



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 6, 2020 – 01:42 PM BST

PDB ID : 6EA5
Title : Structure of BDBV GPcl in complex with the pan-ebolavirus mAb ADI-15878
Authors : King, L.B.; West, B.R.; Moyer, C.L.; Fusco, M.L.; Milligan, J.C.; Hui, S.; Saphire, E.O.
Deposited on : 2018-08-02
Resolution : 4.75 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

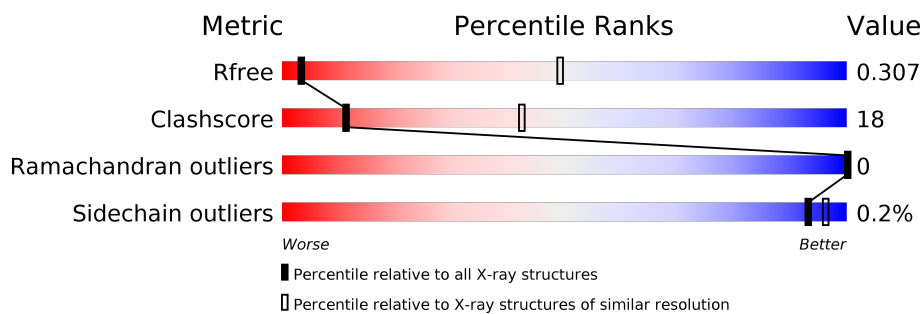
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.75 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}	130704	1089 (5.70-3.80)
Clashscore	141614	1163 (5.70-3.80)
Ramachandran outliers	138981	1098 (5.70-3.80)
Sidechain outliers	138945	1078 (5.70-3.80)

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 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	162	70% 30%
1	C	162	59% 38% .
1	E	162	61% 35% .
2	B	111	44% 50% 6%
2	D	111	59% 35% 6%
2	F	111	63% 30% 7%
3	H	233	66% 25% 9%

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Mol	Chain	Length	Quality of chain
3	M	233	
3	Q	233	
4	L	213	
4	N	213	
4	R	213	
5	G	6	
6	I	5	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	NAG	G	1	-	-	X	-
6	BMA	I	3	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 15944 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 Envelope glycoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	162	Total	C	N	O	S	0	0	0
			1251	798	213	235	5			
1	C	158	Total	C	N	O	S	0	0	0
			1208	767	207	229	5			
1	E	155	Total	C	N	O	S	0	0	0
			1187	755	204	223	5			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	64	ALA	LYS	conflict	UNP B8XCNO
C	64	ALA	LYS	conflict	UNP B8XCNO
E	64	ALA	LYS	conflict	UNP B8XCNO

- Molecule 2 is a protein called Glycoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	104	Total	C	N	O	S	0	0	0
			813	518	142	147	6			
2	D	104	Total	C	N	O	S	0	0	0
			813	518	142	147	6			
2	F	103	Total	C	N	O	S	0	0	0
			808	515	141	146	6			

- Molecule 3 is a protein called ADI-15878 Fab Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	213	Total	C	N	O	S	0	0	0
			1598	1016	269	307	6			
3	M	217	Total	C	N	O	S	0	0	0
			1625	1031	274	314	6			

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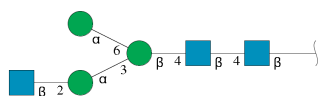
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	Q	222	Total	C	N	O	S	0	0	0
			1655	1047	280	322	6			

- Molecule 4 is a protein called ADI-15878 Fab Light Chain.

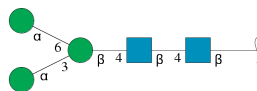
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	L	210	Total	C	N	O	S	0	0	0
			1597	999	261	333	4			
4	N	212	Total	C	N	O	S	0	0	0
			1617	1011	267	335	4			
4	R	211	Total	C	N	O	S	0	0	0
			1608	1006	266	332	4			

- Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]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
5	G	6	Total	C	N	O	0	0	0
			75	42	3	30			

- Molecule 6 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]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
6	I	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).

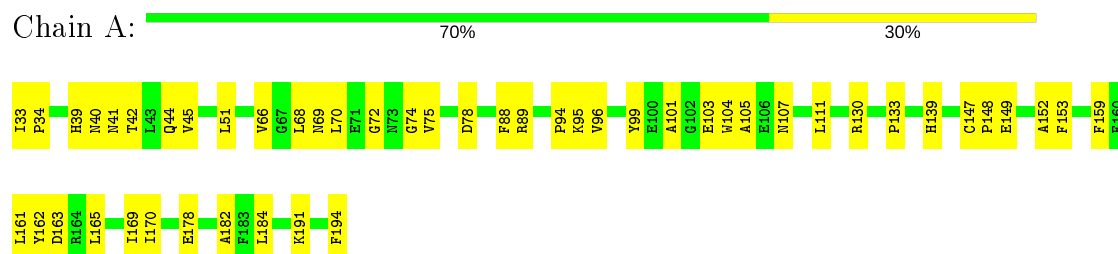


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	N	O	0	0
			14	8	1	5		
7	B	1	Total	C	N	O	0	0
			14	8	1	5		

