Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 02:41 PM GMT

PDB ID	:	4A5W
Title	:	Crystal structure of C5b6
Authors	:	Hadders, M.A.; Bubeck, D.; Forneris, F.; Pangburn, M.; Llorca, O.; Lea, S.M.; Gros, P.
Deposited on	:	2011-10-28
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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

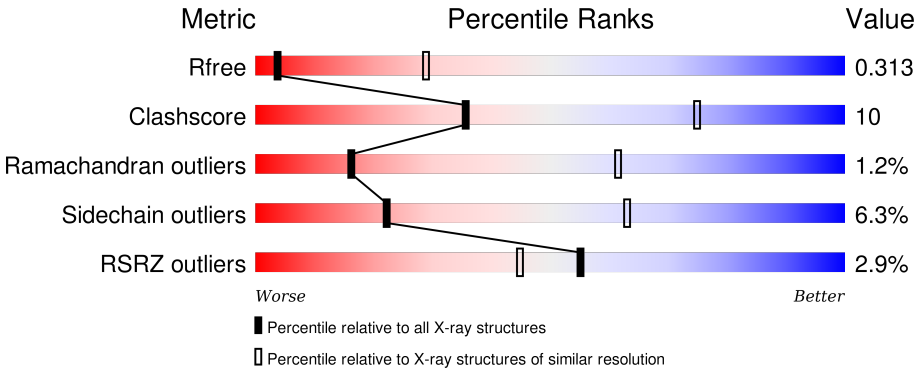
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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}	91344	1051 (3.60-3.40)
Clashscore	102246	1157 (3.60-3.40)
Ramachandran outliers	100387	1120 (3.60-3.40)
Sidechain outliers	100360	1121 (3.60-3.40)
RSRZ outliers	91569	1058 (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. 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 <=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	1580	2% 73% 21%
2	B	913	5% 65% 27% 5%

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
6	BMA	B	1571	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 19028 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.

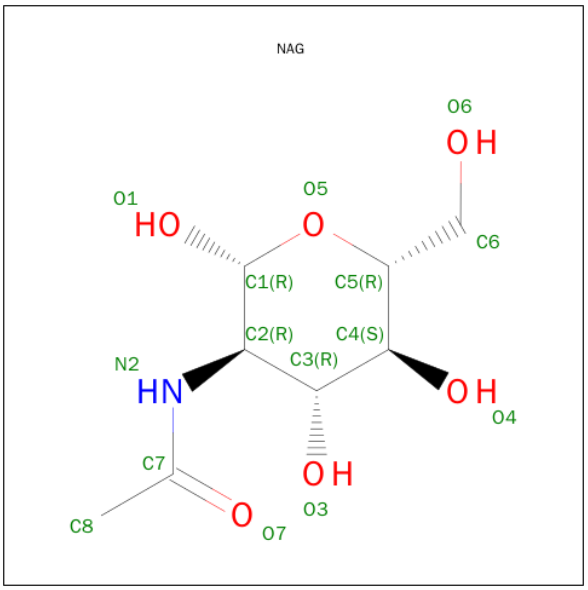
- Molecule 1 is a protein called COMPLEMENT C5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1528	Total	C	N	O	S	0	0	0
			12111	7768	1977	2321	45			

- Molecule 2 is a protein called COMPLEMENT COMPONENT C6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	871	Total	C	N	O	S	0	0	0
			6817	4206	1196	1344	71			

- Molecule 3 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: 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	A	1	Total	C	N	O	0	0
			14	8	1	5		

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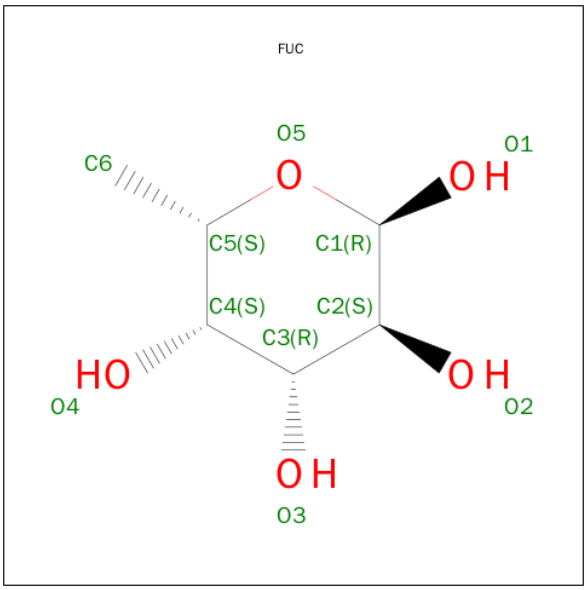
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total C N O 14 8 1 5	0	0
3	B	1	Total C N O 14 8 1 5	0	0

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

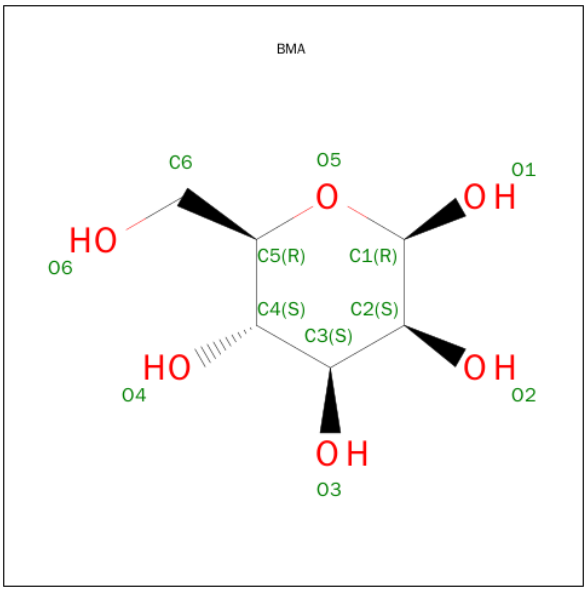
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total Ca 1 1	0	0

- Molecule 5 is SUGAR (ALPHA-L-FUCOSE) (three-letter code: FUC) (formula: $C_6H_{12}O_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total C O 10 6 4	0	0

- Molecule 6 is SUGAR (BETA-D-MANNOSE) (three-letter code: BMA) (formula: $C_6H_{12}O_6$).



