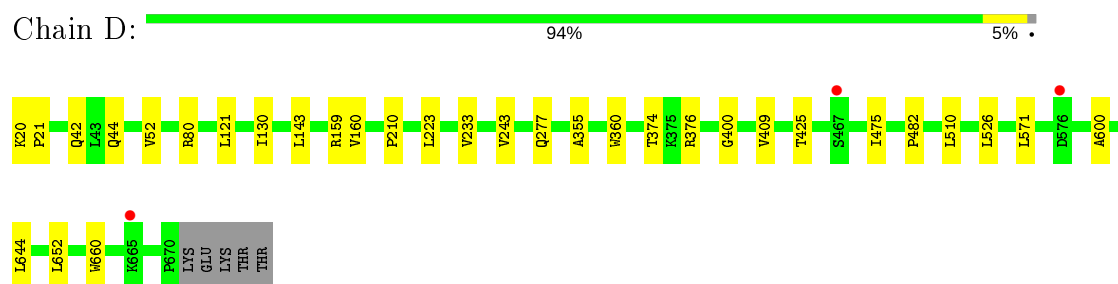
3 Residue-property plots [i](#)

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.

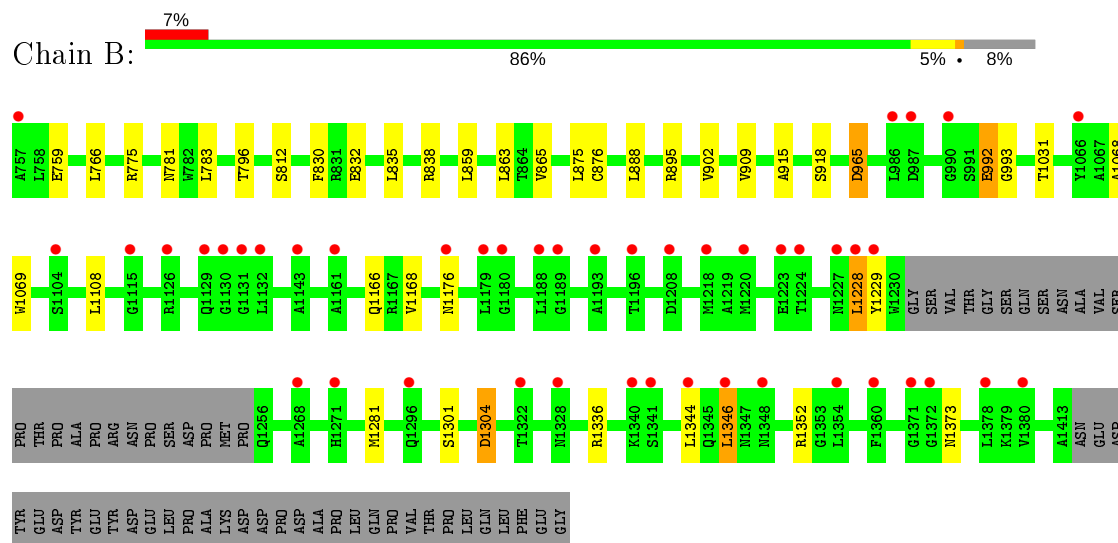
- Molecule 1: Complement C4-A



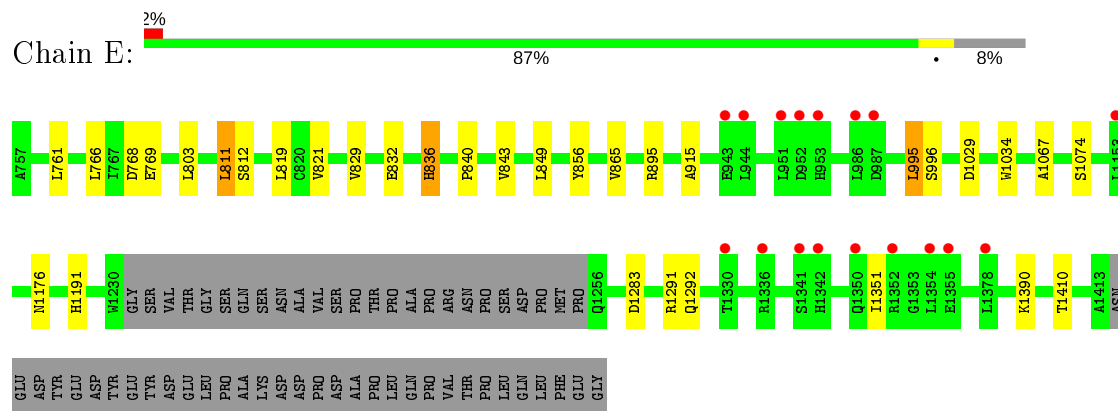
- Molecule 1: Complement C4-A



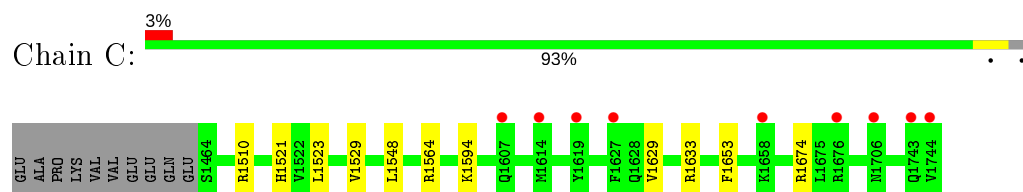
- Molecule 2: Complement C4-A



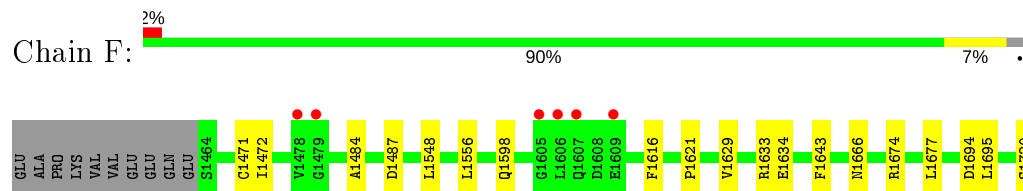
- Molecule 2: Complement C4-A



- Molecule 3: Complement C4-A



- Molecule 3: Complement C4-A



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	121.50Å 161.08Å 131.60Å 90.00° 107.26° 90.00°	Depositor
Resolution (Å)	49.38 – 3.50 49.38 – 3.50	Depositor EDS
% Data completeness (in resolution range)	98.7 (49.38-3.50) 98.7 (49.38-3.50)	Depositor EDS
R_{merge}	0.49	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.14 (at 3.48Å)	Xtriage
Refinement program	PHENIX dev_2376	Depositor
R, R_{free}	0.248 , 0.293 0.248 , 0.293	Depositor DCC
R_{free} test set	2014 reflections (3.34%)	wwPDB-VP
Wilson B-factor (Å ²)	101.3	Xtriage
Anisotropy	0.345	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 76.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	24312	wwPDB-VP
Average B, all atoms (Å ²)	122.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.90% 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	0.29	1/5128 (0.0%)	0.52	1/6961 (0.0%)
1	D	0.26	0/5128	0.52	0/6961
2	B	0.25	0/4975	0.51	0/6765
2	E	0.25	0/4975	0.49	0/6765
3	C	0.26	0/2287	0.53	0/3090
3	F	0.26	0/2287	0.53	0/3090
All	All	0.26	1/24780 (0.0%)	0.51	1/33632 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	433	ILE	C-N	10.15	1.53	1.34

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	22	ARG	NE-CZ-NH2	-5.07	117.76	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	60	ASN	Peptide

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	5012	0	5025	22	1
1	D	5012	0	5025	11	0
2	B	4876	0	4845	18	1
2	E	4876	0	4845	14	0
3	C	2240	0	2184	2	0
3	F	2240	0	2184	6	2
4	A	14	0	13	0	0
4	B	14	0	13	0	0
4	D	14	0	13	0	0
4	E	14	0	13	0	0
All	All	24312	0	24160	68	2

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 1.

