Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 01:10 PM GMT

PDB ID	:	3T5O
Title	:	Crystal Structure of human Complement Component C6
Authors	:	Aleshin, A.E.; Stec, B.; Bankston, L.A.; DiScipio, R.G.; Liddington, R.C.
Deposited on	:	2011-07-27
Resolution	:	2.87 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:

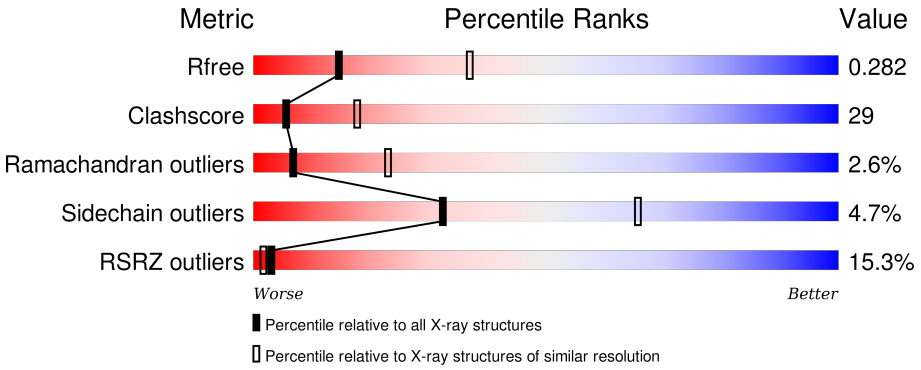
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.87 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	2228 (2.90-2.82)
Clashscore	102246	2499 (2.90-2.82)
Ramachandran outliers	100387	2439 (2.90-2.82)
Sidechain outliers	100360	2442 (2.90-2.82)
RSRZ outliers	91569	2236 (2.90-2.82)

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	913	15%, 52%, 38%, 5%, 5%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 6934 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 component C6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	871	Total	C	N	O	S	0	0	0
			6830	4222	1203	1336	69			

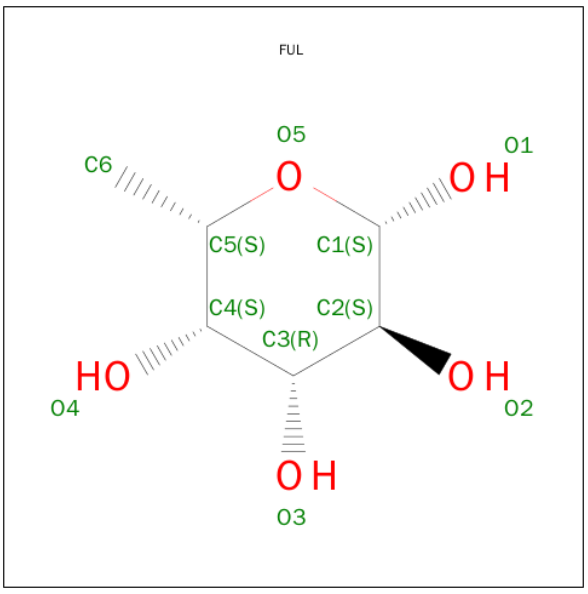
- Molecule 2 is CADMIUM ION (three-letter code: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Cd	0	0
			1	1		

- Molecule 3 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 4 is SUGAR (BETA-L-FUCOSE) (three-letter code: FUL) (formula: $C_6H_{12}O_5$).

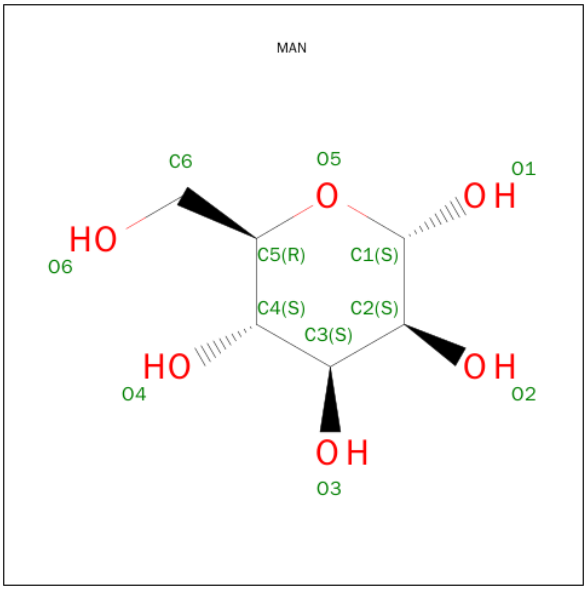


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 10 6 4	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	2	Total C O 21 12 9	0	0

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



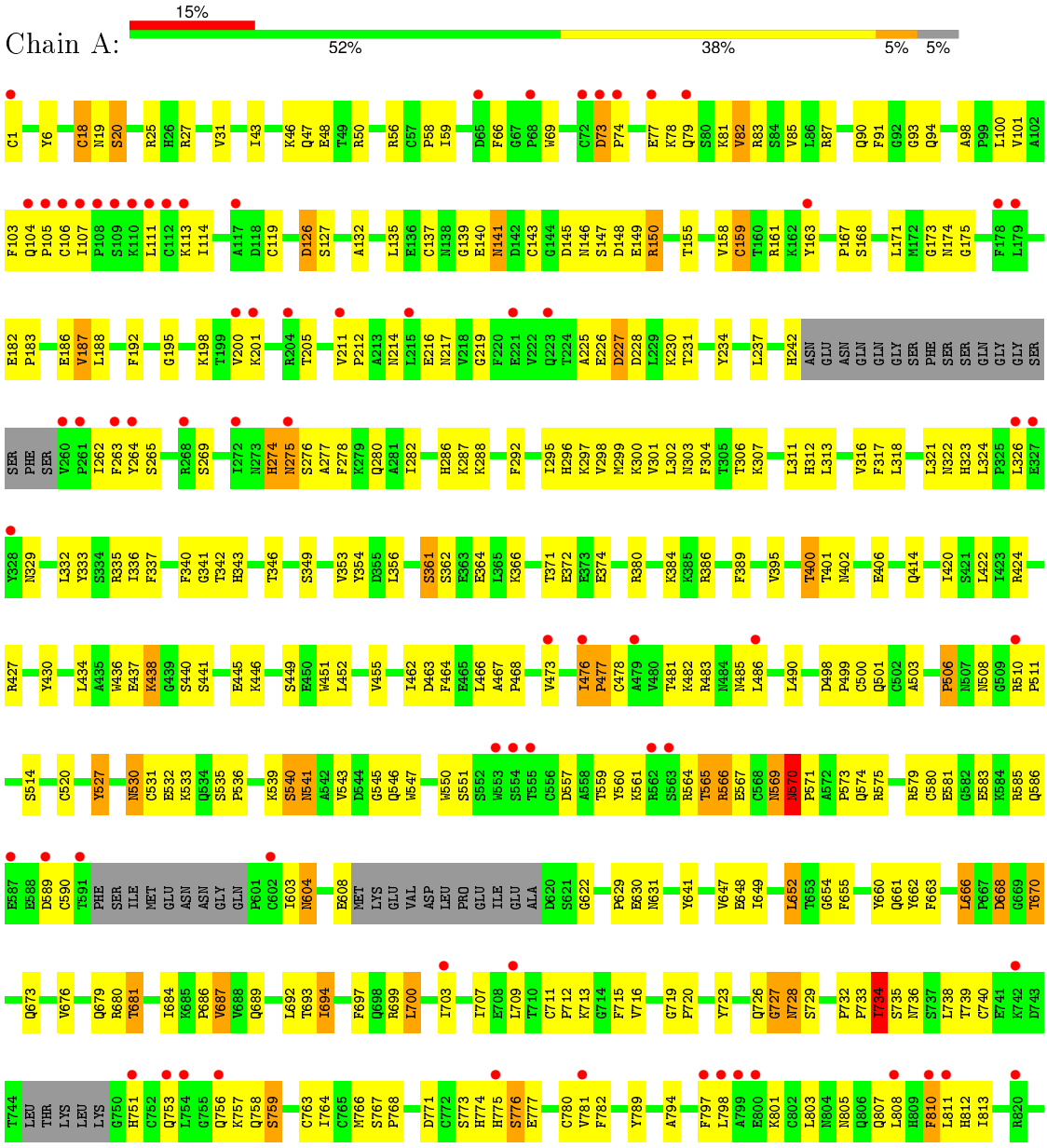
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 11 6 5	0	0
6	A	1	Total C O 11 6 5	0	0
6	A	1	Total C O 11 6 5	0	0
6	A	1	Total C O 11 6 5	0	0