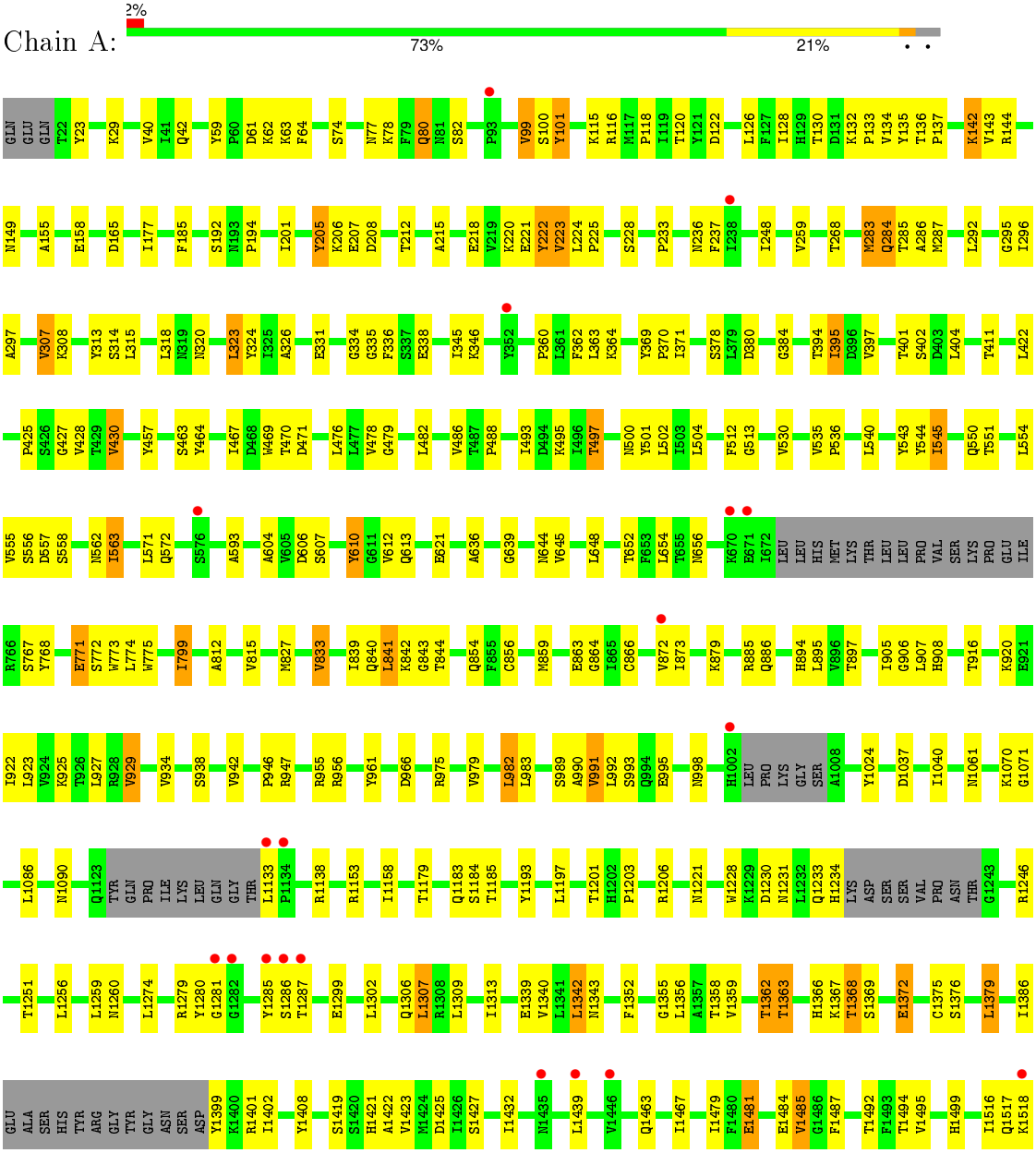
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total C O 11 6 5	0	0
6	B	1	Total C O 11 6 5	0	0
6	B	1	Total C O 11 6 5	0	0

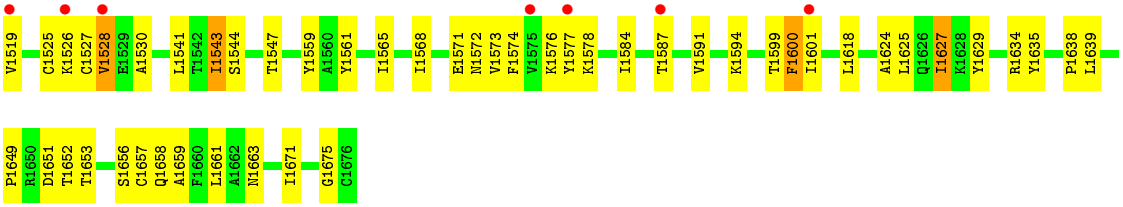
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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 C5

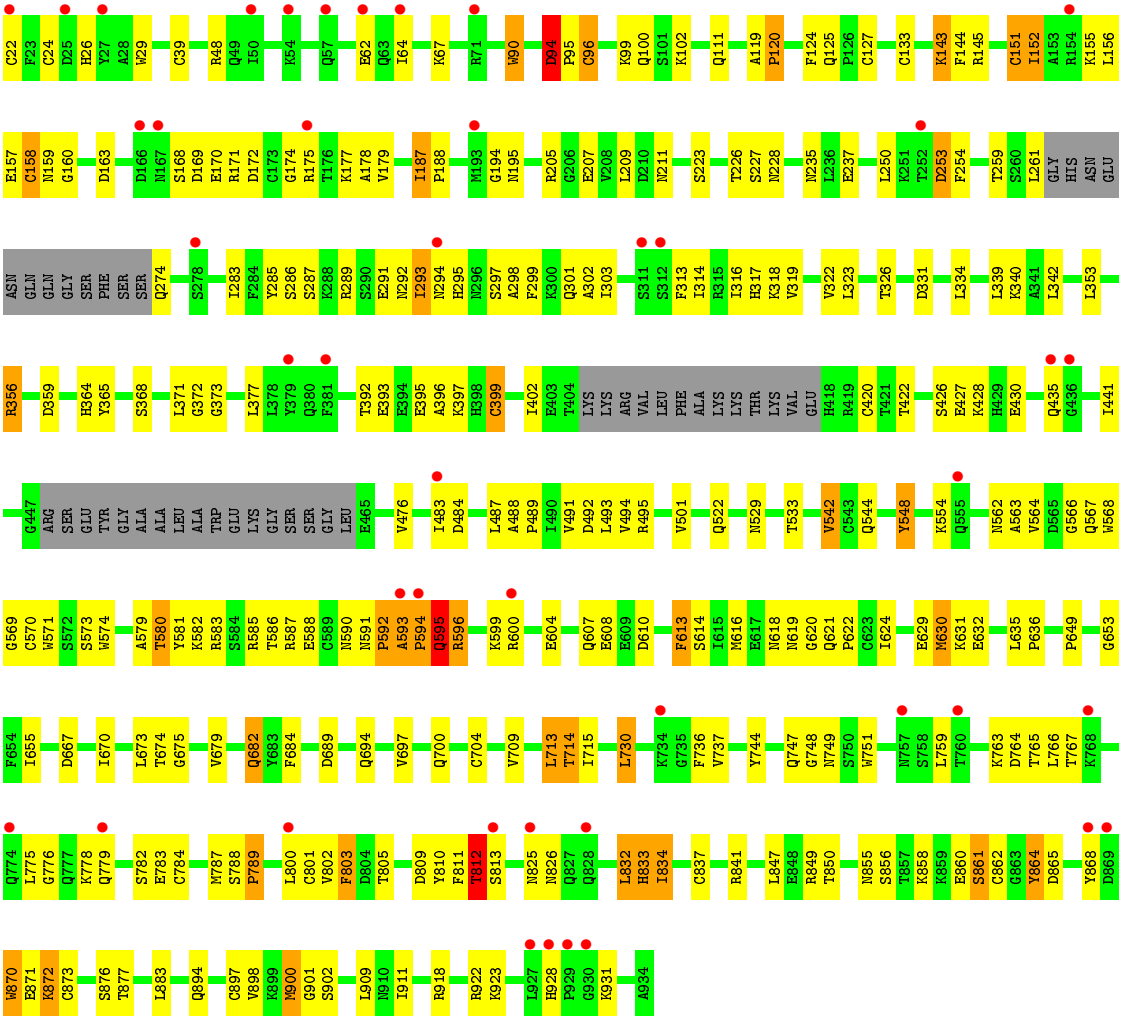
Chain A:





• Molecule 2: COMPLEMENT COMPONENT C6

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	154.22Å 230.75Å 269.98Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.19 – 3.50 46.19 – 3.50	Depositor EDS
% Data completeness (in resolution range)	(Not available) (46.19-3.50) 96.9 (46.19-3.50)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.42 (at 3.48Å)	Xtriage
Refinement program	BUSTER 2.8.0	Depositor
R, R_{free}	0.256 , 0.270 0.300 , 0.313	Depositor DCC
R_{free} test set	3027 reflections (5.40%)	DCC
Wilson B-factor (Å^2)	129.0	Xtriage
Anisotropy	0.245	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.26 , 83.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.39$, $< L^2 > = 0.22$	Xtriage
Outliers	0 of 59024 reflections	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	19028	wwPDB-VP
Average B, all atoms (Å^2)	157.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.12% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: CA, BMA, NAG, FUC

