



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:56 PM UTC

PDB ID : 5I5K / pdb_00005i5k
Title : Structure of complement C5 in complex with eculizumab
Authors : Schatz-Jakobsen, J.A.; Andersen, G.R.
Deposited on : 2016-02-15
Resolution : 4.20 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

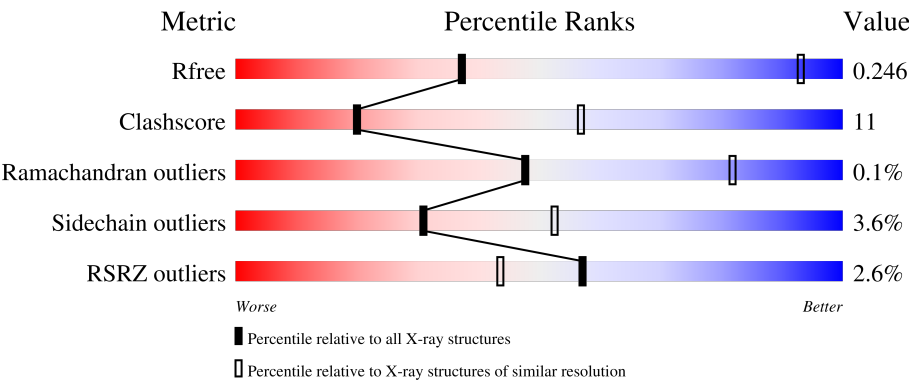
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

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 4.20 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))
R_{free}	180053	1004 (4.52-3.88)
Clashscore	190562	1019 (4.50-3.90)
Ramachandran outliers	187476	1020 (4.56-3.84)
Sidechain outliers	187428	1006 (4.56-3.84)
RSRZ outliers	180081	1001 (4.52-3.88)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1676	4% 70% 26% ..
1	B	1676	% 68% 28% ..
2	H	230	3% 67% 28% ..
2	X	230	% 61% 34% ..
3	L	214	2% 69% 30%

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Mol	Chain	Length	Quality of chain
3	Y	214	 6% 70% 30%
4	C	3	 67% 33%
4	D	3	 67% 33%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 32530 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Complement C5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	1634	Total	C	N	O	S	0	0	0
			12932	8277	2126	2476	53			
1	A	1632	Total	C	N	O	S	0	0	0
			12922	8271	2124	2474	53			

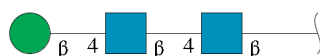
- Molecule 2 is a protein called Eculizumab heavy chain (variable domain).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	221	Total	C	N	O	S	0	0	0
			1679	1064	276	332	7			
2	X	221	Total	C	N	O	S	0	0	0
			1679	1064	276	332	7			

- Molecule 3 is a protein called Eculizumab light chain (variable domain).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	213	Total	C	N	O	S	0	0	0
			1620	1013	270	332	5			
3	Y	213	Total	C	N	O	S	0	0	0
			1620	1013	270	332	5			

- Molecule 4 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



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

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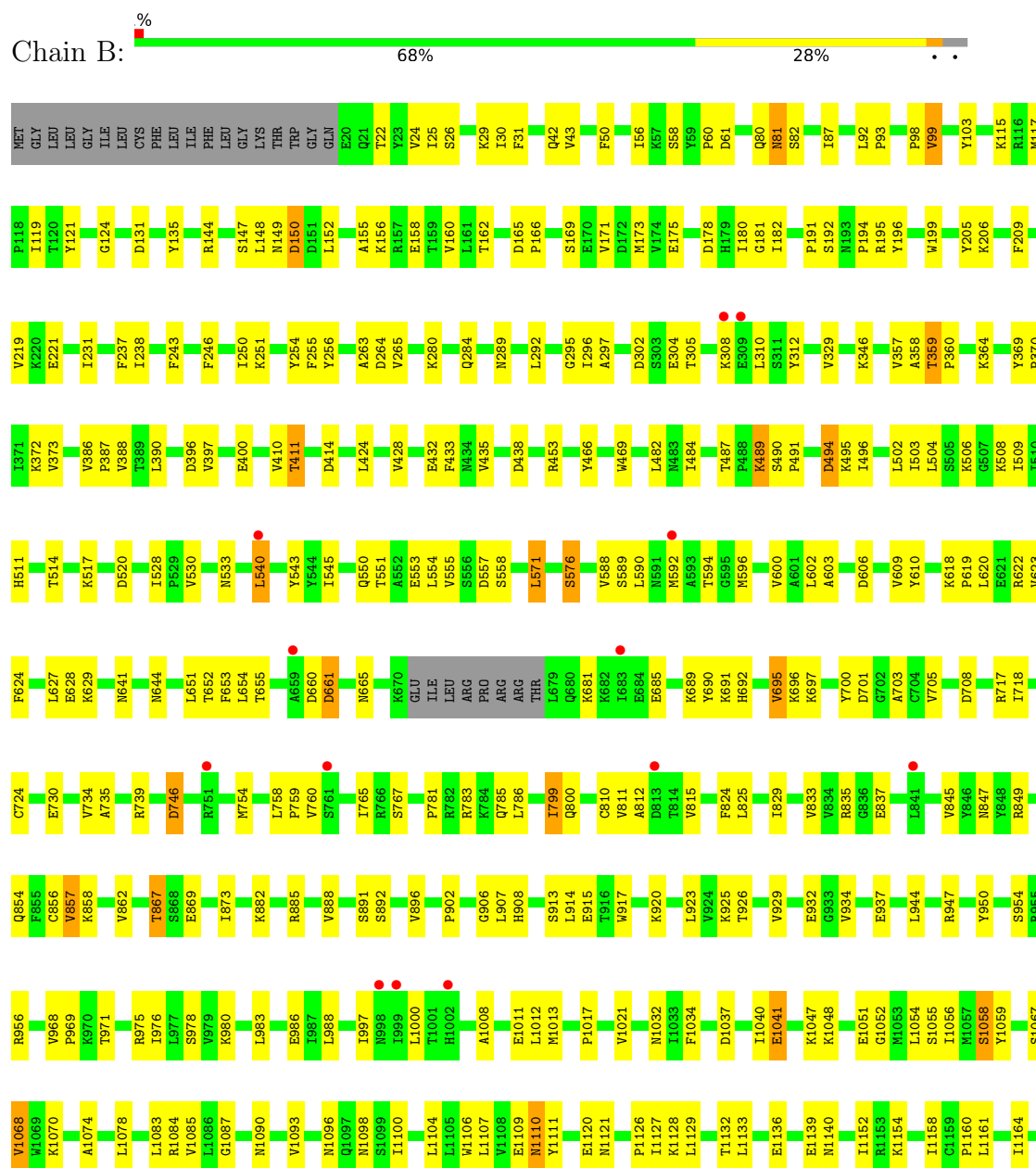
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	D	3	Total	C	N	O	0	0	0
			39	22	2	15			

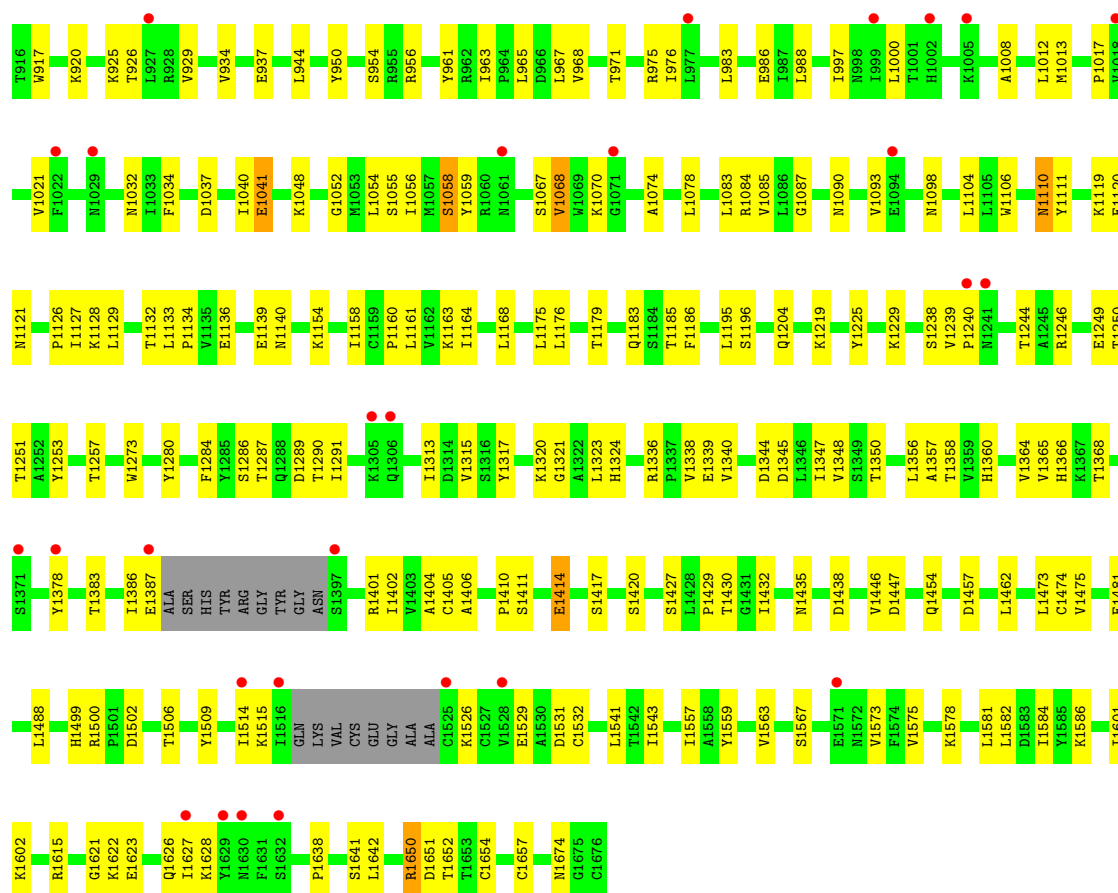
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

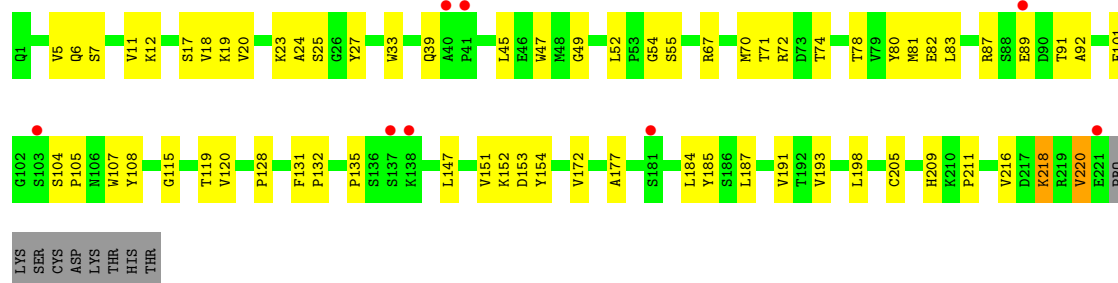
• Molecule 1: Complement C5



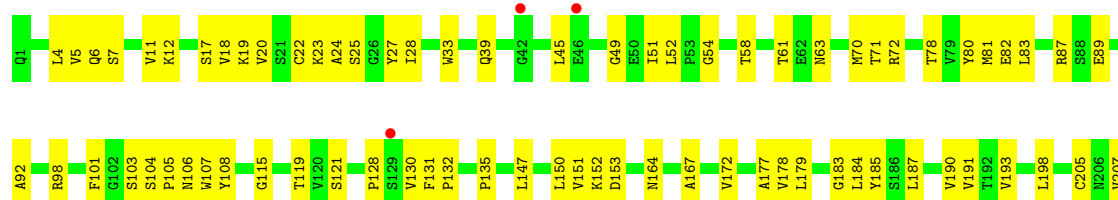


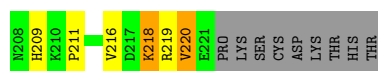


• Molecule 2: Eculizumab heavy chain (variable domain)



• Molecule 2: Eculizumab heavy chain (variable domain)

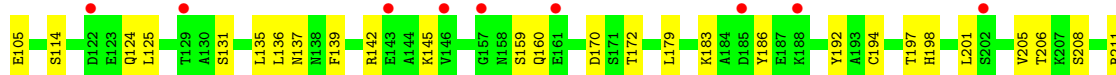
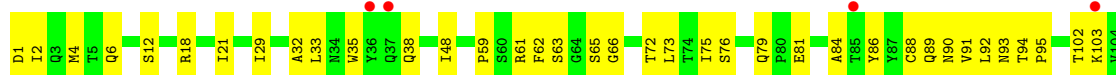