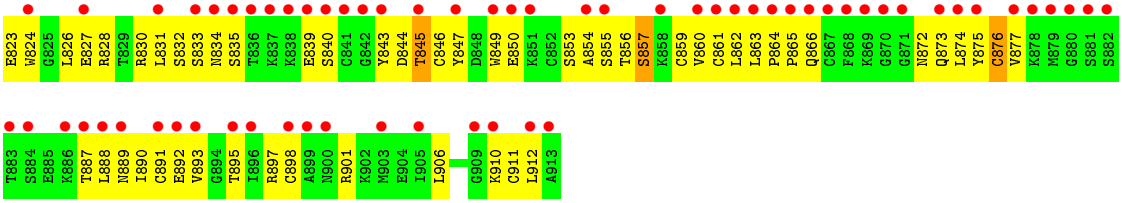
3 Residue-property plots (i)

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 component C6

Chain A:




E823
W824
G825
L826
E827
R828
T829
R830
L831
S832
S833
N834
S835
T836
K837
K838
E839
S840
C841
G842
Y843
D844
T845
C846
Y847
D848
W849
E850
K851
C852
S853
A854
S855
T856
S857
K858
C859
Y860
C861
L862
L863
P864
P865
Q866
C867
F868
K869
G870
G871
N872
Q873
L874
Y875
C876
V877
K878
M879
G880
S881
S882

T883
S884
E885
K886
T887
L888
N889
I890
C891
E892
V893
G894
T895
I896
R897
C898
A899
N900
R901
K902
M903
E904
I905
L906
G909
K910
C911
L912
A913

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	146.81Å 180.15Å 60.53Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.06 – 2.87 47.53 – 2.87	Depositor EDS
% Data completeness (in resolution range)	94.9 (43.06-2.87) 94.9 (47.53-2.87)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	1.66 (at 2.86Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.4_486)	Depositor
R, R_{free}	0.222 , 0.276 0.225 , 0.282	Depositor DCC
R_{free} test set	2179 reflections (6.49%)	DCC
Wilson B-factor (Å^2)	82.3	Xtriage
Anisotropy	0.026	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 81.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 35749 reflections	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	6934	wwPDB-VP
Average B, all atoms (Å^2)	121.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.45% 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: BGC, NAG, CD, FUC, FUL, MAN

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	0.50	1/6973 (0.0%)	0.67	3/9409 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	531	CYS	CB-SG	5.23	1.91	1.82

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	652	LEU	CA-CB-CG	-6.84	99.56	115.30
1	A	570	ASN	N-CA-C	-5.68	95.67	111.00
1	A	666	LEU	CA-CB-CG	-5.07	103.64	115.30

There are no chirality outliers.

There are no planarity outliers.

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	6830	0	6498	398	0
2	A	1	0	0	0	0
3	A	28	0	25	0	0
4	A	10	0	10	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	21	0	19	1	0
6	A	44	0	40	7	0
All	All	6934	0	6592	398	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 29.

