Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 08:38 PM GMT

PDB ID	:	1L5G
Title	:	CRYSTAL STRUCTURE OF THE EXTRACELLULAR SEGMENT OF INTEGRIN AVB3 IN COMPLEX WITH AN ARG-GLY-ASP LIGAND
Authors	:	Xiong, J.-P.; Stehle, T.; Zhang, R.; Joachimiak, A.; Frech, M.; Goodman, S.L.; Arnaout, M.A.
Deposited on	:	2002-03-06
Resolution	:	3.20 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 (i)) were used in the production of this report:

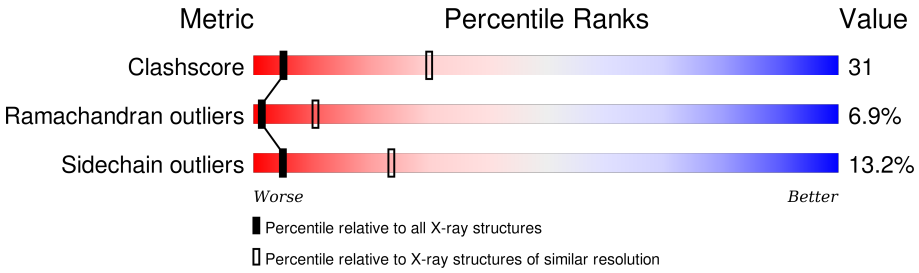
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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 3.20 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))
Clashscore	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	957	47% 41% 8%
2	B	692	29% 37% 10% 22%
3	C	5	20% 60% 20%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 11700 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 INTEGRIN ALPHA V.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	927	Total	C	N	O	S	0	0	0
			7216	4568	1224	1389	35			

- Molecule 2 is a protein called INTEGRIN BETA-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	539	Total	C	N	O	S	0	0	0
			4182	2594	700	842	46			

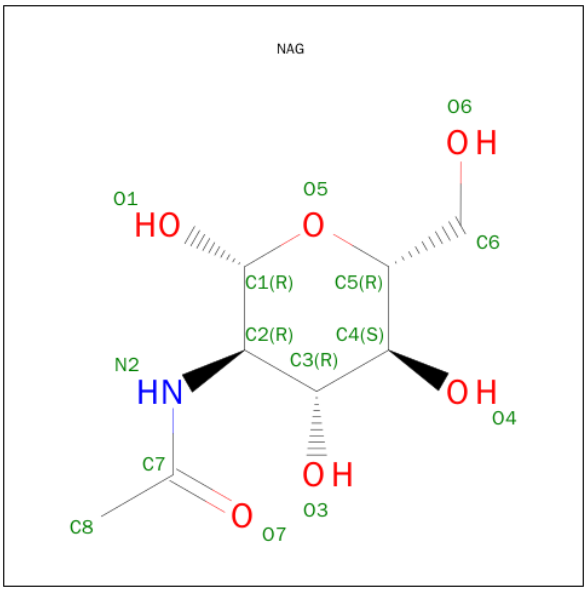
- Molecule 3 is a protein called CYCLIC ARG-GLY-ASP PEPTIDE.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	5	Total	C	N	O	0	0	0
			42	27	8	7			

- Molecule 4 is a polymer of unknown type called SUGAR (2-MER).

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

- Molecule 5 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 6 is a polymer of unknown type called SUGAR (2-MER).

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

- Molecule 7 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	3	Total Mn 3 3	0	0
7	A	5	Total Mn 5 5	0	0

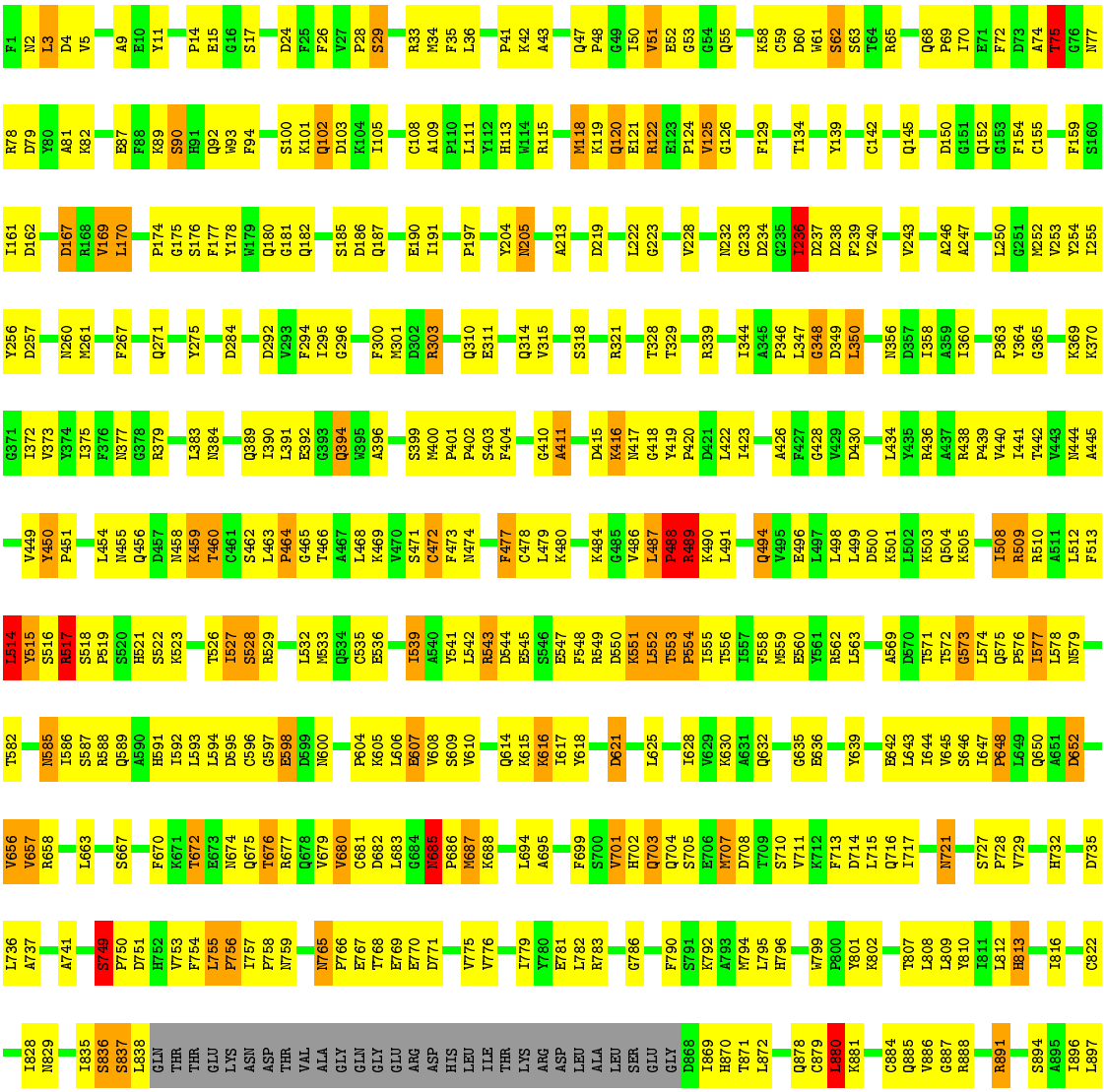
3 Residue-property plots (i)

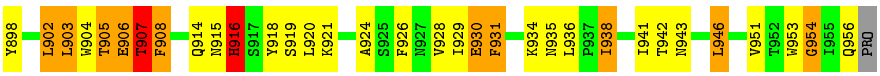
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

Note EDS was not executed.

- Molecule 1: INTEGRIN ALPHA V

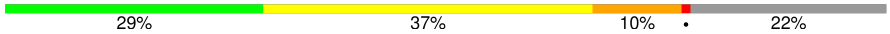
Chain A:

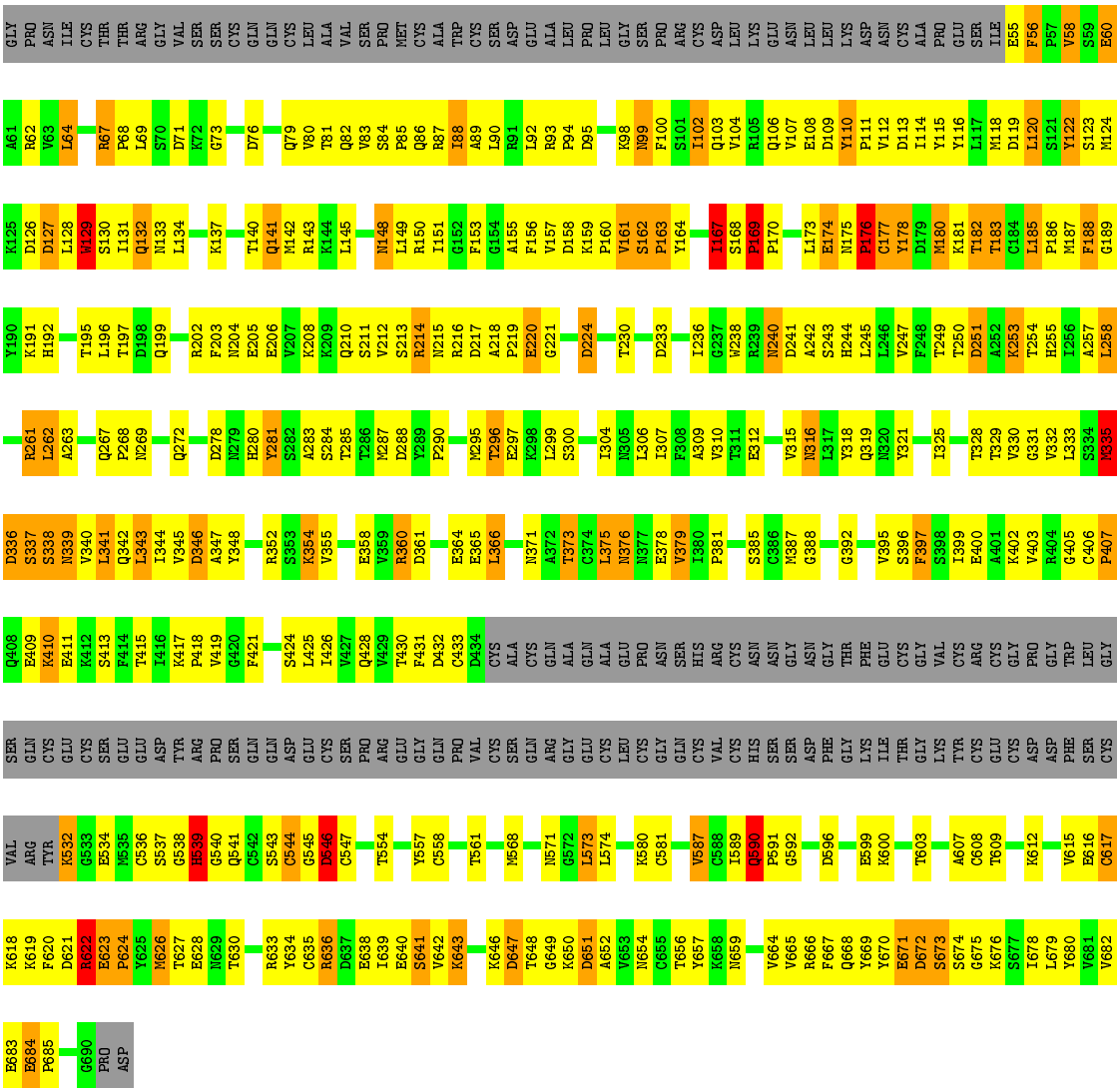




• Molecule 2: INTEGRIN BETA-3

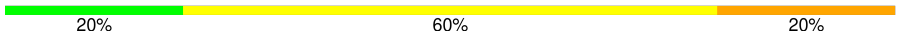
Chain B:





• Molecule 3: CYCLIC ARG-GLY-ASP PEPTIDE

Chain C:



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	129.79Å 129.79Å 308.78Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 3.20	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-3.20)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.16	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.248 , 0.328	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	11700	wwPDB-VP
Average B, all atoms (Å^2)	39.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MVA, MN, NAG, NDG

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	0.48	1/7372 (0.0%)	0.83	13/9994 (0.1%)
2	B	0.48	0/4256	0.85	7/5754 (0.1%)
3	C	0.49	0/34	0.77	0/43
All	All	0.48	1/11662 (0.0%)	0.84	20/15791 (0.1%)

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
3	C	1	0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	75	THR	CA-CB	6.56	1.70	1.53

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	75	THR	N-CA-CB	7.91	125.33	110.30
2	B	336	ASP	N-CA-C	-7.27	91.38	111.00
1	A	553	THR	N-CA-C	-7.17	91.65	111.00
1	A	907	THR	N-CA-C	-7.16	91.68	111.00
1	A	460	THR	N-CA-C	7.02	129.94	111.00
1	A	488	PRO	N-CA-C	7.01	130.32	112.10
1	A	349	ASP	N-CA-C	-6.41	93.69	111.00
2	B	545	GLY	N-CA-C	-6.29	97.37	113.10
2	B	590	GLN	N-CA-C	6.23	127.81	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	169	PRO	N-CA-C	-6.15	96.10	112.10
2	B	622	ARG	N-CA-C	5.84	126.78	111.00
1	A	749	SER	C-N-CD	5.82	140.61	128.40
1	A	672	THR	N-CA-C	-5.72	95.56	111.00
2	B	335	MET	N-CA-C	-5.60	95.89	111.00
1	A	916	HIS	N-CA-C	5.47	125.77	111.00
1	A	597	GLY	N-CA-C	5.33	126.43	113.10
1	A	489	ARG	CB-CA-C	5.19	120.79	110.40
2	B	587	VAL	N-CA-C	-5.16	97.08	111.00
1	A	542	LEU	CA-CB-CG	5.01	126.83	115.30
1	A	880	LEU	N-CA-C	-5.01	97.47	111.00

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	C	5004	PHE	CA

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7216	0	7035	396	0
2	B	4182	0	4029	300	0
3	C	42	0	39	8	0
4	A	112	0	100	11	0
5	A	28	0	26	8	0
5	B	28	0	26	5	0
6	A	28	0	25	7	0
6	B	56	0	50	8	0
7	A	5	0	0	0	0
7	B	3	0	0	0	0
All	All	11700	0	11330	708	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 31.