- Molecule 3: Eculizumab light chain (variable domain)



- Molecule 3: Eculizumab light chain (variable domain)



- Molecule 4: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 4: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	197.70Å 269.32Å 202.82Å 90.00° 98.58° 90.00°	Depositor
Resolution (Å)	49.80 – 4.20 49.80 – 4.20	Depositor EDS
% Data completeness (in resolution range)	99.7 (49.80-4.20) 99.7 (49.80-4.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.17	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.17 (at 4.14Å)	Xtriage
Refinement program	PHENIX (1.10_2152: ???)	Depositor
R, R_{free}	0.204 , 0.244 0.207 , 0.246	Depositor DCC
R_{free} test set	2000 reflections (2.45%)	wwPDB-VP
Wilson B-factor (Å ²)	182.6	Xtriage
Anisotropy	0.110	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 204.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	32530	wwPDB-VP
Average B, all atoms (Å ²)	244.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.77% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.15	1/13201 (0.0%)	0.38	1/17907 (0.0%)
1	B	0.15	1/13211 (0.0%)	0.38	1/17921 (0.0%)
2	H	0.14	0/1723	0.41	0/2350
2	X	0.14	0/1723	0.41	0/2350
3	L	0.16	0/1653	0.40	1/2247 (0.0%)
3	Y	0.14	0/1653	0.39	1/2247 (0.0%)
All	All	0.15	2/33164 (0.0%)	0.39	4/45022 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	2
2	H	0	1
2	X	0	1
All	All	0	6

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	576	SER	C-N	8.49	1.53	1.33
1	B	576	SER	C-N	7.79	1.52	1.33

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	66	GLY	N-CA-C	5.69	126.66	113.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	489	LYS	N-CA-C	5.51	117.70	107.99
3	Y	66	GLY	N-CA-C	5.38	125.93	113.18
1	B	489	LYS	N-CA-C	5.22	117.19	107.99

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	489	LYS	Peptide
1	A	494	ASP	Peptide
1	B	489	LYS	Peptide
1	B	494	ASP	Peptide
2	H	108	TYR	Peptide
2	X	108	TYR	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	12922	0	12866	284	0
1	B	12932	0	12876	296	0
2	H	1679	0	1628	43	0
2	X	1679	0	1628	50	0
3	L	1620	0	1576	44	0
3	Y	1620	0	1576	38	0
4	C	39	0	34	1	0
4	D	39	0	34	1	0
All	All	32530	0	32218	736	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 11.

All (736) 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:B:1106:TRP:O	1:B:1110:ASN:HB2	1.48	1.14