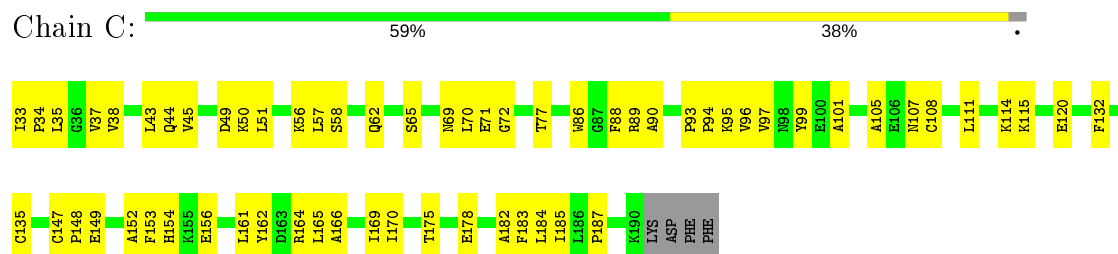
3 Residue-property plots

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. 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. 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.

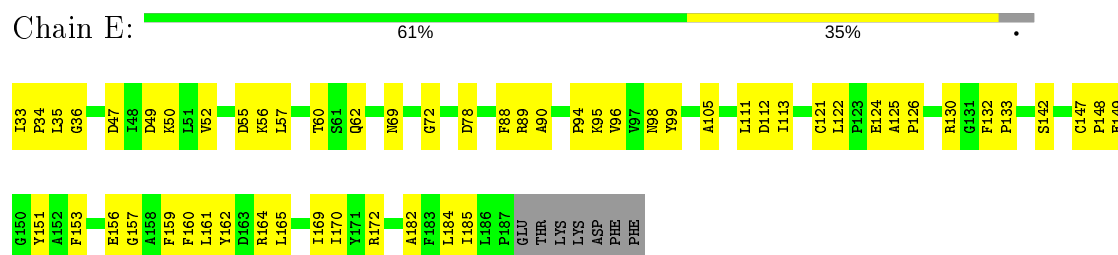
• Molecule 1: Envelope glycoprotein



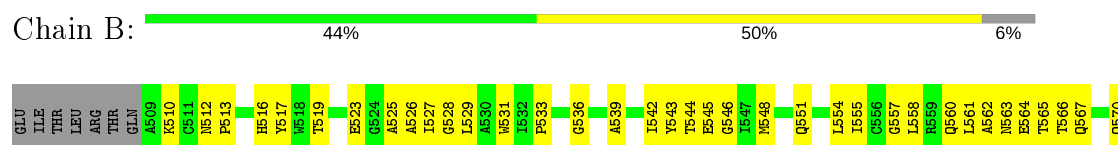
• Molecule 1: Envelope glycoprotein



• Molecule 1: Envelope glycoprotein



• Molecule 2: Glycoprotein





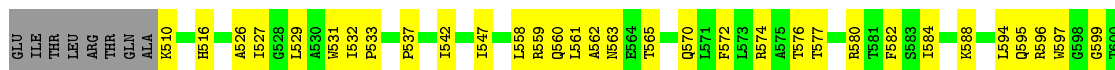
- Molecule 2: Glycoprotein

Chain D: 59% 35% 6%



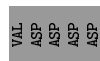
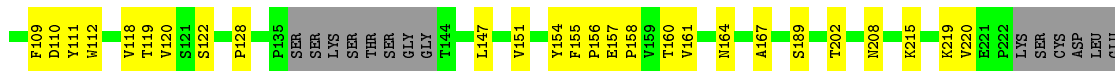
- Molecule 2: Glycoprotein

Chain F: 63% 30% 7%



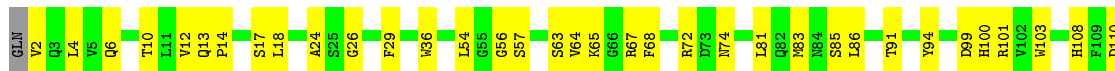
- Molecule 3: ADI-15878 Fab Heavy Chain

Chain H: 66% 25% 9%



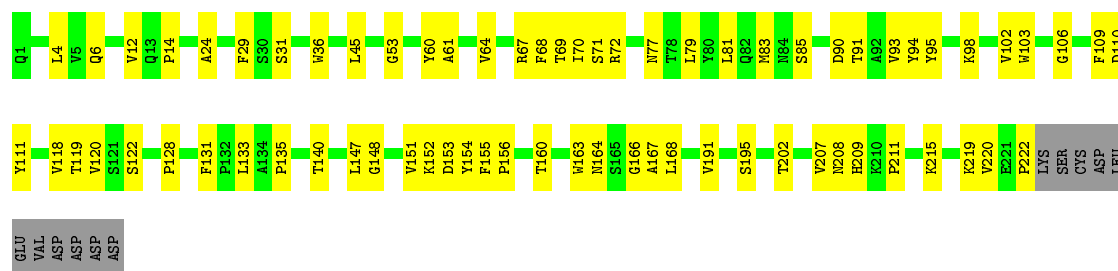
- Molecule 3: ADI-15878 Fab Heavy Chain

Chain M: 67% 26% 7%




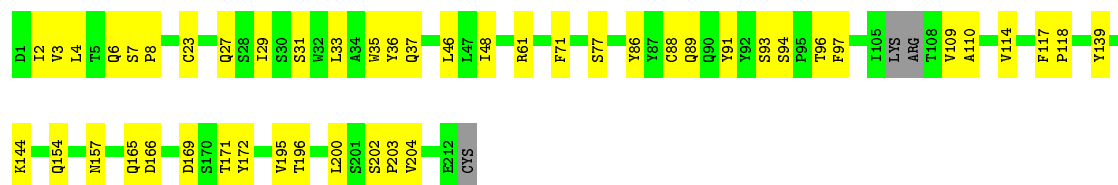
- Molecule 3: ADI-15878 Fab Heavy Chain

Chain Q: 