All (708) 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)
6:A:2943:NAG:H2	6:A:2943:NAG:H61	1.34	1.06
1:A:487:LEU:HD23	1:A:488:PRO:HD3	1.37	1.05
1:A:236:ILE:HD13	1:A:236:ILE:H	1.21	1.02
2:B:69:LEU:HD22	2:B:80:VAL:HA	1.46	0.95
2:B:371:ASN:ND2	5:B:3371:NAG:H62	1.81	0.95
1:A:741:ALA:H	1:A:786:GLY:HA3	1.28	0.93
2:B:185:LEU:HD23	2:B:185:LEU:H	1.32	0.93
2:B:169:PRO:HB2	2:B:170:PRO:HD3	1.48	0.93
2:B:157:VAL:HG11	2:B:188:PHE:H	1.31	0.92
2:B:316:ASN:HD22	2:B:316:ASN:H	1.12	0.92
1:A:416:LYS:H	1:A:416:LYS:HD2	1.38	0.89
2:B:157:VAL:HG12	2:B:189:GLY:H	1.36	0.89
2:B:129:TRP:HB2	2:B:208:LYS:HE3	1.55	0.88
1:A:585:ASN:ND2	4:A:2585:NAG:H61	1.90	0.87
1:A:751:ASP:HB2	4:A:2950:NAG:H81	1.57	0.86
1:A:685:ASN:HB3	1:A:686:PRO:HD3	1.55	0.85
1:A:9:ALA:HB3	1:A:434:LEU:HB3	1.58	0.84
1:A:445:ALA:HB1	1:A:559:MET:HE1	1.60	0.84
1:A:379:ARG:HE	1:A:384:ASN:HB2	1.44	0.83
1:A:608:VAL:HG22	1:A:717:ILE:HG13	1.62	0.82
2:B:99:ASN:H	2:B:99:ASN:HD22	1.25	0.81
1:A:51:VAL:H	1:A:90:SER:HB3	1.45	0.81
1:A:77:ASN:HD21	1:A:89:LYS:H	1.26	0.81
2:B:218:ALA:HB3	2:B:219:PRO:HD3	1.62	0.81
1:A:228:VAL:HG22	1:A:237:ASP:HB3	1.60	0.81
1:A:444:ASN:HB2	1:A:480:LYS:HG2	1.63	0.80
2:B:178:TYR:HA	2:B:181:LYS:HD2	1.62	0.80
2:B:650:LYS:HB2	6:B:3655:NDG:H6C2	1.63	0.79
2:B:316:ASN:ND2	2:B:316:ASN:H	1.79	0.79
2:B:373:THR:HB	2:B:379:VAL:HG12	1.62	0.79
2:B:343:LEU:HD22	2:B:343:LEU:H	1.48	0.78
1:A:236:ILE:CD1	1:A:236:ILE:H	1.96	0.78
6:A:2943:NAG:C2	6:A:2943:NAG:H61	2.13	0.78
2:B:88:ILE:HG22	2:B:425:LEU:HD11	1.65	0.77
2:B:371:ASN:HD22	5:B:3371:NAG:H62	1.47	0.77
2:B:119:ASP:O	2:B:124:MET:HG3	1.84	0.77
1:A:441:ILE:HD11	1:A:563:LEU:HD22	1.67	0.76
2:B:157:VAL:HG13	2:B:158:ASP:H	1.49	0.76
2:B:141:GLN:HB3	2:B:345:VAL:HG21	1.66	0.76
1:A:672:THR:HG22	1:A:677:ARG:HA	1.68	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:315:VAL:HG21	1:A:360:ILE:HD13	1.69	0.75
2:B:157:VAL:CG1	2:B:188:PHE:H	1.98	0.75
2:B:650:LYS:HD2	6:B:3655:NDG:H6C1	1.69	0.74
2:B:64:LEU:HB2	2:B:87:ARG:HB3	1.68	0.74
2:B:141:GLN:HE21	2:B:345:VAL:HG21	1.51	0.74
1:A:608:VAL:HG21	1:A:716:GLN:HA	1.69	0.74
1:A:450:TYR:HB2	1:A:451:PRO:HD3	1.70	0.73
1:A:301:MET:HA	1:A:310:GLN:O	1.88	0.73
1:A:663:LEU:HD23	1:A:694:LEU:HD23	1.70	0.73
2:B:84:SER:HB3	2:B:85:PRO:HD3	1.68	0.73
2:B:112:VAL:HG22	2:B:243:SER:HB3	1.71	0.73
6:A:2944:NDG:H6C1	6:A:2944:NDG:H2	1.70	0.73
1:A:650:GLN:HE21	1:A:711:VAL:HG12	1.55	0.72
1:A:650:GLN:HB3	1:A:701:VAL:HG23	1.69	0.72
1:A:236:ILE:N	1:A:236:ILE:HD13	2.02	0.72
1:A:93:TRP:CD1	1:A:111:LEU:HD12	2.25	0.72
3:C:5005:MVA:HN2	3:C:5005:MVA:HG22	1.72	0.71
1:A:178:TYR:HD2	3:C:5001:ARG:CZ	2.03	0.71
2:B:654:ASN:HD22	6:B:3654:NAG:H62	1.56	0.71
1:A:500:ASP:HB2	1:A:555:ILE:HG23	1.73	0.71
1:A:539:ILE:H	1:A:539:ILE:HD12	1.56	0.71
2:B:157:VAL:CG1	2:B:189:GLY:H	2.03	0.70
1:A:459:LYS:O	1:A:469:LYS:HB3	1.90	0.70
1:A:74:ALA:O	1:A:75:THR:HG23	1.92	0.70
2:B:158:ASP:HB3	2:B:187:MET:HE1	1.74	0.70
2:B:623:GLU:HG2	2:B:624:PRO:HD2	1.71	0.70
2:B:127:ASP:O	2:B:128:LEU:HD12	1.91	0.70
1:A:228:VAL:CG2	1:A:237:ASP:HB3	2.21	0.70
2:B:650:LYS:HD2	6:B:3655:NDG:C6	2.21	0.69
1:A:551:LYS:HB2	1:A:551:LYS:HZ3	1.57	0.69
1:A:741:ALA:H	1:A:786:GLY:CA	2.02	0.69
2:B:642:VAL:HB	2:B:680:TYR:HB3	1.73	0.69
2:B:249:THR:HA	2:B:309:ALA:O	1.93	0.69
1:A:657:VAL:HG23	1:A:658:ARG:H	1.55	0.69
1:A:790:PHE:O	1:A:888:ARG:HA	1.92	0.69
2:B:617:CYS:SG	2:B:618:LYS:N	2.66	0.68
2:B:618:LYS:HB2	2:B:639:ILE:HD12	1.72	0.68
1:A:756:PRO:HD3	1:A:954:GLY:H	1.58	0.68
1:A:710:SER:HA	1:A:736:LEU:HD13	1.75	0.68
1:A:228:VAL:HG23	1:A:238:ASP:O	1.93	0.68
1:A:419:TYR:CE1	1:A:439:PRO:HA	2.29	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:2044:NAG:C6	4:A:2045:NAG:C1	2.72	0.67
1:A:55:GLN:NE2	1:A:69:PRO:HB3	2.09	0.67
2:B:157:VAL:HG11	2:B:188:PHE:N	2.08	0.67
2:B:571:ASN:ND2	2:B:573:LEU:HB2	2.10	0.67
1:A:373:VAL:HB	1:A:391:LEU:HB2	1.77	0.67
2:B:185:LEU:HB2	2:B:186:PRO:HD2	1.76	0.67
2:B:580:LYS:HB2	2:B:580:LYS:NZ	2.10	0.67
1:A:344:ILE:HG22	1:A:358:ILE:HD11	1.77	0.66
1:A:656:VAL:HG23	1:A:657:VAL:H	1.60	0.66
1:A:556:THR:HG22	1:A:589:GLN:HB3	1.78	0.66
2:B:130:SER:HB3	2:B:338:SER:CB	2.24	0.66
2:B:133:ASN:O	2:B:137:LYS:N	2.28	0.65
2:B:122:TYR:HB2	2:B:213:SER:O	1.95	0.65
1:A:670:PHE:CE1	1:A:672:THR:HG23	2.32	0.65
1:A:169:VAL:O	1:A:185:SER:HA	1.96	0.65
1:A:869:ILE:HG13	1:A:870:HIS:HD2	1.61	0.65
1:A:501:LYS:HD2	1:A:509:ARG:HH12	1.61	0.65
1:A:544:ASP:O	1:A:547:GLU:HG2	1.97	0.65
1:A:159:PHE:CZ	2:B:261:ARG:HD2	2.32	0.65
2:B:157:VAL:HG13	2:B:158:ASP:N	2.12	0.64
2:B:616:GLU:HG2	2:B:657:TYR:OH	1.97	0.64
1:A:776:VAL:HB	1:A:809:LEU:HD21	1.79	0.64
6:A:2944:NDG:H2	6:A:2944:NDG:C6	2.27	0.64
2:B:657:TYR:CE2	2:B:665:VAL:HB	2.32	0.64
2:B:366:LEU:HA	2:B:402:LYS:O	1.98	0.64
2:B:140:THR:HG22	2:B:143:ARG:HH21	1.62	0.64
1:A:871:THR:HA	1:A:919:SER:HB3	1.80	0.64
1:A:608:VAL:HG11	1:A:715:LEU:HB3	1.78	0.64
2:B:142:MET:SD	2:B:345:VAL:HG22	2.38	0.64
2:B:243:SER:HG	2:B:348:TYR:HE1	1.44	0.64
1:A:808:LEU:HD13	1:A:920:LEU:HD22	1.80	0.64
2:B:185:LEU:CD2	2:B:185:LEU:H	2.05	0.63
1:A:609:SER:HB3	1:A:630:LYS:HB3	1.80	0.63
1:A:487:LEU:CD2	1:A:488:PRO:HD3	2.21	0.63
1:A:769:GLU:HG2	1:A:902:LEU:HD21	1.80	0.63
1:A:812:LEU:HD21	1:A:902:LEU:HD22	1.80	0.63
1:A:191:ILE:HA	1:A:204:TYR:CE2	2.32	0.63
1:A:578:LEU:HD22	1:A:578:LEU:H	1.64	0.63
1:A:111:LEU:HD21	2:B:262:LEU:O	1.99	0.62
2:B:388:GLY:HA2	2:B:636:ARG:NH1	2.15	0.62
1:A:835:ILE:HG12	1:A:836:SER:N	2.15	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:348:GLY:HA3	1:A:420:PRO:HG2	1.81	0.62
2:B:638:GLU:O	2:B:678:ILE:HD12	2.00	0.62
2:B:120:LEU:HD21	2:B:210:GLN:HB3	1.79	0.62
2:B:534:GLU:HB3	2:B:544:CYS:SG	2.39	0.62
1:A:711:VAL:HG13	1:A:736:LEU:HD11	1.82	0.62
2:B:88:ILE:CG2	2:B:425:LEU:HD11	2.30	0.61
1:A:751:ASP:HB2	4:A:2950:NAG:C8	2.28	0.61
2:B:646:LYS:HD2	2:B:668:GLN:HE21	1.65	0.61
1:A:177:PHE:HB2	1:A:180:GLN:HG3	1.83	0.61
2:B:114:ILE:HD13	2:B:344:ILE:HG21	1.82	0.61
2:B:159:LYS:HE3	2:B:284:SER:O	2.01	0.61
1:A:379:ARG:NE	1:A:384:ASN:HB2	2.13	0.61
1:A:375:ILE:O	1:A:375:ILE:HG13	2.01	0.61
2:B:100:PHE:CE1	2:B:399:ILE:HD13	2.36	0.61
2:B:221:GLY:H	2:B:255:HIS:H	1.48	0.60
1:A:347:LEU:HD13	1:A:350:LEU:HD22	1.82	0.60
1:A:464:PRO:HD3	1:A:514:LEU:HD13	1.81	0.60
1:A:41:PRO:O	1:A:42:LYS:HB2	2.01	0.60
1:A:458:ASN:O	1:A:471:SER:HA	2.01	0.60
1:A:442:THR:HG22	1:A:579:ASN:HB2	1.82	0.60
1:A:539:ILE:N	1:A:539:ILE:HD12	2.15	0.60
1:A:808:LEU:O	1:A:808:LEU:HD12	2.02	0.60
1:A:390:ILE:HG13	1:A:390:ILE:O	1.99	0.60
2:B:129:TRP:C	2:B:131:ILE:H	2.03	0.60
1:A:375:ILE:HG12	1:A:389:GLN:HB3	1.82	0.60
2:B:169:PRO:CB	2:B:170:PRO:HD3	2.28	0.59
1:A:650:GLN:NE2	1:A:711:VAL:HG12	2.15	0.59
2:B:671:GLU:HA	2:B:676:LYS:O	2.01	0.59
2:B:187:MET:HE3	2:B:215:ASN:HB3	1.83	0.59
2:B:104:VAL:HG13	2:B:395:VAL:HG23	1.84	0.59
2:B:161:VAL:HG22	2:B:162:SER:H	1.67	0.59
2:B:62:ARG:HD2	2:B:85:PRO:HB3	1.83	0.59
1:A:474:ASN:OD1	1:A:539:ILE:HG23	2.02	0.59
1:A:415:ASP:HB2	1:A:416:LYS:HD2	1.83	0.59
2:B:64:LEU:HB3	2:B:86:GLN:HB2	1.85	0.59
1:A:727:SER:HB2	1:A:728:PRO:HD2	1.83	0.59
1:A:58:LYS:HB2	1:A:70:ILE:HD11	1.85	0.59
2:B:157:VAL:O	2:B:220:GLU:HG3	2.03	0.59
1:A:510:ARG:HH12	1:A:553:THR:HB	1.67	0.59
1:A:741:ALA:N	1:A:786:GLY:HA3	2.09	0.59
2:B:156:PHE:HB2	2:B:189:GLY:O	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:370:LYS:O	1:A:404:PHE:HB3	2.02	0.59
2:B:371:ASN:OD1	2:B:381:PRO:HA	2.03	0.58
1:A:552:LEU:HD11	1:A:591:HIS:HD2	1.68	0.58
1:A:410:GLY:O	1:A:411:ALA:HB2	2.03	0.58
1:A:903:LEU:HD13	1:A:905:THR:H	1.69	0.58
2:B:185:LEU:HD23	2:B:185:LEU:N	2.13	0.58
1:A:159:PHE:HZ	2:B:261:ARG:HD2	1.69	0.58
2:B:635:CYS:O	2:B:635:CYS:SG	2.61	0.58
2:B:173:LEU:CD1	2:B:178:TYR:HB3	2.34	0.58
1:A:441:ILE:HG23	1:A:487:LEU:HD11	1.86	0.58
1:A:646:SER:HB2	1:A:714:ASP:HB2	1.84	0.58
2:B:620:PHE:O	2:B:622:ARG:HD3	2.04	0.58