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1106:TRP:O	1:A:1110:ASN:HB2	1.49	1.09
1:A:364:LYS:NZ	1:A:557:ASP:OD2	1.85	1.07
1:B:1229:LYS:HZ1	1:B:1240:PRO:HD2	1.28	0.96
1:B:717:ARG:NH1	1:B:1447:ASP:O	1.99	0.94
1:A:150:ASP:OD2	1:A:508:LYS:NZ	2.00	0.94
1:B:1229:LYS:NZ	1:B:1238:SER:O	2.05	0.90
1:A:1229:LYS:HZ1	1:A:1239:VAL:HA	1.37	0.89
1:A:717:ARG:NH1	1:A:1447:ASP:O	2.06	0.89
1:A:1229:LYS:NZ	1:A:1238:SER:O	2.06	0.88
1:B:692:HIS:HB2	1:B:695:VAL:HB	1.56	0.86
2:X:135:PRO:HG3	2:X:198:LEU:HD21	1.56	0.85
2:H:135:PRO:HG3	2:H:198:LEU:HD21	1.57	0.85
1:A:282:MET:HG3	1:A:757:LEU:HD21	1.60	0.83
1:B:1128:LYS:NZ	1:B:1417:SER:OG	2.13	0.81
1:A:1229:LYS:HZ1	1:A:1240:PRO:HD2	1.43	0.81
1:A:692:HIS:HB2	1:A:695:VAL:HB	1.62	0.80
1:A:685:GLU:O	1:A:689:LYS:HB2	1.81	0.80
1:B:506:LYS:NZ	1:B:533:ASN:O	2.15	0.78
1:B:906:GLY:H	1:B:929:VAL:HB	1.49	0.77
1:B:150:ASP:OD2	1:B:508:LYS:NZ	2.14	0.77
1:A:124:GLY:HA3	1:A:148:LEU:O	1.85	0.77
1:B:1160:PRO:O	1:A:1098:ASN:ND2	2.18	0.77
2:H:132:PRO:HB3	2:H:218:LYS:HZ3	1.48	0.76
1:B:835:ARG:HA	1:B:902:PRO:HG2	1.67	0.76
1:A:906:GLY:H	1:A:929:VAL:HB	1.50	0.76
1:B:124:GLY:HA3	1:B:148:LEU:O	1.84	0.74
1:B:1098:ASN:ND2	1:A:1160:PRO:O	2.20	0.74
1:B:685:GLU:O	1:B:689:LYS:HB2	1.87	0.73
1:A:835:ARG:HA	1:A:902:PRO:HG2	1.70	0.73
3:Y:18:ARG:NH1	3:Y:76:SER:OG	2.22	0.73
2:H:132:PRO:HB3	2:H:218:LYS:NZ	2.04	0.73
3:L:61:ARG:HH11	3:L:79:GLN:HG3	1.53	0.73
1:B:976:ILE:HG12	1:B:1339:GLU:HG2	1.71	0.72
1:B:149:ASN:HB3	1:B:155:ALA:HB2	1.71	0.72
1:B:885:ARG:HD2	2:H:101:PHE:HB2	1.70	0.72
1:A:735:ALA:HB1	1:A:739:ARG:HH12	1.55	0.72
1:B:661:ASP:O	1:B:665:ASN:ND2	2.23	0.72
1:B:1383:THR:HG22	1:B:1402:ILE:HG12	1.71	0.72
1:A:885:ARG:HD2	2:X:101:PHE:HB2	1.72	0.72
2:X:132:PRO:HB3	2:X:218:LYS:HZ3	1.54	0.71
2:H:20:VAL:O	2:H:81:MET:HB3	1.89	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Y:114:SER:O	3:Y:136:LEU:HA	1.91	0.71
1:B:944:LEU:HB2	1:B:1357:ALA:HB3	1.73	0.71
1:B:432:GLU:OE2	1:B:453:ARG:NH2	2.23	0.70
1:A:1383:THR:HG22	1:A:1402:ILE:HG12	1.71	0.70
3:L:170:ASP:OD2	3:L:172:THR:OG1	2.08	0.70
1:A:131:ASP:OD1	1:A:135:TYR:OH	2.08	0.70
1:A:1128:LYS:NZ	1:A:1417:SER:OG	2.25	0.70
1:B:735:ALA:HB1	1:B:739:ARG:HH12	1.57	0.70
1:B:144:ARG:NH2	1:B:602:LEU:O	2.25	0.69
3:Y:170:ASP:OD2	3:Y:172:THR:OG1	2.09	0.69
1:B:98:PRO:HB3	1:B:121:TYR:HE2	1.56	0.69
1:B:1229:LYS:HZ1	1:B:1239:VAL:HA	1.56	0.69
1:A:606:ASP:HB3	1:A:609:VAL:HG23	1.74	0.69
1:A:858:LYS:HB2	1:A:913:SER:HB2	1.74	0.69
1:A:1128:LYS:O	1:A:1246:ARG:NH2	2.22	0.69
1:B:1229:LYS:NZ	1:B:1240:PRO:HD2	2.07	0.69
1:A:1229:LYS:NZ	1:A:1240:PRO:HD2	2.07	0.69
1:B:1541:LEU:HB2	1:B:1543:ILE:HG13	1.74	0.69
3:L:114:SER:O	3:L:136:LEU:HA	1.93	0.68
1:A:373:VAL:HG21	1:A:388:VAL:HG11	1.75	0.68
3:Y:114:SER:HB2	3:Y:137:ASN:HB3	1.76	0.68
1:B:1575:VAL:HB	1:B:1602:LYS:HB3	1.76	0.68
2:X:132:PRO:HB3	2:X:218:LYS:NZ	2.08	0.68
1:B:934:VAL:O	1:B:1366:HIS:HA	1.93	0.68
1:B:131:ASP:OD1	1:B:135:TYR:OH	2.12	0.68
2:H:153:ASP:HA	2:H:184:LEU:HB3	1.74	0.67
1:A:1074:ALA:O	1:A:1121:ASN:ND2	2.28	0.67
1:A:1378:TYR:O	1:A:1406:ALA:HA	1.95	0.67
1:B:858:LYS:HB2	1:B:913:SER:HB2	1.77	0.67
3:L:114:SER:HB2	3:L:137:ASN:HB3	1.75	0.67
1:B:857:VAL:HG21	1:B:896:VAL:HG21	1.77	0.67
1:B:606:ASP:HB3	1:B:609:VAL:HG23	1.77	0.66
1:B:1246:ARG:NH1	1:B:1500:ARG:HD3	2.09	0.66
1:A:1084:ARG:HD2	1:A:1154:LYS:HG3	1.76	0.66
1:A:98:PRO:HB3	1:A:121:TYR:HE2	1.60	0.66
1:A:1246:ARG:HH11	1:A:1500:ARG:HD3	1.61	0.66
1:A:1557:ILE:HA	1:A:1622:LYS:HA	1.78	0.66
3:Y:12:SER:HA	3:Y:105:GLU:HB2	1.76	0.66
1:A:441:ASP:OD1	1:A:441:ASP:N	2.29	0.65
1:A:1432:ILE:HG22	1:A:1481:GLU:HA	1.77	0.65
1:B:31:PHE:HB2	1:B:119:ILE:HG22	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:358:ALA:HB2	1:A:474:LYS:HE3	1.78	0.65
1:A:868:SER:HB2	1:A:1526:LYS:HB3	1.77	0.65
1:B:504:LEU:HG	1:B:509:ILE:HA	1.79	0.65
2:H:54:GLY:H	2:H:72:ARG:HE	1.45	0.65
1:A:31:PHE:HB2	1:A:119:ILE:HG22	1.78	0.65
1:A:1622:LYS:NZ	1:A:1642:LEU:HD12	2.12	0.65
1:A:1411:SER:H	1:A:1414:GLU:HG3	1.62	0.65
1:B:988:LEU:HD23	1:B:1021:VAL:HG22	1.78	0.65
1:B:1557:ILE:HA	1:B:1622:LYS:HA	1.78	0.65
1:A:43:VAL:HG11	1:A:50:PHE:HZ	1.62	0.65
3:Y:29:ILE:HB	3:Y:32:ALA:HB3	1.78	0.65
2:H:17:SER:HA	2:H:83:LEU:O	1.97	0.65
1:A:506:LYS:NZ	1:A:533:ASN:O	2.30	0.65
1:A:829:ILE:HD13	1:A:925:LYS:HG2	1.78	0.65
1:B:681:LYS:H	1:B:681:LYS:HD2	1.62	0.64
1:B:799:ILE:HG23	1:B:815:VAL:HB	1.80	0.64
1:B:364:LYS:NZ	1:B:557:ASP:OD2	2.29	0.64
2:X:54:GLY:H	2:X:72:ARG:HE	1.43	0.64
1:B:708:ASP:OD2	1:B:1401:ARG:NH2	2.31	0.64
1:A:825:LEU:HB2	1:A:914:LEU:HD22	1.80	0.64
1:A:944:LEU:HB2	1:A:1357:ALA:HB3	1.77	0.64
1:B:1432:ILE:HG22	1:B:1481:GLU:HA	1.79	0.64
3:L:29:ILE:HB	3:L:32:ALA:HB3	1.79	0.64
1:A:854:GLN:NE2	3:Y:92:LEU:O	2.31	0.64
1:A:1000:LEU:HD11	1:A:1017:PRO:HG3	1.80	0.64
1:A:504:LEU:HD21	1:A:651:LEU:HD21	1.79	0.63
1:A:536:PRO:HB3	1:A:628:GLU:OE2	1.99	0.63
2:X:20:VAL:O	2:X:81:MET:HB3	1.98	0.63
1:B:1411:SER:H	1:B:1414:GLU:HG3	1.61	0.63
1:A:29:LYS:HG3	1:A:30:ILE:HG12	1.80	0.63
1:A:847:ASN:HD21	1:A:849:ARG:HB3	1.64	0.63
3:Y:103:LYS:HD3	3:Y:142:ARG:HH12	1.64	0.63
1:A:1246:ARG:NH1	1:A:1500:ARG:HD3	2.13	0.63
1:A:263:ALA:HB3	1:A:292:LEU:HB3	1.80	0.63
1:A:685:GLU:O	1:A:689:LYS:CB	2.46	0.63
1:B:1128:LYS:O	1:B:1246:ARG:NH2	2.24	0.63
1:A:681:LYS:H	1:A:681:LYS:HD2	1.64	0.63
1:A:976:ILE:HG12	1:A:1339:GLU:HG2	1.80	0.63
2:X:218:LYS:HE3	2:X:220:VAL:HG22	1.81	0.63
1:B:1315:VAL:HG13	1:B:1323:LEU:HB3	1.79	0.62
1:B:653:PHE:CZ	1:B:660:ASP:HB3	2.34	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:661:ASP:O	1:A:665:ASN:ND2	2.32	0.62
1:A:1229:LYS:NZ	1:A:1239:VAL:HA	2.12	0.62
1:B:1000:LEU:HD11	1:B:1017:PRO:HG3	1.82	0.62
1:A:374:GLN:OE1	1:A:376:LYS:NZ	2.29	0.62
3:L:18:ARG:NH1	3:L:76:SER:OG	2.33	0.62
2:X:190:VAL:HG21	3:Y:135:LEU:HD11	1.81	0.62
1:B:691:LYS:HA	1:B:696:LYS:HE3	1.81	0.62
1:B:847:ASN:HD21	1:B:849:ARG:HB3	1.64	0.62
1:A:708:ASP:OD2	1:A:1401:ARG:NH2	2.33	0.62
1:A:387:PRO:HB2	1:A:438:ASP:HB3	1.82	0.61
1:A:432:GLU:OE2	1:A:453:ARG:NH2	2.33	0.61
2:X:153:ASP:HA	2:X:184:LEU:HB3	1.82	0.61
1:B:1246:ARG:HH11	1:B:1500:ARG:HD3	1.66	0.61
1:A:799:ILE:HG23	1:A:815:VAL:HB	1.83	0.61
1:B:396:ASP:OD1	1:B:397:VAL:N	2.34	0.61
1:A:149:ASN:HB3	1:A:155:ALA:HB2	1.83	0.61
1:A:571:LEU:HD12	1:A:812:ALA:HB2	1.83	0.61
1:B:24:VAL:HA	1:B:655:THR:HG22	1.81	0.61
1:A:115:LYS:HB2	1:A:654:LEU:HD11	1.82	0.61
3:Y:1:ASP:OD2	3:Y:95:PRO:HG2	2.01	0.61
1:B:1286:SER:O	1:B:1290:THR:OG1	2.18	0.60
4:C:2:NAG:H83	4:C:2:NAG:H3	1.83	0.60
1:B:1249:GLU:HG2	1:B:1253:TYR:HE2	1.66	0.60
1:B:58:SER:OG	1:B:61:ASP:O	2.18	0.60
1:B:550:GLN:HG2	1:B:551:THR:H	1.67	0.60
1:B:1229:LYS:NZ	1:B:1239:VAL:HA	2.15	0.60
1:A:503:ILE:HB	1:A:511:HIS:HB2	1.83	0.60
1:A:997:ILE:HD11	1:A:1048:LYS:HD3	1.83	0.60
1:B:205:TYR:HB2	1:B:209:PHE:HB2	1.84	0.60
1:B:829:ILE:HD13	1:B:925:LYS:HG2	1.83	0.60
1:A:195:ARG:HG3	1:A:1058:SER:HA	1.83	0.59
1:A:735:ALA:HB1	1:A:739:ARG:NH1	2.16	0.59
1:B:685:GLU:O	1:B:689:LYS:CB	2.51	0.59
1:B:1625:LEU:HB2	1:B:1636:ILE:O	2.03	0.58
1:A:144:ARG:NH1	1:A:775:TRP:O	2.28	0.58
1:A:1249:GLU:HG2	1:A:1253:TYR:HE2	1.67	0.58
1:B:1084:ARG:HD2	1:B:1154:LYS:HG3	1.86	0.58
1:B:1129:LEU:HD13	1:B:1139:GLU:HB3	1.85	0.58
1:A:653:PHE:CZ	1:A:660:ASP:HB3	2.38	0.58
1:A:857:VAL:HG21	1:A:896:VAL:HG21	1.85	0.58
1:B:171:VAL:HG12	1:B:1054:LEU:HD13	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:2:NAG:H3	4:D:2:NAG:H83	1.86	0.58
2:X:19:LYS:HG2	2:X:82:GLU:HG2	1.86	0.58
1:B:25:ILE:O	1:B:653:PHE:HA	2.03	0.58
1:B:1308:ARG:NH1	1:A:103:TYR:OH	2.37	0.58
1:B:1620:MET:HG3	1:B:1644:TRP:HB3	1.86	0.58
1:B:735:ALA:HB1	1:B:739:ARG:NH1	2.17	0.57
1:A:988:LEU:HD23	1:A:1021:VAL:HG22	1.85	0.57
1:B:263:ALA:HB3	1:B:292:LEU:HB3	1.86	0.57
1:B:825:LEU:HB2	1:B:914:LEU:HD22	1.86	0.57
1:B:1012:LEU:HD22	1:B:1085:VAL:HG21	1.85	0.57
1:B:484:ILE:HD12	1:B:528:ILE:HD12	1.86	0.57
2:H:67:ARG:CZ	2:H:87:ARG:HH12	2.17	0.57
1:A:550:GLN:HG2	1:A:551:THR:H	1.69	0.57
2:H:67:ARG:NH2	2:H:87:ARG:HH12	2.02	0.57
1:A:1161:LEU:HB3	1:A:1164:ILE:HG12	1.87	0.57
3:L:125:LEU:HD23	3:L:183:LYS:HE3	1.86	0.57
1:A:758:LEU:HB2	1:A:759:PRO:HD3	1.87	0.57
1:A:1244:THR:HG23	1:A:1502:ASP:OD2	2.04	0.57
1:B:1161:LEU:HB3	1:B:1164:ILE:HG12	1.86	0.57
1:A:156:LYS:HA	1:A:178:ASP:OD2	2.05	0.57
3:Y:4:MET:SD	3:Y:4:MET:N	2.78	0.57
1:B:618:LYS:HE2	1:B:800:GLN:HE22	1.69	0.57