All (68) 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:E:1029:ASP:OD1	2:E:1034:TRP:NE1	2.29	0.61
1:D:374:THR:O	1:D:376:ARG:NH1	2.36	0.59
2:B:775:ARG:NH2	2:B:835:LEU:O	2.37	0.58
1:A:391:ARG:HA	1:A:397:PRO:HA	1.88	0.54
2:E:836:HIS:HD1	2:E:856:TYR:HE1	1.56	0.54
1:A:243:VAL:HG13	1:A:355:ALA:HB2	1.88	0.54
1:A:187:ARG:NH2	1:A:200:ASP:OD2	2.37	0.52
1:A:146:ASP:OD1	2:B:781:ASN:ND2	2.43	0.51
1:D:243:VAL:HG13	1:D:355:ALA:HB2	1.93	0.50
1:A:339:TYR:OH	1:A:356:GLU:OE2	2.23	0.49
1:A:378:LEU:HD22	1:A:379:VAL:H	1.76	0.49
1:D:277:GLN:H	1:D:277:GLN:CD	2.16	0.49
1:A:375:LYS:H	1:A:375:LYS:HD2	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:400:GLY:N	1:D:425:THR:OG1	2.39	0.47
1:A:374:THR:O	1:A:376:ARG:NH1	2.35	0.47
1:A:400:GLY:N	1:A:425:THR:OG1	2.45	0.47
2:E:1067:ALA:HB2	2:E:1074:SER:HA	1.96	0.47
2:E:1291:ARG:NH1	2:E:1292:GLN:OE1	2.43	0.47
2:E:843:VAL:HG21	2:E:849:LEU:HD22	1.96	0.47
1:A:59:ARG:CZ	1:A:65:ASN:HD21	2.28	0.47
1:A:179:GLU:CD	2:B:1352:ARG:HH22	2.19	0.46
1:A:111:VAL:HG13	1:A:127:ILE:HG23	1.98	0.46
2:B:876:CYS:HB3	2:B:902:VAL:HG13	1.98	0.46
2:B:859:LEU:HD12	2:B:863:LEU:HD11	1.97	0.46
2:B:766:LEU:HD22	2:B:918:SER:HA	1.97	0.45
2:B:1346:LEU:HD23	2:B:1346:LEU:H	1.80	0.45
2:B:1228:LEU:HA	2:B:1228:LEU:HD22	1.83	0.45
3:F:1720:SER:O	3:F:1723:GLN:NE2	2.49	0.45
2:B:830:PHE:CZ	2:B:832:GLU:HA	2.52	0.44
2:E:811:LEU:HD11	2:E:819:LEU:HG	1.99	0.44
3:F:1484:ALA:HB1	3:F:1556:LEU:HD21	1.98	0.44
1:D:210:PRO:HA	1:D:233:VAL:HG13	1.99	0.44
2:E:761:LEU:HD12	2:E:1410:THR:HG21	1.99	0.44
2:B:1301:SER:OG	2:B:1304:ASP:OD1	2.29	0.44
1:A:61:PRO:HD3	1:A:68:CYS:SG	2.57	0.44
2:E:811:LEU:HD13	2:E:821:VAL:HB	1.98	0.44
2:E:865:VAL:HG11	2:E:915:ALA:HB1	2.00	0.44
1:A:180:ASN:HA	1:A:213:TRP:CD2	2.54	0.43
1:A:22:ARG:HB2	1:A:44:GLN:HB2	2.01	0.43
1:A:351:GLU:OE1	2:B:838:ARG:NH2	2.49	0.43
2:B:992:GLU:CD	2:B:993:GLY:H	2.21	0.43
1:D:42:GLN:NE2	1:D:44:GLN:OE1	2.35	0.43
1:A:223:LEU:H	1:A:223:LEU:HD23	1.84	0.43
1:D:644:LEU:HD22	1:D:644:LEU:H	1.83	0.43
2:E:803:LEU:HA	2:E:829:VAL:HG23	2.01	0.43
2:B:1228:LEU:HD13	2:B:1229:TYR:H	1.84	0.43
2:E:840:PRO:HG3	2:E:849:LEU:HD21	2.00	0.42
1:A:262:MET:HB3	1:A:360:TRP:CH2	2.55	0.42
1:D:159:ARG:CZ	1:D:600:ALA:HB1	2.50	0.42
1:A:158:TYR:CE1	1:A:200:ASP:HB3	2.55	0.42
2:B:875:LEU:HG	2:B:909:VAL:HG11	2.01	0.42
2:B:865:VAL:HG11	2:B:915:ALA:HB1	2.01	0.42
2:E:768:ASP:O	2:E:769:GLU:HB3	2.20	0.42
3:F:1666:ASN:ND2	3:F:1694:ASP:OD2	2.47	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:1643:PHE:CZ	3:F:1677:LEU:HB2	2.55	0.41
3:C:1510:ARG:HG2	3:C:1510:ARG:H	1.66	0.41
2:B:1068:ALA:HB3	2:B:1069:TRP:CE3	2.54	0.41
2:B:1108:LEU:HD11	2:B:1168:VAL:HG22	2.01	0.41
1:A:149:ILE:HA	1:A:232:GLU:O	2.21	0.41
1:A:571:LEU:HD22	2:B:812:SER:HB2	2.03	0.41
3:F:1616:PHE:CE1	3:F:1621:PRO:HD2	2.55	0.41
1:D:571:LEU:HD22	2:E:812:SER:HB2	2.02	0.41
1:A:74:PHE:HB3	1:A:85:LEU:HD11	2.03	0.40
1:D:20:LYS:HB2	1:D:21:PRO:CD	2.51	0.40
3:C:1521:HIS:CE1	3:C:1523:LEU:HG	2.55	0.40
2:E:995:LEU:HD22	2:E:996:SER:H	1.86	0.40
3:F:1471:CYS:C	3:F:1472:ILE:HD12	2.42	0.40
1:D:510:LEU:HD11	1:D:652:LEU:HG	2.03	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1336:ARG:NH2	3:F:1695:LEU:O[2_555]	2.08	0.12
1:A:155:ARG:NH1	3:F:1634:GLU:OE2[2_555]	2.11	0.09