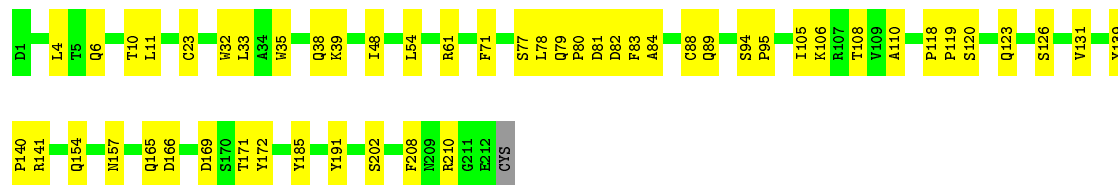
• Molecule 4: ADI-15878 Fab Light Chain

Chain L: 




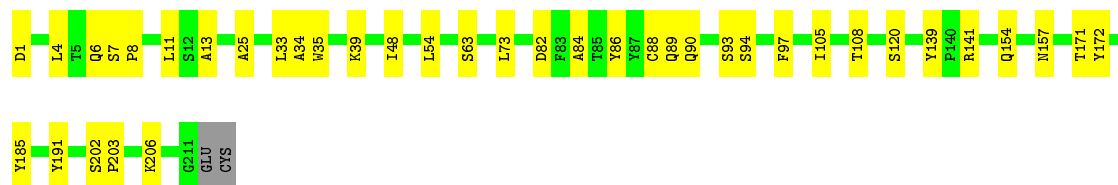
• Molecule 4: ADI-15878 Fab Light Chain

Chain N: 




• Molecule 4: ADI-15878 Fab Light Chain

Chain R: 



• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G: 



- Molecule 6: α -D-mannopyranose-(1-3)-[α -D-mannopyranose-(1-6)] β -D-mannopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose-(1-4)-2-acetamido-2-deoxy- β -D-glucopyranose

Chain I:



MAG1
MAG2
BOA3
MAN4
MAN5

4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	151.62Å 151.62Å 247.10Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	41.26 – 4.75 43.77 – 4.75	Depositor EDS
% Data completeness (in resolution range)	99.4 (41.26-4.75) 99.4 (43.77-4.75)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.21 (at 4.85Å)	Xtriage
Refinement program	PHENIX DEV_1539	Depositor
R, R_{free}	0.295 , 0.305 0.304 , 0.307	Depositor DCC
R_{free} test set	848 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	259.4	Xtriage
Anisotropy	0.392	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 161.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.075 for -h,-k,l	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	15944	wwPDB-VP
Average B, all atoms (Å ²)	203.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.35% 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 [i](#)

5.1 Standard geometry [i](#)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.40	0/1282	0.64	0/1741
1	C	0.38	0/1237	0.71	0/1683
1	E	0.37	0/1216	0.60	0/1654
2	B	0.36	0/833	0.65	0/1134
2	D	0.36	0/833	0.65	0/1134
2	F	0.38	0/828	0.63	0/1127
3	H	0.29	0/1639	0.52	0/2236
3	M	0.32	0/1666	0.52	0/2271
3	Q	0.30	0/1697	0.52	0/2314
4	L	0.31	0/1631	0.51	0/2218
4	N	0.31	0/1652	0.53	0/2246
4	R	0.30	0/1643	0.52	0/2234
All	All	0.33	0/16157	0.57	0/21992

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

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	1251	0	1223	55	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1208	0	1180	72	0
1	E	1187	0	1163	68	0
2	B	813	0	790	73	0
2	D	813	0	790	62	1
2	F	808	0	785	56	0
3	H	1598	0	1560	50	0
3	M	1625	0	1588	64	0
3	Q	1655	0	1618	56	0
4	L	1597	0	1537	35	0
4	N	1617	0	1564	57	0
4	R	1608	0	1558	29	1
5	G	75	0	64	11	0
6	I	61	0	52	11	0
7	A	14	0	13	6	0
7	B	14	0	13	4	0
All	All	15944	0	15498	560	1

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 18.