1:B:997:ILE:HD11	1:B:1048:LYS:HD3	1.86	0.57
2:H:218:LYS:HE3	2:H:220:VAL:HG22	1.87	0.57
1:A:124:GLY:CA	1:A:148:LEU:O	2.52	0.57
1:B:180:ILE:HG13	1:B:182:ILE:H	1.70	0.56
1:A:610:TYR:HE1	1:A:618:LYS:HD3	1.70	0.56
1:A:746:ASP:HA	1:A:749:LEU:HD12	1.87	0.56
1:B:1420:SER:HB3	1:B:1497:GLU:OE2	2.05	0.56
1:B:1435:ASN:ND2	1:B:1438:ASP:OD1	2.37	0.56
1:B:652:THR:HG23	1:B:660:ASP:OD2	2.05	0.56
1:B:1068:VAL:HA	1:B:1078:LEU:HD13	1.87	0.56
1:B:1650:ARG:O	1:B:1652:THR:N	2.39	0.56
1:B:1313:ILE:HG23	1:B:1350:THR:HG22	1.86	0.56
1:B:1429:PRO:HB2	1:B:1432:ILE:HD11	1.87	0.56
1:A:237:PHE:HD1	1:A:346:LYS:HB3	1.71	0.56
1:A:1012:LEU:HD22	1:A:1085:VAL:HG21	1.87	0.56
1:B:195:ARG:HG3	1:B:1058:SER:HA	1.86	0.56
1:B:504:LEU:HD21	1:B:651:LEU:HD21	1.86	0.56
1:A:944:LEU:HD13	1:A:1350:THR:HG21	1.87	0.56
3:Y:103:LYS:HD3	3:Y:142:ARG:NH1	2.19	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:975:ARG:HB2	1:B:1340:VAL:HB	1.87	0.56
2:H:152:LYS:HE3	2:H:153:ASP:OD2	2.05	0.56
1:B:29:LYS:HG3	1:B:30:ILE:HG12	1.88	0.56
1:B:156:LYS:HA	1:B:178:ASP:OD2	2.06	0.56
1:B:620:LEU:HD11	1:B:800:GLN:HB2	1.88	0.56
1:B:1615:ARG:HD3	1:B:1650:ARG:HE	1.70	0.56
2:H:6:GLN:HG2	2:H:115:GLY:C	2.31	0.56
2:X:147:LEU:HD13	2:X:198:LEU:HD13	1.86	0.56
1:B:1219:LYS:HB2	1:B:1225:TYR:HB2	1.88	0.56
1:B:1315:VAL:HG23	1:B:1348:VAL:HG22	1.87	0.55
1:B:1378:TYR:O	1:B:1406:ALA:HA	2.06	0.55
2:H:54:GLY:H	2:H:72:ARG:NE	2.03	0.55
1:A:1013:MET:HE3	1:A:1287:THR:HB	1.89	0.55
1:B:178:ASP:OD1	1:B:181:GLY:N	2.39	0.55
1:B:1629:TYR:HE2	1:B:1634:ARG:HB2	1.71	0.55
1:A:691:LYS:HA	1:A:696:LYS:HE3	1.87	0.55
1:A:1313:ILE:HG23	1:A:1350:THR:HG22	1.87	0.55
1:A:1344:ASP:OD1	1:A:1345:ASP:N	2.39	0.55
1:B:697:LYS:HE3	1:B:701:ASP:OD2	2.05	0.55
2:X:177:ALA:HB1	2:X:185:TYR:HB3	1.88	0.55
1:A:1126:PRO:O	1:A:1499:HIS:ND1	2.39	0.55
3:Y:125:LEU:HD23	3:Y:183:LYS:HE3	1.89	0.55
1:B:135:TYR:HB2	1:B:219:VAL:HG22	1.88	0.55
1:B:237:PHE:HD1	1:B:346:LYS:HB3	1.72	0.55
1:A:956:ARG:HA	1:A:1348:VAL:O	2.06	0.55
1:A:1429:PRO:HB2	1:A:1432:ILE:HD11	1.89	0.55
1:B:854:GLN:NE2	3:L:92:LEU:O	2.39	0.54
1:A:1575:VAL:HB	1:A:1602:LYS:HB3	1.88	0.54
1:A:191:PRO:HD2	1:A:194:PRO:HB3	1.88	0.54
1:A:567:CYS:HB2	1:A:570:GLN:H	1.72	0.54
2:X:6:GLN:HG2	2:X:115:GLY:C	2.32	0.54
2:X:17:SER:HA	2:X:83:LEU:O	2.07	0.54
2:X:147:LEU:HD12	2:X:220:VAL:HB	1.89	0.54
1:A:1650:ARG:O	1:A:1652:THR:N	2.40	0.54
1:B:196:TYR:CZ	1:B:221:GLU:HB2	2.42	0.54
1:A:1410:PRO:HB2	1:A:1414:GLU:HB2	1.88	0.54
1:B:25:ILE:HB	1:B:654:LEU:HB2	1.89	0.54
1:A:833:VAL:HG13	1:A:1430:THR:HG21	1.90	0.54
1:A:934:VAL:O	1:A:1366:HIS:HA	2.07	0.54
1:B:99:VAL:HG23	1:B:119:ILE:HD11	1.90	0.54
1:B:387:PRO:HB2	1:B:438:ASP:HB3	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1229:LYS:HZ1	1:B:1240:PRO:CD	2.12	0.54
1:A:746:ASP:OD1	1:A:746:ASP:N	2.41	0.54
1:A:1087:GLY:HA2	1:A:1158:ILE:HD11	1.88	0.54
1:A:950:TYR:CD2	1:A:1356:LEU:HD21	2.43	0.54
1:A:1249:GLU:HG2	1:A:1253:TYR:CE2	2.42	0.54
3:Y:65:SER:HB3	3:Y:72:THR:OG1	2.08	0.54
1:B:1107:LEU:HD11	1:B:1152:ILE:HD11	1.90	0.53
1:B:1563:VAL:HG12	1:B:1581:LEU:HA	1.90	0.53
1:B:619:PRO:O	1:B:623:VAL:HB	2.09	0.53
2:H:72:ARG:NH2	2:H:74:THR:OG1	2.40	0.53
3:L:21:ILE:HD13	3:L:102:THR:HG21	1.90	0.53
1:B:619:PRO:HA	1:B:622:ARG:HG2	1.89	0.53
1:A:831:TYR:CZ	1:A:1457:ASP:HB3	2.43	0.53
1:A:1315:VAL:HG23	1:A:1348:VAL:HG22	1.90	0.53
3:Y:131:SER:HA	3:Y:179:LEU:O	2.09	0.53
1:B:1622:LYS:NZ	1:B:1642:LEU:HD12	2.24	0.53
1:A:205:TYR:HB2	1:A:209:PHE:HB2	1.89	0.53
1:B:1462:LEU:HD11	1:B:1475:VAL:HG21	1.90	0.53
1:B:758:LEU:HB2	1:B:759:PRO:HD3	1.90	0.53
1:A:507:GLY:HA2	1:A:632:LEU:HG	1.91	0.53
1:A:1068:VAL:HA	1:A:1078:LEU:HD13	1.90	0.53
1:A:1563:VAL:HG12	1:A:1581:LEU:HA	1.89	0.53
1:B:302:ASP:OD2	1:B:305:THR:OG1	2.20	0.53
3:L:194:CYS:O	3:L:206:THR:HA	2.09	0.53
1:A:1175:LEU:O	1:A:1179:THR:OG1	2.19	0.53
1:A:1315:VAL:HG13	1:A:1323:LEU:HB3	1.91	0.53
1:B:1244:THR:HG23	1:B:1502:ASP:OD2	2.09	0.53
1:B:1196:SER:HB2	1:B:1257:THR:HG23	1.91	0.53
1:A:58:SER:OG	1:A:61:ASP:O	2.22	0.53
1:A:873:ILE:HG13	1:A:882:LYS:HE3	1.91	0.53
3:L:61:ARG:HH11	3:L:79:GLN:CG	2.20	0.52
1:A:99:VAL:HG23	1:A:119:ILE:HD11	1.91	0.52
2:X:5:VAL:HB	2:X:23:LYS:HB2	1.90	0.52
1:A:1289:ASP:OD1	1:A:1290:THR:N	2.42	0.52
1:B:1013:MET:HE3	1:B:1287:THR:HB	1.90	0.52
1:B:1559:TYR:CZ	1:B:1621:GLY:HA3	2.45	0.52
1:A:180:ILE:HG13	1:A:182:ILE:H	1.74	0.52
1:A:1111:TYR:HB3	1:A:1119:LYS:HG3	1.91	0.52
1:B:115:LYS:HB2	1:B:654:LEU:HD11	1.90	0.52
1:B:358:ALA:HB1	1:B:469:TRP:HH2	1.75	0.52
1:B:1515:LYS:HD2	1:B:1607:THR:HG21	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:746:ASP:N	1:B:746:ASP:OD1	2.40	0.52
1:B:1249:GLU:HG2	1:B:1253:TYR:CE2	2.44	0.52
1:A:697:LYS:HE3	1:A:701:ASP:OD2	2.10	0.52
2:X:209:HIS:CD2	2:X:211:PRO:HD2	2.44	0.52
1:B:983:LEU:HD21	1:B:1356:LEU:HD13	1.91	0.52
1:B:1420:SER:OG	1:B:1421:HIS:N	2.43	0.52
1:B:854:GLN:HE22	3:L:92:LEU:HD12	1.75	0.52
1:B:1047:LYS:NZ	1:B:1051:GLU:OE2	2.43	0.52
3:L:1:ASP:OD2	3:L:95:PRO:HG2	2.09	0.52
1:A:178:ASP:OD1	1:A:181:GLY:N	2.43	0.52
1:A:1435:ASN:ND2	1:A:1438:ASP:OD1	2.43	0.52
2:X:54:GLY:H	2:X:72:ARG:NE	2.08	0.52
1:B:594:THR:OG1	1:B:596:MET:O	2.18	0.52
1:B:1083:LEU:HD13	1:B:1104:LEU:HD23	1.92	0.52
1:A:1323:LEU:HG	1:A:1324:HIS:H	1.75	0.52
3:Y:201:LEU:HD21	3:Y:205:VAL:HG23	1.92	0.52
1:B:1344:ASP:OD1	1:B:1345:ASP:N	2.44	0.51
3:L:59:PRO:HB2	3:L:61:ARG:HG3	1.92	0.51
2:X:87:ARG:HG3	2:X:89:GLU:HG2	1.91	0.51
1:B:618:LYS:HE3	1:B:619:PRO:HD2	1.93	0.51
2:H:24:ALA:HB1	2:H:27:TYR:HE1	1.75	0.51
3:L:32:ALA:O	3:L:91:VAL:HG22	2.11	0.51
1:A:1427:SER:O	1:A:1509:TYR:OH	2.20	0.51
1:A:975:ARG:HB2	1:A:1340:VAL:HB	1.92	0.51
1:A:1615:ARG:HD3	1:A:1650:ARG:HE	1.75	0.51
2:H:5:VAL:HB	2:H:23:LYS:HB2	1.91	0.51
2:H:87:ARG:HG3	2:H:89:GLU:HG2	1.93	0.51
1:B:503:ILE:HB	1:B:511:HIS:HB2	1.92	0.51
1:A:424:LEU:HD13	1:A:428:VAL:HG21	1.92	0.51
1:A:484:ILE:HD12	1:A:528:ILE:HD12	1.93	0.51
1:A:490:SER:N	1:A:491:PRO:HD3	2.25	0.51
3:Y:145:LYS:HB3	3:Y:197:THR:HB	1.92	0.51
1:B:837:GLU:HG2	1:B:1488:LEU:HA	1.91	0.51
3:Y:194:CYS:O	3:Y:206:THR:HA	2.09	0.51
1:B:944:LEU:HD13	1:B:1350:THR:HG21	1.91	0.51
1:A:858:LYS:HE2	1:A:915:GLU:OE2	2.11	0.51
1:B:590:LEU:HB3	1:B:786:LEU:O	2.11	0.51
3:L:59:PRO:HG2	3:L:62:PHE:HE1	1.75	0.51
1:A:1286:SER:O	1:A:1290:THR:OG1	2.22	0.51
1:A:1622:LYS:HZ2	1:A:1642:LEU:HD12	1.74	0.51
3:Y:32:ALA:O	3:Y:91:VAL:HG22	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:7:SER:HB2	2:H:20:VAL:HG13	1.92	0.51
2:H:147:LEU:HD13	2:H:198:LEU:HD13	1.91	0.51
1:A:284:GLN:H	1:A:310:LEU:HD13	1.75	0.51
1:A:387:PRO:HD2	1:A:439:ALA:HA	1.92	0.51
1:A:824:PHE:CZ	1:A:846:TYR:HB2	2.46	0.50
1:B:550:GLN:H	1:B:550:GLN:CD	2.19	0.50
1:B:950:TYR:CD2	1:B:1356:LEU:HD21	2.46	0.50
1:B:1074:ALA:O	1:B:1121:ASN:ND2	2.44	0.50
2:H:177:ALA:HB1	2:H:185:TYR:HB3	1.92	0.50
1:A:746:ASP:HA	1:A:749:LEU:HB2	1.93	0.50
3:Y:59:PRO:HB2	3:Y:61:ARG:HG3	1.94	0.50
1:B:81:ASN:HD22	1:B:82:SER:H	1.58	0.50
1:B:1558:ALA:HB1	1:B:1588:GLY:HA3	1.94	0.50
3:L:145:LYS:HB3	3:L:197:THR:HB	1.94	0.50
1:A:869:GLU:O	1:A:870:SER:OG	2.28	0.50
1:A:292:LEU:HD21	1:A:295:GLY:HA2	1.94	0.50
1:A:968:VAL:O	1:A:971:THR:OG1	2.29	0.50
1:B:923:LEU:HD11	1:B:925:LYS:HD3	1.92	0.50
3:Y:61:ARG:HH11	3:Y:79:GLN:HG3	1.75	0.50
1:A:25:ILE:HB	1:A:654:LEU:HB2	1.94	0.50
1:B:490:SER:N	1:B:491:PRO:HD3	2.27	0.49
3:L:131:SER:HA	3:L:179:LEU:O	2.12	0.49
1:A:917:TRP:HB2	2:X:107:TRP:CH2	2.46	0.49
1:B:152:LEU:HD22	1:B:627:LEU:HD11	1.93	0.49
3:L:201:LEU:HD21	3:L:205:VAL:HG23	1.94	0.49
1:B:1317:TYR:HB2	1:B:1320:LYS:HB3	1.94	0.49
1:B:1427:SER:O	1:B:1509:TYR:OH	2.18	0.49
1:A:760:VAL:HG23	1:A:761:SER:H	1.77	0.49
1:A:790:LEU:HD13	1:A:819:VAL:HG22	1.94	0.49
1:B:1087:GLY:HA2	1:B:1158:ILE:HD11	1.94	0.49
1:B:906:GLY:N	1:B:929:VAL:HB	2.22	0.49
1:A:1336:ARG:HG3	1:A:1338:VAL:HG23	1.94	0.49
1:B:357:VAL:O	1:B:372:LYS:HB2	2.13	0.49
1:A:1462:LEU:HD11	1:A:1475:VAL:HG21	1.94	0.49
2:X:23:LYS:HG2	2:X:78:THR:HG22	1.94	0.49
1:B:147:SER:HB2	1:B:205:TYR:OH	2.12	0.49
1:B:373:VAL:HG21	1:B:388:VAL:HG11	1.94	0.49
1:B:1126:PRO:O	1:B:1499:HIS:ND1	2.41	0.49
1:A:956:ARG:HH21	1:A:1347:ILE:HG21	1.78	0.49
1:A:983:LEU:HD21	1:A:1356:LEU:HD13	1.94	0.49
3:L:12:SER:HA	3:L:105:GLU:HB2	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:455:ILE:HD12	1:A:640:LEU:HD21	1.94	0.49
1:A:554:LEU:HD11	1:A:655:THR:HG21	1.93	0.49
