



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:43 PM GMT

PDB ID : 4FXK  
Title : Human complement C4  
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Deposited on : 2012-07-03  
Resolution : 3.60 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

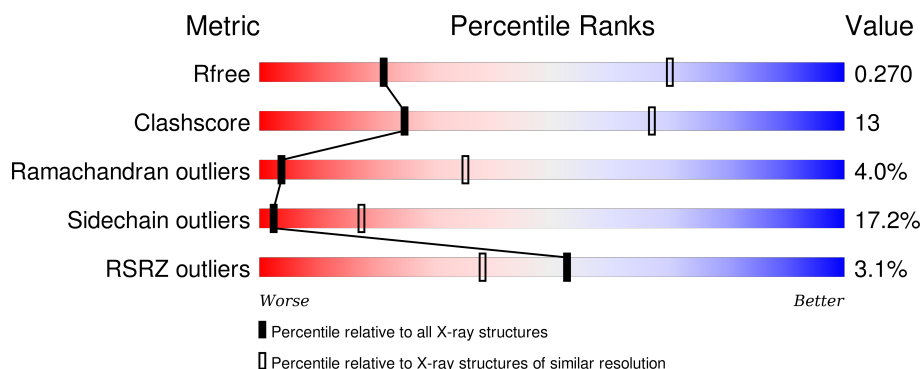
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.60 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))
$R_{free}$	91344	1408 (3.80-3.40)
Clashscore	102246	1010 (3.74-3.46)
Ramachandran outliers	100387	1007 (3.76-3.44)
Sidechain outliers	100360	1007 (3.76-3.44)
RSRZ outliers	91569	1003 (3.78-3.42)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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>4%</div> <div>63%</div> <div>29%</div> <div>7%</div> <div>•</div> </div>
2	B	767	<div> <div>2%</div> <div>54%</div> <div>30%</div> <div>7%</div> <div>9%</div> <div>•</div> </div>
3	C	291	<div> <div>%</div> <div>62%</div> <div>27%</div> <div>10%</div> <div>•</div> </div>

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 12794 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 Beta chain.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	697	Total	C	N	O	S	0	0	0
			5361	3371	943	1023	24			

- Molecule 3 is a protein called Complement C4 gamma chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	290	Total	C	N	O	S	0	0	0
			2312	1451	411	433	17			

- Molecule 4 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



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

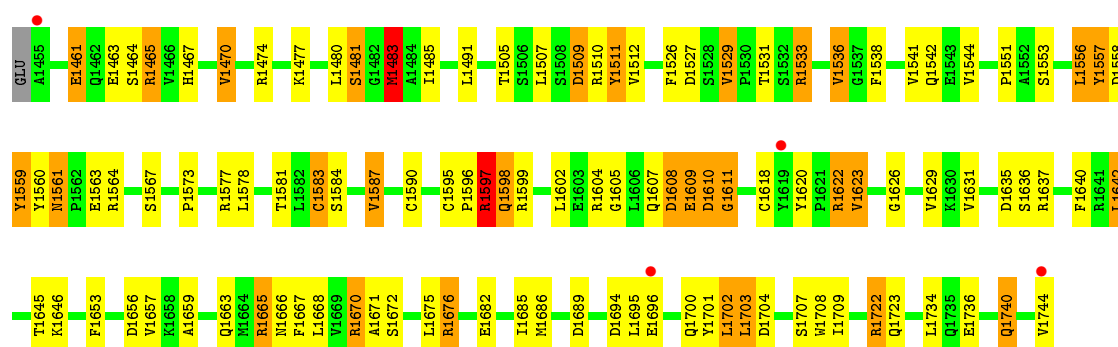
- Molecule 5 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	2	Total	C	N	O	0	0
			28	16	2	10		
5	B	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 6 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	B	3	Total	C	N	O	0	0
			39	22	2	15		





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	85.45Å 103.31Å 256.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.90 – 3.60 45.90 – 3.60	Depositor EDS
% Data completeness (in resolution range)	99.6 (45.90-3.60) 99.7 (45.90-3.60)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.48 (at 3.57Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, $R_{free}$	0.200 , 0.269 0.202 , 0.270	Depositor DCC
$R_{free}$ test set	1347 reflections (5.00%)	DCC
Wilson B-factor (Å <sup>2</sup> )	113.2	Xtriage
Anisotropy	0.501	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 98.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 26955 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	12794	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	131.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.66% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: BMA, 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	0/5128	0.56	1/6961 (0.0%)
2	B	0.26	0/5472	0.54	0/7436
3	C	0.26	0/2360	0.54	0/3188
All	All	0.27	0/12960	0.55	1/17585 (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	3

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	102	LEU	CA-CB-CG	5.23	127.33	115.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	477	ARG	Peptide
1	A	666	ARG	Peptide
1	A	669	CYS	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	120	0
2	B	5361	0	5311	158	0
3	C	2312	0	2253	65	0
4	A	14	0	13	0	0
5	B	56	0	50	0	0
6	B	39	0	34	1	0
All	All	12794	0	12686	326	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 13.