All (560) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:ASN:HB2	7:A:201:NAG:C8	1.57	1.32
1:E:57:LEU:HD12	1:E:62:GLN:NE2	1.50	1.26
2:F:563:ASN:HD21	5:G:1:NAG:C1	1.50	1.23
1:A:41:ASN:HB2	7:A:201:NAG:H81	1.23	1.11
3:M:12:VAL:HG12	3:M:13:GLN:H	1.16	1.09
3:M:12:VAL:HG12	3:M:13:GLN:N	1.69	1.05
3:H:12:VAL:HG12	3:H:13:GLN:H	1.21	1.04
3:M:12:VAL:CG1	3:M:13:GLN:H	1.70	1.04
1:A:41:ASN:HB2	7:A:201:NAG:H82	1.37	1.02
2:F:563:ASN:OD1	5:G:1:NAG:C7	2.11	0.99
3:H:12:VAL:HG12	3:H:13:GLN:N	1.76	0.95
1:E:124:GLU:HG3	1:E:172:ARG:NH1	1.81	0.94
1:E:57:LEU:HD12	1:E:62:GLN:HE21	1.05	0.94
3:H:12:VAL:CG1	3:H:13:GLN:H	1.81	0.92
1:C:77:THR:HB	1:C:107:ASN:HD22	1.32	0.92
2:F:563:ASN:ND2	5:G:1:NAG:C1	2.33	0.91
1:A:41:ASN:CB	7:A:201:NAG:H81	1.99	0.91
1:C:164:ARG:HB2	2:F:577:THR:HG21	1.52	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:563:ASN:OD1	5:G:1:NAG:H82	1.73	0.89
4:R:7:SER:OG	4:R:8:PRO:HD3	1.74	0.88
2:F:527:ILE:HG13	4:L:94:SER:H	1.39	0.87
2:D:531:TRP:CZ3	2:D:532:ILE:HG22	2.10	0.87
1:E:124:GLU:HG3	1:E:172:ARG:HH12	1.36	0.87
1:E:57:LEU:CD1	1:E:62:GLN:HE21	1.86	0.86
1:E:72:GLY:HA3	2:F:559:ARG:NH2	1.91	0.85
1:E:124:GLU:CG	1:E:172:ARG:HH12	1.88	0.85
1:C:94:PRO:HB3	1:C:169:ILE:HD12	1.59	0.85
2:F:563:ASN:OD1	5:G:1:NAG:C8	2.26	0.84
4:N:39:LYS:HE2	4:N:81:ASP:OD1	1.79	0.83
1:E:57:LEU:HA	1:E:62:GLN:HE22	1.43	0.82
2:B:592:PHE:CZ	2:B:596:ARG:NH1	2.49	0.81
3:Q:120:VAL:O	3:Q:120:VAL:HG12	1.79	0.81
1:E:47:ASP:HB3	1:E:50:LYS:HG2	1.63	0.80
3:H:128:PRO:HB3	3:H:154:TYR:HB3	1.62	0.80
2:B:551:GLN:HG2	2:B:554:LEU:HD12	1.64	0.80
1:C:72:GLY:HA3	2:D:559:ARG:NH2	1.97	0.80
1:A:34:PRO:HD2	2:B:565:THR:HG23	1.65	0.79
2:B:599:GLY:HA3	1:E:56:LYS:NZ	1.97	0.79
1:C:184:LEU:HD11	2:D:561:LEU:HD23	1.65	0.79
1:A:88:PHE:HB3	1:A:149:GLU:HB2	1.62	0.78
4:N:39:LYS:CE	4:N:81:ASP:OD1	2.31	0.78
1:E:94:PRO:HB3	1:E:169:ILE:HD12	1.65	0.78
1:E:184:LEU:HD11	2:F:558:LEU:HD13	1.63	0.78
1:E:50:LYS:O	2:F:595:GLN:NE2	2.16	0.78
1:E:72:GLY:HA3	2:F:559:ARG:HH22	1.44	0.78
4:N:33:LEU:HD22	4:N:71:PHE:CD2	2.16	0.78
2:D:531:TRP:HZ3	1:E:157:GLY:HA3	1.49	0.78
2:D:560:GLN:O	2:D:563:ASN:HB3	1.83	0.78
4:R:6:GLN:NE2	4:R:88:CYS:SG	2.57	0.78
2:B:557:GLY:O	2:B:560:GLN:HB2	1.83	0.77
1:E:124:GLU:CG	1:E:172:ARG:NH1	2.49	0.76
4:N:33:LEU:CD2	4:N:71:PHE:CG	2.69	0.75
1:A:41:ASN:CB	7:A:201:NAG:C8	2.52	0.75
1:C:43:LEU:HD12	1:C:43:LEU:O	1.85	0.75
3:H:10:THR:HB	3:H:18:LEU:HD21	1.66	0.75
3:Q:128:PRO:HB3	3:Q:154:TYR:HB3	1.69	0.75
2:D:532:ILE:HD11	2:D:535:PHE:HB2	1.69	0.75
1:C:164:ARG:HB2	2:F:577:THR:CG2	2.17	0.75