1:A:623:VAL:HG21	1:A:809:ILE:HD13	1.93	0.49
1:A:961:TYR:O	1:A:1628:LYS:HD3	2.13	0.49
1:B:360:PRO:O	1:B:369:TYR:OH	2.19	0.49
1:B:833:VAL:HG13	1:B:1430:THR:HG21	1.94	0.49
1:A:269:PHE:HB2	1:A:283:MET:HE2	1.94	0.48
1:A:730:GLU:O	1:A:734:VAL:HG23	2.13	0.48
1:B:250:ILE:HD12	1:B:265:VAL:HG11	1.95	0.48
1:B:858:LYS:HE2	1:B:915:GLU:OE2	2.14	0.48
1:B:908:HIS:O	1:B:926:THR:HA	2.14	0.48
1:A:1601:ILE:HG12	1:A:1638:PRO:HA	1.94	0.48
2:X:152:LYS:HE3	2:X:153:ASP:OD2	2.12	0.48
1:B:703:ALA:HB3	1:B:754:MET:HE1	1.95	0.48
1:A:837:GLU:HG2	1:A:1488:LEU:HA	1.96	0.48
1:A:1622:LYS:HG3	1:A:1623:GLU:HG2	1.95	0.48
1:B:292:LEU:HD21	1:B:295:GLY:HA2	1.94	0.48
1:B:390:LEU:HD13	1:B:435:VAL:HG22	1.96	0.48
1:B:1386:ILE:HG13	1:B:1387:GLU:H	1.78	0.48
1:A:652:THR:HG23	1:A:660:ASP:OD2	2.13	0.48
1:B:1323:LEU:HG	1:B:1324:HIS:H	1.77	0.48
1:A:1404:ALA:O	1:A:1474:CYS:HA	2.14	0.48
1:B:1289:ASP:OD1	1:B:1290:THR:N	2.46	0.48
1:B:1514:ILE:HG22	1:B:1515:LYS:H	1.78	0.48
3:L:65:SER:HB3	3:L:72:THR:OG1	2.13	0.48
1:A:25:ILE:O	1:A:653:PHE:HA	2.14	0.48
2:X:24:ALA:HB1	2:X:27:TYR:HE1	1.79	0.48
1:B:1128:LYS:NZ	1:B:1136:GLU:OE2	2.40	0.48
1:B:1175:LEU:O	1:B:1179:THR:OG1	2.24	0.48
1:A:1358:THR:HB	1:A:1360:HIS:CE1	2.49	0.48
1:A:1674:ASN:O	1:A:1674:ASN:ND2	2.46	0.48
1:B:641:ASN:H	1:B:644:ASN:HB3	1.78	0.48
1:B:968:VAL:O	1:B:971:THR:OG1	2.28	0.48
1:B:1529:GLU:HB3	1:B:1532:CYS:SG	2.54	0.48
1:A:1083:LEU:HD13	1:A:1104:LEU:HD23	1.96	0.48
1:B:1067:SER:HA	1:B:1074:ALA:HA	1.95	0.47
1:A:73:LEU:HD12	1:A:79:PHE:HD1	1.79	0.47
2:H:209:HIS:CD2	2:H:211:PRO:HD2	2.49	0.47
1:A:92:LEU:HD22	1:A:99:VAL:HG21	1.96	0.47
2:X:27:TYR:CD2	2:X:98:ARG:NH1	2.83	0.47
2:X:49:GLY:HA3	2:X:70:MET:HE1	1.94	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1654:CYS:SG	1:A:1657:CYS:N	2.88	0.47
1:A:292:LEU:HA	1:A:297:ALA:HB2	1.96	0.47
1:A:304:GLU:HG3	1:A:308:LYS:HD2	1.97	0.47
3:Y:192:TYR:O	3:Y:208:SER:HA	2.15	0.47
1:B:956:ARG:HH21	1:B:1347:ILE:HG21	1.79	0.47
1:A:250:ILE:HD12	1:A:265:VAL:HG11	1.96	0.47
3:Y:21:ILE:HD13	3:Y:102:THR:HG21	1.95	0.47
1:A:158:GLU:OE2	1:A:206:LYS:HD3	2.15	0.47
1:A:888:VAL:HG22	1:A:892:SER:HB2	1.95	0.47
1:A:1541:LEU:HB2	1:A:1543:ILE:HG13	1.97	0.47
1:B:165:ASP:OD1	1:B:169:SER:N	2.48	0.47
1:B:292:LEU:HA	1:B:297:ALA:HB2	1.97	0.47
1:B:1133:LEU:HD12	1:B:1133:LEU:H	1.80	0.47
1:A:577:PRO:HD2	1:A:588:VAL:HG23	1.95	0.47
1:B:1315:VAL:HG12	1:B:1324:HIS:O	2.15	0.47
3:L:103:LYS:HD3	3:L:142:ARG:HH12	1.79	0.47
1:A:503:ILE:HG12	1:A:540:LEU:HD12	1.95	0.47
1:B:192:SER:HB2	1:B:1011:GLU:OE2	2.15	0.47
1:B:1586:LYS:HE3	1:B:1674:ASN:HA	1.97	0.47
1:A:278:ASP:OD1	1:A:278:ASP:N	2.42	0.47
1:A:1120:GLU:OE2	1:A:1121:ASN:N	2.46	0.47
1:B:124:GLY:CA	1:B:148:LEU:O	2.57	0.47
2:H:71:THR:OG1	2:H:80:TYR:HB2	2.15	0.47
2:H:147:LEU:HD12	2:H:220:VAL:HB	1.97	0.47
1:A:272:ARG:NH2	1:A:277:ASP:O	2.43	0.47
1:B:862:VAL:HG22	1:B:907:LEU:HD21	1.96	0.46
1:B:1032:ASN:HD22	1:A:61:ASP:CG	2.24	0.46
2:H:39:GLN:O	2:H:92:ALA:HB1	2.15	0.46
1:A:1133:LEU:HD12	1:A:1133:LEU:H	1.80	0.46
1:B:191:PRO:HD2	1:B:194:PRO:HB3	1.97	0.46
1:B:1186:PHE:HA	1:B:1250:THR:HG22	1.97	0.46
1:B:1405:CYS:HA	1:B:1473:LEU:O	2.15	0.46
1:B:1358:THR:HB	1:B:1360:HIS:CE1	2.51	0.46
2:X:104:SER:HB2	2:X:105:PRO:HD2	1.97	0.46
2:X:130:VAL:HA	2:X:150:LEU:O	2.15	0.46
1:B:256:TYR:CD2	1:B:824:PHE:HE2	2.34	0.46
1:B:1136:GLU:O	1:B:1140:ASN:HB2	2.16	0.46
1:B:1284:PHE:HD1	1:B:1290:THR:HG23	1.80	0.46
1:B:1410:PRO:HB2	1:B:1414:GLU:HB2	1.96	0.46
1:A:862:VAL:HG22	1:A:907:LEU:HD21	1.97	0.46
3:Y:89:GLN:HG2	3:Y:90:ASN:N	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:698:CYS:SG	1:A:1446:VAL:HG21	2.55	0.46
1:A:1196:SER:HB2	1:A:1257:THR:HG23	1.98	0.46
2:X:12:LYS:HD2	2:X:18:VAL:HA	1.97	0.46
1:B:1400:LYS:NZ	1:B:1481:GLU:OE2	2.23	0.46
2:H:23:LYS:HG2	2:H:78:THR:HG22	1.98	0.46
1:A:308:LYS:HA	1:A:313:TYR:HA	1.97	0.46
1:A:602:LEU:HD12	1:A:774:LEU:HD22	1.97	0.46
1:A:1586:LYS:HE3	1:A:1674:ASN:HA	1.97	0.46
2:X:71:THR:OG1	2:X:80:TYR:HB2	2.15	0.46
1:B:520:ASP:OD1	1:B:520:ASP:N	2.42	0.46
1:B:610:TYR:HE1	1:B:618:LYS:HD3	1.81	0.46
1:B:1650:ARG:C	1:B:1652:THR:H	2.23	0.46
1:A:965:LEU:HA	1:A:1627:ILE:HD13	1.98	0.46
1:B:1268:ASN:OD1	1:B:1300:TYR:OH	2.31	0.46
1:B:1336:ARG:HG3	1:B:1338:VAL:HG23	1.98	0.46
1:B:1524:ALA:HB1	1:B:1528:VAL:HG21	1.98	0.46
3:L:186:TYR:HE2	3:L:211:ARG:HH22	1.64	0.46
1:A:243:PHE:CE2	1:A:304:GLU:HB2	2.51	0.46
1:A:1622:LYS:HZ1	1:A:1642:LEU:HD12	1.79	0.46
1:B:1034:PHE:CE1	1:B:1041:GLU:HG2	2.51	0.46
2:H:104:SER:HB2	2:H:105:PRO:HD2	1.98	0.46
1:B:590:LEU:O	1:B:785:GLN:HA	2.16	0.46
1:B:592:MET:SD	1:B:600:VAL:HG21	2.56	0.46
1:A:1059:TYR:CE2	1:A:1070:LYS:HG2	2.51	0.46
3:Y:2:ILE:HG21	3:Y:93:ASN:HB2	1.96	0.46
1:B:867:THR:C	1:B:869:GLU:H	2.24	0.45
1:A:171:VAL:HG12	1:A:1054:LEU:HD13	1.98	0.45
1:A:1008:ALA:HB3	1:A:1078:LEU:HD11	1.99	0.45
1:A:1317:TYR:HB2	1:A:1320:LYS:HB3	1.97	0.45
1:B:624:PHE:O	1:B:628:GLU:HG2	2.16	0.45
1:B:1132:THR:O	1:B:1136:GLU:N	2.40	0.45
1:A:520:ASP:OD1	1:A:520:ASP:N	2.45	0.45
2:H:49:GLY:HA3	2:H:70:MET:HE1	1.98	0.45
2:H:154:TYR:CE2	2:H:185:TYR:HB2	2.51	0.45
1:A:98:PRO:HB3	1:A:121:TYR:CE2	2.47	0.45
1:A:254:TYR:O	1:A:255:PHE:HD1	1.99	0.45
1:B:571:LEU:HD12	1:B:812:ALA:HB2	1.97	0.45
2:H:11:VAL:HG12	2:H:119:THR:HB	1.99	0.45
3:L:2:ILE:HG21	3:L:93:ASN:HB2	1.97	0.45
1:A:396:ASP:OD1	1:A:397:VAL:N	2.49	0.45
1:A:920:LYS:HE2	2:X:103:SER:O	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:39:GLN:O	2:X:92:ALA:HB1	2.17	0.45
1:B:1531:ASP:OD1	1:B:1641:SER:OG	2.21	0.45
1:A:624:PHE:O	1:A:628:GLU:HG2	2.16	0.45
1:A:963:ILE:O	1:A:1627:ILE:HG23	2.17	0.45
1:A:504:LEU:HG	1:A:509:ILE:HA	1.98	0.45
1:A:1186:PHE:HA	1:A:1250:THR:HG22	1.98	0.45
2:X:7:SER:HB2	2:X:20:VAL:HG13	1.98	0.45
1:B:42:GLN:HG2	1:B:80:GLN:HG2	1.99	0.45
1:B:284:GLN:H	1:B:310:LEU:HD13	1.81	0.45
1:B:469:TRP:HE3	1:B:469:TRP:H	1.65	0.45
1:A:619:PRO:HA	1:A:622:ARG:HG2	1.98	0.45
1:A:1136:GLU:O	1:A:1140:ASN:HB2	2.17	0.45
2:X:193:VAL:HG23	2:X:198:LEU:HB2	1.98	0.45
3:Y:35:TRP:HB2	3:Y:48:ILE:HB	1.98	0.45
2:X:178:VAL:HG21	3:Y:160:GLN:HB3	1.98	0.45
3:Y:159:SER:HB3	3:Y:179:LEU:HD13	1.99	0.45
1:B:873:ILE:HG13	1:B:882:LYS:HE3	1.99	0.45
1:B:1320:LYS:HG3	1:B:1321:GLY:H	1.82	0.45
1:A:147:SER:HB2	1:A:205:TYR:OH	2.17	0.45
1:A:1286:SER:OG	1:A:1287:THR:N	2.50	0.45
1:A:1320:LYS:HG3	1:A:1321:GLY:H	1.81	0.45
1:A:1500:ARG:HB2	1:A:1502:ASP:OD1	2.17	0.45
1:A:1531:ASP:OD1	1:A:1641:SER:OG	2.21	0.45
1:B:304:GLU:HG3	1:B:308:LYS:HD2	1.99	0.45
1:B:1455:ILE:HA	1:B:1459:HIS:O	2.17	0.45
3:L:83:PHE:CG	3:L:106:ILE:HD12	2.52	0.45
1:A:25:ILE:HG13	1:A:106:VAL:HG21	1.99	0.45
1:A:1514:ILE:HG22	1:A:1515:LYS:H	1.81	0.45
1:B:390:LEU:HD11	1:B:433:PHE:HB2	1.98	0.44
1:B:1052:GLY:O	1:B:1055:SER:HB3	2.17	0.44
1:B:1404:ALA:O	1:B:1474:CYS:HA	2.16	0.44
1:B:1581:LEU:HD12	1:B:1582:LEU:H	1.82	0.44
1:A:142:LYS:NZ	1:A:771:GLU:OE2	2.36	0.44
1:A:594:THR:OG1	1:A:596:MET:O	2.29	0.44
1:A:618:LYS:HD2	1:A:618:LYS:HA	1.85	0.44
1:A:1129:LEU:HD13	1:A:1139:GLU:HB3	1.98	0.44
1:B:571:LEU:HD21	1:B:810:CYS:HB3	1.99	0.44
2:H:193:VAL:HG23	2:H:198:LEU:HB2	1.98	0.44
3:L:20:THR:HA	3:L:73:LEU:O	2.17	0.44
3:L:159:SER:HB3	3:L:179:LEU:HD13	1.99	0.44
1:A:722:PRO:HA	1:A:725:ILE:HB	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:166:PRO:HD3	1:B:199:TRP:CE2	2.52	0.44
1:B:1120:GLU:OE2	1:B:1121:ASN:N	2.50	0.44
1:B:1286:SER:OG	1:B:1287:THR:N	2.50	0.44
1:A:908:HIS:O	1:A:926:THR:HA	2.18	0.44
1:A:1132:THR:O	1:A:1136:GLU:N	2.36	0.44
1:B:1109:GLU:OE2	1:A:1163:LYS:HD2	2.17	0.44
1:A:128:ILE:HD13	1:A:201:ILE:HG22	2.00	0.44
1:B:603:ALA:HB3	1:B:800:GLN:HG2	1.99	0.44
1:B:917:TRP:HB2	2:H:107:TRP:CH2	2.52	0.44
1:A:1581:LEU:HD12	1:A:1582:LEU:H	1.82	0.44
1:B:496:ILE:O	1:B:517:LYS:HD2	2.17	0.44
1:B:705:VAL:HG12	1:B:739:ARG:CZ	2.48	0.44
1:B:1176:LEU:HD23	1:B:1195:LEU:HD13	2.00	0.44
1:B:1567:SER:HB3	1:B:1578:LYS:HB2	2.00	0.44
1:A:160:VAL:HG22	1:A:175:GLU:HB3	1.98	0.44
1:A:1037:ASP:OD2	1:A:1040:ILE:HG13	2.17	0.44
1:B:80:GLN:OE1	1:B:514:THR:OG1	2.25	0.44
1:B:251:LYS:HG2	1:B:296:ILE:HG12	2.00	0.44
1:B:370:PRO:HG3	1:B:466:TYR:OH	2.17	0.44
1:B:947:ARG:NH1	1:B:1354:SER:HB3	2.33	0.44
1:B:1096:ASN:O	1:B:1100:ILE:HG12	2.18	0.44
1:B:623:VAL:O	1:B:627:LEU:HB2	2.17	0.44
1:A:1067:SER:HA	1:A:1074:ALA:HA	1.99	0.44
2:X:11:VAL:HA	2:X:119:THR:O	2.18	0.44