All (398) 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:570:ASN:HB3	1:A:571:PRO:CD	1.40	1.41
1:A:824:TRP:HE1	1:A:901:ARG:HD2	1.06	1.17
1:A:570:ASN:HB3	1:A:571:PRO:HD3	1.30	1.13
1:A:476:ILE:HB	1:A:477:PRO:HD2	1.29	1.11
1:A:570:ASN:HB3	1:A:571:PRO:HD2	1.22	1.08
1:A:333:TYR:HE2	1:A:485:ASN:HB3	1.16	1.06
1:A:734:ILE:HD13	1:A:734:ILE:H	0.96	1.06
1:A:570:ASN:CB	1:A:571:PRO:CD	2.33	1.05
1:A:734:ILE:H	1:A:734:ILE:CD1	1.75	0.99
1:A:734:ILE:HD13	1:A:734:ILE:N	1.78	0.98
1:A:715:PHE:HB3	1:A:740:CYS:HB3	1.46	0.98
1:A:1:CYS:HB3	1:A:43:ILE:HD11	1.43	0.97
1:A:333:TYR:CE2	1:A:485:ASN:HB3	2.00	0.96
1:A:567:GLU:O	1:A:569:ASN:OD1	1.84	0.96
1:A:560:TYR:HB3	1:A:589:ASP:HB2	1.51	0.93
1:A:205:THR:O	1:A:205:THR:HG22	1.68	0.90
1:A:840:SER:HA	1:A:844:ASP:HB2	1.52	0.90
1:A:336:ILE:HD11	1:A:486:LEU:HD11	1.53	0.88
1:A:853:SER:HB2	1:A:856:THR:HB	1.54	0.88
1:A:734:ILE:HG13	1:A:738:LEU:HB2	1.56	0.87
1:A:801:LYS:HA	1:A:805:ASN:HB2	1.55	0.87
1:A:824:TRP:NE1	1:A:901:ARG:HD2	1.90	0.85
1:A:756:GLN:HB2	1:A:763:CYS:HB3	1.57	0.85
1:A:546:GLN:HB2	1:A:571:PRO:CG	2.07	0.84
1:A:476:ILE:HB	1:A:477:PRO:CD	2.08	0.83
1:A:757:LYS:HE2	1:A:766:MET:HA	1.61	0.82
1:A:863:LEU:HB3	1:A:865:PRO:HD2	1.59	0.82
1:A:893:VAL:HG12	1:A:897:ARG:CZ	2.11	0.81
1:A:566:ARG:HD2	1:A:583:GLU:O	1.81	0.80
1:A:400:THR:HG22	1:A:401:THR:HG23	1.64	0.80
1:A:560:TYR:CB	1:A:589:ASP:HB2	2.11	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:699:ARG:O	1:A:700:LEU:HD13	1.82	0.79
1:A:79:GLN:HG3	1:A:106:CYS:HB2	1.65	0.78
1:A:824:TRP:O	1:A:828:ARG:HG2	1.84	0.77
1:A:719:GLY:H	1:A:738:LEU:HD13	1.48	0.77
1:A:73:ASP:H	1:A:74:PRO:HD3	1.50	0.76
1:A:126:ASP:OD1	1:A:150:ARG:NH2	2.19	0.76
1:A:570:ASN:CB	1:A:571:PRO:HD3	2.10	0.75
1:A:545:GLY:HA3	1:A:573:PRO:HG3	1.67	0.75
1:A:73:ASP:N	1:A:74:PRO:HD3	2.02	0.75
1:A:342:THR:HG22	1:A:343:HIS:ND1	2.02	0.74
1:A:853:SER:CB	1:A:856:THR:HB	2.17	0.74
1:A:143:CYS:SG	1:A:148:ASP:HB3	2.27	0.73
1:A:476:ILE:HD12	1:A:482:LYS:HE3	1.69	0.73
1:A:874:LEU:HD22	1:A:890:ILE:HG22	1.71	0.72
1:A:372:GLU:H	4:A:1004:FUL:C1	2.03	0.72
1:A:734:ILE:HG13	1:A:738:LEU:CB	2.20	0.72
1:A:581:GLU:HA	1:A:581:GLU:OE1	1.89	0.71
1:A:141:ASN:ND2	1:A:146:ASN:HB2	2.05	0.71
1:A:231:THR:HG22	1:A:295:ILE:HG13	1.73	0.71
1:A:274:HIS:HB3	1:A:277:ALA:HB3	1.73	0.71
1:A:476:ILE:CD1	1:A:482:LYS:HE3	2.21	0.70
1:A:560:TYR:HA	1:A:590:CYS:O	1.92	0.70
1:A:570:ASN:CB	1:A:571:PRO:HD2	2.11	0.69
1:A:897:ARG:HA	1:A:901:ARG:HA	1.75	0.69
1:A:482:LYS:HA	1:A:485:ASN:HB2	1.73	0.69
1:A:380:ARG:HH11	1:A:380:ARG:HG2	1.55	0.69
1:A:297:LYS:HG2	1:A:299:MET:HE2	1.71	0.69
1:A:66:PHE:HB3	1:A:81:LYS:HE2	1.73	0.69
1:A:876:CYS:SG	1:A:906:LEU:HD12	2.33	0.68
1:A:79:GLN:O	1:A:103:PHE:HA	1.94	0.68
1:A:828:ARG:HG3	1:A:847:TYR:CZ	2.28	0.67
1:A:801:LYS:O	1:A:805:ASN:HB2	1.95	0.67
1:A:843:TYR:N	1:A:844:ASP:HA	2.10	0.67
1:A:668:ASP:HB3	1:A:670:THR:HB	1.77	0.67
1:A:547:TRP:H	6:A:1010:MAN:H2	1.60	0.67
1:A:274:HIS:HB3	1:A:277:ALA:CB	2.24	0.67
1:A:692:LEU:HD12	1:A:692:LEU:H	1.59	0.67
1:A:187:VAL:HG13	1:A:188:LEU:HD13	1.76	0.67
1:A:277:ALA:HB1	1:A:422:LEU:CD2	2.25	0.66
1:A:546:GLN:HB2	1:A:571:PRO:HG3	1.78	0.66
1:A:801:LYS:CA	1:A:805:ASN:HB2	2.23	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:91:PHE:HD1	1:A:530:ASN:ND2	1.93	0.66
1:A:780:CYS:O	1:A:811:LEU:HB3	1.95	0.66
1:A:733:PRO:O	1:A:735:SER:N	2.28	0.66
1:A:498:ASP:O	1:A:501:GLN:HG3	1.96	0.65
1:A:342:THR:HG22	1:A:343:HIS:CE1	2.31	0.65
1:A:111:LEU:O	1:A:113:LYS:HG2	1.95	0.65
1:A:569:ASN:OD1	1:A:569:ASN:N	2.30	0.65
1:A:801:LYS:HG3	1:A:805:ASN:CG	2.17	0.65
1:A:301:VAL:O	1:A:302:LEU:HD12	1.97	0.65
1:A:333:TYR:O	1:A:336:ILE:HG12	1.97	0.65
1:A:726:GLN:O	1:A:728:ASN:N	2.30	0.64
1:A:887:THR:C	1:A:888:LEU:HD22	2.18	0.64
1:A:739:THR:HG22	1:A:740:CYS:N	2.13	0.64
1:A:140:GLU:CD	1:A:158:VAL:HG21	2.17	0.64
1:A:237:LEU:HD21	1:A:292:PHE:CE1	2.32	0.64
1:A:205:THR:O	1:A:205:THR:CG2	2.42	0.63
1:A:893:VAL:HG12	1:A:897:ARG:NH2	2.14	0.63
1:A:66:PHE:CB	1:A:81:LYS:HE2	2.29	0.63
1:A:104:GLN:HB3	1:A:105:PRO:HD2	1.79	0.62
1:A:532:GLU:HG2	1:A:533:LYS:N	2.14	0.62
1:A:681:THR:OG1	1:A:703:ILE:HD11	2.00	0.62
1:A:888:LEU:HD12	1:A:892:GLU:CD	2.20	0.61
1:A:875:TYR:HB2	1:A:910:LYS:HA	1.83	0.61
1:A:757:LYS:HG2	1:A:766:MET:HB3	1.82	0.61
1:A:728:ASN:C	1:A:728:ASN:OD1	2.38	0.60
1:A:329:ASN:HD22	1:A:332:LEU:HB2	1.65	0.60
1:A:798:LEU:O	1:A:801:LYS:HB3	2.01	0.60
1:A:498:ASP:CG	1:A:499:PRO:HD2	2.22	0.60
1:A:59:ILE:O	1:A:93:GLY:HA3	2.00	0.60
1:A:211:VAL:HG12	1:A:212:PRO:O	2.02	0.60
1:A:139:GLY:N	1:A:149:GLU:OE2	2.35	0.60
1:A:73:ASP:N	1:A:74:PRO:CD	2.65	0.59
1:A:876:CYS:HA	1:A:911:CYS:HB2	1.84	0.59
1:A:343:HIS:HB3	1:A:466:LEU:HB3	1.85	0.59
1:A:296:HIS:HA	1:A:354:TYR:O	2.03	0.59
1:A:875:TYR:CG	1:A:910:LYS:HA	2.37	0.59
1:A:557:ASP:HB2	1:A:561:LYS:O	2.02	0.59
1:A:288:LYS:HA	1:A:527:TYR:CD1	2.38	0.59
1:A:716:VAL:O	1:A:740:CYS:HA	2.02	0.59
1:A:216:GLU:HB2	1:A:307:LYS:HB2	1.85	0.59
1:A:715:PHE:CB	1:A:740:CYS:HB3	2.28	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:550:TRP:CE3	1:A:564:ARG:HG2	2.38	0.58
1:A:386:ARG:HH12	1:A:414:GLN:NE2	2.01	0.58
1:A:689:GLN:NE2	1:A:736:ASN:HA	2.19	0.58
1:A:464:PHE:O	1:A:464:PHE:CD1	2.57	0.58
1:A:694:ILE:CG2	1:A:709:LEU:HD11	2.34	0.58
1:A:274:HIS:O	1:A:276:SER:N	2.37	0.58
1:A:532:GLU:HG2	1:A:533:LYS:H	1.69	0.58
1:A:81:LYS:O	1:A:101:VAL:HG23	2.05	0.57
1:A:630:GLU:O	1:A:631:ASN:HB2	2.05	0.57
1:A:69:TRP:HZ3	1:A:79:GLN:O	1.88	0.57
1:A:77:GLU:O	1:A:77:GLU:HG3	2.03	0.57
1:A:887:THR:O	1:A:888:LEU:HD13	2.04	0.57
1:A:810:PHE:CD2	1:A:811:LEU:N	2.73	0.57
1:A:580:CYS:HB2	6:A:1010:MAN:H3	1.87	0.57
1:A:756:GLN:CB	1:A:763:CYS:HB3	2.32	0.56
1:A:876:CYS:HA	1:A:911:CYS:CB	2.30	0.56
1:A:386:ARG:HH12	1:A:414:GLN:HE21	1.54	0.56
1:A:313:LEU:HD12	1:A:318:LEU:HD13	1.88	0.56
1:A:389:PHE:CE1	1:A:445:GLU:HB3	2.41	0.56