All (326) 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:124:THR:HG22	1:A:126:ASN:H	1.41	0.85
1:A:252:ILE:HB	1:A:362:PHE:HB3	1.59	0.82
1:A:287:LEU:H	1:A:339:TYR:HA	1.44	0.82
1:A:669:CYS:HB2	1:A:670:PRO:HD2	1.63	0.81
2:B:1336:ARG:HD3	2:B:1359:GLN:HB3	1.62	0.81
1:A:425:THR:HG23	1:A:431:VAL:HB	1.62	0.79
2:B:1022:LEU:HD21	2:B:1089:ALA:HB2	1.66	0.77
1:A:408:THR:HB	1:A:445:GLN:HG3	1.69	0.74
2:B:1327:LEU:HA	2:B:1370:VAL:HG13	1.70	0.73
2:B:965:ASP:HB3	2:B:966:PRO:HD2	1.70	0.72
1:A:368:SER:HB2	1:A:391:ARG:HG3	1.71	0.72
2:B:950:PRO:HG3	2:B:1370:VAL:HB	1.72	0.71
2:B:1335:GLY:HA3	2:B:1359:GLN:HB2	1.73	0.71
2:B:1031:THR:HG23	2:B:1033:GLN:HG3	1.72	0.70
1:A:24:LEU:HD21	1:A:548:TYR:HE1	1.56	0.69
2:B:994:ALA:HA	2:B:1000:VAL:HG23	1.74	0.68
3:C:1686:MET:HG3	3:C:1708:TRP:HB3	1.76	0.68
2:B:980:VAL:HG22	2:B:1380:VAL:HG22	1.76	0.68
2:B:907:ALA:H	2:B:933:ILE:HG13	1.59	0.67
2:B:1351:ILE:HG23	2:B:1354:LEU:HB3	1.76	0.67
3:C:1703:LEU:HG	3:C:1709:ILE:HD11	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1207:VAL:HA	2:B:1210:LEU:HD12	1.76	0.66
2:B:961:PRO:HB3	2:B:1365:LYS:HD3	1.79	0.65
2:B:1010:CYS:SG	2:B:1013:GLN:N	2.67	0.65
1:A:544:VAL:HG12	1:A:557:SER:HB3	1.78	0.65
2:B:949:ASN:HB3	2:B:953:HIS:CD2	2.32	0.65
1:A:162:ALA:HB3	1:A:193:MET:HE1	1.79	0.64
1:A:571:LEU:HD12	2:B:822:ALA:HB2	1.77	0.64
1:A:609:TYR:HE2	1:A:616:HIS:HB2	1.62	0.64
2:B:1227:ASN:ND2	2:B:1254:MET:SD	2.70	0.64
1:A:323:LEU:HD13	1:A:330:ILE:HG12	1.78	0.64
2:B:970:PRO:HB3	2:B:1388:ASP:H	1.63	0.64
2:B:726:PRO:HA	2:B:729:ARG:HB3	1.79	0.64
1:A:444:LEU:HB3	1:A:462:VAL:HB	1.81	0.63
1:A:375:LYS:HD3	1:A:377:HIS:HD2	1.64	0.63
2:B:1149:LEU:HB2	2:B:1172:ILE:HD11	1.81	0.63
1:A:475:ILE:HD11	1:A:545:ALA:HB3	1.80	0.62
1:A:374:THR:H	1:A:387:GLN:HG3	1.63	0.62
1:A:644:LEU:HD11	1:A:659:GLN:HB3	1.81	0.61
6:B:1807:BMA:O2	3:C:1696:GLU:HA	1.99	0.61
2:B:921:PHE:HB3	2:B:923:VAL:HG23	1.82	0.61
2:B:1327:LEU:HD12	2:B:1370:VAL:HG11	1.83	0.61
1:A:148:PRO:HG2	1:A:149:ILE:HD12	1.82	0.60
1:A:409:VAL:HG13	1:A:441:ILE:HD12	1.83	0.60
1:A:218:ARG:HB2	1:A:225:SER:HB2	1.83	0.60
3:C:1666:ASN:HB2	3:C:1700:GLN:HG2	1.84	0.59
2:B:953:HIS:CD2	2:B:957:THR:HB	2.38	0.59
2:B:1261:TRP:O	2:B:1265:THR:HG22	2.03	0.59
2:B:978:VAL:HG13	2:B:1360:PHE:CD2	2.38	0.58
1:A:288:ASP:HB2	1:A:292:LYS:HG3	1.85	0.58
2:B:710:LEU:HD13	3:C:1507:LEU:HD12	1.85	0.58
1:A:100:HIS:HE1	1:A:103:LEU:HB3	1.69	0.58
1:A:130:ILE:HG23	1:A:655:SER:HB2	1.85	0.58
2:B:1124:LEU:HD21	2:B:1126:ARG:HH21	1.67	0.58
1:A:617:LYS:HD2	1:A:623:LYS:HE3	1.84	0.58
1:A:576:ASP:HB3	1:A:588:LYS:HB2	1.86	0.58
2:B:775:ARG:NH1	2:B:777:PHE:O	2.37	0.58
1:A:147:GLN:HG3	1:A:148:PRO:HD2	1.86	0.58
3:C:1637:ARG:HG3	3:C:1642:LEU:HD23	1.85	0.57
1:A:336:LEU:HD13	1:A:337:ARG:HH11	1.69	0.57
1:A:286:LEU:N	1:A:294:THR:O	2.27	0.57
1:A:110:LEU:HB2	1:A:132:LEU:HD11	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:101:GLN:HB3	1:A:223:LEU:HD13	1.87	0.57
2:B:1334:THR:HG22	2:B:1339:PHE:HD1	1.70	0.57
2:B:1389:MET:HE2	3:C:1567:SER:HB2	1.86	0.56
1:A:439:GLN:OE1	1:A:439:GLN:N	2.38	0.56
3:C:1597:ARG:NE	3:C:1599:ARG:HH21	2.02	0.56
1:A:477:ARG:HE	1:A:489:LEU:HD11	1.71	0.56
2:B:791:ARG:O	2:B:792:PHE:HB3	2.04	0.56
2:B:955:GLY:HA2	2:B:958:LEU:HB2	1.88	0.56
2:B:1337:ASN:HB2	2:B:1359:GLN:HE21	1.71	0.56
1:A:446:LEU:HB3	1:A:460:LEU:HB3	1.88	0.56
2:B:1267:TYR:HA	2:B:1270:LEU:HD12	1.87	0.56
2:B:1083:LEU:O	2:B:1087:SER:HB3	2.05	0.56
2:B:1090:GLN:HG3	2:B:1155:VAL:HG13	1.88	0.56
3:C:1465:ARG:HB3	3:C:1541:VAL:HG12	1.88	0.56
1:A:379:VAL:HB	1:A:382:ALA:HB3	1.88	0.55
1:A:238:LEU:HD12	1:A:239:PRO:HD2	1.88	0.55
1:A:124:THR:HB	1:A:127:ILE:HG23	1.87	0.55
2:B:941:ARG:HG3	2:B:1383:THR:HB	1.87	0.55
1:A:253:LEU:HD21	1:A:454:HIS:NE2	2.20	0.55
2:B:989:LEU:HD11	2:B:1351:ILE:HB	1.87	0.55
2:B:1244:THR:CG2	2:B:1245:PRO:HD2	2.37	0.55
1:A:296:PHE:HD2	1:A:299:LEU:H	1.54	0.55
3:C:1631:VAL:HA	3:C:1645:THR:HG22	1.88	0.55
2:B:948:LEU:HD11	2:B:1378:LEU:HB2	1.89	0.54
3:C:1656:ASP:CG	3:C:1659:ALA:HB2	2.28	0.54
2:B:1272:LEU:HD11	2:B:1281:MET:HB2	1.89	0.54
1:A:669:CYS:HB2	1:A:670:PRO:CD	2.35	0.54
1:A:150:TYR:CZ	1:A:156:VAL:HB	2.42	0.54
2:B:1328:ASN:HB2	2:B:1369:LYS:O	2.07	0.53
2:B:843:VAL:HB	2:B:933:ILE:HG22	1.90	0.53
1:A:473:LEU:HB2	1:A:547:TYR:HE2	1.73	0.53
3:C:1559:TYR:HD2	3:C:1560:TYR:H	1.54	0.53
2:B:1287:ALA:O	2:B:1291:ARG:HG2	2.09	0.53
3:C:1558:ASP:OD1	3:C:1561:ASN:ND2	2.41	0.53
3:C:1676:ARG:HD3	3:C:1676:ARG:H	1.73	0.53
1:A:117:LEU:O	1:A:121:LEU:HB2	2.07	0.53
2:B:953:HIS:HB3	2:B:956:ARG:HB2	1.91	0.53
1:A:407:ALA:HB3	1:A:419:GLN:HB2	1.90	0.53
1:A:484:ARG:O	1:A:486:GLY:N	2.41	0.52
2:B:1346:LEU:HD22	2:B:1349:ARG:HH21	1.74	0.52
2:B:1126:ARG:NH2	2:B:1263:GLU:OE1	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1105:ASN:OD1	2:B:1167:ARG:NH2	2.43	0.52
2:B:703:CYS:HB2	2:B:731:PRO:HB2	1.92	0.52
1:A:578:ALA:HB3	1:A:587:VAL:HA	1.91	0.52
3:C:1485:ILE:HB	3:C:1557:TYR:CE2	2.45	0.52
1:A:336:LEU:HD12	1:A:336:LEU:H	1.75	0.52
3:C:1509:ASP:OD1	3:C:1509:ASP:N	2.35	0.52