2:X:151:VAL:HB	2:X:187:LEU:HG	1.99	0.44
1:B:1358:THR:HB	1:B:1360:HIS:HE1	1.83	0.44
1:B:1674:ASN:ND2	1:B:1674:ASN:O	2.50	0.44
3:L:1:ASP:CG	3:L:2:ILE:H	2.25	0.44
3:L:59:PRO:HG2	3:L:62:PHE:CE1	2.52	0.44
1:A:543:TYR:HA	1:A:555:VAL:O	2.18	0.43
1:A:1650:ARG:C	1:A:1652:THR:H	2.25	0.43
1:B:1037:ASP:OD2	1:B:1040:ILE:HG13	2.18	0.43
3:L:4:MET:SD	3:L:4:MET:N	2.91	0.43
1:B:1639:LEU:HD12	1:B:1639:LEU:HA	1.90	0.43
1:A:765:ILE:HG13	1:A:767:SER:H	1.82	0.43
1:A:1034:PHE:CE1	1:A:1041:GLU:HG2	2.54	0.43
1:B:986:GLU:OE2	1:B:1280:TYR:O	2.36	0.43
1:A:270:GLY:HA2	1:A:283:MET:HG3	2.01	0.43
1:A:1251:THR:HG21	1:A:1273:TRP:CZ3	2.54	0.43
1:A:619:PRO:O	1:A:623:VAL:HB	2.18	0.43
1:B:503:ILE:HG12	1:B:540:LEU:HD12	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:956:ARG:HA	1:B:1348:VAL:O	2.19	0.43
1:B:1438:ASP:OD2	1:B:1478:ARG:HG3	2.19	0.43
1:A:857:VAL:HA	1:A:913:SER:O	2.19	0.43
1:A:1623:GLU:HB2	1:A:1638:PRO:HG2	2.01	0.43
1:A:424:LEU:HD11	1:A:431:LEU:HD22	2.01	0.43
1:A:963:ILE:HD12	1:A:1626:GLN:O	2.19	0.43
3:Y:18:ARG:HG3	3:Y:76:SER:HA	2.01	0.43
1:B:1008:ALA:HB3	1:B:1078:LEU:HD11	2.01	0.43
2:H:19:LYS:HG2	2:H:82:GLU:HG2	1.99	0.43
2:H:47:TRP:HB2	3:L:98:PHE:CD2	2.54	0.43
3:L:38:GLN:O	3:L:84:ALA:HB1	2.19	0.43
1:A:864:GLY:O	1:A:903:LEU:HB2	2.19	0.43
1:A:986:GLU:OE2	1:A:1280:TYR:O	2.36	0.43
2:X:51:ILE:HG13	2:X:58:THR:HG22	2.01	0.43
1:B:1090:ASN:HA	1:B:1093:VAL:O	2.19	0.43
1:B:1500:ARG:HB2	1:B:1502:ASP:OD1	2.18	0.43
1:A:1133:LEU:HB2	1:A:1134:PRO:HD3	2.01	0.43
1:A:1386:ILE:HG13	1:A:1387:GLU:H	1.84	0.43
1:B:162:THR:HG22	1:B:173:MET:HB2	2.00	0.43
1:B:730:GLU:O	1:B:734:VAL:HG23	2.18	0.43
3:L:18:ARG:HG3	3:L:76:SER:HA	2.01	0.43
3:L:192:TYR:O	3:L:208:SER:HA	2.18	0.43
3:Y:139:PHE:HB2	3:Y:198:HIS:NE2	2.33	0.43
3:L:89:GLN:HG2	3:L:90:ASN:N	2.34	0.42
2:X:106:ASN:O	2:X:107:TRP:HD1	2.01	0.42
2:H:52:LEU:HD13	2:H:55:SER:HB2	2.01	0.42
2:X:172:VAL:HG22	2:X:191:VAL:HG23	2.01	0.42
1:B:414:ASP:OD1	1:B:414:ASP:N	2.52	0.42
1:B:980:LYS:HD3	1:B:1333:PHE:O	2.19	0.42
1:B:1525:CYS:HB2	1:B:1526:LYS:HD2	2.01	0.42
1:A:545:ILE:HG12	1:A:554:LEU:HD23	2.00	0.42
1:A:1405:CYS:HA	1:A:1473:LEU:O	2.19	0.42
2:X:11:VAL:HB	2:X:121:SER:HB2	2.01	0.42
1:B:357:VAL:O	1:B:359:THR:HG22	2.20	0.42
1:B:386:VAL:H	1:B:411:THR:HG23	1.84	0.42
1:B:387:PRO:HA	1:B:410:VAL:HG22	2.01	0.42
1:B:1110:ASN:HB3	1:B:1111:TYR:CD2	2.55	0.42
1:A:265:VAL:HG13	1:A:329:VAL:HG22	2.00	0.42
1:A:364:LYS:HG3	1:A:466:TYR:HB2	2.01	0.42
1:A:496:ILE:O	1:A:517:LYS:HD2	2.19	0.42
3:Y:38:GLN:O	3:Y:84:ALA:HB1	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:160:VAL:HG22	1:B:175:GLU:HB3	2.00	0.42
1:B:424:LEU:HD13	1:B:428:VAL:HG21	2.00	0.42
1:B:1290:THR:O	1:B:1294:ILE:HG12	2.20	0.42
1:A:165:ASP:OD1	1:A:169:SER:N	2.44	0.42
1:A:1110:ASN:HB3	1:A:1111:TYR:CD2	2.55	0.42
1:B:1622:LYS:HZ1	1:B:1642:LEU:HD12	1.84	0.42
3:L:21:ILE:O	3:L:73:LEU:HB3	2.20	0.42
1:A:835:ARG:HE	1:A:905:ILE:HD11	1.84	0.42
1:A:1175:LEU:HB2	1:A:1195:LEU:HD21	2.00	0.42
2:X:218:LYS:HZ2	2:X:219:ARG:C	2.26	0.42
1:B:718:ILE:HG12	1:B:1446:VAL:HG12	2.01	0.42
2:H:172:VAL:HG22	2:H:191:VAL:HG23	2.02	0.42
1:A:868:SER:CB	1:A:1526:LYS:HB3	2.48	0.42
1:A:1559:TYR:CZ	1:A:1621:GLY:HA3	2.55	0.42
1:A:1567:SER:HB3	1:A:1578:LYS:HB2	2.02	0.42
2:X:128:PRO:HG3	2:X:209:HIS:HB2	2.02	0.42
3:Y:186:TYR:HE2	3:Y:211:ARG:HH22	1.67	0.42
1:B:92:LEU:HB3	1:B:93:PRO:HD2	2.01	0.42
1:B:254:TYR:O	1:B:255:PHE:HD1	2.02	0.42
1:B:557:ASP:OD1	1:B:558:SER:N	2.53	0.42
1:B:915:GLU:HG2	1:B:920:LYS:HG2	2.02	0.42
1:B:1562:LYS:NZ	1:B:1648:TRP:CZ2	2.85	0.42
1:A:623:VAL:O	1:A:627:LEU:HB2	2.20	0.42
1:A:967:LEU:HD13	1:A:1365:VAL:HG22	2.01	0.42
1:B:835:ARG:NH2	1:B:969:PRO:O	2.52	0.42
1:B:1629:TYR:CE2	1:B:1634:ARG:HB2	2.53	0.42
1:A:1090:ASN:HA	1:A:1093:VAL:O	2.20	0.42
2:X:131:PHE:HB3	3:Y:124:GLN:HB2	2.01	0.42
1:B:43:VAL:HG11	1:B:50:PHE:HZ	1.85	0.42
2:H:12:LYS:HD2	2:H:18:VAL:HA	2.02	0.42
1:B:250:ILE:CD1	1:B:265:VAL:HG11	2.49	0.41
1:B:396:ASP:HB3	1:B:400:GLU:H	1.85	0.41
1:B:937:GLU:HG2	1:B:1364:VAL:HG22	2.02	0.41
3:L:139:PHE:HB2	3:L:198:HIS:NE2	2.35	0.41
3:L:160:GLN:HE21	3:L:160:GLN:HB2	1.68	0.41
1:A:550:GLN:HG2	1:A:551:THR:N	2.35	0.41
2:X:61:THR:HG22	2:X:63:ASN:H	1.85	0.41
1:B:495:LYS:HA	1:B:495:LYS:HD3	1.75	0.41
3:L:139:PHE:HB2	3:L:198:HIS:CE1	2.55	0.41
1:A:29:LYS:HE3	1:A:30:ILE:HD11	2.01	0.41
1:A:569:ASN:ND2	1:A:805:SER:OG	2.38	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1176:LEU:HD23	1:A:1195:LEU:HD13	2.01	0.41
1:A:1581:LEU:HD21	1:A:1584:ILE:HG12	2.01	0.41
3:Y:63:SER:O	3:Y:73:LEU:HD12	2.20	0.41
1:B:60:PRO:HB2	1:A:1032:ASN:ND2	2.35	0.41
1:B:238:ILE:HG12	1:B:246:PHE:CE2	2.55	0.41
1:B:550:GLN:HG2	1:B:551:THR:N	2.35	0.41
1:A:718:ILE:HG12	1:A:1446:VAL:HG12	2.02	0.41
1:A:1219:LYS:HB2	1:A:1225:TYR:HB2	2.01	0.41
1:B:888:VAL:HG22	1:B:892:SER:HB2	2.01	0.41
3:L:22:THR:OG1	3:L:71:PHE:O	2.37	0.41
1:B:243:PHE:CE2	1:B:304:GLU:HB2	2.55	0.41
1:B:700:TYR:HB2	1:B:758:LEU:HD13	2.01	0.41
2:H:128:PRO:HD3	2:H:209:HIS:ND1	2.35	0.41
2:H:151:VAL:HB	2:H:187:LEU:HG	2.03	0.41
3:L:106:ILE:HG12	3:L:166:GLN:NE2	2.35	0.41
1:A:270:GLY:O	1:A:323:LEU:HD12	2.19	0.41
1:A:618:LYS:HE3	1:A:619:PRO:HD2	2.03	0.41
1:B:265:VAL:HG13	1:B:329:VAL:HG22	2.03	0.41
1:B:781:PRO:C	1:B:783:ARG:H	2.28	0.41
1:B:1387:GLU:H	1:B:1387:GLU:HG3	1.72	0.41
1:B:1537:GLU:HB2	1:B:1541:LEU:HD11	2.01	0.41
1:A:557:ASP:OD1	1:A:558:SER:N	2.53	0.41
2:X:33:TRP:CZ2	2:X:52:LEU:HD12	2.55	0.41
2:X:130:VAL:HG21	2:X:207:VAL:HG21	2.02	0.41
2:X:164:ASN:HB2	2:X:167:ALA:HB3	2.01	0.41
1:B:56:ILE:HD12	1:B:87:ILE:HG12	2.03	0.41
1:B:592:MET:HE2	1:B:602:LEU:HD11	2.02	0.41
1:A:868:SER:HB2	1:A:1526:LYS:CB	2.49	0.41
1:A:873:ILE:CG1	1:A:882:LYS:HE3	2.50	0.41
1:B:1594:LYS:HE3	1:B:1595:ASP:HB3	2.03	0.41
1:A:238:ILE:HG12	1:A:246:PHE:CE2	2.56	0.41
3:Y:86:TYR:HB2	3:Y:102:THR:HB	2.03	0.41
1:B:158:GLU:OE2	1:B:206:LYS:HD3	2.19	0.41
1:B:543:TYR:HA	1:B:555:VAL:O	2.21	0.41
1:B:765:ILE:HG13	1:B:767:SER:H	1.85	0.41
2:H:47:TRP:HD1	3:L:98:PHE:HE2	1.69	0.41
1:A:196:TYR:CZ	1:A:221:GLU:HB2	2.56	0.41
1:A:854:GLN:CD	1:A:854:GLN:H	2.29	0.41
1:A:1358:THR:HB	1:A:1360:HIS:HE1	1.85	0.41
1:B:545:ILE:HG12	1:B:554:LEU:HD23	2.03	0.41
1:B:978:SER:OG	1:B:986:GLU:OE1	2.33	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1331:LYS:HD3	1:B:1331:LYS:HA	1.88	0.41
2:H:33:TRP:CZ2	2:H:52:LEU:HD12	2.56	0.41
2:H:91:THR:HG21	2:H:120:VAL:HB	2.02	0.41
3:Y:6:GLN:NE2	3:Y:102:THR:OG1	2.54	0.41
3:Y:59:PRO:HG2	3:Y:62:PHE:HE1	1.86	0.41
1:B:1572:ASN:C	1:B:1574:PHE:H	2.28	0.40
1:B:1640:ASP:HB2	1:B:1643:THR:HG23	2.03	0.40
1:A:50:PHE:CZ	1:A:73:LEU:HD11	2.55	0.40
1:A:1139:GLU:CD	1:A:1183:GLN:HB3	2.46	0.40
1:A:882:LYS:NZ	2:X:28:ILE:HD13	2.37	0.40
1:A:1529:GLU:HB3	1:A:1532:CYS:SG	2.61	0.40
3:Y:62:PHE:CD2	3:Y:75:ILE:HD11	2.57	0.40
1:B:620:LEU:HD22	1:B:811:VAL:HG13	2.03	0.40
1:B:629:LYS:HD3	1:B:629:LYS:HA	1.92	0.40
1:B:847:ASN:O	1:B:891:SER:HA	2.22	0.40
1:B:1601:ILE:HG12	1:B:1638:PRO:HA	2.03	0.40
1:B:1654:CYS:SG	1:B:1657:CYS:N	2.95	0.40
2:H:131:PHE:HB3	3:L:124:GLN:HB2	2.02	0.40
3:L:61:ARG:HH11	3:L:79:GLN:CD	2.29	0.40
1:A:24:VAL:HA	1:A:655:THR:HG22	2.03	0.40
1:A:103:TYR:HD1	1:A:103:TYR:HA	1.78	0.40
1:A:284:GLN:N	1:A:310:LEU:HD13	2.36	0.40
1:A:641:ASN:O	1:A:645:VAL:HG23	2.22	0.40
1:A:906:GLY:N	1:A:929:VAL:HB	2.26	0.40
1:A:1251:THR:HG21	1:A:1273:TRP:HZ3	1.87	0.40
2:X:4:LEU:HD11	2:X:22:CYS:HB3	2.02	0.40
2:X:179:LEU:HD11	2:X:183:GLY:HA2	2.04	0.40
1:B:833:VAL:O	1:B:929:VAL:HA	2.21	0.40
1:B:1320:LYS:HB2	1:B:1344:ASP:OD2	2.22	0.40
1:B:1577:TYR:CZ	1:B:1611:LEU:HD12	2.56	0.40
1:A:166:PRO:HD3	1:A:199:TRP:CE2	2.56	0.40
1:A:968:VAL:HG22	1:A:1368:THR:HG22	2.04	0.40
1:A:1052:GLY:O	1:A:1055:SER:HB3	2.21	0.40
1:A:1284:PHE:HD1	1:A:1290:THR:HG23	1.87	0.40
1:A:1315:VAL:HG12	1:A:1324:HIS:O	2.21	0.40
1:B:1059:TYR:CE2	1:B:1070:LYS:HG2	2.57	0.40
1:A:357:VAL:O	1:A:372:LYS:HB2	2.22	0.40
1:A:937:GLU:HG2	1:A:1364:VAL:HG22	2.03	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	1624/1676 (97%)	1552 (96%)	70 (4%)	2 (0%)	48	82
1	B	1626/1676 (97%)	1553 (96%)	71 (4%)	2 (0%)	48	82
2	H	219/230 (95%)	207 (94%)	12 (6%)	0	100	100
2	X	219/230 (95%)	208 (95%)	11 (5%)	0	100	100
3	L	211/214 (99%)	197 (93%)	14 (7%)	0	100	100
3	Y	211/214 (99%)	196 (93%)	15 (7%)	0	100	100
All	All	4110/4240 (97%)	3913 (95%)	193 (5%)	4 (0%)	48	82