1:A:61:TRP:C	1:A:63:SER:H	2.08	0.58
1:A:2:ASN:HA	1:A:389:GLN:OE1	2.04	0.58
1:A:929:ILE:O	1:A:930:GLU:HB2	2.04	0.58
2:B:219:PRO:HB2	2:B:255:HIS:CE1	2.39	0.57
2:B:151:ILE:O	2:B:196:LEU:HA	2.04	0.57
2:B:623:GLU:CG	2:B:624:PRO:HD2	2.34	0.57
1:A:621:ASP:HB3	1:A:891:ARG:NH2	2.20	0.57
2:B:127:ASP:HB3	2:B:337:SER:HB3	1.85	0.57
2:B:102:ILE:HG22	2:B:399:ILE:HD11	1.87	0.57
1:A:489:ARG:HA	1:A:528:SER:OG	2.05	0.57
1:A:61:TRP:CH2	1:A:415:ASP:HB3	2.39	0.57
2:B:316:ASN:ND2	2:B:316:ASN:N	2.53	0.57
1:A:472:CYS:N	5:A:2458:NAG:H61	2.19	0.57
2:B:103:GLN:HG3	2:B:396:SER:HB3	1.87	0.57
6:A:2944:NDG:C2	6:A:2944:NDG:C6	2.80	0.57
2:B:536:CYS:SG	2:B:543:SER:O	2.62	0.57
1:A:813:HIS:HA	1:A:828:ILE:HD12	1.86	0.57
1:A:688:LYS:HA	1:A:688:LYS:HE2	1.86	0.57
2:B:672:ASP:HB3	2:B:676:LYS:HE2	1.87	0.56
2:B:554:THR:O	2:B:558:CYS:HA	2.04	0.56
2:B:99:ASN:HD22	2:B:99:ASN:N	1.98	0.56
1:A:438:ARG:NH2	1:A:577:ILE:HG23	2.21	0.56
2:B:219:PRO:HG3	2:B:253:LYS:HD2	1.85	0.56
2:B:173:LEU:HD13	2:B:178:TYR:HB3	1.86	0.56
2:B:73:GLY:HA3	2:B:109:ASP:HB3	1.88	0.56
1:A:606:LEU:HB2	1:A:727:SER:HB3	1.88	0.56
1:A:543:ARG:O	1:A:548:PHE:HE2	1.88	0.56
2:B:130:SER:C	2:B:132:GLN:H	2.07	0.56
2:B:249:THR:HG22	2:B:309:ALA:HB3	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3:LEU:HD11	1:A:350:LEU:HD21	1.87	0.56
2:B:333:LEU:HA	2:B:340:VAL:HG12	1.87	0.56
2:B:124:MET:SD	2:B:251:ASP:HB2	2.46	0.55
4:A:2045:NAG:HN2	4:A:2045:NAG:H5	1.71	0.55
2:B:352:ARG:HH11	2:B:421:PHE:HZ	1.54	0.55
2:B:111:PRO:HG2	2:B:242:ALA:HA	1.89	0.55
1:A:271:GLN:HE22	1:A:301:MET:HB2	1.71	0.55
1:A:756:PRO:HD3	1:A:954:GLY:N	2.22	0.55
1:A:373:VAL:HG23	1:A:404:PHE:CE2	2.42	0.55
1:A:593:LEU:HD21	1:A:596:CYS:HB2	1.87	0.55
1:A:180:GLN:HE22	1:A:213:ALA:HB3	1.70	0.55
1:A:462:SER:HA	1:A:468:LEU:O	2.06	0.55
2:B:589:ILE:O	2:B:591:PRO:HD3	2.06	0.55
2:B:684:GLU:H	2:B:685:PRO:HD3	1.71	0.55
1:A:529:ARG:HB2	1:A:532:LEU:HB2	1.89	0.55
1:A:881:LYS:NZ	1:A:881:LYS:HB2	2.22	0.55
1:A:749:SER:CB	1:A:750:PRO:HD3	2.37	0.55
1:A:253:VAL:HG21	1:A:295:ILE:HG12	1.88	0.55
1:A:702:HIS:O	1:A:703:GLN:HB3	2.07	0.55
2:B:630:THR:O	2:B:634:TYR:HB3	2.06	0.55
2:B:58:VAL:CG1	2:B:93:ARG:H	2.20	0.55
2:B:654:ASN:HD22	6:B:3654:NAG:C6	2.19	0.55
2:B:250:THR:HG22	2:B:310:VAL:HG12	1.89	0.55
2:B:94:PRO:O	2:B:95:ASP:HB2	2.07	0.55
2:B:169:PRO:HB2	2:B:170:PRO:CD	2.25	0.55
2:B:131:ILE:HG12	2:B:338:SER:O	2.07	0.54
1:A:751:ASP:CB	4:A:2950:NAG:H81	2.34	0.54
2:B:657:TYR:O	2:B:664:VAL:HA	2.06	0.54
1:A:513:PHE:CE1	1:A:521:HIS:HB3	2.42	0.54
1:A:645:VAL:HB	1:A:679:VAL:HB	1.88	0.54
2:B:230:THR:HG23	2:B:304:ILE:HD12	1.89	0.54
1:A:783:ARG:HB2	1:A:894:SER:OG	2.07	0.54
2:B:360:ARG:O	2:B:361:ASP:HB2	2.07	0.54
1:A:928:VAL:HB	1:A:941:ILE:HB	1.88	0.54
2:B:410:LYS:HG2	2:B:411:GLU:H	1.73	0.54
1:A:78:ARG:HG3	1:A:87:GLU:OE2	2.07	0.54
1:A:451:PRO:HD2	1:A:473:PHE:HB2	1.88	0.54
2:B:683:GLU:O	2:B:684:GLU:HB3	2.07	0.54
1:A:802:LYS:HG2	1:A:807:THR:HA	1.90	0.54
1:A:543:ARG:HD3	1:A:547:GLU:HG3	1.90	0.54
1:A:496:GLU:OE2	1:A:522:SER:HB3	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:99:ASN:H	2:B:99:ASN:ND2	2.02	0.54
2:B:110:TYR:CD1	2:B:111:PRO:HD2	2.43	0.54
1:A:639:TYR:CD2	1:A:721:ASN:ND2	2.76	0.54
1:A:749:SER:HB3	1:A:750:PRO:HD3	1.89	0.54
2:B:622:ARG:NH2	2:B:659:ASN:HB2	2.22	0.54
1:A:458:ASN:HB3	5:A:2458:NAG:H62	1.91	0.53
1:A:529:ARG:HH11	1:A:529:ARG:HG2	1.74	0.53
2:B:71:ASP:HA	2:B:108:GLU:H	1.73	0.53
1:A:758:PRO:HG2	2:B:666:ARG:NH1	2.23	0.53
2:B:652:ALA:HB1	2:B:669:TYR:O	2.08	0.53
1:A:170:LEU:HG	1:A:239:PHE:CD2	2.44	0.53
6:A:2944:NDG:H6C1	6:A:2944:NDG:C2	2.32	0.53
2:B:571:ASN:HD21	2:B:573:LEU:HB2	1.72	0.53
2:B:615:VAL:HG23	2:B:657:TYR:OH	2.09	0.53
1:A:812:LEU:O	1:A:829:ASN:HB2	2.08	0.53
2:B:683:GLU:O	2:B:684:GLU:CB	2.56	0.53
1:A:11:TYR:HE2	1:A:65:ARG:HA	1.73	0.53
1:A:477:PHE:CD2	1:A:477:PHE:N	2.76	0.53
2:B:309:ALA:HA	2:B:331:GLY:O	2.08	0.53
4:A:2044:NAG:H62	4:A:2045:NAG:C1	2.38	0.53
2:B:403:VAL:HG11	2:B:431:PHE:CE2	2.44	0.53
1:A:643:LEU:O	1:A:680:VAL:HA	2.08	0.53
1:A:498:LEU:HB2	1:A:558:PHE:HB3	1.89	0.53
1:A:363:PRO:HA	1:A:404:PHE:O	2.09	0.53
2:B:82:GLN:O	2:B:104:VAL:HA	2.09	0.53
1:A:456:GLN:NE2	1:A:545:GLU:HB3	2.24	0.53
2:B:162:SER:OG	2:B:163:PRO:HD3	2.09	0.53
1:A:238:ASP:HB3	1:A:256:TYR:O	2.09	0.53
1:A:621:ASP:HB3	1:A:891:ARG:HH22	1.74	0.53
1:A:450:TYR:CB	1:A:451:PRO:HD3	2.39	0.53
2:B:375:LEU:HA	2:B:633:ARG:HH21	1.74	0.53
1:A:118:MET:SD	1:A:118:MET:N	2.82	0.53
2:B:127:ASP:CB	2:B:337:SER:HB3	2.39	0.52
2:B:60:GLU:HB3	2:B:90:LEU:HD23	1.91	0.52
1:A:347:LEU:HD22	1:A:422:LEU:HD12	1.91	0.52
2:B:426:ILE:HD12	2:B:426:ILE:N	2.23	0.52
2:B:607:ALA:C	2:B:609:THR:H	2.11	0.52
1:A:444:ASN:O	1:A:479:LEU:HD12	2.10	0.52
2:B:532:LYS:HD2	2:B:532:LYS:O	2.09	0.52
2:B:185:LEU:HD21	2:B:211:SER:OG	2.10	0.52
1:A:422:LEU:HD23	1:A:423:ILE:N	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:134:LEU:HB3	2:B:203:PHE:HE2	1.75	0.52
2:B:178:TYR:HB2	2:B:181:LYS:HZ3	1.75	0.52
2:B:536:CYS:HB2	2:B:546:ASP:HA	1.92	0.52
1:A:926:PHE:HE2	1:A:943:ASN:HB3	1.75	0.52
2:B:158:ASP:OD1	2:B:159:LYS:N	2.39	0.52
2:B:340:VAL:HG22	2:B:341:LEU:HG	1.92	0.52
1:A:139:TYR:OH	1:A:186:ASP:HB2	2.09	0.52
1:A:328:THR:HG22	1:A:329:THR:N	2.24	0.52
2:B:64:LEU:HD22	2:B:86:GLN:HB2	1.92	0.52
1:A:178:TYR:HB2	3:C:5001:ARG:NH2	2.25	0.52
1:A:346:PRO:O	1:A:410:GLY:O	2.27	0.52
2:B:88:ILE:HG13	2:B:89:ALA:N	2.25	0.52
2:B:540:GLY:O	2:B:558:CYS:HB2	2.08	0.52
2:B:192:HIS:NE2	2:B:195:THR:HG22	2.24	0.52
2:B:134:LEU:CB	2:B:203:PHE:HE2	2.23	0.52
2:B:131:ILE:HG22	2:B:131:ILE:O	2.11	0.51
2:B:332:VAL:O	2:B:343:LEU:HD11	2.09	0.51
1:A:628:ILE:HD12	1:A:663:LEU:HD21	1.92	0.51
1:A:494:GLN:HE21	1:A:494:GLN:HA	1.74	0.51
2:B:417:LYS:HE2	2:B:424:SER:HB3	1.92	0.51
1:A:775:VAL:HG22	1:A:902:LEU:CD1	2.41	0.51
2:B:670:TYR:HB3	2:B:678:ILE:HG23	1.92	0.51
6:A:2943:NAG:H2	6:A:2943:NAG:C6	2.16	0.51
2:B:167:ILE:O	2:B:169:PRO:CD	2.59	0.51
1:A:642:GLU:HA	1:A:681:CYS:O	2.10	0.51
2:B:88:ILE:CG1	2:B:89:ALA:N	2.74	0.51
1:A:459:LYS:CB	1:A:469:LYS:HB3	2.41	0.51
1:A:586:ILE:HD12	1:A:587:SER:H	1.75	0.51
2:B:240:ASN:N	2:B:240:ASN:HD22	2.08	0.51
1:A:794:MET:O	1:A:926:PHE:HA	2.10	0.51
1:A:571:THR:C	1:A:573:GLY:H	2.14	0.51
1:A:799:TRP:HB3	1:A:880:LEU:HB3	1.93	0.51
2:B:358:GLU:CD	2:B:419:VAL:HG12	2.32	0.51
2:B:167:ILE:O	2:B:169:PRO:HD3	2.10	0.51
1:A:257:ASP:HB3	1:A:261:MET:H	1.76	0.51
2:B:88:ILE:HG13	2:B:89:ALA:H	1.76	0.50
1:A:113:HIS:HD2	1:A:122:ARG:O	1.94	0.50
2:B:233:ASP:HA	2:B:238:TRP:HD1	1.75	0.50
1:A:578:LEU:HD22	1:A:578:LEU:N	2.25	0.50
1:A:560:GLU:OE2	4:A:2585:NAG:H83	2.12	0.50
1:A:150:ASP:O	1:A:177:PHE:HA	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:557:TYR:O	2:B:558:CYS:HB2	2.12	0.50
1:A:460:THR:OG1	5:A:2458:NAG:O5	2.29	0.50
2:B:684:GLU:N	2:B:685:PRO:HD3	2.26	0.50
2:B:164:TYR:CE1	2:B:263:ALA:HB2	2.46	0.50
1:A:125:VAL:HG22	1:A:142:CYS:HB3	1.94	0.50
1:A:554:PRO:HG3	1:A:591:HIS:CD2	2.47	0.50
2:B:257:ALA:O	2:B:258:LEU:HB2	2.12	0.50
4:A:2045:NAG:H5	4:A:2045:NAG:N2	2.26	0.50
2:B:620:PHE:HB3	2:B:622:ARG:HE	1.77	0.50
2:B:185:LEU:CB	2:B:186:PRO:HD2	2.42	0.50
2:B:373:THR:HA	2:B:379:VAL:HA	1.94	0.50
1:A:869:ILE:HG13	1:A:870:HIS:CD2	2.45	0.50
2:B:129:TRP:CD1	2:B:130:SER:N	2.80	0.50
2:B:399:ILE:H	2:B:399:ILE:HD12	1.75	0.50
2:B:188:PHE:N	2:B:188:PHE:CD1	2.80	0.49
2:B:373:THR:CB	2:B:379:VAL:HG12	2.38	0.49
2:B:162:SER:CB	2:B:163:PRO:HD3	2.42	0.49
1:A:685:ASN:HB3	1:A:686:PRO:CD	2.34	0.49
2:B:173:LEU:C	2:B:175:ASN:H	2.14	0.49
2:B:373:THR:HB	2:B:379:VAL:CG1	2.40	0.49
1:A:801:TYR:HB2	1:A:880:LEU:HB2	1.94	0.49
1:A:650:GLN:CG	1:A:704:GLN:HB2	2.43	0.49
1:A:240:VAL:HG22	1:A:255:ILE:HG12	1.94	0.49
1:A:441:ILE:O	1:A:578:LEU:HA	2.12	0.49
2:B:580:LYS:HB2	2:B:580:LYS:HZ2	1.77	0.49
1:A:604:PRO:HB3	1:A:636:GLU:O	2.12	0.49
2:B:338:SER:O	2:B:339:ASN:HB2	2.13	0.49
2:B:623:GLU:HG2	2:B:624:PRO:CD	2.41	0.49