2:B:722:ARG:HG2	3:C:1510:ARG:H	1.75	0.52
2:B:951:LEU:HD13	2:B:1373:ASN:HD22	1.75	0.52
3:C:1702:LEU:HD22	3:C:1703:LEU:H	1.74	0.52
3:C:1583:CYS:HB2	3:C:1587:VAL:HG22	1.91	0.51
2:B:890:PRO:HB2	2:B:893:SER:HB3	1.93	0.51
2:B:1327:LEU:HD22	2:B:1376:GLY:HA3	1.93	0.51
3:C:1604:ARG:HD3	3:C:1608:ASP:HA	1.92	0.51
1:A:338:LEU:HA	1:A:361:TYR:HA	1.92	0.51
2:B:977:TYR:CE1	2:B:1357:GLU:HG3	2.46	0.51
2:B:1325:ARG:HB3	2:B:1374:SER:HB3	1.92	0.51
2:B:1265:THR:HG21	2:B:1288:TRP:CZ3	2.46	0.51
2:B:1312:LEU:HD12	2:B:1316:TRP:CZ2	2.46	0.51
2:B:950:PRO:HG3	2:B:1370:VAL:CB	2.39	0.50
3:C:1609:GLU:O	3:C:1611:GLY:N	2.37	0.50
3:C:1477:LYS:HE2	3:C:1531:THR:HB	1.93	0.50
2:B:1027:TYR:HA	2:B:1317:ILE:HG12	1.92	0.50
1:A:509:ILE:HG13	1:A:517:PHE:HB3	1.94	0.50
2:B:1370:VAL:HG12	2:B:1371:GLY:H	1.76	0.50
2:B:965:ASP:OD2	2:B:978:VAL:HG11	2.11	0.50
1:A:642:SER:OG	1:A:643:ALA:N	2.43	0.50
2:B:1100:LEU:HD12	2:B:1155:VAL:HG11	1.92	0.50
3:C:1463:GLU:OE1	3:C:1464:SER:N	2.41	0.50
1:A:507:TYR:CZ	1:A:519:ASN:HB3	2.46	0.50
1:A:33:LEU:HD21	1:A:134:PHE:CE2	2.47	0.50
1:A:641:ASP:N	1:A:641:ASP:OD1	2.44	0.50
3:C:1598:GLN:O	3:C:1676:ARG:NH1	2.45	0.49
2:B:1397:LEU:HD12	3:C:1564:ARG:O	2.12	0.49
2:B:1066:TYR:CZ	2:B:1082:VAL:HG11	2.48	0.49
2:B:984:ASP:HB3	2:B:1346:LEU:HB2	1.93	0.49
1:A:151:ASN:ND2	1:A:154:GLN:OE1	2.44	0.49
1:A:414:SER:O	1:A:415:VAL:HB	2.13	0.49
3:C:1623:VAL:HG21	3:C:1686:MET:HB2	1.94	0.49
1:A:546:PHE:HB3	1:A:555:ALA:HB2	1.95	0.49
1:A:140:HIS:NE2	1:A:628:MET:HA	2.26	0.49
3:C:1505:THR:O	3:C:1510:ARG:NH2	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1208:ASP:O	2:B:1212:VAL:HG13	2.13	0.49
1:A:144:GLN:HG3	1:A:159:ARG:HD3	1.95	0.49
1:A:524:ARG:HE	1:A:527:THR:HG23	1.78	0.49
2:B:843:VAL:O	2:B:933:ILE:HA	2.13	0.49
2:B:992:GLU:O	2:B:996:SER:N	2.46	0.49
2:B:985:PRO:O	2:B:989:LEU:HB2	2.13	0.48
3:C:1663:GLN:OE1	3:C:1665:ARG:NH2	2.45	0.48
2:B:985:PRO:HD2	2:B:989:LEU:HD23	1.94	0.48
3:C:1526:PHE:HZ	3:C:1536:VAL:HG21	1.77	0.48
3:C:1608:ASP:N	3:C:1608:ASP:OD1	2.46	0.48
1:A:286:LEU:HA	1:A:339:TYR:HB2	1.96	0.48
2:B:1227:ASN:HB3	2:B:1288:TRP:HB2	1.95	0.48
2:B:805:THR:HB	2:B:828:ARG:HD3	1.95	0.48
2:B:966:PRO:HB2	2:B:968:MET:HB2	1.96	0.48
1:A:36:PRO:O	1:A:514:GLN:NE2	2.47	0.48
2:B:875:LEU:HD11	2:B:911:LEU:HD11	1.96	0.48
1:A:185:ARG:H	1:A:185:ARG:HG2	1.44	0.48
2:B:949:ASN:CG	2:B:1375:LYS:HG2	2.34	0.48
2:B:1406:HIS:HB3	3:C:1465:ARG:HG3	1.96	0.48
3:C:1736:GLU:OE2	3:C:1740:GLN:NE2	2.47	0.48
1:A:133:LEU:HD11	1:A:664:ARG:O	2.13	0.48
3:C:1509:ASP:HB2	3:C:1511:TYR:CE1	2.49	0.47
2:B:1370:VAL:HG12	2:B:1371:GLY:N	2.29	0.47
2:B:1403:VAL:HG23	3:C:1573:PRO:HD3	1.96	0.47
2:B:1205:ALA:HB1	2:B:1206:PRO:HD2	1.96	0.47
1:A:223:LEU:O	1:A:224:GLU:HG2	2.14	0.47
1:A:253:LEU:HD21	1:A:454:HIS:CE1	2.49	0.47
1:A:163:LEU:HB3	1:A:169:PRO:HA	1.96	0.47
1:A:392:GLU:HB3	1:A:396:SER:C	2.34	0.47
2:B:781:ASN:O	2:B:783:LEU:N	2.46	0.47
1:A:247:PRO:HB3	1:A:360:TRP:CH2	2.50	0.47
2:B:809:HIS:CD2	2:B:824:PRO:HB3	2.49	0.47
2:B:1337:ASN:HB2	2:B:1359:GLN:NE2	2.30	0.47
2:B:1201:SER:HA	2:B:1210:LEU:HD21	1.97	0.47
1:A:606:THR:C	1:A:608:LEU:H	2.18	0.47
2:B:1125:ASP:O	3:C:1480:LEU:HD23	2.15	0.47
2:B:1399:ILE:HB	3:C:1556:LEU:HB2	1.96	0.47
2:B:1150:HIS:CD2	2:B:1202:LEU:HG	2.50	0.47
2:B:992:GLU:OE2	2:B:1352:ARG:NH2	2.48	0.46
1:A:26:PHE:CD2	1:A:654:PHE:HB2	2.49	0.46
2:B:857:ASN:ND2	2:B:891:ALA:HA	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1254:MET:HE1	2:B:1288:TRP:NE1	2.29	0.46
2:B:1244:THR:HG22	2:B:1245:PRO:HD2	1.97	0.46
2:B:1078:LEU:O	2:B:1082:VAL:HG23	2.15	0.46
2:B:1038:PRO:O	2:B:1041:THR:HG22	2.15	0.46
3:C:1480:LEU:HD12	3:C:1564:ARG:NH1	2.31	0.46
1:A:296:PHE:HD2	1:A:299:LEU:N	2.13	0.46
2:B:789:VAL:HG13	2:B:793:GLN:HB2	1.96	0.46
2:B:1217:LEU:HD22	2:B:1230:TRP:CZ3	2.50	0.46
2:B:969:ILE:HB	2:B:970:PRO:HD3	1.97	0.46
3:C:1609:GLU:H	3:C:1609:GLU:HG2	1.55	0.46
1:A:146:ASP:O	1:A:604:LEU:HD21	2.16	0.46
2:B:1397:LEU:HD23	2:B:1397:LEU:HA	1.83	0.46
1:A:559:ARG:NH1	1:A:637:PRO:HA	2.31	0.46
2:B:847:GLU:O	2:B:903:PRO:HD2	2.17	0.45
1:A:375:LYS:HD3	1:A:377:HIS:CD2	2.49	0.45
3:C:1467:HIS:HD2	3:C:1538:PHE:O	1.98	0.45
2:B:1255:PRO:O	2:B:1292:GLN:NE2	2.50	0.45
1:A:664:ARG:HA	1:A:664:ARG:HD2	1.72	0.45
2:B:1001:ALA:HB2	2:B:1016:ILE:HG23	1.97	0.45
2:B:868:HIS:CE1	2:B:914:VAL:HB	2.51	0.45
1:A:143:LEU:HB2	1:A:229:THR:OG1	2.17	0.45
2:B:970:PRO:HB2	2:B:1386:VAL:HG13	1.97	0.45
3:C:1483:MET:N	3:C:1527:ASP:O	2.50	0.45
2:B:965:ASP:HB2	2:B:1361:SER:O	2.17	0.45
2:B:973:ASP:OD2	3:C:1702:LEU:HG	2.17	0.45
2:B:1126:ARG:HD2	2:B:1260:LEU:HD13	1.97	0.45
3:C:1602:LEU:HD13	3:C:1723:GLN:HB3	1.99	0.45
2:B:1176:ASN:OD1	2:B:1205:ALA:HB2	2.17	0.45
2:B:833:PHE:HE1	2:B:855:LEU:HD22	1.82	0.45
3:C:1740:GLN:O	3:C:1744:VAL:HA	2.17	0.45
2:B:1124:LEU:HD21	2:B:1126:ARG:NH2	2.30	0.45
1:A:57:PHE:HB3	1:A:71:LYS:HA	1.99	0.45
1:A:388:ALA:HB3	1:A:431:VAL:HG12	2.00	0.44
1:A:571:LEU:HA	1:A:571:LEU:HD22	1.81	0.44
2:B:1401:VAL:HG22	3:C:1470:VAL:HG22	1.99	0.44