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	1573	VAL
1	A	1573	VAL
1	B	1651	ASP
1	A	1651	ASP

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1450/1484 (98%)	1397 (96%)	53 (4%)	30	51
1	B	1450/1484 (98%)	1392 (96%)	58 (4%)	28	49
2	H	190/199 (96%)	184 (97%)	6 (3%)	34	56

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	X	190/199 (96%)	184 (97%)	6 (3%)	34	56
3	L	184/185 (100%)	178 (97%)	6 (3%)	33	55
3	Y	184/185 (100%)	180 (98%)	4 (2%)	45	64
All	All	3648/3736 (98%)	3515 (96%)	133 (4%)	31	52

All (133) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	22	THR
1	B	26	SER
1	B	81	ASN
1	B	99	VAL
1	B	103	TYR
1	B	117	MET
1	B	150	ASP
1	B	231	ILE
1	B	264	ASP
1	B	280	LYS
1	B	289	ASN
1	B	312	TYR
1	B	359	THR
1	B	411	THR
1	B	482	LEU
1	B	487	THR
1	B	494	ASP
1	B	502	LEU
1	B	530	VAL
1	B	540	LEU
1	B	553	GLU
1	B	571	LEU
1	B	576	SER
1	B	588	VAL
1	B	589	SER
1	B	661	ASP
1	B	690	TYR
1	B	695	VAL
1	B	724	CYS
1	B	746	ASP
1	B	760	VAL
1	B	799	ILE
1	B	845	VAL

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Mol	Chain	Res	Type
1	B	856	CYS
1	B	857	VAL
1	B	867	THR
1	B	932	GLU
1	B	954	SER
1	B	1041	GLU
1	B	1056	ILE
1	B	1058	SER
1	B	1068	VAL
1	B	1110	ASN
1	B	1127	ILE
1	B	1168	LEU
1	B	1185	THR
1	B	1291	ILE
1	B	1370	THR
1	B	1381	ILE
1	B	1414	GLU
1	B	1420	SER
1	B	1432	ILE
1	B	1454	GLN
1	B	1506	THR
1	B	1525	CYS
1	B	1528	VAL
1	B	1620	MET
1	B	1650	ARG
2	H	25	SER
2	H	45	LEU
2	H	205	CYS
2	H	216	VAL
2	H	218	LYS
2	H	220	VAL
3	L	2	ILE
3	L	33	LEU
3	L	81	GLU
3	L	88	CYS
3	L	94	THR
3	L	97	THR
1	A	22	THR
1	A	81	ASN
1	A	99	VAL
1	A	103	TYR
1	A	117	MET

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Mol	Chain	Res	Type
1	A	180	ILE
1	A	208	ASP
1	A	231	ILE
1	A	264	ASP
1	A	280	LYS
1	A	289	ASN
1	A	312	TYR
1	A	348	VAL
1	A	359	THR
1	A	411	THR
1	A	441	ASP
1	A	482	LEU
1	A	494	ASP
1	A	502	LEU
1	A	530	VAL
1	A	535	VAL
1	A	540	LEU
1	A	553	GLU
1	A	571	LEU
1	A	576	SER
1	A	589	SER
1	A	661	ASP
1	A	690	TYR
1	A	695	VAL
1	A	724	CYS
1	A	746	ASP
1	A	760	VAL
1	A	799	ILE
1	A	845	VAL
1	A	856	CYS
1	A	857	VAL
1	A	867	THR
1	A	954	SER
1	A	1041	GLU
1	A	1056	ILE
1	A	1058	SER
1	A	1068	VAL
1	A	1110	ASN
1	A	1127	ILE
1	A	1168	LEU
1	A	1185	THR
1	A	1204	GLN

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Mol	Chain	Res	Type
1	A	1291	ILE
1	A	1414	GLU
1	A	1420	SER
1	A	1454	GLN
1	A	1506	THR
1	A	1650	ARG
2	X	25	SER
2	X	45	LEU
2	X	205	CYS
2	X	216	VAL
2	X	218	LYS
2	X	220	VAL
3	Y	33	LEU
3	Y	81	GLU
3	Y	88	CYS
3	Y	94	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	81	ASN
1	B	97	ASN
1	B	500	ASN
1	B	569	ASN
1	B	647	HIS
1	B	656	ASN
1	B	800	GLN
1	B	838	GLN
1	B	840	GLN
1	B	1454	GLN
1	B	1536	GLN
1	B	1616	GLN
2	H	35	GLN
2	H	180	GLN
3	L	38	GLN
1	A	38	ASN
1	A	391	ASN
1	A	472	ASN
1	A	500	ASN
1	A	665	ASN
1	A	875	HIS
1	A	1435	ASN

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Mol	Chain	Res	Type
2	X	6	GLN
2	X	35	GLN
3	Y	38	GLN
3	Y	210	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

6 monosaccharides 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	C	1	4,1	14,14,15	0.58	0	17,19,21	0.44	0
4	NAG	C	2	4	14,14,15	0.70	1 (7%)	17,19,21	1.33	2 (11%)
4	BMA	C	3	4	11,11,12	0.60	0	15,15,17	0.67	0
4	NAG	D	1	4,1	14,14,15	0.68	0	17,19,21	0.49	0
4	NAG	D	2	4	14,14,15	0.59	0	17,19,21	1.42	2 (11%)
4	BMA	D	3	4	11,11,12	0.53	0	15,15,17	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
4	NAG	C	1	4,1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	C	2	4	-	6/6/23/26	0/1/1/1
4	BMA	C	3	4	-	0/2/19/22	0/1/1/1
4	NAG	D	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	D	2	4	-	6/6/23/26	0/1/1/1
4	BMA	D	3	4	-	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)
4	C	2	NAG	C1-C2	2.40	1.55	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	2	NAG	C2-N2-C7	4.58	129.04	122.90
4	C	2	NAG	C2-N2-C7	4.54	128.99	122.90
4	D	2	NAG	C1-C2-N2	2.37	114.17	110.43
4	C	2	NAG	C1-C2-N2	2.04	113.65	110.43

There are no chirality outliers.

All (16) torsion outliers are listed below:

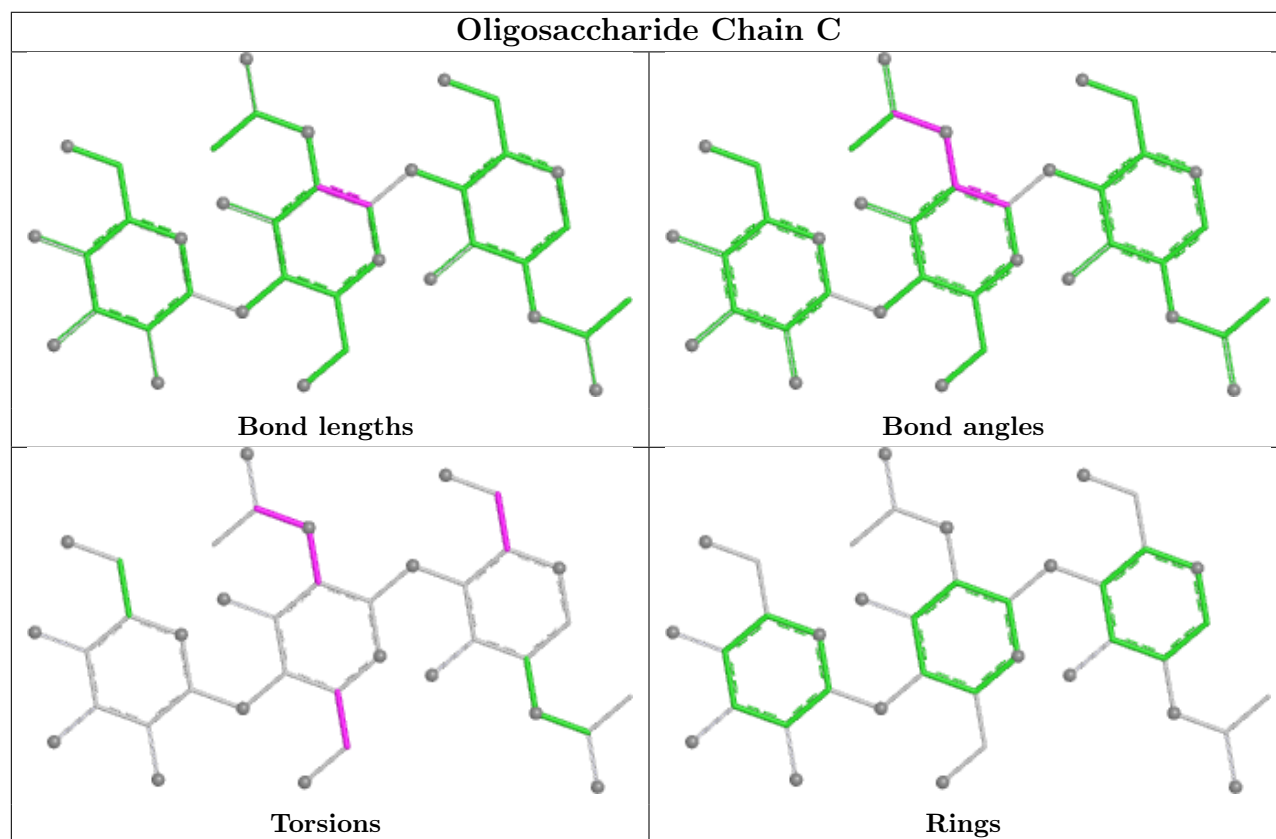
Mol	Chain	Res	Type	Atoms
4	D	2	NAG	O5-C5-C6-O6
4	D	2	NAG	C4-C5-C6-O6
4	C	2	NAG	C8-C7-N2-C2
4	C	2	NAG	O7-C7-N2-C2
4	D	2	NAG	C8-C7-N2-C2
4	D	2	NAG	O7-C7-N2-C2
4	C	2	NAG	O5-C5-C6-O6
4	D	1	NAG	O5-C5-C6-O6
4	C	1	NAG	O5-C5-C6-O6
4	C	2	NAG	C4-C5-C6-O6
4	D	1	NAG	C4-C5-C6-O6
4	C	1	NAG	C4-C5-C6-O6
4	C	2	NAG	C1-C2-N2-C7
4	D	2	NAG	C1-C2-N2-C7
4	C	2	NAG	C3-C2-N2-C7
4	D	2	NAG	C3-C2-N2-C7