1:A:3:LEU:HD21	1:A:350:LEU:HD11	1.93	0.49
2:B:355:VAL:O	2:B:385:SER:HA	2.11	0.49
1:A:931:PHE:CD2	1:A:931:PHE:N	2.80	0.49
2:B:673:SER:C	2:B:675:GLY:H	2.14	0.49
2:B:129:TRP:C	2:B:131:ILE:N	2.66	0.49
2:B:409:GLU:O	2:B:410:LYS:HB2	2.13	0.49
1:A:450:TYR:HD1	1:A:474:ASN:HB2	1.77	0.49
1:A:526:THR:HG22	1:A:527:ILE:H	1.78	0.49
2:B:590:GLN:C	2:B:592:GLY:H	2.15	0.49
2:B:346:ASP:OD1	2:B:346:ASP:N	2.46	0.49
1:A:683:LEU:HB3	1:A:687:MET:SD	2.53	0.49
1:A:663:LEU:HD22	1:A:695:ALA:C	2.33	0.49
1:A:663:LEU:CD2	1:A:694:LEU:HD23	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:178:TYR:HB2	3:C:5001:ARG:HH21	1.78	0.49
1:A:499:LEU:HD12	1:A:519:PRO:HA	1.94	0.49
1:A:191:ILE:HA	1:A:204:TYR:HE2	1.75	0.48
1:A:792:LYS:HB3	1:A:930:GLU:HB3	1.95	0.48
1:A:491:LEU:O	1:A:526:THR:HA	2.13	0.48
1:A:35:PHE:HB3	1:A:59:CYS:O	2.13	0.48
1:A:400:MET:HB2	1:A:401:PRO:HD2	1.95	0.48
1:A:578:LEU:H	1:A:578:LEU:CD2	2.26	0.48
1:A:914:GLN:HE21	1:A:916:HIS:HB3	1.78	0.48
1:A:750:PRO:HD2	1:A:776:VAL:HA	1.96	0.48
2:B:587:VAL:HG23	2:B:587:VAL:O	2.13	0.48
2:B:67:ARG:O	2:B:69:LEU:HD12	2.13	0.48
1:A:372:ILE:HD12	1:A:392:GLU:HG2	1.94	0.48
1:A:487:LEU:H	1:A:488:PRO:HD2	1.77	0.48
1:A:579:ASN:HB3	1:A:582:THR:HG23	1.95	0.48
2:B:319:GLN:HA	2:B:330:VAL:HG21	1.94	0.48
1:A:303:ARG:HH11	1:A:303:ARG:HG3	1.78	0.48
1:A:243:VAL:CG1	1:A:246:ALA:HB2	2.42	0.48
5:B:3371:NAG:H3	5:B:3371:NAG:O7	2.13	0.48
1:A:454:LEU:HD22	1:A:473:PHE:HB3	1.96	0.48
1:A:463:LEU:HG	1:A:464:PRO:HD2	1.95	0.48
2:B:371:ASN:ND2	5:B:3371:NAG:C6	2.63	0.48
2:B:174:GLU:O	2:B:186:PRO:HB3	2.14	0.48
2:B:316:ASN:HB2	5:B:3320:NAG:H82	1.96	0.48
1:A:478:CYS:HB3	1:A:533:MET:HE2	1.96	0.48
2:B:267:GLN:HA	2:B:268:PRO:HD3	1.78	0.48
1:A:938:ILE:HD13	1:A:938:ILE:N	2.29	0.48
1:A:72:PHE:HD2	1:A:129:PHE:HB3	1.78	0.48
1:A:295:ILE:HD12	1:A:295:ILE:N	2.28	0.48
2:B:115:TYR:OH	2:B:192:HIS:ND1	2.45	0.48
1:A:300:PHE:CE2	1:A:314:GLN:NE2	2.81	0.48
1:A:439:PRO:HB2	1:A:487:LEU:HD13	1.96	0.47
2:B:181:LYS:CE	2:B:181:LYS:HA	2.44	0.47
2:B:180:MET:HG3	2:B:181:LYS:N	2.29	0.47
1:A:648:PRO:O	1:A:677:ARG:HD3	2.14	0.47
1:A:449:VAL:HG23	1:A:474:ASN:O	2.14	0.47
1:A:377:ASN:O	1:A:383:LEU:HD12	2.14	0.47
1:A:60:ASP:C	1:A:62:SER:H	2.15	0.47
2:B:306:LEU:O	2:B:328:THR:HG23	2.15	0.47
2:B:343:LEU:O	2:B:347:ALA:N	2.43	0.47
1:A:816:ILE:HD11	1:A:822:CYS:SG	2.54	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:594:LEU:HD23	1:A:595:ASP:N	2.29	0.47
2:B:574:LEU:HD11	2:B:581:CYS:HB2	1.96	0.47
1:A:886:VAL:HG12	1:A:887:GLY:N	2.30	0.47
2:B:181:LYS:HZ1	2:B:183:THR:HA	1.79	0.47
1:A:271:GLN:NE2	1:A:301:MET:H	2.11	0.47
1:A:512:LEU:HD11	1:A:543:ARG:NH2	2.28	0.47
2:B:620:PHE:HB3	2:B:622:ARG:HD3	1.97	0.47
1:A:102:GLN:HB2	1:A:103:ASP:H	1.55	0.47
2:B:221:GLY:HA2	2:B:255:HIS:HB2	1.97	0.47
1:A:672:THR:HG22	1:A:677:ARG:CA	2.42	0.47
2:B:325:ILE:HG22	2:B:328:THR:HG1	1.79	0.47
2:B:410:LYS:HG2	2:B:411:GLU:N	2.29	0.47
2:B:411:GLU:OE1	2:B:428:GLN:HB3	2.13	0.47
1:A:271:GLN:HE22	1:A:301:MET:N	2.12	0.47
1:A:650:GLN:HE21	1:A:711:VAL:CG1	2.25	0.47
2:B:538:GLY:O	2:B:539:HIS:HB2	2.14	0.47
1:A:779:ILE:HD12	1:A:898:TYR:CD2	2.50	0.47
2:B:118:MET:SD	2:B:153:PHE:CD1	3.08	0.47
2:B:118:MET:SD	2:B:153:PHE:HD1	2.38	0.47
2:B:129:TRP:HD1	2:B:130:SER:H	1.63	0.47
1:A:674:ASN:HB3	1:A:676:THR:HG22	1.96	0.47
2:B:187:MET:CE	2:B:215:ASN:HB3	2.45	0.47
2:B:646:LYS:HD2	2:B:668:GLN:NE2	2.30	0.47
1:A:441:ILE:HG23	1:A:487:LEU:CD1	2.44	0.46
1:A:527:ILE:O	1:A:528:SER:HB2	2.15	0.46
1:A:598:GLU:C	1:A:600:ASN:N	2.67	0.46
2:B:318:TYR:HA	2:B:321:TYR:HB2	1.98	0.46
1:A:178:TYR:CD2	3:C:5001:ARG:CZ	2.93	0.46
1:A:170:LEU:HD11	1:A:239:PHE:HB3	1.97	0.46
1:A:754:PHE:CD1	2:B:656:THR:HG22	2.50	0.46
1:A:921:LYS:CE	1:A:946:LEU:HD12	2.45	0.46
2:B:178:TYR:C	2:B:180:MET:H	2.18	0.46
2:B:141:GLN:CD	2:B:342:GLN:HE21	2.19	0.46
2:B:411:GLU:HG3	2:B:413:SER:OG	2.15	0.46
1:A:569:ALA:O	1:A:573:GLY:HA2	2.15	0.46
1:A:575:GLN:HA	1:A:576:PRO:HD3	1.68	0.46
1:A:625:LEU:HD23	1:A:699:PHE:HB2	1.97	0.46
2:B:544:CYS:C	2:B:546:ASP:H	2.17	0.46
1:A:390:ILE:HD12	1:A:392:GLU:HG2	1.98	0.46
2:B:205:GLU:HG3	2:B:206:GLU:H	1.80	0.46
1:A:5:VAL:O	1:A:5:VAL:HG12	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:906:GLU:C	1:A:908:PHE:N	2.68	0.46
1:A:42:LYS:O	1:A:52:GLU:HG2	2.15	0.46
2:B:267:GLN:HE21	2:B:287:MET:HB2	1.81	0.46
1:A:53:GLY:O	1:A:94:PHE:HB3	2.16	0.46
2:B:599:GLU:HG2	2:B:600:LYS:N	2.31	0.46
1:A:42:LYS:HA	1:A:52:GLU:HB3	1.97	0.46
1:A:260:ASN:O	1:A:261:MET:HB3	2.16	0.46
2:B:148:ASN:HD22	2:B:149:LEU:N	2.13	0.46
2:B:262:LEU:HD23	2:B:262:LEU:N	2.31	0.46
1:A:260:ASN:ND2	5:A:2260:NAG:C6	2.79	0.46
1:A:674:ASN:O	1:A:676:THR:N	2.42	0.46
1:A:68:GLN:NE2	1:A:69:PRO:HD2	2.31	0.46
1:A:26:PHE:O	1:A:28:PRO:HD3	2.16	0.46
1:A:667:SER:HB2	1:A:682:ASP:HB2	1.97	0.46
1:A:154:PHE:O	1:A:175:GLY:HA3	2.16	0.46
2:B:378:GLU:O	2:B:379:VAL:HG22	2.15	0.46
1:A:647:ILE:HD11	1:A:670:PHE:HE2	1.81	0.46
2:B:82:GLN:HG2	2:B:107:VAL:HG23	1.98	0.46
2:B:621:ASP:O	2:B:626:MET:SD	2.74	0.46
2:B:169:PRO:CB	2:B:170:PRO:CD	2.93	0.45
2:B:337:SER:O	2:B:338:SER:OG	2.27	0.45
1:A:271:GLN:HE22	1:A:301:MET:CB	2.29	0.45
1:A:606:LEU:CB	1:A:727:SER:HB3	2.46	0.45
2:B:333:LEU:HA	2:B:340:VAL:CG1	2.46	0.45
2:B:131:ILE:HG23	2:B:134:LEU:HG	1.98	0.45
1:A:74:ALA:O	1:A:75:THR:CG2	2.62	0.45
2:B:417:LYS:HB3	2:B:424:SER:HB3	1.98	0.45
1:A:934:LYS:O	1:A:935:ASN:HB2	2.16	0.45
2:B:269:ASN:ND2	2:B:290:PRO:HB3	2.30	0.45
1:A:647:ILE:HG21	1:A:699:PHE:CE1	2.51	0.45
6:B:3654:NAG:H62	6:B:3654:NAG:O3	2.15	0.45
2:B:612:LYS:O	2:B:615:VAL:HG22	2.17	0.45
1:A:508:ILE:O	1:A:510:ARG:N	2.49	0.45
1:A:121:GLU:O	1:A:122:ARG:HB2	2.17	0.45
1:A:77:ASN:ND2	1:A:89:LYS:H	2.03	0.45
2:B:648:THR:O	2:B:650:LYS:N	2.50	0.45
2:B:654:ASN:ND2	6:B:3654:NAG:C6	2.79	0.45
2:B:106:GLN:HB2	2:B:392:GLY:H	1.81	0.45
1:A:516:SER:O	1:A:518:SER:N	2.49	0.45
2:B:224:ASP:CG	2:B:281:TYR:HE2	2.20	0.45
1:A:756:PRO:HA	1:A:953:TRP:HZ3	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:366:LEU:H	2:B:366:LEU:HD23	1.81	0.45
2:B:647:ASP:O	6:B:3655:NDG:C1	2.64	0.45
1:A:903:LEU:HD13	1:A:905:THR:N	2.30	0.45
1:A:552:LEU:CD2	1:A:592:ILE:H	2.29	0.45
2:B:64:LEU:HD22	2:B:86:GLN:CB	2.47	0.45
1:A:301:MET:HG2	1:A:311:GLU:HA	1.98	0.45
1:A:347:LEU:CD2	1:A:422:LEU:HD12	2.46	0.45
2:B:641:SER:OG	2:B:683:GLU:HB2	2.16	0.45
1:A:644:ILE:HD12	1:A:680:VAL:HG22	1.99	0.45
1:A:29:SER:HB2	1:A:103:ASP:OD1	2.17	0.45
2:B:244:HIS:O	2:B:245:LEU:HD23	2.16	0.45
2:B:312:GLU:HA	2:B:315:VAL:HG23	1.99	0.45
2:B:281:TYR:HE1	2:B:283:ALA:HB3	1.82	0.45
1:A:61:TRP:O	1:A:61:TRP:CG	2.70	0.45
1:A:464:PRO:HG2	1:A:517:ARG:HE	1.80	0.45
2:B:365:GLU:HG3	2:B:407:PRO:HD3	1.99	0.45
2:B:169:PRO:HD2	2:B:170:PRO:CD	2.47	0.45
1:A:100:SER:CB	1:A:105:ILE:HG22	2.47	0.45
1:A:252:MET:CE	1:A:254:TYR:HE1	2.29	0.45
1:A:252:MET:HA	1:A:267:PHE:O	2.17	0.44
1:A:284:ASP:O	1:A:356:ASN:HB2	2.17	0.44
1:A:796:HIS:O	1:A:924:ALA:HA	2.17	0.44
1:A:604:PRO:HD3	1:A:721:ASN:OD1	2.17	0.44
2:B:299:LEU:HA	2:B:299:LEU:HD12	1.70	0.44
1:A:487:LEU:H	1:A:488:PRO:CD	2.31	0.44
1:A:716:GLN:NE2	1:A:729:VAL:HG22	2.33	0.44
2:B:173:LEU:HD11	2:B:176:PRO:HA	1.99	0.44
2:B:607:ALA:O	2:B:609:THR:N	2.50	0.44
1:A:942:THR:O	1:A:943:ASN:HB2	2.16	0.44
1:A:33:ARG:NH1	1:A:62:SER:HB2	2.32	0.44
2:B:296:THR:HG22	2:B:297:GLU:N	2.32	0.44
1:A:487:LEU:N	1:A:488:PRO:CD	2.81	0.44
2:B:58:VAL:O	2:B:98:LYS:HE2	2.18	0.44
2:B:58:VAL:HG12	2:B:92:LEU:HA	1.99	0.44
1:A:101:LYS:HB3	1:A:102:GLN:H	1.69	0.44
1:A:449:VAL:HG21	1:A:473:PHE:HD1	1.82	0.44
1:A:465:GLY:HA3	1:A:517:ARG:NH2	2.33	0.44
1:A:552:LEU:HD12	1:A:686:PRO:HG3	1.99	0.44
2:B:141:GLN:HE21	2:B:141:GLN:HB3	1.56	0.44
1:A:795:LEU:HB3	1:A:884:CYS:HB2	1.99	0.44
1:A:795:LEU:HD23	1:A:796:HIS:N	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:176:SER:CB	1:A:182:GLN:HE21	2.31	0.44
2:B:344:ILE:N	2:B:344:ILE:HD13	2.33	0.44