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	0.35	0/12375	0.52	1/16792 (0.0%)
2	B	0.36	0/6957	0.68	4/9392 (0.0%)
All	All	0.35	0/19332	0.58	5/26184 (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
2	B	0	1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	94	ASP	C-N-CD	-6.74	105.78	120.60
2	B	630	MET	C-N-CA	5.80	136.20	121.70
2	B	592	PRO	N-CA-C	-5.70	97.29	112.10
2	B	594	PRO	C-N-CA	5.57	135.63	121.70
1	A	1368	THR	C-N-CA	5.37	135.13	121.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	94	ASP	Peptide

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	12111	0	12029	195	0
2	B	6817	0	6472	173	0
3	A	28	0	26	0	0
3	B	28	0	26	0	0
4	B	1	0	0	0	0
5	B	10	0	10	1	0
6	B	33	0	30	3	0
All	All	19028	0	18593	364	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 (364) 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:992:LEU:HB3	1:A:993:SER:HA	1.42	1.02
1:A:1280:TYR:HB2	1:A:1281:GLY:HA2	1.51	0.90
2:B:294:ASN:HB3	2:B:295:HIS:HA	1.56	0.85
1:A:1286:SER:HB2	1:A:1287:THR:HA	1.65	0.79
1:A:1571:GLU:HB2	1:A:1572:ASN:HA	1.65	0.79
2:B:876:SER:HB2	2:B:877:THR:HA	1.64	0.79
2:B:599:LYS:HD3	2:B:600:ARG:H	1.49	0.78
1:A:1627:ILE:HA	1:A:1634:ARG:H	1.48	0.77
2:B:143:LYS:HB2	2:B:144:PHE:HA	1.67	0.75
1:A:767:SER:HB2	1:A:768:TYR:HA	1.72	0.71
2:B:592:PRO:HA	2:B:593:ALA:HB3	1.73	0.69
1:A:467:ILE:HG22	1:A:486:VAL:HG12	1.72	0.69
1:A:120:THR:HG22	1:A:122:ASP:H	1.57	0.69
2:B:588:GLU:HB2	2:B:590:ASN:HD22	1.57	0.69
2:B:571:TRP:HB2	6:B:1571:BMA:H2	1.75	0.69
1:A:982:LEU:HD11	1:A:1307:LEU:HB3	1.75	0.69
2:B:649:PRO:HB2	2:B:653:GLY:HA2	1.73	0.69
2:B:177:LYS:HB2	2:B:178:ALA:HB2	1.76	0.68
1:A:982:LEU:HD22	1:A:1309:LEU:HB2	1.75	0.67
1:A:62:LYS:N	1:A:63:LYS:HA	2.08	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1432:ILE:HG12	1:A:1481:GLU:HB3	1.77	0.66
2:B:291:GLU:HB2	2:B:292:ASN:HA	1.75	0.66
1:A:1578:LYS:HA	1:A:1599:THR:HG22	1.76	0.66
2:B:655:ILE:HG12	2:B:670:ILE:HG22	1.76	0.66
2:B:94:ASP:HB2	2:B:99:LYS:H	1.61	0.66
2:B:782:SER:N	2:B:783:GLU:HA	2.11	0.66
1:A:1624:ALA:HA	1:A:1638:PRO:HD3	1.77	0.65
1:A:827:MET:HG2	1:A:843:GLY:HA3	1.78	0.65
2:B:778:LYS:HB2	2:B:784:CYS:HB3	1.80	0.63
1:A:268:THR:HB	1:A:326:ALA:HB3	1.80	0.63
1:A:430:VAL:HG22	2:B:175:ARG:HG2	1.81	0.62
1:A:360:PRO:HG3	1:A:636:ALA:HB3	1.81	0.62
2:B:195:ASN:HA	2:B:207:GLU:HA	1.80	0.62
1:A:612:VAL:HG23	1:A:613:GLN:HB2	1.82	0.62
1:A:286:ALA:HA	1:A:287:MET:HB2	1.82	0.61
1:A:1368:THR:HA	1:A:1369:SER:HB3	1.83	0.61
2:B:39:CYS:SG	5:B:1005:FUC:H3	2.40	0.61
2:B:94:ASP:O	2:B:96:CYS:N	2.34	0.61
1:A:975:ARG:HB2	1:A:1340:VAL:HB	1.83	0.61
1:A:992:LEU:HB3	1:A:993:SER:CA	2.25	0.61
1:A:192:SER:HB2	1:A:1339:GLU:HG2	1.83	0.60
1:A:308:LYS:HA	1:A:314:SER:HB3	1.83	0.60
1:A:78:LYS:O	1:A:80:GLN:NE2	2.33	0.60
2:B:614:SER:HB3	2:B:616:MET:HB2	1.84	0.60
2:B:629:GLU:HB3	2:B:632:GLU:HB2	1.84	0.60
2:B:591:ASN:HD22	2:B:592:PRO:HD3	1.67	0.60
1:A:1518:LYS:HE2	1:A:1573:VAL:HB	1.84	0.60
1:A:842:LYS:HG2	1:A:897:THR:HG22	1.83	0.60
2:B:159:ASN:HB3	2:B:160:GLY:HA2	1.84	0.59
2:B:876:SER:CB	2:B:877:THR:HA	2.31	0.59
1:A:395:ILE:HA	1:A:401:THR:HA	1.85	0.59
1:A:1274:LEU:O	1:A:1279:ARG:NH2	2.35	0.59
2:B:776:GLY:HA3	2:B:784:CYS:HB2	1.84	0.59
1:A:1484:GLU:HB3	1:A:1485:VAL:HA	1.83	0.59
2:B:227:SER:N	2:B:228:ASN:O	2.27	0.59
1:A:966:ASP:HB2	1:A:1367:LYS:HD2	1.85	0.58
2:B:573:SER:HB2	2:B:586:THR:H	1.67	0.58
2:B:187:ILE:HD12	2:B:188:PRO:HD2	1.85	0.58
1:A:394:THR:HG21	1:A:425:PRO:HD2	1.85	0.58
1:A:128:ILE:HB	1:A:215:ALA:HB2	1.85	0.58
1:A:315:LEU:HB3	1:A:318:LEU:HB2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1525:CYS:HA	1:A:1526:LYS:HB2	1.86	0.58
2:B:285:TYR:HB3	2:B:489:PRO:HD3	1.86	0.57
1:A:1421:HIS:HE1	1:A:1463:GLN:HB3	1.67	0.57
1:A:1584:ILE:HG12	1:A:1594:LYS:HE3	1.85	0.57
2:B:29:TRP:HA	2:B:48:ARG:HA	1.85	0.57
2:B:314:ILE:HD11	2:B:397:LYS:HG3	1.87	0.57
2:B:872:LYS:HB3	2:B:876:SER:HB3	1.86	0.57
2:B:649:PRO:HB3	2:B:655:ILE:HG13	1.85	0.57
1:A:535:VAL:HG23	1:A:536:PRO:HD3	1.87	0.57
2:B:748:GLY:N	2:B:749:ASN:HB2	2.19	0.56
1:A:1259:LEU:HD13	1:A:1299:GLU:HB3	1.87	0.56
2:B:902:SER:HB2	2:B:923:LYS:HG2	1.86	0.56
2:B:860:GLU:OE2	2:B:894:GLN:NE2	2.38	0.56
1:A:101:TYR:HB3	1:A:118:PRO:HA	1.88	0.56
2:B:373:GLY:HA3	2:B:476:VAL:HG21	1.88	0.56
2:B:620:GLY:H	2:B:621:GLN:HA	1.72	0.55