1:C:99:TYR:OH	1:C:162:TYR:O	2.04	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:113:ILE:HG23	1:E:121:CYS:HB2	1.69	0.74
4:N:154:GLN:HB3	4:N:157:ASN:HD21	1.52	0.74
4:N:108:THR:HB	4:N:139:TYR:CE2	2.22	0.74
1:A:42:THR:HG22	1:A:44:GLN:NE2	2.03	0.73
3:Q:53:GLY:O	3:Q:72:ARG:NH2	2.21	0.73
2:F:563:ASN:O	5:G:1:NAG:H82	1.89	0.73
4:L:110:ALA:H	4:L:139:TYR:HB2	1.54	0.72
1:A:51:LEU:HD21	2:B:596:ARG:HG2	1.71	0.72
3:H:61:ALA:HB3	3:H:64:VAL:HG22	1.70	0.72
2:B:592:PHE:CE1	2:B:596:ARG:NH1	2.58	0.71
1:C:58:SER:OG	1:C:62:GLN:NE2	2.23	0.71
3:Q:67:ARG:NH2	3:Q:90:ASP:OD2	2.23	0.71
1:C:88:PHE:HB3	1:C:149:GLU:HB2	1.72	0.71
3:H:12:VAL:HG12	3:H:13:GLN:O	1.91	0.70
2:D:521:GLN:NE2	2:D:524:GLY:HA3	2.06	0.70
1:C:77:THR:CB	1:C:107:ASN:HD22	2.04	0.70
4:N:33:LEU:HD23	4:N:71:PHE:CD1	2.26	0.70
1:A:184:LEU:HD21	2:B:558:LEU:HD13	1.74	0.70
1:A:39:HIS:HB3	1:A:42:THR:HB	1.72	0.70
2:F:527:ILE:HG13	4:L:94:SER:N	2.05	0.70
4:R:35:TRP:HB2	4:R:48:ILE:HG22	1.73	0.70
3:H:2:VAL:N	3:H:27:PHE:HB2	2.07	0.70
2:D:531:TRP:CH2	2:D:532:ILE:HG22	2.27	0.69
2:F:563:ASN:OD1	5:G:1:NAG:N2	2.25	0.69
4:L:144:LYS:HB3	4:L:196:THR:HB	1.73	0.69
4:L:89:GLN:OE1	4:L:97:PHE:CE1	2.46	0.69
3:M:101:ARG:NH1	6:I:3:BMA:C6	2.57	0.68
4:N:105:ILE:HG13	4:N:165:GLN:OE1	1.94	0.68
1:E:99:TYR:OH	1:E:162:TYR:O	2.12	0.68
2:F:529:LEU:HD22	4:L:91:TYR:CE1	2.29	0.68
3:Q:163:TRP:O	3:Q:166:GLY:N	2.26	0.67
1:E:122:LEU:HB2	1:E:172:ARG:HG3	1.76	0.67
2:B:599:GLY:HA3	1:E:56:LYS:HZ3	1.58	0.67
3:M:12:VAL:HG11	3:M:86:LEU:HD12	1.77	0.66
4:L:35:TRP:HB2	4:L:48:ILE:HG22	1.77	0.66
1:A:40:ASN:O	7:A:201:NAG:H82	1.96	0.66
4:L:4:LEU:C	4:L:4:LEU:HD12	2.16	0.66
3:M:72:ARG:NH1	3:M:74:ASN:OD1	2.29	0.66
2:F:529:LEU:HD11	3:H:106:GLY:HA2	1.78	0.65
3:H:102:VAL:HG11	3:H:106:GLY:HA3	1.77	0.65
1:C:51:LEU:HD22	2:D:595:GLN:HG3	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:90:ASP:O	3:Q:94:TYR:OH	2.14	0.65
2:D:532:ILE:CD1	2:D:535:PHE:HB2	2.27	0.65
2:D:531:TRP:CZ3	1:E:157:GLY:HA3	2.31	0.64
4:N:106:LYS:HB2	4:N:139:TYR:HB2	1.78	0.64
2:D:593:LEU:HD21	2:F:594:LEU:HD23	1.79	0.64
4:N:119:PRO:HD3	4:N:131:VAL:HG22	1.79	0.64
1:C:69:ASN:ND2	1:C:105:ALA:HB2	2.13	0.64
1:C:152:ALA:O	1:C:169:ILE:HA	1.97	0.64
1:E:147:CYS:N	1:E:148:PRO:HD3	2.12	0.64
2:D:554:LEU:HD23	2:D:554:LEU:C	2.17	0.64
2:B:533:PRO:HB2	1:C:153:PHE:CD2	2.33	0.63
3:M:135:PRO:HG3	3:M:147:LEU:HB3	1.80	0.63
1:C:43:LEU:HD21	2:D:557:GLY:HA3	1.80	0.63
1:E:52:VAL:O	2:F:596:ARG:NH2	2.30	0.63
4:R:108:THR:H	4:R:139:TYR:HE2	1.45	0.63
1:E:111:LEU:HD12	1:E:170:ILE:HG21	1.81	0.63
1:C:45:VAL:HG21	3:M:54:LEU:HG	1.80	0.63
1:C:71:GLU:OE2	1:C:107:ASN:N	2.21	0.63
3:M:36:TRP:CE2	3:M:81:LEU:HB2	2.34	0.63