2:B:1080:ALA:HA	2:B:1107:LEU:HD21	1.99	0.44
1:A:625:PHE:O	1:A:628:MET:HG2	2.17	0.44
2:B:1162:GLU:HG3	2:B:1165:LYS:HD3	2.00	0.44
2:B:710:LEU:HA	2:B:710:LEU:HD12	1.79	0.44
1:A:22:ARG:NH1	1:A:658:ASP:OD2	2.36	0.44
2:B:1379:LYS:HB3	2:B:1379:LYS:HE2	1.75	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:336:LEU:HD13	1:A:337:ARG:NH1	2.32	0.44
2:B:1008:ARG:HD3	2:B:1008:ARG:N	2.33	0.44
2:B:955:GLY:H	2:B:958:LEU:HD12	1.82	0.44
2:B:1269:LEU:HD12	2:B:1311:ALA:HB1	1.99	0.44
1:A:252:ILE:HD12	1:A:362:PHE:HD2	1.83	0.44
1:A:33:LEU:HD13	1:A:33:LEU:HA	1.86	0.44
1:A:484:ARG:HG2	1:A:563:GLN:HE22	1.82	0.44
1:A:411:SER:HA	1:A:412:PRO:HD2	1.76	0.44
2:B:986:LEU:HD21	2:B:1377:THR:HB	2.00	0.44
1:A:487:ASP:O	1:A:533:VAL:HG22	2.18	0.44
3:C:1667:PHE:CD2	3:C:1701:TYR:HB2	2.53	0.44
2:B:949:ASN:ND2	2:B:952:ASP:HB2	2.33	0.43
2:B:853:PRO:HD2	2:B:897:VAL:O	2.18	0.43
2:B:1327:LEU:HB3	2:B:1346:LEU:HD12	2.00	0.43
2:B:1368:VAL:O	2:B:1370:VAL:HG23	2.18	0.43
2:B:1070:LEU:HA	2:B:1070:LEU:HD22	1.81	0.43
2:B:697:PRO:HB2	2:B:698:THR:H	1.54	0.43
2:B:1180:GLY:HA3	2:B:1209:LEU:HG	2.01	0.43
1:A:608:LEU:HD23	1:A:609:TYR:N	2.33	0.43
1:A:330:ILE:HG13	1:A:330:ILE:H	1.49	0.43
2:B:1360:PHE:HZ	2:B:1384:TYR:CD2	2.37	0.43
3:C:1629:VAL:O	3:C:1682:GLU:HA	2.18	0.43
3:C:1702:LEU:HD22	3:C:1703:LEU:N	2.34	0.43
3:C:1604:ARG:HG2	3:C:1605:GLY:H	1.83	0.43
1:A:35:VAL:HG13	1:A:165:GLN:HG3	2.00	0.43
1:A:210:PRO:HB3	1:A:234:LYS:HA	2.01	0.43
1:A:656:ASP:OD1	1:A:656:ASP:N	2.49	0.43
2:B:968:MET:SD	2:B:970:PRO:HD2	2.59	0.43
2:B:1162:GLU:HG3	2:B:1165:LYS:HB3	1.99	0.43
1:A:155:ARG:HB2	1:A:155:ARG:HE	1.80	0.43
2:B:1119:ASP:HA	2:B:1120:PRO:HD2	1.87	0.43
1:A:487:ASP:OD1	1:A:487:ASP:N	2.52	0.43
1:A:33:LEU:HD23	1:A:136:SER:HA	2.00	0.43
3:C:1646:LYS:HE2	3:C:1646:LYS:HB3	1.80	0.43
2:B:868:HIS:HB3	2:B:884:ALA:HB2	2.01	0.42
3:C:1474:ARG:NH1	3:C:1529:VAL:O	2.51	0.42
1:A:268:ALA:HB2	1:A:345:ILE:HD13	2.01	0.42
3:C:1597:ARG:HE	3:C:1599:ARG:HH21	1.66	0.42
1:A:563:GLN:O	1:A:565:GLY:N	2.52	0.42
2:B:830:PHE:O	2:B:830:PHE:HD1	2.01	0.42
2:B:1360:PHE:HA	2:B:1360:PHE:HD2	1.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1206:PRO:HG2	2:B:1209:LEU:HD22	2.00	0.42
1:A:415:VAL:HG13	1:A:416:PRO:HD2	2.02	0.42
2:B:871:PRO:HG3	2:B:881:GLY:HA3	2.01	0.42
2:B:845:ARG:NH1	2:B:936:GLU:OE1	2.52	0.42
2:B:1360:PHE:HB3	2:B:1361:SER:H	1.60	0.42
2:B:953:HIS:HB3	2:B:957:THR:H	1.84	0.42
2:B:977:TYR:HB2	2:B:1358:LEU:O	2.20	0.42
1:A:302:GLN:HG3	1:A:302:GLN:O	2.20	0.42
3:C:1667:PHE:CZ	3:C:1685:ILE:HD11	2.54	0.42
2:B:870:SER:HA	2:B:871:PRO:HD3	1.87	0.42
2:B:974:PHE:HE2	3:C:1640:PHE:HE1	1.68	0.42
1:A:411:SER:HB2	1:A:414:SER:OG	2.20	0.42
1:A:376:ARG:HD2	1:A:376:ARG:N	2.35	0.42
2:B:1258:PRO:HA	3:C:1563:GLU:HG3	2.02	0.42
2:B:778:PHE:HA	2:B:779:PRO:HD3	1.94	0.42
1:A:117:LEU:HG	1:A:121:LEU:HD12	2.02	0.41
1:A:169:PRO:HG3	2:B:815:LYS:HD3	2.01	0.41
2:B:738:PHE:O	2:B:742:LEU:HG	2.20	0.41
1:A:605:ASP:OD2	1:A:606:THR:N	2.54	0.41
1:A:606:THR:O	1:A:608:LEU:N	2.50	0.41
2:B:720:ALA:O	2:B:723:VAL:HG22	2.20	0.41
2:B:1400:GLU:OE2	3:C:1533:ARG:NH1	2.53	0.41
1:A:106:PRO:HG2	1:A:134:PHE:HB3	2.02	0.41
2:B:1207:VAL:O	2:B:1210:LEU:HB2	2.20	0.41
1:A:136:SER:OG	1:A:223:LEU:HD12	2.20	0.41
2:B:1086:LEU:HB3	2:B:1100:LEU:HD21	2.02	0.41
1:A:274:LYS:HD2	1:A:275:PRO:HD2	2.03	0.41
1:A:296:PHE:HE1	1:A:325:LYS:HB3	1.84	0.41
3:C:1583:CYS:SG	3:C:1584:SER:N	2.94	0.41
1:A:38:SER:OG	1:A:514:GLN:HG3	2.20	0.41
2:B:920:GLU:HG2	2:B:921:PHE:CD1	2.55	0.41
1:A:100:HIS:CE1	1:A:103:LEU:HB3	2.53	0.41
3:C:1480:LEU:HD22	3:C:1481:SER:N	2.35	0.41
1:A:509:ILE:O	1:A:516:VAL:HG13	2.21	0.41
1:A:296:PHE:CD1	1:A:322:ALA:HA	2.56	0.41
1:A:407:ALA:HB2	1:A:435:ILE:HD13	2.03	0.41
2:B:1289:LEU:HD12	2:B:1312:LEU:CD2	2.51	0.41
1:A:654:PHE:H	1:A:661:THR:HG1	1.65	0.41
2:B:1221:ALA:HB2	2:B:1230:TRP:CH2	2.56	0.41
2:B:986:LEU:HD22	2:B:1290:THR:HG23	2.03	0.41
1:A:21:PRO:HA	1:A:45:ASP:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:835:LEU:HD11	2:B:853:PRO:HB3	2.03	0.41
2:B:1042:LYS:O	2:B:1046:VAL:HG12	2.21	0.41
2:B:919:PHE:O	2:B:920:GLU:HB3	2.20	0.40
2:B:969:ILE:HD12	3:C:1694:ASP:C	2.42	0.40
3:C:1626:GLY:HA2	3:C:1686:MET:HB3	2.02	0.40
1:A:576:ASP:HB2	1:A:590:HIS:CD2	2.56	0.40
1:A:33:LEU:HB2	1:A:136:SER:HA	2.03	0.40
2:B:1289:LEU:HB3	2:B:1312:LEU:HD21	2.03	0.40
3:C:1704:ASP:O	3:C:1707:SER:HB2	2.21	0.40
2:B:1206:PRO:HB2	2:B:1207:VAL:H	1.69	0.40
3:C:1599:ARG:HH12	3:C:1607:GLN:NE2	2.20	0.40
1:A:392:GLU:HG2	1:A:392:GLU:H	1.55	0.40
3:C:1595:CYS:HB3	3:C:1596:PRO:HD2	2.04	0.40
2:B:948:LEU:HB2	2:B:1376:GLY:C	2.40	0.40
2:B:969:ILE:HG13	3:C:1695:LEU:HD12	2.02	0.40
1:A:295:PHE:CE1	1:A:297:ARG:HG2	2.56	0.40
3:C:1653:PHE:CE2	3:C:1657:VAL:HA	2.57	0.40
3:C:1670:ARG:O	3:C:1672:SER:N	2.45	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	649/656 (99%)	547 (84%)	75 (12%)	27 (4%)	3	33
2	B	693/767 (90%)	587 (85%)	81 (12%)	25 (4%)	4	39
3	C	288/291 (99%)	239 (83%)	35 (12%)	14 (5%)	3	29
All	All	1630/1714 (95%)	1373 (84%)	191 (12%)	66 (4%)	4	35