1:A:1519:VAL:HA	1:A:1525:CYS:HB2	1.89	0.55
1:A:149:ASN:HB2	1:A:155:ALA:HB2	1.88	0.55
2:B:99:LYS:HD3	2:B:124:PHE:HB3	1.88	0.55
1:A:283:MET:HA	1:A:284:GLN:HB2	1.88	0.55
1:A:982:LEU:HD12	1:A:1356:LEU:H	1.71	0.55
1:A:133:PRO:HG3	1:A:610:TYR:CD2	2.43	0.54
2:B:548:TYR:HB3	2:B:554:LYS:HB2	1.88	0.54
2:B:62:GLU:O	2:B:67:LYS:NZ	2.40	0.54
2:B:800:LEU:O	2:B:813:SER:N	2.41	0.54
2:B:847:LEU:HA	2:B:850:THR:HG23	1.90	0.54
2:B:898:VAL:HG21	2:B:909:LEU:O	2.08	0.54
1:A:799:ILE:HG13	1:A:815:VAL:HB	1.90	0.54
1:A:1203:PRO:HA	2:B:673:LEU:HD13	1.90	0.54
2:B:392:THR:HB	2:B:395:GLU:HB3	1.90	0.54
2:B:571:TRP:HB2	6:B:1571:BMA:C2	2.38	0.53
1:A:1576:LYS:HA	1:A:1601:ILE:HG22	1.90	0.53
1:A:1379:LEU:HD23	1:A:1495:VAL:HG12	1.90	0.53
2:B:100:GLN:N	2:B:125:GLN:O	2.32	0.53
2:B:825:ASN:ND2	2:B:826:ASN:OD1	2.42	0.53
2:B:567:GLN:H	2:B:592:PRO:HD2	1.74	0.53
1:A:572:GLN:HG3	1:A:593:ALA:HB3	1.90	0.52
1:A:1342:LEU:H	1:A:1342:LEU:HD23	1.74	0.52
1:A:283:MET:HA	1:A:284:GLN:CB	2.40	0.52
1:A:1653:THR:HB	1:A:1658:GLN:HG3	1.91	0.52
1:A:550:GLN:HG2	1:A:551:THR:HG23	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:LYS:HB2	1:A:654:LEU:HD21	1.90	0.52
2:B:803:PHE:N	2:B:832:LEU:O	2.42	0.52
2:B:566:GLY:HA2	2:B:592:PRO:HB2	1.92	0.52
1:A:283:MET:HB2	1:A:285:THR:HG22	1.91	0.52
2:B:801:CYS:HA	2:B:812:THR:HA	1.90	0.52
2:B:211:ASN:HD22	2:B:235:ASN:HB2	1.74	0.52
2:B:862:CYS:SG	2:B:883:LEU:HB2	2.50	0.52
1:A:29:LYS:HA	1:A:652:THR:HG22	1.92	0.52
1:A:1656:SER:N	1:A:1657:CYS:HA	2.25	0.51
1:A:768:TYR:OH	1:A:922:ILE:O	2.28	0.51
2:B:261:LEU:HB2	2:B:544:GLN:HB3	1.92	0.51
2:B:630:MET:HB2	2:B:631:LYS:C	2.31	0.51
2:B:594:PRO:HA	2:B:595:GLN:CB	2.41	0.51
2:B:594:PRO:HA	2:B:595:GLN:HG2	1.92	0.51
2:B:871:GLU:HB2	2:B:873:CYS:SG	2.51	0.51
2:B:396:ALA:HA	2:B:399:CYS:HB2	1.92	0.51
1:A:1256:LEU:O	1:A:1260:ASN:ND2	2.37	0.51
2:B:254:PHE:HD1	2:B:316:ILE:HB	1.75	0.51
2:B:293:ILE:HD12	2:B:294:ASN:H	1.76	0.51
1:A:1625:LEU:HD23	1:A:1638:PRO:HB3	1.92	0.51
2:B:168:SER:O	2:B:170:GLU:N	2.44	0.51
1:A:502:LEU:HD13	1:A:543:TYR:HE1	1.76	0.51
2:B:145:ARG:HA	2:B:151:CYS:HA	1.92	0.50
1:A:464:TYR:HA	1:A:555:VAL:HG11	1.92	0.50
1:A:1153:ARG:HG2	1:A:1197:LEU:HB3	1.92	0.50
1:A:1527:CYS:HA	1:A:1528:VAL:HB	1.93	0.50
2:B:143:LYS:CB	2:B:144:PHE:HA	2.40	0.50
2:B:607:GLN:HA	2:B:608:GLU:HB3	1.93	0.50
2:B:291:GLU:HB2	2:B:292:ASN:CA	2.40	0.50
2:B:619:ASN:N	2:B:620:GLY:HA2	2.25	0.50
1:A:1372:GLU:O	1:A:1376:SER:N	2.41	0.50
2:B:489:PRO:HB2	2:B:491:VAL:HG12	1.93	0.50
1:A:1571:GLU:HA	1:A:1574:PHE:H	1.77	0.50
1:A:23:TYR:CZ	1:A:656:ASN:HB2	2.47	0.50
1:A:854:GLN:HB3	1:A:885:ARG:HB3	1.93	0.50
1:A:335:GLY:H	1:A:895:LEU:HD13	1.77	0.50
2:B:294:ASN:CB	2:B:295:HIS:HA	2.36	0.50
2:B:90:TRP:HB3	2:B:100:GLN:HG3	1.93	0.49
1:A:476:LEU:HD11	1:A:482:LEU:HD22	1.94	0.49
2:B:297:SER:HB3	2:B:299:PHE:HD1	1.77	0.49
2:B:861:SER:HB2	2:B:864:TYR:HB2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:259:VAL:HB	1:A:295:GLY:HA3	1.95	0.49
1:A:886:GLN:HG2	1:A:894:HIS:CE1	2.48	0.49
2:B:832:LEU:HD23	2:B:833:HIS:HB2	1.94	0.49
1:A:99:VAL:HG13	1:A:100:SER:H	1.77	0.49
2:B:259:THR:HB	2:B:313:PHE:HB2	1.95	0.49
2:B:803:PHE:HB2	2:B:809:ASP:O	2.13	0.49
2:B:334:LEU:HD22	2:B:339:LEU:HD13	1.93	0.49
2:B:133:CYS:SG	2:B:133:CYS:O	2.71	0.49
2:B:585:ARG:HH21	2:B:607:GLN:HB2	1.78	0.49
1:A:501:TYR:CZ	1:A:513:GLY:HA3	2.48	0.49
2:B:501:VAL:HB	2:B:624:ILE:HG23	1.95	0.49
2:B:90:TRP:HE1	2:B:102:LYS:HD3	1.78	0.49
1:A:1086:LEU:O	1:A:1090:ASN:ND2	2.46	0.49
1:A:1422:ALA:HB3	1:A:1467:ILE:HD11	1.95	0.49
1:A:1657:CYS:SG	1:A:1658:GLN:N	2.85	0.49
1:A:1185:THR:HB	1:A:1230:ASP:HA	1.95	0.49
1:A:134:VAL:HG22	1:A:218:GLU:HB3	1.93	0.48
1:A:307:VAL:HG23	1:A:308:LYS:H	1.77	0.48
1:A:1649:PRO:HG2	1:A:1661:LEU:HD13	1.94	0.48
2:B:736:PHE:HA	2:B:764:ASP:H	1.78	0.48
1:A:143:VAL:HG13	1:A:185:PHE:HB2	1.95	0.48
2:B:174:GLY:HA3	2:B:175:ARG:HA	1.70	0.48
2:B:621:GLN:N	2:B:622:PRO:HA	2.29	0.48
2:B:832:LEU:HA	2:B:833:HIS:CG	2.49	0.48
2:B:788:SER:HB2	2:B:789:PRO:HA	1.96	0.48
1:A:906:GLY:H	1:A:929:VAL:HG22	1.78	0.48
2:B:713:LEU:HD13	2:B:715:ILE:HB	1.95	0.48
1:A:907:LEU:H	1:A:907:LEU:HD23	1.79	0.48
2:B:763:LYS:NZ	2:B:767:THR:OG1	2.44	0.48
1:A:397:VAL:N	1:A:427:GLY:O	2.43	0.48
1:A:1228:TRP:H	1:A:1251:THR:HG22	1.79	0.48
1:A:1037:ASP:HB2	1:A:1040:ILE:HG12	1.96	0.48