1:A:546:GLN:HB2	1:A:571:PRO:CD	2.36	0.56
1:A:875:TYR:CB	1:A:910:LYS:HA	2.35	0.56
1:A:876:CYS:CA	1:A:911:CYS:HB2	2.36	0.56
1:A:440:SER:OG	1:A:441:SER:N	2.39	0.56
1:A:847:TYR:HB3	1:A:849:TRP:CE2	2.41	0.55
1:A:402:ASN:O	1:A:406:GLU:HB2	2.07	0.55
1:A:82:VAL:HG22	1:A:101:VAL:HB	1.88	0.55
1:A:322:ASN:C	1:A:324:LEU:H	2.10	0.55
1:A:863:LEU:H	1:A:866:GLN:HE21	1.53	0.55
1:A:872:ASN:H	1:A:890:ILE:HD13	1.71	0.55
1:A:336:ILE:HD11	1:A:486:LEU:CD1	2.34	0.55
1:A:227:ASP:O	1:A:230:LYS:HE2	2.07	0.54
1:A:280:GLN:NE2	1:A:420:ILE:HG23	2.22	0.54
1:A:300:LYS:HG2	1:A:349:SER:HB3	1.89	0.54
1:A:812:HIS:CD2	1:A:813:ILE:O	2.60	0.54
1:A:689:GLN:HE21	1:A:736:ASN:HA	1.72	0.54
1:A:564:ARG:NH2	1:A:586:GLN:OE1	2.40	0.54
1:A:839:GLU:HG3	1:A:846:CYS:HB3	1.89	0.54
1:A:877:VAL:CG2	1:A:888:LEU:HD23	2.38	0.53
1:A:307:LYS:O	1:A:311:LEU:HD21	2.08	0.53
1:A:832:SER:OG	1:A:833:SER:N	2.39	0.53
1:A:6:TYR:O	1:A:27:ARG:HD3	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:801:LYS:NZ	1:A:844:ASP:OD1	2.40	0.53
1:A:498:ASP:OD2	1:A:499:PRO:HD2	2.09	0.53
1:A:132:ALA:N	1:A:135:LEU:HD12	2.23	0.53
1:A:82:VAL:CG2	1:A:101:VAL:HB	2.39	0.53
1:A:663:PHE:CD1	1:A:673:GLN:HG2	2.43	0.53
1:A:354:TYR:CE1	1:A:434:LEU:HD13	2.43	0.53
1:A:751:HIS:O	1:A:753:GLN:HG3	2.10	0.52
1:A:298:VAL:HG23	1:A:353:VAL:HG22	1.91	0.52
1:A:372:GLU:HB2	4:A:1004:FUL:O2	2.10	0.52
1:A:776:SER:HB2	1:A:794:ALA:HB3	1.90	0.52
1:A:774:HIS:O	1:A:775:HIS:C	2.48	0.52
1:A:161:ARG:HD3	1:A:163:TYR:HE2	1.74	0.52
1:A:168:SER:HB3	1:A:171:LEU:HD22	1.90	0.52
1:A:833:SER:O	1:A:834:ASN:HB2	2.09	0.52
1:A:100:LEU:H	1:A:100:LEU:HD12	1.74	0.52
1:A:694:ILE:HG22	1:A:709:LEU:CD1	2.39	0.52
1:A:175:GLY:HA3	1:A:340:PHE:O	2.09	0.52
1:A:739:THR:HG22	1:A:740:CYS:H	1.75	0.52
1:A:182:GLU:HG2	1:A:183:PRO:HD2	1.91	0.52
1:A:173:GLY:O	1:A:187:VAL:HG12	2.09	0.52
1:A:47:GLN:HG2	1:A:48:GLU:N	2.24	0.52
1:A:856:THR:O	1:A:857:SER:HB2	2.10	0.51
1:A:337:PHE:HA	1:A:341:GLY:O	2.10	0.51
1:A:451:TRP:O	1:A:455:VAL:HG23	2.10	0.51
1:A:901:ARG:O	1:A:901:ARG:HG2	2.10	0.51
1:A:726:GLN:NE2	1:A:729:SER:OG	2.29	0.51
1:A:567:GLU:C	1:A:569:ASN:OD1	2.48	0.51
1:A:476:ILE:CB	1:A:477:PRO:HD2	2.19	0.51
1:A:336:ILE:CD1	1:A:486:LEU:HD11	2.33	0.51
1:A:473:VAL:HG13	1:A:473:VAL:O	2.11	0.51
1:A:850:GLU:HB3	1:A:859:CYS:HB3	1.93	0.51
1:A:739:THR:CG2	1:A:740:CYS:N	2.74	0.51
1:A:59:ILE:CG2	1:A:87:ARG:HD2	2.41	0.51
1:A:85:VAL:HG23	1:A:85:VAL:O	2.11	0.51
1:A:546:GLN:O	1:A:571:PRO:HD2	2.11	0.51
1:A:473:VAL:O	1:A:483:ARG:HG3	2.10	0.51
1:A:274:HIS:O	1:A:277:ALA:N	2.45	0.50
1:A:287:LYS:O	1:A:288:LYS:HB3	2.10	0.50
1:A:306:THR:HB	1:A:346:THR:O	2.11	0.50
1:A:380:ARG:HH11	1:A:380:ARG:CG	2.23	0.50
1:A:83:ARG:NH2	1:A:98:ALA:O	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:278:PHE:CE2	1:A:282:ILE:HD11	2.46	0.50
1:A:876:CYS:N	1:A:911:CYS:HB2	2.27	0.50
1:A:808:LEU:HD12	1:A:808:LEU:N	2.27	0.50
1:A:751:HIS:CG	1:A:751:HIS:O	2.65	0.50
1:A:234:TYR:HB2	1:A:292:PHE:HB2	1.93	0.50
1:A:301:VAL:O	1:A:302:LEU:CD1	2.60	0.49
1:A:362:SER:O	1:A:366:LYS:HG3	2.11	0.49
1:A:56:ARG:O	1:A:58:PRO:HD3	2.11	0.49
1:A:333:TYR:HE2	1:A:485:ASN:CB	2.07	0.49
1:A:276:SER:O	1:A:280:GLN:HG3	2.12	0.49
1:A:427:ARG:HB2	1:A:430:TYR:HD2	1.76	0.49
1:A:242:HIS:CE1	1:A:269:SER:HA	2.47	0.49
1:A:372:GLU:N	4:A:1004:FUL:C1	2.75	0.49
1:A:158:VAL:HG23	1:A:159:CYS:N	2.27	0.49
1:A:371:THR:HG22	1:A:374:GLU:HG3	1.94	0.49
1:A:106:CYS:SG	1:A:107:ILE:N	2.85	0.49
1:A:527:TYR:CD2	1:A:527:TYR:N	2.80	0.49
1:A:478:CYS:HB3	1:A:481:THR:HB	1.94	0.49
1:A:663:PHE:CG	1:A:673:GLN:HG2	2.48	0.49
1:A:734:ILE:O	1:A:735:SER:C	2.51	0.49
1:A:477:PRO:HG2	1:A:478:CYS:H	1.78	0.49
1:A:873:GLN:NE2	1:A:875:TYR:CE1	2.81	0.49
1:A:727:GLY:O	1:A:728:ASN:OD1	2.30	0.49
1:A:198:LYS:HG3	1:A:211:VAL:HB	1.95	0.49
1:A:547:TRP:HE1	6:A:1010:MAN:H5	1.78	0.48
1:A:147:SER:C	1:A:149:GLU:H	2.16	0.48
1:A:263:PHE:H	1:A:263:PHE:HD2	1.61	0.48
1:A:541:ASN:O	1:A:575:ARG:HD2	2.14	0.48
1:A:263:PHE:HB3	1:A:468:PRO:HD3	1.95	0.48
1:A:874:LEU:CD2	1:A:890:ILE:HG22	2.43	0.48
1:A:550:TRP:HB2	6:A:1009:MAN:H5	1.94	0.48
1:A:354:TYR:HE1	1:A:434:LEU:HD13	1.79	0.48
1:A:303:ASN:O	1:A:304:PHE:HB3	2.14	0.48
1:A:476:ILE:CB	1:A:477:PRO:CD	2.87	0.48
1:A:336:ILE:HD11	1:A:486:LEU:HD21	1.95	0.48
1:A:107:ILE:HG13	1:A:107:ILE:O	2.14	0.48
1:A:78:LYS:HA	1:A:104:GLN:O	2.14	0.48
1:A:498:ASP:OD1	1:A:500:CYS:HB3	2.14	0.48
1:A:371:THR:HG23	1:A:374:GLU:H	1.77	0.48
1:A:758:GLN:HG2	1:A:759:SER:N	2.28	0.48
1:A:828:ARG:HD2	1:A:849:TRP:HZ2	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:158:VAL:HG11	1:A:195:GLY:HA2	1.95	0.48
1:A:735:SER:O	1:A:736:ASN:HB2	2.13	0.48
1:A:739:THR:CG2	1:A:740:CYS:H	2.27	0.48
1:A:803:LEU:HD12	1:A:803:LEU:N	2.29	0.48
1:A:324:LEU:HB3	1:A:333:TYR:HE1	1.79	0.47
1:A:684:ILE:O	1:A:686:PRO:HD3	2.15	0.47
1:A:78:LYS:HD3	1:A:103:PHE:CE1	2.50	0.47
1:A:876:CYS:CA	1:A:911:CYS:CB	2.93	0.47
1:A:27:ARG:HG3	1:A:46:LYS:HA	1.96	0.47
1:A:719:GLY:H	1:A:738:LEU:CD1	2.21	0.47
1:A:805:ASN:C	1:A:807:GLN:H	2.17	0.47
1:A:50:ARG:HH22	6:A:1007:MAN:H5	1.78	0.47
1:A:863:LEU:C	1:A:865:PRO:HD2	2.35	0.47
1:A:546:GLN:N	1:A:571:PRO:HG2	2.29	0.47
1:A:113:LYS:O	1:A:114:ILE:HD13	2.14	0.47
1:A:776:SER:O	1:A:777:GLU:C	2.53	0.47
1:A:889:ASN:O	1:A:893:VAL:HG23	2.14	0.47
1:A:827:GLU:HA	1:A:830:ARG:NH1	2.30	0.47
1:A:756:GLN:HE21	1:A:763:CYS:CB	2.28	0.47
1:A:864:PRO:N	1:A:865:PRO:HD2	2.30	0.47
1:A:875:TYR:CE2	1:A:910:LYS:HG2	2.50	0.47
1:A:569:ASN:O	1:A:570:ASN:C	2.52	0.47
1:A:694:ILE:HG23	1:A:709:LEU:HD11	1.96	0.47
1:A:912:LEU:N	1:A:912:LEU:HD12	2.30	0.47
1:A:343:HIS:HA	1:A:467:ALA:O	2.15	0.46
1:A:579:ARG:H	1:A:579:ARG:HG3	1.52	0.46
1:A:264:TYR:CD1	1:A:265:SER:O	2.68	0.46
1:A:380:ARG:NH1	1:A:380:ARG:CG	2.79	0.46
1:A:569:ASN:O	1:A:571:PRO:HD2	2.15	0.46
1:A:237:LEU:HD21	1:A:292:PHE:CD1	2.50	0.46