3:H:10:THR:CB	3:H:18:LEU:HD21	2.29	0.62
3:H:83:MET:HB3	3:H:86:LEU:HD21	1.81	0.62
1:A:66:VAL:HG22	1:A:101:ALA:HB3	1.81	0.62
4:N:33:LEU:HD22	4:N:71:PHE:CG	2.32	0.62
1:A:45:VAL:HG21	3:H:56:GLY:CA	2.29	0.62
2:B:576:THR:HG21	2:B:581:THR:HG21	1.79	0.62
7:B:701:NAG:H83	2:F:531:TRP:HH2	1.62	0.62
2:F:563:ASN:CG	5:G:1:NAG:C7	2.66	0.62
3:Q:140:THR:O	3:Q:140:THR:HG23	1.99	0.62
2:D:537:PRO:HG2	2:D:542:ILE:HG22	1.82	0.61
3:M:144:THR:N	3:M:195:SER:HG	1.98	0.61
1:A:99:TYR:OH	1:A:162:TYR:O	2.12	0.61
1:A:99:TYR:CZ	1:A:161:LEU:HD22	2.37	0.60
2:B:536:GLY:O	1:C:89:ARG:NH2	2.31	0.60
1:A:40:ASN:OD1	1:A:40:ASN:O	2.20	0.60
3:H:147:LEU:HB2	3:H:220:VAL:HG11	1.84	0.60
1:A:182:ALA:HB2	2:B:562:ALA:HB2	1.83	0.60
4:L:4:LEU:O	4:L:4:LEU:HD12	2.02	0.60
4:N:105:ILE:HG13	4:N:105:ILE:O	2.01	0.60
2:F:558:LEU:O	2:F:558:LEU:HD12	2.01	0.60
3:M:101:ARG:HH12	6:I:3:BMA:H62	1.68	0.59
1:E:55:ASP:OD1	2:F:596:ARG:NH2	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:4:LEU:HA	4:R:25:ALA:HA	1.85	0.59
1:A:103:GLU:HA	2:B:517:TYR:HA	1.84	0.59
2:B:563:ASN:HD21	7:B:701:NAG:C1	2.14	0.59
3:Q:120:VAL:O	3:Q:120:VAL:CG1	2.50	0.59
2:D:532:ILE:HD12	2:D:535:PHE:HD2	1.67	0.58
2:D:561:LEU:HD13	3:M:54:LEU:HD23	1.85	0.58
1:C:97:VAL:HG23	2:D:584:ILE:HD12	1.84	0.58
3:M:125:THR:HG22	3:M:156:PRO:HD3	1.86	0.58
3:M:101:ARG:NH1	6:I:3:BMA:H62	2.19	0.58
4:N:35:TRP:HB2	4:N:48:ILE:HG22	1.85	0.57
3:M:103:TRP:HB3	6:I:1:NAG:H62	1.86	0.57
1:A:107:ASN:OD1	1:A:139:HIS:NE2	2.36	0.57
4:N:106:LYS:HD2	4:N:141:ARG:H	1.68	0.57
1:C:69:ASN:HD22	1:C:105:ALA:HB2	1.69	0.57
2:F:576:THR:O	2:F:576:THR:HG23	2.05	0.57
1:A:130:ARG:NH2	2:D:577:THR:OG1	2.38	0.57
1:E:57:LEU:HD12	1:E:62:GLN:HE22	1.61	0.57
1:E:89:ARG:HB3	1:E:153:PHE:CD1	2.39	0.57
3:H:102:VAL:HB	3:H:106:GLY:H	1.70	0.57
2:B:551:GLN:HG2	2:B:554:LEU:CD1	2.34	0.56
2:F:516:HIS:HA	2:F:547:ILE:HG22	1.87	0.56
3:M:135:PRO:HD2	3:M:222:PRO:HB3	1.87	0.56
2:B:528:GLY:O	2:B:531:TRP:NE1	2.38	0.56
2:B:539:ALA:HB2	1:C:93:PRO:HD3	1.87	0.56
2:B:548:MET:HG3	2:B:555:ILE:HD11	1.88	0.56
4:R:1:ASP:HB2	4:R:94:SER:CB	2.35	0.56
1:C:154:HIS:CD2	1:C:156:GLU:HB2	2.41	0.56
1:C:51:LEU:HD11	2:D:596:ARG:CZ	2.35	0.56
2:D:532:ILE:O	2:D:532:ILE:HG13	2.06	0.56
1:E:88:PHE:HB3	1:E:149:GLU:HB2	1.88	0.56
1:E:96:VAL:HB	2:F:580:ARG:HG2	1.87	0.56
4:N:105:ILE:CG1	4:N:165:GLN:OE1	2.53	0.56
1:A:152:ALA:O	1:A:169:ILE:HA	2.06	0.56
3:Q:168:LEU:HD21	3:Q:191:VAL:HG21	1.88	0.56
1:C:115:LYS:HD3	1:C:147:CYS:H	1.70	0.55
2:B:582:PHE:CE2	2:D:578:GLU:HG2	2.40	0.55
1:E:57:LEU:HA	1:E:62:GLN:NE2	2.17	0.55
4:R:1:ASP:HB2	4:R:94:SER:HB2	1.89	0.55