1:A:371:ILE:HD12	1:A:422:LEU:HD13	1.96	0.48
1:A:331:GLU:HB2	1:A:334:GLY:O	2.14	0.48
1:A:493:ILE:HG13	1:A:495:LYS:H	1.79	0.48
2:B:227:SER:HB3	2:B:228:ASN:HB2	1.96	0.47
2:B:194:GLY:HA2	2:B:209:LEU:HD12	1.95	0.47
1:A:132:LYS:NZ	1:A:134:VAL:O	2.47	0.47
1:A:363:LEU:HD21	1:A:428:VAL:HG13	1.95	0.47
2:B:582:LYS:NZ	2:B:610:ASP:OD1	2.42	0.47
2:B:834:ILE:HG22	2:B:870:TRP:HZ2	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:975:ARG:HG2	1:A:1363:THR:HB	1.96	0.47
1:A:946:PRO:HB3	1:A:1352:PHE:O	2.15	0.47
1:A:543:TYR:HB3	1:A:556:SER:HB3	1.97	0.47
1:A:1372:GLU:HA	1:A:1375:CYS:HB3	1.95	0.47
1:A:1600:PHE:HB2	1:A:1639:LEU:HB2	1.95	0.47
1:A:1571:GLU:CB	1:A:1572:ASN:HA	2.42	0.47
2:B:529:ASN:HB2	2:B:564:VAL:H	1.80	0.46
1:A:839:ILE:HD12	1:A:841:LEU:HD23	1.96	0.46
1:A:207:GLU:HA	1:A:208:ASP:HA	1.66	0.46
2:B:562:ASN:O	2:B:596:ARG:HB3	2.15	0.46
2:B:100:GLN:HB2	2:B:127:CYS:HB3	1.97	0.46
1:A:998:ASN:HB3	2:B:613:PHE:HE1	1.80	0.46
1:A:946:PRO:HD2	1:A:1355:GLY:O	2.15	0.46
2:B:682:GLN:HB3	2:B:697:VAL:HG21	1.98	0.46
2:B:302:ALA:HB2	2:B:441:ILE:HD13	1.96	0.46
1:A:133:PRO:HG3	1:A:610:TYR:HD2	1.81	0.46
1:A:604:ALA:O	1:A:772:SER:OG	2.33	0.46
2:B:152:ILE:HB	2:B:156:LEU:HD13	1.96	0.46
1:A:934:VAL:HG22	1:A:1366:HIS:CD2	2.51	0.46
2:B:670:ILE:HD11	2:B:697:VAL:HG21	1.98	0.46
1:A:1659:ALA:O	1:A:1663:ASN:ND2	2.49	0.46
2:B:849:ARG:HD3	2:B:918:ARG:HG3	1.97	0.46
1:A:1517:GLN:HB2	1:A:1530:ALA:HB2	1.98	0.46
2:B:226:THR:HA	2:B:227:SER:HA	1.68	0.46
2:B:900:MET:HB3	2:B:901:GLY:H	1.58	0.46
1:A:991:VAL:HG12	1:A:1024:TYR:CZ	2.51	0.45
2:B:766:LEU:HA	2:B:872:LYS:HE2	1.98	0.45
1:A:767:SER:CB	1:A:768:TYR:HA	2.44	0.45
1:A:1565:ILE:HD12	1:A:1578:LYS:O	2.17	0.45
2:B:574:TRP:HZ3	2:B:583:ARG:HD2	1.81	0.45
2:B:323:LEU:HB2	2:B:371:LEU:HG	1.97	0.45
2:B:855:ASN:HA	2:B:856:SER:HA	1.68	0.45
2:B:587:ARG:NH2	6:B:1568:BMA:O5	2.49	0.45
2:B:620:GLY:N	2:B:621:GLN:HA	2.32	0.45
2:B:585:ARG:HB3	2:B:607:GLN:O	2.16	0.45
1:A:394:THR:O	1:A:402:SER:N	2.48	0.45
1:A:1061:ASN:HD21	1:A:1071:GLY:HA3	1.82	0.45
1:A:604:ALA:HA	1:A:799:ILE:HA	1.98	0.45
1:A:771:GLU:HA	1:A:772:SER:HA	1.74	0.45
2:B:170:GLU:O	2:B:172:ASP:HB2	2.16	0.45
1:A:1541:LEU:O	1:A:1543:ILE:HG12	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1307:LEU:HA	1:A:1355:GLY:HA2	1.98	0.45
2:B:736:PHE:HA	2:B:764:ASP:N	2.31	0.45
2:B:342:LEU:HD21	2:B:494:VAL:HG13	1.98	0.45
1:A:773:TRP:CE3	1:A:774:LEU:HB2	2.52	0.45
1:A:992:LEU:HG	1:A:995:GLU:HB3	1.99	0.45
2:B:847:LEU:O	2:B:850:THR:OG1	2.31	0.45
1:A:989:SER:OG	1:A:990:ALA:N	2.49	0.45
2:B:483:ILE:HG13	2:B:484:ASP:H	1.83	0.44
1:A:863:GLU:HA	1:A:864:GLY:HA2	1.53	0.44
1:A:323:LEU:N	1:A:345:ILE:O	2.49	0.44
2:B:427:GLU:N	2:B:428:LYS:HA	2.32	0.44
2:B:568:TRP:HA	2:B:569:GLY:HA3	1.86	0.44
2:B:298:ALA:O	2:B:301:GLN:HG2	2.18	0.44
1:A:457:TYR:CZ	1:A:555:VAL:HG13	2.53	0.44
2:B:713:LEU:HD22	2:B:730:LEU:HB2	2.00	0.44
1:A:938:SER:HA	1:A:1362:THR:HA	1.99	0.44
1:A:606:ASP:OD1	1:A:607:SER:N	2.51	0.44
2:B:594:PRO:HA	2:B:595:GLN:HB2	2.00	0.44
2:B:96:CYS:SG	2:B:340:LYS:HG2	2.57	0.44
1:A:362:PHE:CZ	1:A:639:GLY:HA2	2.53	0.44
1:A:1302:LEU:O	1:A:1306:GLN:HG2	2.18	0.44
2:B:326:THR:HA	2:B:368:SER:HA	1.98	0.44
2:B:747:GLN:H	2:B:749:ASN:HB2	1.83	0.44
1:A:101:TYR:CD2	1:A:116:ARG:HD3	2.53	0.44
2:B:574:TRP:CZ2	2:B:585:ARG:HD3	2.52	0.44
1:A:479:GLY:H	1:A:530:VAL:HG23	1.83	0.44
1:A:40:VAL:HG21	1:A:512:PHE:HB3	1.99	0.44
1:A:201:ILE:HB	1:A:215:ALA:HB3	2.00	0.44
1:A:74:SER:HB2	1:A:77:ASN:HD22	1.81	0.44
2:B:604:GLU:OE2	2:B:607:GLN:NE2	2.51	0.44
1:A:1184:SER:OG	1:A:1230:ASP:OD1	2.35	0.44
2:B:303:ILE:HG12	2:B:542:VAL:HB	1.98	0.44
2:B:331:ASP:OD2	2:B:495:ARG:NH2	2.51	0.44
1:A:137:PRO:HB3	1:A:194:PRO:HG2	2.00	0.44
1:A:557:ASP:OD1	1:A:558:SER:N	2.50	0.43
1:A:1231:ASN:HB3	1:A:1234:HIS:HB3	2.01	0.43
2:B:564:VAL:O	2:B:595:GLN:NE2	2.51	0.43
2:B:24:CYS:O	2:B:48:ARG:NH1	2.51	0.43
2:B:254:PHE:HA	2:B:317:HIS:H	1.81	0.43
2:B:323:LEU:HD13	2:B:371:LEU:HD11	1.99	0.43
1:A:571:LEU:HD22	1:A:812:ALA:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:644:ASN:O	1:A:648:LEU:HB2	2.17	0.43
1:A:833:VAL:HG21	1:A:927:LEU:HD11	2.00	0.43
1:A:224:LEU:HA	1:A:225:PRO:HD2	1.83	0.43
1:A:42:GLN:HE22	1:A:500:ASN:HB3	1.84	0.43
1:A:612:VAL:HA	1:A:613:GLN:HA	1.75	0.43
1:A:840:GLN:NE2	1:A:1487:PHE:HA	2.33	0.43