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	649/656 (99%)	623 (96%)	25 (4%)	1 (0%)	47 81
1	D	649/656 (99%)	626 (96%)	23 (4%)	0	100 100
2	B	628/690 (91%)	579 (92%)	48 (8%)	1 (0%)	47 81
2	E	628/690 (91%)	598 (95%)	30 (5%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	279/291 (96%)	260 (93%)	19 (7%)	0	100	100
3	F	279/291 (96%)	260 (93%)	19 (7%)	0	100	100
All	All	3112/3274 (95%)	2946 (95%)	164 (5%)	2 (0%)	51	84

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	60	ASN
2	B	965	ASP

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	557/562 (99%)	545 (98%)	12 (2%)	52	78
1	D	557/562 (99%)	544 (98%)	13 (2%)	50	77
2	B	524/575 (91%)	508 (97%)	16 (3%)	40	70
2	E	524/575 (91%)	513 (98%)	11 (2%)	53	79
3	C	240/249 (96%)	232 (97%)	8 (3%)	38	68
3	F	240/249 (96%)	234 (98%)	6 (2%)	47	75
All	All	2642/2772 (95%)	2576 (98%)	66 (2%)	47	75

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	130	ILE
1	A	143	LEU
1	A	160	VAL
1	A	223	LEU
1	A	235	LYS
1	A	314	LEU
1	A	375	LYS
1	A	409	VAL

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Mol	Chain	Res	Type
1	A	493	LEU
1	A	527	THR
1	A	529	VAL
1	A	551	ASP
2	B	759	GLU
2	B	783	LEU
2	B	796	THR
2	B	888	LEU
2	B	895	ARG
2	B	965	ASP
2	B	992	GLU
2	B	1031	THR
2	B	1166	GLN
2	B	1176	ASN
2	B	1228	LEU
2	B	1281	MET
2	B	1304	ASP
2	B	1344	LEU
2	B	1346	LEU
2	B	1373	ASN
3	C	1529	VAL
3	C	1548	LEU
3	C	1564	ARG
3	C	1594	LYS
3	C	1629	VAL
3	C	1633	ARG
3	C	1653	PHE
3	C	1674	ARG
1	D	52	VAL
1	D	80	ARG
1	D	121	LEU
1	D	130	ILE
1	D	143	LEU
1	D	160	VAL
1	D	223	LEU
1	D	360	TRP
1	D	409	VAL
1	D	475	ILE
1	D	482	PRO
1	D	526	LEU
1	D	660	TRP
2	E	766	LEU

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Mol	Chain	Res	Type
2	E	811	LEU
2	E	832	GLU
2	E	836	HIS
2	E	895	ARG
2	E	995	LEU
2	E	1176	ASN
2	E	1191	HIS
2	E	1283	ASP
2	E	1351	ILE
2	E	1390	LYS
3	F	1487	ASP
3	F	1548	LEU
3	F	1598	GLN
3	F	1629	VAL
3	F	1633	ARG
3	F	1674	ARG