1:C:162:TYR:HB2	1:C:165:LEU:O	2.05	0.55
4:L:29:ILE:HD11	4:L:33:LEU:HD12	1.88	0.55
3:Q:147:LEU:HB2	3:Q:220:VAL:HG11	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:164:ASN:CB	3:Q:167:ALA:HB3	2.36	0.55
1:A:42:THR:CG2	1:A:44:GLN:NE2	2.70	0.55
4:N:106:LYS:HA	4:N:139:TYR:CD2	2.42	0.55
2:B:599:GLY:HA3	1:E:56:LYS:HZ2	1.72	0.55
1:E:159:PHE:CZ	2:F:570:GLN:NE2	2.75	0.54
3:M:91:THR:HG23	3:M:119:THR:HA	1.90	0.54
2:D:521:GLN:NE2	2:D:524:GLY:CA	2.69	0.54
2:D:531:TRP:CH2	2:D:532:ILE:CG2	2.90	0.54
1:A:70:LEU:HD21	1:A:75:VAL:HG11	1.88	0.54
2:F:560:GLN:O	2:F:563:ASN:HB3	2.08	0.54
3:M:110:ASP:OD1	3:M:111:TYR:N	2.40	0.54
1:E:36:GLY:HA3	2:F:561:LEU:HD21	1.89	0.54
4:R:33:LEU:HD22	4:R:89:GLN:O	2.08	0.54
3:M:36:TRP:CZ2	3:M:81:LEU:HB2	2.43	0.54
1:A:111:LEU:HD12	1:A:170:ILE:HG21	1.90	0.54
2:D:521:GLN:HB3	2:D:524:GLY:HA3	1.90	0.53
3:H:110:ASP:OD1	3:H:111:TYR:N	2.40	0.53
3:M:2:VAL:HG13	3:M:2:VAL:O	2.08	0.53
3:Q:94:TYR:HE2	3:Q:118:VAL:HB	1.73	0.53
2:B:599:GLY:O	2:B:600:THR:C	2.46	0.53
3:M:198:LEU:HD21	3:M:222:PRO:HG3	1.90	0.53
3:M:6:GLN:HB3	3:M:116:ALA:HB2	1.89	0.53
4:R:154:GLN:HB3	4:R:157:ASN:HD21	1.74	0.53
1:A:45:VAL:HG21	3:H:56:GLY:HA3	1.90	0.53
4:N:202:SER:HB3	4:R:11:LEU:HD13	1.91	0.53
2:B:531:TRP:CD1	2:D:567:GLN:HG3	2.44	0.53
3:M:4:LEU:CD2	3:M:24:ALA:HA	2.39	0.53
1:E:112:ASP:O	1:E:142:SER:HA	2.08	0.53
4:N:48:ILE:HG13	4:N:54:LEU:HD23	1.91	0.53
1:A:94:PRO:HB3	1:A:169:ILE:HD13	1.90	0.52
1:A:130:ARG:HH11	1:C:93:PRO:CB	2.21	0.52
1:A:95:LYS:NZ	2:B:574:ARG:HA	2.24	0.52
3:H:30:SER:HB3	3:H:74:ASN:HB3	1.90	0.52
1:C:96:VAL:HB	2:D:580:ARG:HA	1.91	0.52
3:Q:6:GLN:HA	3:Q:6:GLN:OE1	2.08	0.52
1:A:159:PHE:CE2	2:B:566:THR:HG23	2.43	0.52
2:B:531:TRP:HE3	2:D:570:GLN:HG3	1.74	0.52
1:A:78:ASP:N	1:A:78:ASP:OD1	2.43	0.52
2:D:597:TRP:CE2	2:F:597:TRP:HB3	2.44	0.52
1:C:77:THR:CB	1:C:107:ASN:ND2	2.73	0.52
3:H:95:TYR:HB3	3:H:112:TRP:HE3	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:36:TYR:CZ	4:L:46:LEU:HD23	2.45	0.52
3:M:202:THR:HB	3:M:219:LYS:HE3	1.90	0.52
1:E:151:TYR:CG	1:E:169:ILE:HD13	2.45	0.52
4:R:1:ASP:HB2	4:R:94:SER:OG	2.09	0.52
3:H:160:THR:OG1	3:H:208:ASN:HB3	2.10	0.52
2:D:521:GLN:NE2	2:D:524:GLY:C	2.64	0.51
2:D:531:TRP:CH2	1:E:156:GLU:O	2.63	0.51
4:N:185:TYR:HA	4:N:191:TYR:OH	2.10	0.51
4:R:185:TYR:HA	4:R:191:TYR:OH	2.10	0.51
3:Q:164:ASN:HB2	3:Q:167:ALA:HB3	1.92	0.51
3:Q:93:VAL:HG11	3:Q:95:TYR:OH	2.09	0.51
1:A:72:GLY:O	2:B:512:ASN:HB2	2.10	0.51
3:H:12:VAL:CG1	3:H:16:GLY:HA3	2.39	0.51
3:H:35:SER:HB3	3:H:109:PHE:CZ	2.46	0.51
3:Q:12:VAL:HG23	3:Q:120:VAL:HA	1.92	0.51
2:B:563:ASN:ND2	7:B:701:NAG:C1	2.73	0.51