1:A:375:ILE:CD1	1:A:389:GLN:HB3	2.48	0.44
2:B:71:ASP:HB3	2:B:108:GLU:CB	2.48	0.44
1:A:113:HIS:CD2	1:A:124:PRO:HD3	2.53	0.44
1:A:402:PRO:HA	1:A:428:GLY:HA3	2.00	0.44
2:B:62:ARG:CD	2:B:85:PRO:HB3	2.48	0.44
3:C:5001:ARG:N	3:C:5005:MVA:HN3	2.32	0.44
1:A:579:ASN:HB3	1:A:582:THR:CG2	2.48	0.44
1:A:11:TYR:CE2	1:A:65:ARG:HA	2.51	0.44
2:B:295:MET:O	2:B:299:LEU:HB2	2.17	0.44
1:A:15:GLU:HA	1:A:430:ASP:OD1	2.18	0.44
1:A:439:PRO:CB	1:A:487:LEU:HD13	2.48	0.43
2:B:215:ASN:O	3:C:5003:ASP:HB3	2.19	0.43
1:A:253:VAL:HG21	1:A:295:ILE:CG1	2.47	0.43
1:A:526:THR:O	1:A:527:ILE:HG23	2.17	0.43
1:A:417:ASN:O	1:A:419:TYR:N	2.46	0.43
2:B:130:SER:HB3	2:B:338:SER:OG	2.17	0.43
2:B:132:GLN:O	2:B:204:ASN:ND2	2.50	0.43
1:A:26:PHE:CZ	1:A:28:PRO:HG3	2.53	0.43
2:B:182:THR:HG22	2:B:182:THR:O	2.18	0.43
2:B:67:ARG:H	2:B:67:ARG:HD2	1.83	0.43
2:B:173:LEU:HD13	2:B:178:TYR:CG	2.53	0.43
1:A:410:GLY:O	1:A:411:ALA:CB	2.66	0.43
2:B:620:PHE:HB3	2:B:622:ARG:NE	2.33	0.43
2:B:148:ASN:C	2:B:148:ASN:HD22	2.22	0.43
1:A:607:GLU:HG2	1:A:632:GLN:HB2	2.00	0.43
1:A:222:LEU:HD12	1:A:223:GLY:N	2.32	0.43
1:A:472:CYS:H	5:A:2458:NAG:H61	1.82	0.43
2:B:127:ASP:HA	2:B:337:SER:HB3	2.00	0.43
1:A:440:VAL:HG22	1:A:577:ILE:CD1	2.49	0.43
1:A:451:PRO:HG2	1:A:473:PHE:HA	1.99	0.43
1:A:449:VAL:CG2	1:A:473:PHE:HD1	2.32	0.43
2:B:213:SER:O	2:B:214:ARG:HB2	2.17	0.43
1:A:170:LEU:HA	1:A:170:LEU:HD23	1.81	0.43
1:A:605:LYS:H	1:A:635:GLY:H	1.66	0.43
1:A:610:VAL:HG11	1:A:732:HIS:HB2	2.01	0.43
1:A:533:MET:HG3	1:A:533:MET:O	2.19	0.43
1:A:271:GLN:HE22	1:A:301:MET:H	1.66	0.43
1:A:650:GLN:CB	1:A:701:VAL:HG23	2.45	0.43
1:A:375:ILE:CG1	1:A:389:GLN:HB3	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:83:VAL:HA	2:B:103:GLN:O	2.19	0.43
1:A:456:GLN:HE22	1:A:545:GLU:HB3	1.84	0.43
2:B:177:CYS:HB2	2:B:180:MET:SD	2.59	0.43
1:A:672:THR:HG22	1:A:677:ARG:CB	2.49	0.43
1:A:915:ASN:ND2	1:A:953:TRP:HE1	2.15	0.43
1:A:14:PRO:HG2	1:A:17:SER:OG	2.19	0.43
1:A:526:THR:HG22	1:A:527:ILE:N	2.34	0.43
1:A:125:VAL:HG23	1:A:152:GLN:O	2.18	0.43
1:A:459:LYS:H	1:A:459:LYS:HG3	1.52	0.43
2:B:102:ILE:CG2	2:B:399:ILE:HD11	2.47	0.43
2:B:191:LYS:HD3	2:B:280:HIS:NE2	2.33	0.43
1:A:394:GLN:O	1:A:394:GLN:HG2	2.18	0.43
2:B:157:VAL:HG13	2:B:187:MET:HE2	2.01	0.42
1:A:510:ARG:NH2	1:A:553:THR:O	2.45	0.42
1:A:781:GLU:HB2	1:A:896:ILE:HG23	1.99	0.42
1:A:704:GLN:HB3	1:A:707:MET:CB	2.49	0.42
1:A:869:ILE:HG23	1:A:870:HIS:N	2.34	0.42
1:A:783:ARG:NE	1:A:894:SER:OG	2.33	0.42
2:B:115:TYR:HH	2:B:192:HIS:CE1	2.35	0.42
1:A:523:LYS:HG2	1:A:536:GLU:OE2	2.19	0.42
1:A:404:PHE:HA	1:A:426:ALA:HB2	2.01	0.42
1:A:36:LEU:HB2	1:A:59:CYS:HB2	2.01	0.42
1:A:174:PRO:O	1:A:181:GLY:HA2	2.18	0.42
1:A:17:SER:O	1:A:41:PRO:O	2.36	0.42
1:A:436:ARG:CZ	1:A:574:LEU:HD13	2.49	0.42
1:A:364:TYR:O	1:A:369:LYS:HG2	2.19	0.42
2:B:130:SER:C	2:B:132:GLN:N	2.71	0.42
2:B:131:ILE:CG2	2:B:131:ILE:O	2.67	0.42
2:B:173:LEU:HD13	2:B:178:TYR:CD1	2.54	0.42
2:B:87:ARG:NH2	2:B:428:GLN:OE1	2.53	0.42
1:A:17:SER:HB2	1:A:43:ALA:HB2	2.02	0.42
1:A:364:TYR:HE2	1:A:403:SER:HG	1.68	0.42
1:A:47:GLN:HA	1:A:48:PRO:HD3	1.83	0.42
1:A:92:GLN:HG3	1:A:109:ALA:HB1	2.01	0.42
2:B:342:GLN:CD	2:B:342:GLN:N	2.73	0.42
2:B:247:VAL:HG21	2:B:344:ILE:HD12	2.02	0.42
1:A:239:PHE:HD1	1:A:261:MET:SD	2.43	0.42
1:A:176:SER:OG	1:A:182:GLN:NE2	2.51	0.42
1:A:753:VAL:O	1:A:951:VAL:HA	2.19	0.42
1:A:439:PRO:O	1:A:576:PRO:HB3	2.19	0.42
1:A:657:VAL:HG11	1:A:663:LEU:CD1	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:104:VAL:HG11	2:B:355:VAL:HG11	2.02	0.42
2:B:358:GLU:HG3	2:B:358:GLU:O	2.20	0.42
1:A:907:THR:HG22	1:A:918:TYR:CD2	2.55	0.42
1:A:872:LEU:HA	1:A:872:LEU:HD23	1.76	0.42
1:A:503:LYS:HE3	1:A:510:ARG:HD3	2.02	0.42
2:B:115:TYR:CD1	2:B:236:ILE:HG23	2.55	0.42
2:B:379:VAL:HG23	2:B:379:VAL:O	2.20	0.41
1:A:916:HIS:HA	1:A:953:TRP:HD1	1.85	0.41
1:A:810:TYR:HE2	1:A:812:LEU:HD23	1.84	0.41
1:A:527:ILE:HB	1:A:528:SER:H	1.66	0.41
1:A:837:SER:HB3	1:A:838:LEU:H	1.53	0.41
1:A:490:LYS:HG3	1:A:490:LYS:O	2.20	0.41
1:A:552:LEU:HD11	1:A:591:HIS:CD2	2.51	0.41
3:C:5004:PHE:HA	3:C:5005:MVA:HN1	1.57	0.41
4:A:2045:NAG:C5	4:A:2045:NAG:N2	2.81	0.41
2:B:120:LEU:HD22	2:B:155:ALA:CB	2.50	0.41
1:A:455:ASN:HB3	5:A:2458:NAG:H4	2.02	0.41
1:A:260:ASN:HD22	5:A:2260:NAG:C6	2.33	0.41
2:B:55:GLU:O	2:B:56:PHE:HB2	2.20	0.41
2:B:354:LYS:HD2	2:B:354:LYS:C	2.41	0.41
2:B:62:ARG:CZ	2:B:85:PRO:HB3	2.50	0.41
2:B:571:ASN:HD21	2:B:573:LEU:CB	2.33	0.41
1:A:808:LEU:O	1:A:809:LEU:HB2	2.20	0.41
1:A:295:ILE:HG22	1:A:296:GLY:N	2.34	0.41
2:B:628:GLU:O	2:B:630:THR:HG23	2.20	0.41
1:A:552:LEU:HD12	1:A:686:PRO:CG	2.50	0.41
1:A:50:ILE:HG23	1:A:90:SER:N	2.36	0.41
2:B:160:PRO:HG2	2:B:285:THR:HG22	2.02	0.41
1:A:247:ALA:O	1:A:250:LEU:HB2	2.21	0.41
1:A:486:VAL:O	1:A:487:LEU:HB3	2.19	0.41
1:A:243:VAL:HG12	1:A:246:ALA:HB2	2.01	0.41
2:B:679:LEU:HD12	2:B:679:LEU:N	2.35	0.41
1:A:562:ARG:HG2	1:A:563:LEU:N	2.34	0.41
1:A:61:TRP:O	1:A:61:TRP:CD2	2.73	0.41
1:A:585:ASN:ND2	4:A:2585:NAG:C6	2.74	0.41
2:B:62:ARG:NH1	2:B:85:PRO:HB3	2.36	0.41
1:A:463:LEU:HB3	1:A:466:THR:O	2.21	0.41
1:A:113:HIS:CD2	1:A:122:ARG:O	2.74	0.41
1:A:119:LYS:HG2	1:A:120:GLN:H	1.86	0.41
1:A:232:ASN:O	1:A:233:GLY:C	2.59	0.41
1:A:480:LYS:HB3	1:A:533:MET:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:657:VAL:O	1:A:658:ARG:HB2	2.21	0.41
2:B:534:GLU:CB	2:B:544:CYS:SG	3.06	0.41
2:B:355:VAL:HG12	2:B:397:PHE:HZ	1.86	0.41
1:A:108:CYS:SG	1:A:161:ILE:HD13	2.61	0.41
2:B:627:THR:O	2:B:627:THR:HG22	2.20	0.41
2:B:418:PRO:HG2	2:B:421:PHE:HB2	2.03	0.41
1:A:505:LYS:HB3	1:A:505:LYS:HE3	1.88	0.41
2:B:159:LYS:O	2:B:161:VAL:N	2.52	0.41
2:B:60:GLU:HB2	2:B:88:ILE:HD11	2.03	0.41
1:A:656:VAL:HG23	1:A:657:VAL:N	2.30	0.41
1:A:512:LEU:HD12	1:A:541:TYR:OH	2.21	0.41
1:A:514:LEU:HB3	1:A:515:TYR:H	1.71	0.41
2:B:406:CYS:HB2	2:B:431:PHE:HB3	2.02	0.41
1:A:765:ASN:HA	1:A:766:PRO:HD2	1.89	0.41
1:A:617:ILE:O	1:A:617:ILE:HG13	2.21	0.41
1:A:79:ASP:HB3	1:A:81:ALA:O	2.21	0.41
2:B:173:LEU:CD1	2:B:176:PRO:HA	2.51	0.41
1:A:749:SER:CB	1:A:750:PRO:CD	2.97	0.41
1:A:328:THR:CG2	1:A:329:THR:N	2.84	0.41
1:A:181:GLY:HA3	1:A:222:LEU:HB3	2.02	0.41
1:A:614:GLN:HE21	1:A:616:LYS:NZ	2.19	0.41
2:B:157:VAL:CG1	2:B:158:ASP:H	2.25	0.40
2:B:343:LEU:CD2	2:B:343:LEU:H	2.25	0.40
1:A:459:LYS:HB3	1:A:469:LYS:HB3	2.01	0.40
2:B:114:ILE:HB	2:B:151:ILE:HG22	2.03	0.40
1:A:571:THR:O	1:A:573:GLY:N	2.54	0.40
1:A:292:ASP:O	1:A:294:PHE:CE1	2.74	0.40
2:B:128:LEU:O	2:B:130:SER:N	2.55	0.40
2:B:178:TYR:CD1	2:B:178:TYR:C	2.95	0.40
1:A:652:ASP:O	1:A:699:PHE:HA	2.21	0.40
1:A:541:TYR:HE2	1:A:543:ARG:HA	1.87	0.40
1:A:260:ASN:ND2	5:A:2260:NAG:H62	2.36	0.40
2:B:278:ASP:OD1	2:B:280:HIS:HB2	2.21	0.40
1:A:618:TYR:CD2	1:A:737:ALA:HB3	2.56	0.40
1:A:419:TYR:HA	1:A:420:PRO:HD3	1.83	0.40
1:A:552:LEU:HD21	1:A:591:HIS:HA	2.02	0.40
1:A:647:ILE:HG22	1:A:713:PHE:CE2	2.56	0.40
2:B:624:PRO:O	2:B:627:THR:N	2.54	0.40
1:A:644:ILE:CD1	1:A:680:VAL:HG22	2.52	0.40
1:A:365:GLY:O	1:A:369:LYS:HA	2.20	0.40
2:B:160:PRO:HG2	2:B:285:THR:CG2	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:484:LYS:H	1:A:487:LEU:HD21	1.86	0.40
1:A:236:ILE:N	1:A:236:ILE:CD1	2.71	0.40
1:A:679:VAL:HG21	1:A:699:PHE:HZ	1.85	0.40
1:A:464:PRO:HD3	1:A:514:LEU:CD1	2.48	0.40
1:A:755:LEU:CD2	1:A:951:VAL:HB	2.51	0.40
1:A:766:PRO:O	1:A:767:GLU:HG3	2.21	0.40
2:B:281:TYR:O	2:B:284:SER:HB2	2.22	0.40
1:A:812:LEU:HD21	1:A:902:LEU:CD2	2.49	0.40
1:A:688:LYS:HA	1:A:688:LYS:CE	2.51	0.40
2:B:150:ARG:HA	2:B:197:THR:O	2.20	0.40
1:A:190:GLU:OE2	1:A:205:ASN:HB2	2.22	0.40
1:A:936:LEU:HA	1:A:936:LEU:HD13	1.86	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	923/957 (96%)	743 (80%)	125 (14%)	55 (6%)	2 16
2	B	535/692 (77%)	392 (73%)	98 (18%)	45 (8%)	1 6
3	C	3/5 (60%)	2 (67%)	0	1 (33%)	0 0
All	All	1461/1654 (88%)	1137 (78%)	223 (15%)	101 (7%)	1 10