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

Mol	Chain	Res	Type
1	A	65	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

4 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	$\# Z > 2$
4	NAG	A	1801	1	14,14,15	0.41	0	17,19,21	0.44	0
4	NAG	D	1801	1	14,14,15	0.38	0	17,19,21	0.40	0
4	NAG	E	1501	2	14,14,15	0.46	0	17,19,21	0.43	0
4	NAG	B	1501	2	14,14,15	0.55	0	17,19,21	0.47	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	NAG	A	1801	1	-	0/6/23/26	0/1/1/1
4	NAG	D	1801	1	-	0/6/23/26	0/1/1/1
4	NAG	E	1501	2	-	0/6/23/26	0/1/1/1
4	NAG	B	1501	2	-	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.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	651/656 (99%)	-0.20	8 (1%) 79 73	42, 108, 160, 194	0
1	D	651/656 (99%)	-0.29	3 (0%) 91 88	51, 93, 137, 177	0
2	B	632/690 (91%)	0.24	45 (7%) 16 15	42, 156, 239, 275	0
2	E	632/690 (91%)	-0.04	17 (2%) 54 48	77, 124, 180, 246	0
3	C	281/291 (96%)	0.05	9 (3%) 47 42	59, 120, 190, 225	0
3	F	281/291 (96%)	-0.03	6 (2%) 63 58	93, 130, 186, 219	0
All	All	3128/3274 (95%)	-0.06	88 (2%) 53 47	42, 115, 200, 275	0

All (88) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	F	1605	GLY	9.0
3	C	1744	VAL	6.7
2	B	1176	ASN	5.1
2	B	1179	LEU	5.1
3	C	1619	TYR	4.6
2	B	1348	ASN	4.6
2	B	1229	TYR	4.5
2	B	1322	THR	4.5
2	E	986	LEU	4.4
2	E	951	LEU	4.2
2	B	757	ALA	4.1
2	B	1296	GLN	4.1
2	B	987	ASP	4.0
2	E	1378	LEU	3.9
3	F	1478	VAL	3.9
2	E	953	HIS	3.8
2	B	1130	GLY	3.8
1	A	526	LEU	3.8
2	B	1271	HIS	3.7

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Mol	Chain	Res	Type	RSRZ
2	E	1341	SER	3.6
2	B	1131	GLY	3.6
2	B	1268	ALA	3.5
2	B	1228	LEU	3.4
3	C	1607	GLN	3.4
3	F	1479	GLY	3.3
2	B	1372	GLY	3.2
2	B	1223	GLU	3.2
3	C	1706	ASN	3.2
3	F	1606	LEU	3.1
2	B	1066	TYR	3.1
2	B	1193	ALA	3.1
3	F	1607	GLN	3.0
2	E	1354	LEU	3.0
2	B	1224	THR	2.9
2	B	1220	MET	2.9
1	A	670	PRO	2.8
2	E	1352	ARG	2.8
2	B	1180	GLY	2.8
2	B	990	GLY	2.7
2	B	1189	GLY	2.7
2	E	987	ASP	2.7
2	E	1330	THR	2.7
2	B	1126	ARG	2.7
3	F	1609	GLU	2.6
2	B	1129	GLN	2.6
3	C	1676	ARG	2.5
2	B	1115	GLY	2.5
2	B	1208	ASP	2.5
2	B	1344	LEU	2.5
2	E	1342	HIS	2.5
2	B	1346	LEU	2.5
2	B	1354	LEU	2.4
2	E	1350	GLN	2.4
2	B	1218	MET	2.4
2	B	1380	VAL	2.4
1	A	435	ILE	2.4
3	C	1614	MET	2.4
1	A	454	HIS	2.3
2	E	1355	GLU	2.3
1	A	505	TYR	2.3
3	C	1743	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	369	LEU	2.3
2	B	1360	PHE	2.3
2	E	1336	ARG	2.3
1	D	665	LYS	2.3
2	B	986	LEU	2.2
2	B	1161	ALA	2.2
2	B	1340	LYS	2.2
3	C	1627	PHE	2.2
2	E	1153	LEU	2.2
2	B	1341	SER	2.2
2	B	1328	ASN	2.1
2	E	943	GLU	2.1
2	B	1132	LEU	2.1
2	B	1196	THR	2.1
2	E	944	LEU	2.1
2	B	1143	ALA	2.1
1	A	293	LYS	2.1
3	C	1658	LYS	2.1
2	B	1188	LEU	2.1
2	B	1371	GLY	2.1
1	D	576	ASP	2.1
2	B	1227	ASN	2.1
2	B	1378	LEU	2.1
2	E	952	ASP	2.0
1	A	462	VAL	2.0
1	D	467	SER	2.0
2	B	1104	SER	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 monosaccharides 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(\AA^2)	Q<0.9
4	NAG	A	1801	14/15	0.76	0.41	90,148,184,193	0
4	NAG	D	1801	14/15	0.82	0.26	132,158,172,184	0
4	NAG	B	1501	14/15	0.84	0.27	124,143,158,158	0
4	NAG	E	1501	14/15	0.85	0.19	142,159,173,178	0

6.5 Other polymers [i](#)

There are no such residues in this entry.