1:A:142:LYS:HB3	1:A:775:TRP:CE2	2.53	0.43
1:A:979:VAL:HG12	1:A:1359:VAL:HB	2.01	0.43
1:A:982:LEU:HB2	1:A:1309:LEU:HD13	2.01	0.43
1:A:463:SER:OG	1:A:544:TYR:OH	2.29	0.43
1:A:955:ARG:HG3	1:A:956:ARG:H	1.83	0.43
2:B:599:LYS:HD2	2:B:600:ARG:HG3	2.01	0.43
1:A:323:LEU:H	1:A:345:ILE:H	1.67	0.43
2:B:253:ASP:OD2	2:B:319:VAL:HG12	2.18	0.43
2:B:286:SER:HA	2:B:287:SER:HB2	1.99	0.43
2:B:928:HIS:O	2:B:931:LYS:HB2	2.18	0.43
2:B:635:LEU:HA	2:B:636:PRO:HD3	1.92	0.43
1:A:1419:SER:HB3	1:A:1467:ILE:HB	2.01	0.43
1:A:1221:ASN:HD21	2:B:636:PRO:HG3	1.84	0.43
2:B:580:THR:N	2:B:581:TYR:HB2	2.34	0.43
1:A:872:VAL:HG12	1:A:879:LYS:HA	2.00	0.43
1:A:1427:SER:HB3	1:A:1492:THR:H	1.83	0.43
1:A:313:TYR:HB2	1:A:318:LEU:HD13	2.01	0.43
2:B:667:ASP:OD1	2:B:667:ASP:N	2.52	0.43
2:B:119:ALA:HA	2:B:120:PRO:HD2	1.88	0.43
2:B:775:LEU:O	2:B:787:MET:HB2	2.19	0.43
2:B:684:PHE:CD1	2:B:694:GLN:HA	2.54	0.43
1:A:1565:ILE:HD11	1:A:1568:ILE:HG23	2.00	0.42
2:B:163:ASP:HA	2:B:168:SER:HA	2.01	0.42
1:A:82:SER:HG	1:A:512:PHE:HE1	1.65	0.42
1:A:991:VAL:HG22	1:A:992:LEU:H	1.84	0.42
1:A:982:LEU:HD23	1:A:983:LEU:N	2.34	0.42
2:B:353:LEU:HD23	2:B:356:ARG:HH21	1.84	0.42
2:B:223:SER:OG	2:B:226:THR:O	2.31	0.42
1:A:1577:TYR:HB2	1:A:1600:PHE:O	2.19	0.42
2:B:426:SER:C	2:B:428:LYS:HA	2.39	0.42
1:A:469:TRP:HB3	1:A:470:THR:H	1.69	0.42
1:A:961:TYR:CZ	1:A:1343:ASN:HB3	2.55	0.42
2:B:422:THR:HG21	2:B:430:GLU:HG2	2.02	0.42
2:B:365:TYR:CE1	2:B:488:ALA:HB3	2.54	0.42
2:B:237:GLU:N	2:B:326:THR:O	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:679:VAL:HG11	2:B:700:GLN:HG2	2.01	0.42
1:A:1544:SER:HB3	1:A:1547:THR:HG23	2.02	0.42
1:A:292:LEU:HA	1:A:297:ALA:HB2	2.00	0.42
1:A:346:LYS:HE2	1:A:378:SER:HB3	2.01	0.42
2:B:713:LEU:HA	2:B:714:THR:OG1	2.19	0.42
2:B:365:TYR:CG	2:B:493:LEU:HD11	2.54	0.42
1:A:384:GLY:HA2	1:A:411:THR:HG23	2.01	0.42
2:B:802:VAL:O	2:B:811:PHE:HB2	2.20	0.41
1:A:471:ASP:CG	1:A:562:ASN:H	2.20	0.41
1:A:905:ILE:H	1:A:905:ILE:HD12	1.84	0.41
1:A:237:PHE:CD1	1:A:378:SER:HB2	2.55	0.41
1:A:369:TYR:HA	1:A:370:PRO:HD3	1.89	0.41
1:A:923:LEU:HD12	1:A:925:LYS:HD3	2.01	0.41
2:B:250:LEU:HD23	2:B:318:LYS:HE3	2.00	0.41
1:A:130:THR:OG1	1:A:135:TYR:OH	2.38	0.41
1:A:1425:ASP:HB3	1:A:1494:THR:HG23	2.03	0.41
1:A:906:GLY:HA2	1:A:908:HIS:CD2	2.55	0.41
2:B:194:GLY:HA2	2:B:209:LEU:HB2	2.01	0.41
2:B:205:ARG:HD3	2:B:359:ASP:O	2.21	0.41
1:A:233:PRO:HA	1:A:248:ILE:HG13	2.02	0.41
1:A:982:LEU:HD23	1:A:983:LEU:H	1.85	0.41
2:B:764:ASP:OD1	2:B:765:THR:N	2.52	0.41
2:B:580:THR:HG23	2:B:581:TYR:HD1	1.86	0.41
2:B:847:LEU:HD23	2:B:850:THR:HG21	2.02	0.41
1:A:136:THR:HG1	1:A:136:THR:H	1.66	0.41
1:A:222:TYR:HD1	1:A:223:VAL:N	2.19	0.41
2:B:574:TRP:CZ3	2:B:583:ARG:HD2	2.55	0.41
2:B:872:LYS:N	2:B:873:CYS:HA	2.36	0.41
1:A:144:ARG:HG2	1:A:775:TRP:CZ2	2.55	0.41
1:A:1423:VAL:HG22	1:A:1463:GLN:HG2	2.03	0.41
1:A:1651:ASP:O	1:A:1653:THR:HG23	2.21	0.41
1:A:1386:ILE:HD11	1:A:1401:ARG:HH21	1.86	0.41
1:A:158:GLU:HG3	1:A:206:LYS:HE2	2.03	0.41
1:A:1671:ILE:HD12	1:A:1675:GLY:HA2	2.01	0.41
1:A:220:LYS:HG2	1:A:221:GLU:H	1.85	0.41
2:B:157:GLU:HA	2:B:158:CYS:HA	1.64	0.41
1:A:126:LEU:HD21	1:A:205:TYR:CE1	2.56	0.41
2:B:322:VAL:HG22	2:B:372:GLY:HA2	2.03	0.41
1:A:859:MET:HE2	1:A:859:MET:HB3	1.94	0.41
2:B:571:TRP:CZ3	2:B:587:ARG:HB2	2.55	0.41
2:B:594:PRO:HA	2:B:595:GLN:CG	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:593:ALA:HA	2:B:594:PRO:HD3	1.80	0.40
1:A:1193:TYR:CE1	1:A:1256:LEU:HB3	2.55	0.40
1:A:1408:TYR:HB2	1:A:1419:SER:HB2	2.03	0.40
2:B:684:PHE:CE1	2:B:694:GLN:HA	2.56	0.40
2:B:250:LEU:HD23	2:B:318:LYS:HB3	2.02	0.40
2:B:22:CYS:HB3	2:B:64:ILE:HD11	2.02	0.40
2:B:674:THR:HA	2:B:675:GLY:HA2	1.55	0.40
1:A:982:LEU:CD1	1:A:1356:LEU:H	2.34	0.40
2:B:90:TRP:NE1	2:B:102:LYS:HD3	2.35	0.40
1:A:478:VAL:HG22	1:A:563:ILE:HD11	2.03	0.40
1:A:61:ASP:HB2	1:A:62:LYS:HB3	2.03	0.40
1:A:545:ILE:HG22	1:A:554:LEU:HB3	2.03	0.40
2:B:364:HIS:CG	2:B:487:LEU:HD13	2.56	0.40
2:B:800:LEU:N	2:B:813:SER:O	2.45	0.40
1:A:1138:ARG:NH2	1:A:1183:GLN:OE1	2.54	0.40
1:A:1402:ILE:HD11	1:A:1479:ILE:HD13	2.03	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	1516/1580 (96%)	1390 (92%)	113 (8%)	13 (1%)	21	68
2	B	863/913 (94%)	699 (81%)	148 (17%)	16 (2%)	10	51
All	All	2379/2493 (95%)	2089 (88%)	261 (11%)	29 (1%)	16	61