All (66) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	52	VAL
1	A	412	PRO
1	A	453	PRO
1	A	467	SER
1	A	478	PRO
1	A	564	ALA
2	B	792	PHE
2	B	801	ASP
2	B	961	PRO
2	B	1092	GLN
2	B	1206	PRO
2	B	1243	PRO
2	B	1249	ASN
2	B	1250	PRO
1	A	65	ASN
1	A	228	SER
1	A	275	PRO
1	A	427	GLY
1	A	485	VAL
1	A	606	THR
1	A	667	LEU
2	B	712	MET
2	B	713	MET
2	B	782	TRP
2	B	1218	MET
2	B	1373	ASN
3	C	1483	MET
3	C	1610	ASP
1	A	66	VAL
1	A	102	LEU
1	A	394	SER
1	A	612	GLY
2	B	1347	ASN
2	B	1375	LYS
3	C	1583	CYS
3	C	1740	GLN
1	A	236	TYR
1	A	330	ILE
1	A	415	VAL
1	A	504	HIS
1	A	643	ALA
2	B	985	PRO
2	B	1070	LEU

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Mol	Chain	Res	Type
2	B	1245	PRO
3	C	1512	VAL
3	C	1533	ARG
3	C	1622	ARG
3	C	1722	ARG
1	A	104	ARG
1	A	607	ALA
2	B	724	GLN
2	B	1154	ALA
3	C	1461	GLU
3	C	1597	ARG
3	C	1620	TYR
3	C	1671	ALA
2	B	1093	VAL
3	C	1611	GLY
2	B	1225	GLY
2	B	950	PRO
1	A	363	VAL
2	B	1207	VAL
1	A	49	GLY
1	A	617	LYS
2	B	1162	GLU
3	C	1551	PRO