1:A:603:ILE:HG22	1:A:604:ASN:O	2.16	0.46
1:A:546:GLN:CB	1:A:571:PRO:CG	2.87	0.46
1:A:400:THR:HG22	1:A:401:THR:CG2	2.42	0.46
1:A:912:LEU:H	1:A:912:LEU:HD12	1.80	0.46
1:A:317:PHE:CE1	1:A:321:LEU:HD22	2.50	0.46
1:A:326:LEU:N	1:A:326:LEU:HD12	2.31	0.45
1:A:782:PHE:CD1	1:A:789:TYR:HB3	2.51	0.45
1:A:69:TRP:CE3	1:A:79:GLN:HB3	2.51	0.45
1:A:386:ARG:HH22	1:A:414:GLN:NE2	2.14	0.45
1:A:862:LEU:O	1:A:895:THR:HB	2.16	0.45
1:A:535:SER:HB2	1:A:536:PRO:HD2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:648:GLU:HB2	1:A:662:TYR:CE1	2.52	0.45
1:A:389:PHE:HZ	1:A:449:SER:HB2	1.81	0.45
1:A:839:GLU:HG3	1:A:846:CYS:CB	2.46	0.45
1:A:187:VAL:HG13	1:A:188:LEU:CD1	2.46	0.45
1:A:486:LEU:HD12	1:A:486:LEU:HA	1.76	0.45
1:A:629:PRO:O	1:A:630:GLU:C	2.55	0.45
1:A:380:ARG:NH1	1:A:380:ARG:HG2	2.26	0.45
1:A:692:LEU:HD12	1:A:692:LEU:N	2.31	0.45
1:A:31:VAL:HG12	1:A:31:VAL:O	2.15	0.45
1:A:873:GLN:HB3	1:A:875:TYR:CE1	2.52	0.44
1:A:302:LEU:O	1:A:349:SER:HB3	2.17	0.44
1:A:18:CYS:SG	5:A:1005:FUC:H5	2.57	0.44
1:A:654:GLY:O	1:A:681:THR:HG23	2.18	0.44
1:A:652:LEU:HA	1:A:652:LEU:HD23	1.56	0.44
1:A:192:PHE:CE2	1:A:312:HIS:CD2	3.05	0.44
1:A:831:LEU:HD12	1:A:835:SER:HB2	1.98	0.44
1:A:354:TYR:CZ	1:A:356:LEU:CD1	3.01	0.44
1:A:226:GLU:O	1:A:228:ASP:N	2.51	0.44
1:A:277:ALA:HB1	1:A:422:LEU:HD23	1.99	0.44
1:A:335:ARG:HA	1:A:335:ARG:HD2	1.78	0.44
1:A:560:TYR:O	1:A:590:CYS:N	2.51	0.44
1:A:694:ILE:H	1:A:694:ILE:HG12	1.53	0.44
1:A:767:SER:HA	1:A:768:PRO:HD3	1.88	0.44
1:A:550:TRP:CD2	1:A:566:ARG:HG2	2.53	0.44
1:A:329:ASN:ND2	1:A:332:LEU:HB2	2.31	0.44
1:A:214:ASN:H	1:A:214:ASN:HD22	1.66	0.44
1:A:361:SER:OG	1:A:364:GLU:HG2	2.18	0.44
1:A:424:ARG:HH11	1:A:424:ARG:HG2	1.83	0.44
1:A:19:ASN:O	1:A:20:SER:HB3	2.16	0.44
1:A:767:SER:N	1:A:771:ASP:OD2	2.48	0.44
1:A:545:GLY:O	1:A:580:CYS:HB3	2.18	0.43
1:A:810:PHE:CG	1:A:811:LEU:N	2.86	0.43
1:A:856:THR:O	1:A:857:SER:CB	2.66	0.43
1:A:622:GLY:HA3	1:A:641:TYR:O	2.19	0.43
1:A:127:SER:HB3	1:A:145:ASP:OD1	2.18	0.43
1:A:828:ARG:HG3	1:A:847:TYR:CE2	2.53	0.43
1:A:264:TYR:HD1	1:A:265:SER:O	2.01	0.43
1:A:891:CYS:O	1:A:895:THR:HG23	2.18	0.43
1:A:801:LYS:C	1:A:805:ASN:HB2	2.38	0.43
1:A:559:THR:C	1:A:561:LYS:N	2.71	0.43
1:A:171:LEU:CD1	1:A:171:LEU:N	2.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:875:TYR:CG	1:A:887:THR:HG23	2.54	0.43
1:A:697:PHE:CD2	1:A:697:PHE:C	2.92	0.43
1:A:550:TRP:CZ2	1:A:566:ARG:NE	2.87	0.43
1:A:666:LEU:HD23	1:A:666:LEU:HA	1.46	0.43
1:A:216:GLU:O	1:A:217:ASN:ND2	2.51	0.43
1:A:694:ILE:CG2	1:A:709:LEU:CD1	2.95	0.43
1:A:843:TYR:HD2	1:A:845:THR:O	2.02	0.43
1:A:585:ARG:HG2	1:A:586:GLN:N	2.34	0.43
1:A:354:TYR:CZ	1:A:356:LEU:HD11	2.54	0.43
1:A:641:TYR:CE1	1:A:647:VAL:HG11	2.54	0.43
1:A:508:ASN:OD1	1:A:543:VAL:HA	2.19	0.43
1:A:781:VAL:HG11	1:A:797:PHE:CD1	2.54	0.43
1:A:436:TRP:C	1:A:437:GLU:HG3	2.38	0.43
1:A:860:VAL:HG12	1:A:861:CYS:N	2.34	0.43
1:A:560:TYR:HB3	1:A:589:ASP:CB	2.36	0.43
1:A:561:LYS:HA	1:A:561:LYS:HD3	1.68	0.43
1:A:864:PRO:N	1:A:865:PRO:CD	2.81	0.42
1:A:655:PHE:CE1	1:A:680:ARG:HG3	2.54	0.42
1:A:756:GLN:HB3	1:A:764:ILE:O	2.19	0.42
1:A:543:VAL:HB	1:A:574:GLN:HB2	2.01	0.42
1:A:455:VAL:HG12	1:A:455:VAL:O	2.19	0.42
1:A:437:GLU:O	1:A:438:LYS:C	2.56	0.42
1:A:452:LEU:HA	1:A:452:LEU:HD12	1.76	0.42
1:A:219:GLY:O	1:A:302:LEU:HA	2.19	0.42
1:A:226:GLU:O	1:A:227:ASP:C	2.57	0.42
1:A:608:GLU:H	1:A:608:GLU:HG2	1.67	0.42
1:A:324:LEU:HB3	1:A:333:TYR:CE1	2.54	0.42
1:A:462:ILE:O	1:A:463:ASP:C	2.57	0.42
1:A:823:GLU:O	1:A:826:LEU:HB3	2.18	0.42
1:A:551:SER:HB2	1:A:565:THR:O	2.20	0.42
1:A:843:TYR:CB	1:A:844:ASP:HA	2.50	0.42
1:A:322:ASN:C	1:A:324:LEU:N	2.72	0.42
1:A:158:VAL:HB	1:A:195:GLY:O	2.20	0.42
1:A:776:SER:CB	1:A:794:ALA:HB3	2.50	0.42
1:A:604:ASN:ND2	1:A:604:ASN:H	2.17	0.42
1:A:302:LEU:O	1:A:349:SER:HA	2.20	0.41
1:A:25:ARG:HH12	6:A:1008:MAN:H61	1.84	0.41
1:A:873:GLN:NE2	1:A:875:TYR:HE1	2.16	0.41
1:A:854:ALA:O	1:A:855:SER:HB2	2.19	0.41
1:A:90:GLN:HE22	1:A:503:ALA:N	2.18	0.41
1:A:286:HIS:HE1	1:A:520:CYS:O	2.04	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:167:PRO:O	1:A:168:SER:HB2	2.20	0.41
1:A:337:PHE:CZ	1:A:490:LEU:HB2	2.55	0.41
1:A:510:ARG:HA	1:A:511:PRO:HD2	1.96	0.41
1:A:539:LYS:O	1:A:540:SER:O	2.38	0.41
1:A:893:VAL:HG12	1:A:897:ARG:NE	2.35	0.41
1:A:550:TRP:CE3	1:A:566:ARG:HG2	2.55	0.41
1:A:603:ILE:N	1:A:603:ILE:HD12	2.35	0.41
1:A:201:LYS:HB2	1:A:201:LYS:HE3	1.83	0.41
1:A:853:SER:HB3	1:A:856:THR:HB	2.01	0.41
1:A:158:VAL:HG23	1:A:159:CYS:HB2	2.01	0.41
1:A:687:VAL:HG21	1:A:735:SER:HA	2.02	0.41
1:A:801:LYS:HG3	1:A:805:ASN:CB	2.50	0.41
1:A:81:LYS:O	1:A:101:VAL:HA	2.20	0.41
1:A:298:VAL:CG2	1:A:462:ILE:HD12	2.50	0.41
1:A:773:SER:OG	1:A:774:HIS:N	2.53	0.41
1:A:686:PRO:HG2	1:A:707:ILE:CD1	2.50	0.41
1:A:332:LEU:O	1:A:335:ARG:HB2	2.21	0.41
1:A:262:ILE:HG22	1:A:263:PHE:CD2	2.55	0.41
1:A:316:VAL:HG13	1:A:317:PHE:N	2.36	0.41
1:A:137:CYS:HB3	1:A:155:THR:HG22	2.02	0.41
1:A:545:GLY:O	1:A:546:GLN:HG2	2.21	0.41
1:A:434:LEU:HA	1:A:434:LEU:HD23	1.84	0.41
1:A:713:LYS:HD3	1:A:713:LYS:N	2.35	0.41
1:A:550:TRP:HB2	6:A:1009:MAN:C5	2.51	0.41
1:A:875:TYR:HB3	1:A:911:CYS:H	1.86	0.41
1:A:666:LEU:HB2	1:A:670:THR:O	2.21	0.41
1:A:225:ALA:O	1:A:228:ASP:HB2	2.20	0.41
1:A:263:PHE:N	1:A:263:PHE:CD2	2.88	0.41
1:A:720:PRO:HG2	1:A:723:TYR:CZ	2.56	0.41
1:A:100:LEU:N	1:A:100:LEU:HD12	2.35	0.40
1:A:660:TYR:O	1:A:676:VAL:HB	2.21	0.40
1:A:843:TYR:N	1:A:844:ASP:CA	2.83	0.40
1:A:828:ARG:NH2	1:A:898:CYS:HA	2.35	0.40
1:A:801:LYS:O	1:A:805:ASN:CB	2.67	0.40
1:A:464:PHE:CE1	1:A:466:LEU:HD21	2.57	0.40
1:A:445:GLU:O	1:A:446:LYS:C	2.60	0.40
1:A:322:ASN:O	1:A:324:LEU:N	2.54	0.40
1:A:274:HIS:O	1:A:275:ASN:C	2.60	0.40
1:A:174:ASN:ND2	1:A:186:GLU:HA	2.36	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	861/913 (94%)	734 (85%)	105 (12%)	22 (3%)	7 23