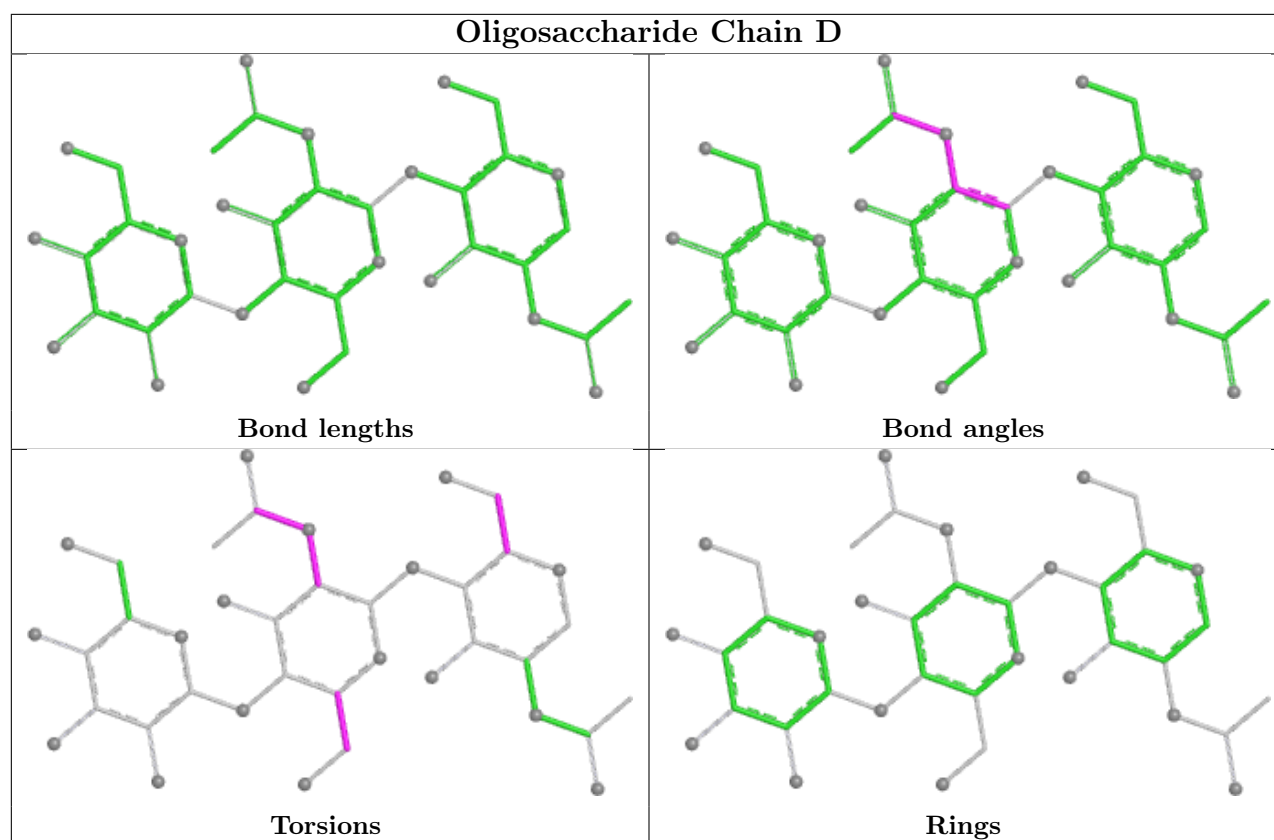
There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	2	NAG	1	0
4	D	2	NAG	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.





5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	1632/1676 (97%)	0.24	60 (3%) 45 36	120, 256, 409, 564	0
1	B	1634/1676 (97%)	0.04	17 (1%) 79 63	122, 185, 271, 483	0
2	H	221/230 (96%)	0.17	8 (3%) 46 37	177, 262, 403, 459	0
2	X	221/230 (96%)	0.10	3 (1%) 73 57	207, 297, 454, 565	0
3	L	213/214 (99%)	0.21	5 (2%) 61 47	181, 289, 424, 499	0
3	Y	213/214 (99%)	0.42	13 (6%) 27 27	183, 315, 423, 494	0
All	All	4134/4240 (97%)	0.16	106 (2%) 57 43	120, 225, 399, 565	0

All (106) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	529	PRO	4.5
1	A	1071	GLY	4.3
1	B	1002	HIS	4.0
1	A	530	VAL	3.9
1	A	1306	GLN	3.9
1	A	1632	SER	3.7
1	A	1525	CYS	3.7
1	A	1005	LYS	3.4
1	A	531	THR	3.3
1	A	52	ALA	3.3
1	A	658	ASN	3.3
1	A	1629	TYR	3.3
3	L	36	TYR	3.2
1	A	63	LYS	3.1
1	A	999	ILE	3.1
1	B	999	ILE	3.1
1	A	654	LEU	3.1
3	Y	85	THR	3.1
1	A	465	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
2	H	89	GLU	3.0
1	A	267	ILE	3.0
3	Y	157	GLY	3.0
1	B	309	GLU	3.0
1	B	659	ALA	3.0
1	A	788	PHE	3.0
1	A	1002	HIS	2.9
1	B	308	LYS	2.9
3	Y	36	TYR	2.8
1	B	1241	ASN	2.8
1	A	1397	SER	2.8
1	A	509	ILE	2.7
1	A	549	GLU	2.7
3	Y	103	LYS	2.6
1	A	1240	PRO	2.6
2	H	221	GLU	2.6
1	A	512	PHE	2.6
2	H	137	SER	2.6
1	A	977	LEU	2.6
3	Y	122	ASP	2.5
1	A	265	VAL	2.5
1	B	751	ARG	2.5
1	A	1627	ILE	2.5
2	H	40	ALA	2.5
1	A	76	GLU	2.4
1	B	1397	SER	2.4
1	B	841	LEU	2.4
1	A	47	THR	2.4
1	A	1514	ILE	2.4
1	A	481	HIS	2.4
1	B	998	ASN	2.4
1	B	813	ASP	2.3
1	A	532	GLN	2.3
3	Y	161	GLU	2.3
1	B	540	LEU	2.3
1	A	869	GLU	2.3
3	Y	146	VAL	2.3
1	A	480	GLU	2.3
3	Y	37	GLN	2.3
1	A	1029	ASN	2.3
1	B	1230	ASP	2.3
3	Y	185	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	1061	ASN	2.2
1	B	761	SER	2.2
1	A	927	LEU	2.2
1	A	1571	GLU	2.2
1	A	1630	ASN	2.2
2	H	138	LYS	2.2
3	Y	188	LYS	2.2
1	A	1241	ASN	2.2
1	A	479	GLY	2.2
1	A	1371	SER	2.2
1	A	1018	VAL	2.2
1	A	1387	GLU	2.2
1	A	75	SER	2.2
2	X	42	GLY	2.1
1	A	467	ILE	2.1
1	A	1305	LYS	2.1
1	A	1516	ILE	2.1
1	A	870	SER	2.1
1	A	664	GLU	2.1
2	X	46	GLU	2.1
2	H	41	PRO	2.1
1	B	592	MET	2.1
1	A	540	LEU	2.1
1	A	1378	TYR	2.1
3	L	135	LEU	2.1
3	Y	202	SER	2.1
1	B	1240	PRO	2.1
3	L	205	VAL	2.1
3	L	193	ALA	2.1
2	H	181	SER	2.1
1	A	597	ASP	2.1
3	Y	129	THR	2.1
1	A	902	PRO	2.1
2	H	103	SER	2.1
2	X	129	SER	2.1
1	A	1528	VAL	2.1
1	A	244	LYS	2.0
1	B	683	ILE	2.0
1	A	151	ASP	2.0
3	L	57	GLY	2.0
1	A	397	VAL	2.0
1	A	497	THR	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	1094	GLU	2.0
3	Y	143	GLU	2.0
1	A	1022	PHE	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](#)

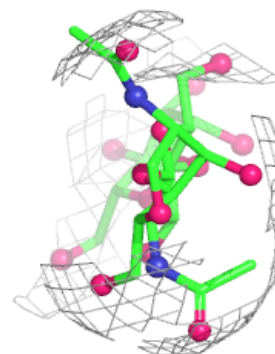
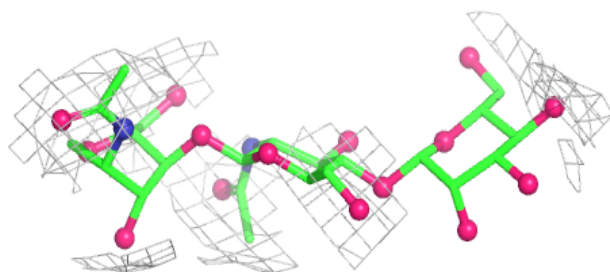
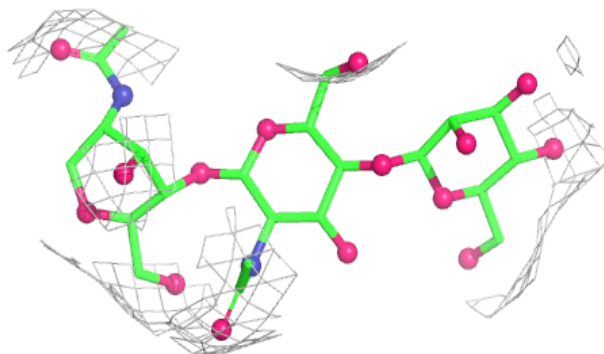
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	NAG	C	1	14/15	-	-	149,202,253,254	0
4	NAG	C	2	14/15	-	-	242,277,305,310	0
4	BMA	C	3	11/12	-	-	188,266,294,295	0
4	NAG	D	1	14/15	-	-	167,236,272,278	0
4	NAG	D	2	14/15	-	-	220,281,316,337	0
4	BMA	D	3	11/12	-	-	302,324,338,340	0

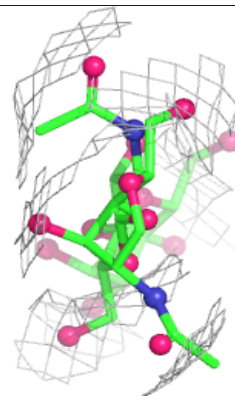
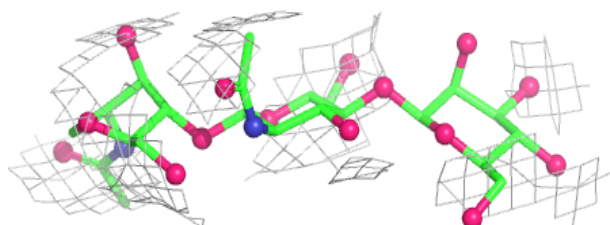
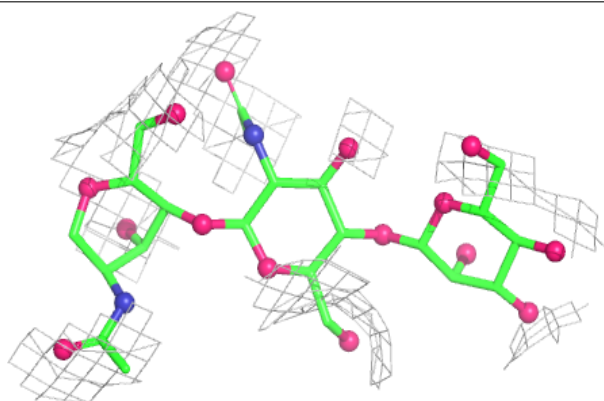
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain C:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around Chain D:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.