### 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%)	463 (83%)	94 (17%)	2	18
2	B	581/641 (91%)	479 (82%)	102 (18%)	2	16
3	C	248/249 (100%)	205 (83%)	43 (17%)	2	17
All	All	1386/1452 (96%)	1147 (83%)	239 (17%)	2	17

All (239) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	LYS
1	A	22	ARG
1	A	27	SER
1	A	41	VAL
1	A	50	GLN
1	A	71	LYS
1	A	74	PHE
1	A	79	GLU
1	A	80	ARG
1	A	86	SER
1	A	87	LEU
1	A	91	LEU
1	A	96	SER
1	A	102	LEU
1	A	103	LEU
1	A	104	ARG
1	A	117	LEU
1	A	130	ILE
1	A	134	PHE
1	A	141	LEU
1	A	143	LEU
1	A	155	ARG
1	A	156	VAL
1	A	159	ARG
1	A	160	VAL
1	A	163	LEU
1	A	166	LYS
1	A	173	THR
1	A	185	ARG
1	A	187	ARG
1	A	190	GLU
1	A	206	ASP
1	A	212	THR
1	A	223	LEU
1	A	233	VAL
1	A	242	GLU
1	A	260	ASP
1	A	269	ARG
1	A	277	GLN
1	A	299	LEU
1	A	302	GLN
1	A	303	THR
1	A	304	LYS