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	150	ARG
1	A	540	SER
1	A	570	ASN
1	A	712	PRO
1	A	727	GLY
1	A	734	ILE
1	A	141	ASN
1	A	275	ASN
1	A	323	HIS
1	A	668	ASP
1	A	857	SER
1	A	227	ASP
1	A	810	PHE
1	A	438	LYS
1	A	759	SER
1	A	506	PRO
1	A	687	VAL
1	A	20	SER
1	A	476	ILE
1	A	477	PRO
1	A	73	ASP
1	A	732	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	772/810 (95%)	736 (95%)	36 (5%)	32 66

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	CYS
1	A	82	VAL
1	A	94	GLN
1	A	119	CYS
1	A	126	ASP
1	A	159	CYS
1	A	187	VAL
1	A	200	VAL
1	A	274	HIS
1	A	361	SER
1	A	384	LYS
1	A	395	VAL
1	A	400	THR
1	A	506	PRO
1	A	514	SER
1	A	527	TYR
1	A	530	ASN
1	A	541	ASN
1	A	565	THR
1	A	566	ARG
1	A	569	ASN
1	A	604	ASN
1	A	649	ILE
1	A	661	GLN
1	A	670	THR
1	A	679	GLN
1	A	681	THR
1	A	693	THR
1	A	694	ILE
1	A	700	LEU
1	A	711	CYS
1	A	728	ASN
1	A	734	ILE
1	A	776	SER
1	A	845	THR