All (101) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	122	ARG
1	A	236	ILE
1	A	396	ALA
1	A	411	ALA
1	A	487	LEU

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Mol	Chain	Res	Type
1	A	488	PRO
1	A	489	ARG
1	A	504	GLN
1	A	514	LEU
1	A	517	ARG
1	A	527	ILE
1	A	703	GLN
1	A	707	MET
1	A	749	SER
1	A	891	ARG
1	A	916	HIS
2	B	123	SER
2	B	129	TRP
2	B	162	SER
2	B	169	PRO
2	B	176	PRO
2	B	241	ASP
2	B	253	LYS
2	B	338	SER
2	B	339	ASN
2	B	546	ASP
3	C	5004	PHE
1	A	75	THR
1	A	82	LYS
1	A	167	ASP
1	A	350	LEU
1	A	399	SER
1	A	416	LYS
1	A	509	ARG
1	A	528	SER
1	A	615	LYS
1	A	648	PRO
1	A	657	VAL
1	A	759	ASN
1	A	836	SER
1	A	837	SER
2	B	177	CYS
2	B	288	ASP
2	B	337	SER
2	B	341	LEU
2	B	376	ASN
2	B	410	LYS

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Mol	Chain	Res	Type
2	B	537	SER
2	B	539	HIS
2	B	547	CYS
2	B	608	CYS
2	B	641	SER
2	B	643	LYS
2	B	649	GLY
2	B	672	ASP
2	B	682	VAL
2	B	684	GLU
1	A	205	ASN
1	A	552	LEU
1	A	621	ASP
1	A	656	VAL
1	A	680	VAL
1	A	705	SER
2	B	163	PRO
2	B	180	MET
2	B	182	THR
2	B	590	GLN
2	B	636	ARG
1	A	515	TYR
1	A	930	GLU
2	B	76	ASP
2	B	79	GLN
2	B	122	TYR
2	B	258	LEU
2	B	335	MET
2	B	407	PRO
2	B	647	ASP
2	B	651	ASP
1	A	62	SER
1	A	550	ASP
1	A	572	THR
1	A	685	ASN
1	A	687	MET
1	A	708	ASP
1	A	757	ILE
1	A	954	GLY
2	B	379	VAL
1	A	126	GLY
1	A	418	GLY