All (29) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	223	VAL
1	A	833	VAL

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Mol	Chain	Res	Type
2	B	95	PRO
2	B	169	ASP
1	A	1627	ILE
2	B	171	ARG
2	B	595	GLN
2	B	834	ILE
2	B	861	SER
2	B	152	ILE
2	B	283	ILE
2	B	563	ALA
1	A	99	VAL
1	A	380	ASP
1	A	1070	LYS
1	A	1372	GLU
1	A	1635	TYR
2	B	402	ILE
2	B	709	VAL
2	B	812	THR
1	A	488	PRO
1	A	497	THR
2	B	579	ALA
1	A	307	VAL
1	A	1528	VAL
1	A	1543	ILE
2	B	120	PRO
2	B	593	ALA
2	B	789	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	1356/1403 (97%)	1281 (94%)	75 (6%)	27	67
2	B	775/810 (96%)	715 (92%)	60 (8%)	16	54
All	All	2131/2213 (96%)	1996 (94%)	135 (6%)	22	63

All (135) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	59	TYR
1	A	64	PHE
1	A	80	GLN
1	A	101	TYR
1	A	142	LYS
1	A	165	ASP
1	A	177	ILE
1	A	205	TYR
1	A	212	THR
1	A	222	TYR
1	A	228	SER
1	A	236	ASN
1	A	283	MET
1	A	284	GLN
1	A	296	ILE
1	A	320	ASN
1	A	323	LEU
1	A	324	TYR
1	A	336	PHE
1	A	338	GLU
1	A	364	LYS
1	A	395	ILE
1	A	404	LEU
1	A	430	VAL
1	A	497	THR
1	A	504	LEU
1	A	540	LEU
1	A	545	ILE
1	A	563	ILE
1	A	610	TYR
1	A	621	GLU
1	A	645	VAL
1	A	771	GLU
1	A	799	ILE
1	A	841	LEU
1	A	844	THR
1	A	856	CYS
1	A	866	CYS
1	A	873	ILE
1	A	916	THR
1	A	920	LYS
1	A	929	VAL

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Mol	Chain	Res	Type
1	A	942	VAL
1	A	947	ARG
1	A	982	LEU
1	A	991	VAL
1	A	1133	LEU
1	A	1158	ILE
1	A	1179	THR
1	A	1201	THR
1	A	1206	ARG
1	A	1233	GLN
1	A	1246	ARG
1	A	1285	TYR
1	A	1307	LEU
1	A	1313	ILE
1	A	1342	LEU
1	A	1358	THR
1	A	1362	THR
1	A	1363	THR
1	A	1379	LEU
1	A	1399	TYR
1	A	1439	LEU
1	A	1481	GLU
1	A	1485	VAL
1	A	1499	HIS
1	A	1516	ILE
1	A	1559	TYR
1	A	1561	TYR
1	A	1587	THR
1	A	1591	VAL
1	A	1600	PHE
1	A	1618	LEU
1	A	1629	TYR
1	A	1652	THR
2	B	26	HIS
2	B	90	TRP
2	B	96	CYS
2	B	111	GLN
2	B	143	LYS
2	B	151	CYS
2	B	155	LYS
2	B	158	CYS
2	B	179	VAL

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Mol	Chain	Res	Type
2	B	187	ILE
2	B	253	ASP
2	B	274	GLN
2	B	289	ARG
2	B	293	ILE
2	B	356	ARG
2	B	377	LEU
2	B	393	GLU
2	B	399	CYS
2	B	420	CYS
2	B	435	GLN
2	B	492	ASP
2	B	522	GLN
2	B	533	THR
2	B	542	VAL
2	B	548	TYR
2	B	570	CYS
2	B	580	THR
2	B	595	GLN
2	B	596	ARG
2	B	613	PHE
2	B	618	ASN
2	B	682	GLN
2	B	689	ASP
2	B	704	CYS
2	B	713	LEU
2	B	714	THR
2	B	730	LEU
2	B	737	VAL
2	B	744	TYR
2	B	751	TRP
2	B	759	LEU
2	B	779	GLN
2	B	803	PHE
2	B	805	THR
2	B	810	TYR
2	B	812	THR
2	B	832	LEU
2	B	833	HIS
2	B	837	CYS
2	B	841	ARG
2	B	858	LYS

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Mol	Chain	Res	Type
2	B	864	TYR
2	B	865	ASP
2	B	868	TYR
2	B	870	TRP
2	B	872	LYS
2	B	897	CYS
2	B	900	MET
2	B	911	ILE
2	B	922	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	42	GLN
1	A	77	ASN
1	A	399	GLN
1	A	642	ASN
1	A	838	GLN
1	A	876	GLN
1	A	1366	HIS
1	A	1421	HIS
1	A	1663	ASN
2	B	26	HIS
2	B	63	GLN
2	B	81	ASN
2	B	111	GLN
2	B	211	ASN
2	B	274	GLN
2	B	292	ASN
2	B	294	ASN
2	B	296	ASN
2	B	364	HIS
2	B	388	ASN
2	B	435	GLN
2	B	522	GLN
2	B	544	GLN
2	B	590	ASN
2	B	591	ASN
2	B	625	ASN
2	B	777	GLN
2	B	779	GLN
2	B	894	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

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 9 ligands modelled in this entry, 1 is monoatomic - leaving 8 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	NAG	A	1911	1	14,14,15	2.38	6 (42%)	15,19,21	1.79	4 (26%)
3	NAG	A	2630	1	14,14,15	2.17	2 (14%)	15,19,21	1.13	1 (6%)
5	FUC	B	1005	2	10,10,11	0.97	1 (10%)	14,14,16	2.75	6 (42%)
3	NAG	B	1324	2	14,14,15	3.37	3 (21%)	15,19,21	2.91	8 (53%)
6	BMA	B	1568	2	11,11,12	1.45	1 (9%)	14,15,17	4.35	7 (50%)
6	BMA	B	1571	2	11,11,12	1.51	2 (18%)	14,15,17	3.80	7 (50%)
6	BMA	B	1574	2	11,11,12	1.34	1 (9%)	14,15,17	2.01	5 (35%)
3	NAG	B	1855	2	14,14,15	1.65	2 (14%)	15,19,21	3.55	4 (26%)

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	1911	1	-	0/6/23/26	0/1/1/1
3	NAG	A	2630	1	-	0/6/23/26	0/1/1/1
5	FUC	B	1005	2	-	0/0/17/20	0/1/1/1
3	NAG	B	1324	2	-	0/6/23/26	0/1/1/1
6	BMA	B	1568	2	-	0/2/19/22	0/1/1/1
6	BMA	B	1571	2	-	0/2/19/22	0/1/1/1
6	BMA	B	1574	2	-	0/2/19/22	0/1/1/1
3	NAG	B	1855	2	-	0/6/23/26	0/1/1/1