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Mol	Chain	Res	Type
1	A	876	CYS

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	36	GLN
1	A	79	GLN
1	A	90	GLN
1	A	174	ASN
1	A	190	ASN
1	A	207	ASN
1	A	223	GLN
1	A	242	HIS
1	A	271	ASN
1	A	275	ASN
1	A	280	GLN
1	A	286	HIS
1	A	296	HIS
1	A	312	HIS
1	A	329	ASN
1	A	377	HIS
1	A	408	HIS
1	A	414	GLN
1	A	530	ASN
1	A	574	GLN
1	A	604	ASN
1	A	679	GLN
1	A	753	GLN
1	A	756	GLN
1	A	804	ASN
1	A	812	HIS
1	A	817	GLN
1	A	866	GLN
1	A	873	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

4 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	$\#\|Z\|>2$
3	NAG	A	1002	1,3	14,14,15	0.58	0	15,19,21	0.71	0
3	NAG	A	1003	3	14,14,15	0.50	0	15,19,21	0.61	0
5	FUC	A	1005	1,5	10,10,11	0.81	0	14,14,16	1.84	4 (28%)
5	BGC	A	1006	5	11,11,12	1.12	1 (9%)	14,15,17	1.61	3 (21%)

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	1002	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	1003	3	-	0/6/23/26	0/1/1/1
5	FUC	A	1005	1,5	-	0/0/17/20	0/1/1/1
5	BGC	A	1006	5	-	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	A	1006	BGC	O5-C1	-3.22	1.38	1.43

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	1006	BGC	C1-C2-C3	-3.85	104.99	109.54
5	A	1005	FUC	C6-C5-C4	-2.73	107.70	113.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	1006	BGC	O5-C1-C2	-2.18	107.32	110.86
5	A	1006	BGC	C3-C4-C5	-2.16	106.44	110.20
5	A	1005	FUC	O4-C4-C5	-2.15	104.78	109.84
5	A	1005	FUC	C1-C2-C3	2.57	112.59	109.54
5	A	1005	FUC	O5-C5-C6	4.25	113.17	106.13

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
5	A	1005	FUC	1	0

5.6 Ligand geometry (i)

Of 6 ligands modelled in this entry, 1 is monoatomic - leaving 5 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	$\#\|Z\| > 2$
4	FUL	A	1004	1	10,10,11	0.65	0	14,14,16	1.25	2 (14%)
6	MAN	A	1007	1	11,11,12	0.86	0	14,15,17	1.23	2 (14%)
6	MAN	A	1008	1	11,11,12	1.16	0	14,15,17	1.73	3 (21%)
6	MAN	A	1009	1	11,11,12	0.62	0	14,15,17	1.51	3 (21%)
6	MAN	A	1010	1	11,11,12	0.46	0	14,15,17	1.39	2 (14%)