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Mol	Chain	Res	Type
1	A	314	LEU
1	A	319	PHE
1	A	330	ILE
1	A	336	LEU
1	A	338	LEU
1	A	344	ILE
1	A	361	TYR
1	A	362	PHE
1	A	363	VAL
1	A	370	ASP
1	A	373	LYS
1	A	379	VAL
1	A	386	LEU
1	A	387	GLN
1	A	391	ARG
1	A	392	GLU
1	A	414	SER
1	A	422	GLN
1	A	439	GLN
1	A	441	ILE
1	A	474	SER
1	A	509	ILE
1	A	510	LEU
1	A	514	GLN
1	A	516	VAL
1	A	517	PHE
1	A	520	ARG
1	A	524	ARG
1	A	530	SER
1	A	552	HIS
1	A	562	VAL
1	A	563	GLN
1	A	567	CYS
1	A	571	LEU
1	A	572	GLU
1	A	574	SER
1	A	576	ASP
1	A	580	GLN
1	A	592	GLU
1	A	594	ASP
1	A	596	LEU
1	A	598	LEU

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Mol	Chain	Res	Type
1	A	608	LEU
1	A	624	VAL
1	A	625	PHE
1	A	635	CYS
1	A	641	ASP
1	A	654	PHE
1	A	655	SER
1	A	661	THR
1	A	669	CYS
2	B	698	THR
2	B	710	LEU
2	B	713	MET
2	B	724	GLN
2	B	725	GLN
2	B	738	PHE
2	B	769	GLU
2	B	771	ASP
2	B	772	ILE
2	B	774	VAL
2	B	775	ARG
2	B	780	GLU
2	B	786	VAL
2	B	802	SER
2	B	805	THR
2	B	813	LEU
2	B	821	VAL
2	B	830	PHE
2	B	831	ARG
2	B	833	PHE
2	B	834	HIS
2	B	838	ARG
2	B	841	MET
2	B	845	ARG
2	B	854	VAL
2	B	860	ASP
2	B	866	SER
2	B	883	LEU
2	B	888	LEU
2	B	919	PHE
2	B	920	GLU
2	B	923	VAL
2	B	931	LEU

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Mol	Chain	Res	Type
2	B	941	ARG
2	B	944	LEU
2	B	968	MET
2	B	976	SER
2	B	979	ARG
2	B	983	SER
2	B	984	ASP
2	B	988	THR
2	B	989	LEU
2	B	992	GLU
2	B	996	SER
2	B	1005	ARG
2	B	1008	ARG
2	B	1013	GLN
2	B	1018	LEU
2	B	1022	LEU
2	B	1030	LYS
2	B	1033	GLN
2	B	1050	GLN
2	B	1055	ARG
2	B	1070	LEU
2	B	1073	ASP
2	B	1087	SER
2	B	1088	LEU
2	B	1090	GLN
2	B	1091	GLU
2	B	1093	VAL
2	B	1104	SER
2	B	1107	LEU
2	B	1108	LEU
2	B	1109	SER
2	B	1112	GLN
2	B	1114	ASP
2	B	1118	GLN
2	B	1124	LEU
2	B	1136	ASP
2	B	1141	LEU
2	B	1153	LEU
2	B	1156	PHE
2	B	1167	ARG
2	B	1168	VAL
2	B	1176	ASN

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Mol	Chain	Res	Type
2	B	1187	LEU
2	B	1212	VAL
2	B	1217	LEU
2	B	1232	SER
2	B	1233	VAL
2	B	1263	GLU
2	B	1272	LEU
2	B	1274	LEU
2	B	1284	GLN
2	B	1289	LEU
2	B	1301	SER
2	B	1304	ASP
2	B	1306	VAL
2	B	1322	THR
2	B	1336	ARG
2	B	1346	LEU
2	B	1348	ASN
2	B	1349	ARG
2	B	1350	GLN
2	B	1360	PHE
2	B	1367	ASN
2	B	1379	LYS
2	B	1388	ASP
2	B	1390	LYS
2	B	1392	THR
2	B	1407	VAL
2	B	1415	GLU
3	C	1461	GLU
3	C	1465	ARG
3	C	1470	VAL
3	C	1481	SER
3	C	1483	MET
3	C	1491	LEU
3	C	1509	ASP
3	C	1511	TYR
3	C	1529	VAL
3	C	1536	VAL
3	C	1542	GLN
3	C	1544	VAL
3	C	1553	SER
3	C	1556	LEU
3	C	1557	TYR