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Mol	Chain	Res	Type
1	A	554	PRO
2	B	56	PHE
2	B	168	SER
2	B	405	GLY
2	B	541	GLN
1	A	348	GLY
1	A	450	TYR
1	A	464	PRO
1	A	508	ILE
1	A	197	PRO
1	A	573	GLY
2	B	167	ILE

5.3.2 Protein sidechains (i)

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	787/812 (97%)	707 (90%)	80 (10%)	9 36
2	B	484/616 (79%)	396 (82%)	88 (18%)	2 10
3	C	3/3 (100%)	3 (100%)	0	100 100
All	All	1274/1431 (89%)	1106 (87%)	168 (13%)	5 23

All (168) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LEU
1	A	4	ASP
1	A	24	ASP
1	A	29	SER
1	A	34	MET
1	A	51	VAL
1	A	90	SER
1	A	102	GLN
1	A	115	ARG
1	A	118	MET

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Mol	Chain	Res	Type
1	A	120	GLN
1	A	125	VAL
1	A	134	THR
1	A	145	GLN
1	A	155	CYS
1	A	162	ASP
1	A	167	ASP
1	A	169	VAL
1	A	170	LEU
1	A	187	GLN
1	A	219	ASP
1	A	234	ASP
1	A	236	ILE
1	A	275	TYR
1	A	303	ARG
1	A	318	SER
1	A	321	ARG
1	A	339	ARG
1	A	394	GLN
1	A	459	LYS
1	A	472	CYS
1	A	477	PHE
1	A	488	PRO
1	A	489	ARG
1	A	494	GLN
1	A	514	LEU
1	A	517	ARG
1	A	535	CYS
1	A	539	ILE
1	A	543	ARG
1	A	549	ARG
1	A	551	LYS
1	A	577	ILE
1	A	585	ASN
1	A	588	ARG
1	A	598	GLU
1	A	607	GLU
1	A	616	LYS
1	A	652	ASP
1	A	675	GLN
1	A	676	THR
1	A	685	ASN

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Mol	Chain	Res	Type
1	A	701	VAL
1	A	721	ASN
1	A	735	ASP
1	A	755	LEU
1	A	756	PRO
1	A	765	ASN
1	A	768	THR
1	A	770	GLU
1	A	771	ASP
1	A	782	LEU
1	A	813	HIS
1	A	878	GLN
1	A	879	CYS
1	A	880	LEU
1	A	885	GLN
1	A	897	LEU
1	A	902	LEU
1	A	903	LEU
1	A	904	TRP
1	A	905	THR
1	A	906	GLU
1	A	907	THR
1	A	908	PHE
1	A	916	HIS
1	A	931	PHE
1	A	938	ILE
1	A	946	LEU
1	A	956	GLN
2	B	58	VAL
2	B	60	GLU
2	B	64	LEU
2	B	67	ARG
2	B	68	PRO
2	B	81	THR
2	B	88	ILE
2	B	99	ASN
2	B	102	ILE
2	B	110	TYR
2	B	113	ASP
2	B	116	TYR
2	B	120	LEU
2	B	126	ASP

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Mol	Chain	Res	Type
2	B	127	ASP
2	B	129	TRP
2	B	132	GLN
2	B	141	GLN
2	B	145	LEU
2	B	148	ASN
2	B	161	VAL
2	B	167	ILE
2	B	174	GLU
2	B	176	PRO
2	B	178	TYR
2	B	183	THR
2	B	185	LEU
2	B	188	PHE
2	B	199	GLN
2	B	202	ARG
2	B	212	VAL
2	B	214	ARG
2	B	216	ARG
2	B	217	ASP
2	B	220	GLU
2	B	224	ASP
2	B	240	ASN
2	B	251	ASP
2	B	254	THR
2	B	261	ARG
2	B	262	LEU
2	B	272	GLN
2	B	281	TYR
2	B	296	THR
2	B	300	SER
2	B	307	ILE
2	B	316	ASN
2	B	329	THR
2	B	335	MET
2	B	336	ASP
2	B	343	LEU
2	B	346	ASP
2	B	354	LYS
2	B	360	ARG
2	B	364	GLU
2	B	366	LEU

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Mol	Chain	Res	Type
2	B	373	THR
2	B	375	LEU
2	B	376	ASN
2	B	387	MET
2	B	397	PHE
2	B	400	GLU
2	B	415	THR
2	B	430	THR
2	B	432	ASP
2	B	433	CYS
2	B	532	LYS
2	B	539	HIS
2	B	544	CYS
2	B	546	ASP
2	B	561	THR
2	B	568	MET
2	B	573	LEU
2	B	596	ASP
2	B	603	THR
2	B	617	CYS
2	B	619	LYS
2	B	622	ARG
2	B	623	GLU
2	B	624	PRO
2	B	626	MET
2	B	640	GLU
2	B	643	LYS
2	B	651	ASP
2	B	667	PHE
2	B	671	GLU
2	B	673	SER
2	B	674	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	68	GLN
1	A	77	ASN
1	A	102	GLN
1	A	113	HIS
1	A	120	GLN
1	A	131	GLN

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Mol	Chain	Res	Type
1	A	152	GLN
1	A	180	GLN
1	A	182	GLN
1	A	271	GLN
1	A	314	GLN
1	A	377	ASN
1	A	394	GLN
1	A	492	ASN
1	A	494	GLN
1	A	589	GLN
1	A	591	HIS
1	A	614	GLN
1	A	623	ASN
1	A	685	ASN
1	A	716	GLN
1	A	718	GLN
1	A	765	ASN
1	A	778	HIS
1	A	798	GLN
1	A	870	HIS
1	A	885	GLN
1	A	914	GLN
1	A	927	ASN
1	A	935	ASN
2	B	99	ASN
2	B	133	ASN
2	B	141	GLN
2	B	148	ASN
2	B	175	ASN
2	B	215	ASN
2	B	240	ASN
2	B	267	GLN
2	B	269	ASN
2	B	272	GLN
2	B	279	ASN
2	B	316	ASN
2	B	339	ASN
2	B	342	GLN
2	B	571	ASN
2	B	629	ASN
2	B	668	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue 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	$\#\|Z\| > 2$
3	MVA	C	5005	3	6,7,8	1.35	1 (16%)	6,8,10	1.23	1 (16%)

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	MVA	C	5005	3	-	0/5/8/10	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	5005	MVA	CN-N	-2.42	1.40	1.46

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	5005	MVA	CN-N-CA	2.17	120.33	113.65

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	5005	MVA	3	0

5.5 Carbohydrates (i)

14 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	$\#\|Z\| > 2$
4	NAG	A	2044	1,4	14,14,15	0.47	0	15,19,21	0.70	0
4	NAG	A	2045	4	14,14,15	0.40	0	15,19,21	0.88	1 (6%)
4	NAG	A	2266	1,4	14,14,15	0.51	0	15,19,21	0.80	0
4	NAG	A	2267	4	14,14,15	0.38	0	15,19,21	0.67	0
4	NAG	A	2585	1,4	14,14,15	0.74	0	15,19,21	0.70	0
4	NAG	A	2586	4	14,14,15	0.53	0	15,19,21	0.76	0
6	NAG	A	2943	1,6	14,14,15	0.47	0	15,19,21	0.83	1 (6%)
6	NDG	A	2944	6	14,14,15	0.67	0	15,19,21	0.62	0
4	NAG	A	2950	1,4	14,14,15	0.49	0	15,19,21	1.38	2 (13%)
4	NAG	A	2951	4	14,14,15	0.42	0	15,19,21	0.62	0
6	NAG	B	3559	2,6	14,14,15	0.79	0	15,19,21	0.77	1 (6%)
6	NDG	B	3560	6	14,14,15	0.78	1 (7%)	15,19,21	1.15	2 (13%)
6	NAG	B	3654	2,6	14,14,15	0.60	0	15,19,21	0.80	0
6	NDG	B	3655	6	14,14,15	0.47	0	15,19,21	0.84	1 (6%)

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	2044	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	2045	4	-	0/6/23/26	0/1/1/1
4	NAG	A	2266	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	2267	4	-	0/6/23/26	0/1/1/1
4	NAG	A	2585	1,4	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	2586	4	-	0/6/23/26	0/1/1/1
6	NAG	A	2943	1,6	-	0/6/23/26	0/1/1/1
6	NDG	A	2944	6	-	0/6/23/26	0/1/1/1
4	NAG	A	2950	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	2951	4	-	0/6/23/26	0/1/1/1
6	NAG	B	3559	2,6	-	0/6/23/26	0/1/1/1
6	NDG	B	3560	6	-	0/6/23/26	0/1/1/1
6	NAG	B	3654	2,6	-	0/6/23/26	0/1/1/1
6	NDG	B	3655	6	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	3560	NDG	C1-C2	2.25	1.55	1.52

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	B	3560	NDG	C2-N2-C7	-2.57	119.73	123.04
4	A	2045	NAG	C2-N2-C7	-2.53	119.79	123.04
6	A	2943	NAG	C2-N2-C7	-2.28	120.11	123.04
6	B	3559	NAG	C2-N2-C7	-2.19	120.22	123.04
6	B	3655	NDG	C2-N2-C7	-2.19	120.23	123.04
4	A	2950	NAG	C4-C3-C2	2.78	115.55	111.23
6	B	3560	NDG	C1-O-C5	2.83	115.84	112.25
4	A	2950	NAG	C3-C4-C5	3.35	116.04	110.20

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	2044	NAG	2	0
4	A	2045	NAG	5	0
4	A	2585	NAG	3	0
6	A	2943	NAG	3	0
6	A	2944	NDG	4	0
4	A	2950	NAG	3	0
6	B	3654	NAG	4	0
6	B	3655	NDG	4	0

5.6 Ligand geometry (i)

Of 12 ligands modelled in this entry, 8 are monoatomic - leaving 4 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	$\#\|Z\| > 2$
5	NAG	A	2260	1	14,14,15	0.65	0	15,19,21	0.80	0
5	NAG	A	2458	1	14,14,15	0.46	0	15,19,21	0.88	1 (6%)
5	NAG	B	3320	2	14,14,15	0.54	0	15,19,21	0.90	1 (6%)
5	NAG	B	3371	2	14,14,15	0.50	0	15,19,21	0.71	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	A	2260	1	-	0/6/23/26	0/1/1/1
5	NAG	A	2458	1	-	0/6/23/26	0/1/1/1
5	NAG	B	3320	2	-	0/6/23/26	0/1/1/1
5	NAG	B	3371	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	3320	NAG	C2-N2-C7	-2.35	120.03	123.04
5	A	2458	NAG	C2-N2-C7	-2.13	120.30	123.04

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	2260	NAG	3	0
5	A	2458	NAG	5	0
5	B	3320	NAG	1	0
5	B	3371	NAG	4	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section will therefore be empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.