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	FUL	A	1004	1	-	0/0/17/20	0/1/1/1
6	MAN	A	1007	1	-	0/2/19/22	0/1/1/1
6	MAN	A	1008	1	-	0/2/19/22	1/1/1/1
6	MAN	A	1009	1	-	0/2/19/22	0/1/1/1
6	MAN	A	1010	1	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	1010	MAN	C2-C3-C4	-3.32	105.40	111.04
6	A	1008	MAN	C1-C2-C3	-3.24	105.70	109.54
6	A	1008	MAN	O4-C4-C3	-3.19	103.16	110.34
6	A	1007	MAN	O4-C4-C3	-2.52	104.65	110.34
6	A	1007	MAN	O5-C1-C2	-2.33	107.08	110.86
6	A	1008	MAN	O4-C4-C5	-2.21	103.37	109.24
6	A	1010	MAN	C1-C2-C3	-2.18	106.96	109.54
6	A	1009	MAN	O5-C1-C2	-2.12	107.42	110.86
4	A	1004	FUL	C1-C2-C3	2.23	112.18	109.54
4	A	1004	FUL	O5-C5-C6	3.06	111.19	106.13
6	A	1009	MAN	C1-O5-C5	3.09	116.17	112.25
6	A	1009	MAN	C3-C4-C5	3.27	115.90	110.20

There are no chirality outliers.

There are no torsion outliers.

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	1008	MAN	C1-C2-C3-C4-C5-O5

5 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1004	FUL	3	0
6	A	1007	MAN	1	0
6	A	1008	MAN	1	0
6	A	1009	MAN	2	0
6	A	1010	MAN	3	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	871/913 (95%)	0.98	133 (15%)	3	2	41, 107, 238, 291	0

All (133) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	840	SER	15.1
1	A	861	CYS	12.1
1	A	892	GLU	10.4
1	A	913	ALA	10.1
1	A	879	MET	9.9
1	A	843	TYR	9.8
1	A	834	ASN	9.7
1	A	870	GLY	9.6
1	A	888	LEU	9.4
1	A	842	GLY	9.4
1	A	865	PRO	9.1
1	A	873	GLN	8.8
1	A	838	LYS	7.9
1	A	111	LEU	7.6
1	A	862	LEU	7.6
1	A	775	HIS	7.6
1	A	871	GLY	7.5
1	A	860	VAL	7.5
1	A	73	ASP	7.0
1	A	105	PRO	7.0
1	A	875	TYR	6.8
1	A	753	GLN	6.7
1	A	264	TYR	6.7
1	A	905	ILE	6.7
1	A	880	GLY	6.7
1	A	893	VAL	6.6
1	A	899	ALA	6.6

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Mol	Chain	Res	Type	RSRZ
1	A	874	LEU	6.6
1	A	110	LYS	6.2
1	A	882	SER	6.2
1	A	864	PRO	5.8
1	A	903	MET	5.7
1	A	836	THR	5.5
1	A	555	THR	5.4
1	A	835	SER	5.4
1	A	887	THR	5.4
1	A	884	SER	5.1
1	A	563	SER	5.1
1	A	889	ASN	5.1
1	A	847	TYR	4.9
1	A	839	GLU	4.9
1	A	754	LEU	4.9
1	A	808	LEU	4.8
1	A	756	GLN	4.8
1	A	896	ILE	4.8
1	A	827	GLU	4.7
1	A	820	ARG	4.7
1	A	200	VAL	4.6
1	A	912	LEU	4.5
1	A	868	PHE	4.5
1	A	591	THR	4.4
1	A	112	CYS	4.4
1	A	473	VAL	4.3
1	A	824	TRP	4.3
1	A	878	LYS	4.3
1	A	811	LEU	4.2
1	A	831	LEU	4.2
1	A	854	ALA	4.2
1	A	117	ALA	4.1
1	A	223	GLN	4.1
1	A	866	GLN	4.1
1	A	107	ILE	4.1
1	A	869	LYS	4.0
1	A	72	CYS	3.9
1	A	742	LYS	3.9
1	A	833	SER	3.8
1	A	877	VAL	3.8
1	A	587	GLU	3.8
1	A	895	THR	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	106	CYS	3.5
1	A	851	LYS	3.4
1	A	204	ARG	3.4
1	A	553	TRP	3.3
1	A	562	ARG	3.3
1	A	910	LYS	3.3
1	A	602	CYS	3.3
1	A	797	PHE	3.2
1	A	275	ASN	3.2
1	A	221	GLU	3.2
1	A	837	LYS	3.2
1	A	104	GLN	3.2
1	A	909	GLY	3.2
1	A	900	ASN	3.1
1	A	261	PRO	3.0
1	A	891	CYS	3.0
1	A	800	GLU	2.9
1	A	268	ARG	2.9
1	A	486	LEU	2.8
1	A	77	GLU	2.8
1	A	326	LEU	2.8
1	A	849	TRP	2.8
1	A	798	LEU	2.8
1	A	109	SER	2.7
1	A	479	ALA	2.7
1	A	867	CYS	2.7
1	A	260	VAL	2.6
1	A	781	VAL	2.6
1	A	841	CYS	2.5
1	A	179	LEU	2.5
1	A	263	PHE	2.5
1	A	65	ASP	2.5
1	A	810	PHE	2.5
1	A	858	LYS	2.5
1	A	845	THR	2.5
1	A	328	TYR	2.5
1	A	68	PRO	2.5
1	A	215	LEU	2.5
1	A	476	ILE	2.5
1	A	211	VAL	2.5
1	A	272	ILE	2.5
1	A	113	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	327	GLU	2.4
1	A	589	ASP	2.4
1	A	201	LYS	2.4
1	A	850	GLU	2.4
1	A	886	LYS	2.4
1	A	178	PHE	2.4
1	A	709	LEU	2.3
1	A	1	CYS	2.3
1	A	883	THR	2.3
1	A	881	SER	2.3
1	A	79	GLN	2.2
1	A	751	HIS	2.2
1	A	799	ALA	2.2
1	A	163	TYR	2.2
1	A	108	PRO	2.2
1	A	898	CYS	2.1
1	A	554	SER	2.1
1	A	855	SER	2.1
1	A	74	PRO	2.1
1	A	863	LEU	2.1
1	A	510	ARG	2.0
1	A	703	ILE	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^{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
5	BGC	A	1006	11/12	0.97	0.20	0.49	51,62,72,80	0
5	FUC	A	1005	10/11	0.98	0.19	-	47,56,68,78	0
3	NAG	A	1003	14/15	0.77	0.54	-	148,174,183,187	0
3	NAG	A	1002	14/15	0.90	0.25	-	120,151,163,169	0

6.4 Ligands

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	MAN	A	1010	11/12	0.88	0.23	-0.00	127,137,142,143	0
6	MAN	A	1009	11/12	0.92	0.19	-0.20	152,162,169,172	0
6	MAN	A	1008	11/12	0.96	0.22	-0.26	58,71,81,107	0
2	CD	A	1001	1/1	0.97	0.18	-0.29	133,133,133,133	0
4	FUL	A	1004	10/11	0.81	0.32	-	154,162,169,172	0
6	MAN	A	1007	11/12	0.95	0.22	-	73,87,95,102	0

6.5 Other polymers

There are no such residues in this entry.