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1324	NAG	O5-C1	-2.21	1.40	1.43
6	B	1568	BMA	C2-C3	2.00	1.55	1.52
3	A	1911	NAG	C7-N2	2.05	1.42	1.34
3	A	1911	NAG	C3-C2	2.11	1.57	1.52
3	A	1911	NAG	O3-C3	2.30	1.48	1.43
3	A	2630	NAG	C2-N2	2.35	1.50	1.46
3	A	1911	NAG	C8-C7	2.40	1.55	1.50
5	B	1005	FUC	C1-C2	2.43	1.58	1.52
6	B	1571	BMA	C4-C5	2.64	1.58	1.53
6	B	1571	BMA	O5-C5	2.80	1.49	1.43
6	B	1574	BMA	C2-C3	3.04	1.56	1.52
3	B	1855	NAG	C3-C2	3.09	1.59	1.52
3	A	1911	NAG	O5-C5	3.24	1.50	1.43
3	B	1324	NAG	C3-C2	3.44	1.60	1.52
3	B	1855	NAG	C1-C2	4.67	1.58	1.52
3	A	1911	NAG	C1-C2	5.96	1.60	1.52
3	A	2630	NAG	C1-C2	7.05	1.62	1.52
3	B	1324	NAG	C1-C2	11.52	1.68	1.52

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	B	1571	BMA	O4-C4-C3	-7.02	94.54	110.34
6	B	1571	BMA	O5-C1-C2	-4.81	103.06	110.86
6	B	1568	BMA	O3-C3-C2	-4.21	102.39	110.00
3	B	1324	NAG	O5-C5-C6	-3.41	99.96	107.35
6	B	1571	BMA	O5-C5-C6	-3.22	100.39	107.35
6	B	1574	BMA	O4-C4-C3	-3.07	103.42	110.34
3	A	2630	NAG	O3-C3-C2	-2.74	103.69	109.11
3	B	1855	NAG	O5-C5-C6	-2.68	101.54	107.35
3	B	1855	NAG	C3-C4-C5	-2.65	105.58	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	1324	NAG	C4-C3-C2	-2.62	107.16	111.23
3	B	1855	NAG	C8-C7-N2	-2.50	111.33	116.11
3	B	1324	NAG	C3-C4-C5	-2.42	105.98	110.20
3	B	1324	NAG	O3-C3-C4	-2.33	105.09	110.34
6	B	1568	BMA	O5-C1-C2	-2.33	107.08	110.86
3	A	1911	NAG	C6-C5-C4	-2.20	107.58	113.02
3	A	1911	NAG	C1-O5-C5	-2.09	109.59	112.25
6	B	1574	BMA	C3-C4-C5	2.07	113.81	110.20
3	B	1324	NAG	O7-C7-N2	2.12	126.19	121.86
6	B	1568	BMA	O3-C3-C4	2.22	115.33	110.34
6	B	1571	BMA	O2-C2-C3	2.24	114.63	110.12
3	A	1911	NAG	C4-C3-C2	2.30	114.81	111.23
6	B	1571	BMA	C6-C5-C4	2.53	119.25	113.02
3	B	1324	NAG	O4-C4-C3	2.59	116.17	110.34
5	B	1005	FUC	C1-C2-C3	2.64	112.67	109.54
6	B	1574	BMA	O2-C2-C3	2.85	115.84	110.12
5	B	1005	FUC	C2-C3-C4	2.90	115.97	111.04
3	B	1324	NAG	C3-C2-N2	2.91	117.53	110.56
5	B	1005	FUC	O2-C2-C1	3.11	115.44	109.21
6	B	1568	BMA	O2-C2-C1	3.39	115.99	109.21
6	B	1568	BMA	C6-C5-C4	3.68	122.09	113.02
5	B	1005	FUC	C3-C4-C5	3.73	116.01	109.72
6	B	1574	BMA	O2-C2-C1	3.77	116.76	109.21
6	B	1574	BMA	C2-C3-C4	3.87	117.62	111.04
5	B	1005	FUC	C1-O5-C5	4.10	118.70	112.38
6	B	1571	BMA	C2-C3-C4	4.69	119.00	111.04
3	A	1911	NAG	O5-C5-C6	5.41	119.06	107.35
5	B	1005	FUC	O5-C1-C2	6.27	121.03	110.86
6	B	1568	BMA	C1-C2-C3	8.14	119.17	109.54
3	B	1324	NAG	C1-O5-C5	8.23	122.69	112.25
6	B	1571	BMA	C1-O5-C5	8.81	123.42	112.25
6	B	1568	BMA	C1-O5-C5	11.79	127.22	112.25
3	B	1855	NAG	C1-O5-C5	12.52	128.14	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	1005	FUC	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	1568	BMA	1	0
6	B	1571	BMA	2	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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^{th} 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	1528/1580 (96%)	-0.05	26 (1%)	73	64	66, 142, 207, 242	0
2	B	871/913 (95%)	0.21	44 (5%)	32	24	85, 183, 243, 264	0
All	All	2399/2493 (96%)	0.04	70 (2%)	55	45	66, 154, 231, 264	0

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1282	GLY	7.8
2	B	869	ASP	6.5
1	A	1286	SER	6.5
2	B	22	CYS	5.7
2	B	594	PRO	5.3
2	B	175	ARG	4.8
1	A	872	VAL	4.6
2	B	779	GLN	4.4
1	A	1002	HIS	4.3
2	B	929	PRO	4.1
1	A	1133	LEU	4.1
1	A	1285	TYR	4.0
1	A	671	GLU	3.7
2	B	813	SER	3.6
2	B	928	HIS	3.6
1	A	1287	THR	3.6
1	A	238	ILE	3.4
2	B	800	LEU	3.2
1	A	1519	VAL	3.1
2	B	154	ARG	2.9
2	B	868	TYR	2.9
2	B	825	ASN	2.9
2	B	483	ILE	2.8
2	B	167	ASN	2.8

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Mol	Chain	Res	Type	RSRZ
2	B	927	LEU	2.8
2	B	774	GLN	2.8
2	B	62	GLU	2.7
2	B	278	SER	2.7
2	B	436	GLY	2.7
2	B	381	PHE	2.7
2	B	555	GLN	2.7
1	A	1435	ASN	2.7
1	A	1575	VAL	2.6
1	A	1446	VAL	2.6
1	A	93	PRO	2.6
2	B	828	GLN	2.6
2	B	27	TYR	2.6
2	B	379	TYR	2.6
2	B	757	ASN	2.6
1	A	1518	LYS	2.5
2	B	57	GLN	2.5
2	B	593	ALA	2.5
2	B	64	ILE	2.4
2	B	435	GLN	2.4
2	B	25	ASP	2.4
1	A	1528	VAL	2.4
1	A	670	LYS	2.4
1	A	576	SER	2.3
2	B	734	LYS	2.3
1	A	1601	ILE	2.3
2	B	930	GLY	2.3
2	B	768	LYS	2.3
2	B	312	SER	2.3
1	A	1526	LYS	2.3
1	A	1439	LEU	2.3
2	B	166	ASP	2.3
2	B	294	ASN	2.3
1	A	1281	GLY	2.3
1	A	1134	PRO	2.2
2	B	600	ARG	2.2
2	B	54	LYS	2.2
2	B	311	SER	2.2
1	A	1587	THR	2.2
2	B	193	MET	2.1
1	A	352	TYR	2.1
2	B	252	THR	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	50	ILE	2.0
2	B	71	ARG	2.0
2	B	760	THR	2.0
1	A	1577	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)

There are no carbohydrates 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. 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^{th} 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(Å^2)	Q<0.9
6	BMA	B	1571	11/12	0.83	0.26	2.14	153,156,157,158	0
3	NAG	B	1324	14/15	0.72	0.40	1.95	190,194,197,197	0
5	FUC	B	1005	10/11	0.83	0.23	-0.36	166,166,168,168	0
4	CA	B	1000	1/1	0.93	0.17	-0.71	146,146,146,146	0
3	NAG	A	1911	14/15	0.89	0.15	-1.01	118,122,124,125	0
6	BMA	B	1568	11/12	0.95	0.15	-1.39	169,172,173,174	0
6	BMA	B	1574	11/12	0.80	0.20	-1.61	188,190,191,193	0
3	NAG	A	2630	14/15	0.18	0.58	-	227,231,233,233	0
3	NAG	B	1855	14/15	0.85	0.18	-	198,201,204,204	0

6.5 Other polymers (i)

There are no such residues in this entry.