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Mol	Chain	Res	Type
3	C	1559	TYR
3	C	1561	ASN
3	C	1577	ARG
3	C	1578	LEU
3	C	1581	THR
3	C	1587	VAL
3	C	1590	CYS
3	C	1597	ARG
3	C	1598	GLN
3	C	1608	ASP
3	C	1609	GLU
3	C	1610	ASP
3	C	1618	CYS
3	C	1622	ARG
3	C	1623	VAL
3	C	1635	ASP
3	C	1636	SER
3	C	1642	LEU
3	C	1665	ARG
3	C	1668	LEU
3	C	1670	ARG
3	C	1675	LEU
3	C	1676	ARG
3	C	1689	ASP
3	C	1702	LEU
3	C	1703	LEU
3	C	1722	ARG
3	C	1734	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	556	ASN
2	B	857	ASN
2	B	940	HIS
2	B	1176	ASN
2	B	1214	HIS
3	C	1740	GLN

### 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 ⓘ

7 carbohydrates 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	$\# Z  > 2$
5	NAG	B	1801	2,5	14,14,15	0.84	0	15,19,21	1.00	1 (6%)
5	NAG	B	1802	5	14,14,15	0.80	0	15,19,21	0.71	0
5	NAG	B	1803	2,5	14,14,15	0.94	1 (7%)	15,19,21	1.10	2 (13%)
5	NAG	B	1804	5	14,14,15	0.78	0	15,19,21	0.65	0
6	NAG	B	1805	2,6	14,14,15	0.81	0	15,19,21	1.01	1 (6%)
6	NAG	B	1806	6	14,14,15	0.76	0	15,19,21	0.66	0
6	BMA	B	1807	6	11,11,12	0.94	0	14,15,17	1.06	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
5	NAG	B	1801	2,5	-	0/6/23/26	0/1/1/1
5	NAG	B	1802	5	-	0/6/23/26	0/1/1/1
5	NAG	B	1803	2,5	-	0/6/23/26	0/1/1/1
5	NAG	B	1804	5	-	0/6/23/26	0/1/1/1
6	NAG	B	1805	2,6	-	0/6/23/26	0/1/1/1
6	NAG	B	1806	6	-	0/6/23/26	0/1/1/1
6	BMA	B	1807	6	-	0/2/19/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1803	NAG	C1-C2	2.23	1.55	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1803	NAG	O4-C4-C3	-2.65	104.36	110.34
6	B	1805	NAG	C2-N2-C7	-2.29	120.10	123.04
5	B	1801	NAG	C2-N2-C7	-2.16	120.26	123.04
5	B	1803	NAG	C4-C3-C2	2.06	114.44	111.23

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	1807	BMA	1	0

## 5.6 Ligand geometry

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	NAG	A	701	1	14,14,15	0.76	0	15,19,21	0.88	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	701	1	-	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	651/656 (99%)	0.16	28 (4%) 39 27	76, 132, 198, 242	0
2	B	697/767 (90%)	0.11	19 (2%) 58 43	69, 120, 186, 240	0
3	C	290/291 (99%)	-0.01	4 (1%) 78 65	87, 119, 162, 202	0
All	All	1638/1714 (95%)	0.11	51 (3%) 52 38	69, 123, 192, 242	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	1236	SER	5.7
2	B	1237	GLN	5.4
2	B	957	THR	5.3
2	B	1235	GLY	5.2
2	B	1238	SER	4.3
3	C	1744	VAL	4.0
2	B	1239	ASN	3.9
1	A	326	LEU	3.6
1	A	258	HIS	3.5
2	B	952	ASP	3.3
1	A	332	ASP	3.2
2	B	1371	GLY	3.2
2	B	1234	THR	3.2
1	A	284	PHE	3.1
2	B	1130	GLY	3.0
2	B	1332	SER	2.7
1	A	296	PHE	2.7
1	A	287	LEU	2.7
1	A	282	VAL	2.7
1	A	288	ASP	2.6
1	A	328	MET	2.6
1	A	325	LYS	2.6
1	A	420	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
2	B	1131	GLY	2.6
1	A	339	TYR	2.5
1	A	429	GLY	2.5
2	B	1367	ASN	2.4
3	C	1619	TYR	2.4
1	A	290	ASP	2.4
2	B	736	CYS	2.4
1	A	327	ASN	2.4
1	A	126	ASN	2.4
1	A	329	GLY	2.4
1	A	345	ILE	2.4
1	A	260	ASP	2.3
1	A	268	ALA	2.3
1	A	241	PHE	2.3
1	A	415	VAL	2.2
2	B	742	LEU	2.2
1	A	266	ILE	2.2
2	B	1129	GLN	2.2
2	B	1405	GLY	2.2
1	A	334	GLN	2.1
2	B	1159	GLU	2.1
3	C	1696	GLU	2.1
1	A	411	SER	2.1
3	C	1455	ALA	2.1
1	A	281	TYR	2.1
2	B	1370	VAL	2.0
1	A	343	ALA	2.0
1	A	272	TYR	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](#)

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
5	NAG	B	1803	14/15	0.86	0.25	-1.29	162,184,193,198	0
5	NAG	B	1804	14/15	0.75	0.47	-	173,193,214,225	0
5	NAG	B	1801	14/15	0.76	0.32	-	186,221,228,233	0
6	NAG	B	1805	14/15	0.79	0.38	-	217,233,260,269	0
5	NAG	B	1802	14/15	0.67	0.46	-	184,212,241,243	0
6	NAG	B	1806	14/15	0.77	0.51	-	216,233,248,260	0
6	BMA	B	1807	11/12	0.46	0.44	-	216,225,231,234	0

## 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	NAG	A	701	14/15	0.78	0.36	-	158,188,216,223	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.