1:E:113:ILE:HG12	1:E:121:CYS:SG	2.50	0.51
4:N:108:THR:HB	4:N:139:TYR:CZ	2.45	0.51
1:A:104:TRP:N	2:B:516:HIS:O	2.37	0.51
3:M:64:VAL:HB	3:M:68:PHE:CD2	2.46	0.51
4:N:165:GLN:HB2	4:N:172:TYR:CZ	2.46	0.51
2:F:510:LYS:HE3	5:G:2:NAG:H82	1.92	0.51
4:N:39:LYS:HE3	4:N:81:ASP:OD1	2.08	0.51
4:L:169:ASP:OD2	4:L:171:THR:OG1	2.21	0.51
4:R:82:ASP:O	4:R:86:TYR:OH	2.24	0.51
1:C:95:LYS:NZ	2:D:574:ARG:HA	2.26	0.51
3:M:14:PRO:HD3	3:M:122:SER:HB2	1.93	0.51
1:E:33:ILE:HB	2:F:588:LYS:CE	2.41	0.51
4:N:11:LEU:HD13	4:R:202:SER:HB3	1.93	0.50
2:D:515:LEU:CB	2:D:555:ILE:HD12	2.42	0.50
3:Q:110:ASP:OD1	3:Q:111:TYR:N	2.44	0.50
3:Q:93:VAL:CG1	3:Q:95:TYR:CZ	2.94	0.50
1:A:39:HIS:HB2	1:A:44:GLN:OE1	2.12	0.50
4:N:6:GLN:NE2	4:N:88:CYS:SG	2.85	0.50
4:L:31:SER:HA	4:L:71:PHE:HZ	1.76	0.50
4:L:6:GLN:NE2	4:L:88:CYS:SG	2.84	0.50
3:M:94:TYR:HE2	3:M:118:VAL:HB	1.76	0.50
2:B:544:THR:HG22	2:B:545:GLU:N	2.26	0.50
1:C:77:THR:HB	1:C:107:ASN:ND2	2.14	0.50
3:M:99:ASP:HA	3:M:108:HIS:O	2.12	0.50
1:E:182:ALA:HB2	2:F:562:ALA:HB2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:34:PRO:HG3	3:M:57:SER:OG	2.12	0.50
3:Q:202:THR:HB	3:Q:219:LYS:HE3	1.94	0.50
1:C:182:ALA:HB2	2:D:562:ALA:HA	1.94	0.49
3:M:12:VAL:CG1	3:M:13:GLN:N	2.34	0.49
2:B:603:ILE:HG12	2:B:610:ILE:HG21	1.94	0.49
2:D:528:GLY:O	2:D:529:LEU:HB3	2.12	0.49
2:B:594:LEU:HD22	1:E:57:LEU:HB3	1.93	0.49
4:L:3:VAL:HG23	4:L:96:THR:HG21	1.93	0.49
1:A:45:VAL:CG2	3:H:56:GLY:CA	2.90	0.49
4:N:38:GLN:O	4:N:84:ALA:HB1	2.12	0.49
2:B:593:LEU:HD21	2:D:594:LEU:HD23	1.94	0.49
1:C:97:VAL:HG13	1:C:166:ALA:HB3	1.95	0.49
3:M:10:THR:OG1	3:M:117:LEU:O	2.27	0.49
3:M:12:VAL:HG13	3:M:13:GLN:H	1.71	0.49
2:B:513:PRO:O	2:B:555:ILE:HG21	2.13	0.49
1:C:183:PHE:C	1:C:184:LEU:HD12	2.33	0.49
3:Q:93:VAL:HG12	3:Q:95:TYR:CZ	2.47	0.49
3:Q:207:VAL:O	3:Q:215:LYS:HA	2.13	0.49
3:H:10:THR:HB	3:H:18:LEU:CD2	2.39	0.49
4:L:109:VAL:HA	4:L:139:TYR:HB2	1.95	0.49
3:Q:12:VAL:CG2	3:Q:120:VAL:HG22	2.42	0.49
4:R:1:ASP:CB	4:R:94:SER:OG	2.61	0.49
1:C:38:VAL:O	1:C:187:PRO:HG3	2.13	0.48
1:E:160:PHE:CE2	1:E:170:ILE:HG12	2.48	0.48
4:N:139:TYR:CE1	4:N:171:THR:HG22	2.48	0.48
2:B:527:ILE:HG12	4:N:94:SER:N	2.28	0.48
1:A:184:LEU:HD21	2:B:558:LEU:CD1	2.42	0.48
2:B:529:LEU:HD21	4:N:32:TRP:CG	2.47	0.48
3:M:100:HIS:HB3	3:M:108:HIS:HB3	1.95	0.48
3:Q:156:PRO:HD2	3:Q:211:PRO:HG2	1.94	0.48
2:D:531:TRP:CZ3	2:D:532:ILE:CG2	2.91	0.48
4:L:165:GLN:HG2	4:L:172:TYR:CE2	2.49	0.48
1:A:162:TYR:HB2	1:A:165:LEU:O	2.14	0.48
1:C:33:ILE:HB	2:D:588:LYS:CE	2.43	0.48
3:M:67:ARG:HB2	3:M:85:SER:HB2	1.94	0.48
1:E:99:TYR:CZ	1:E:161:LEU:HD22	2.49	0.48
4:L:2:ILE:CG2	4:L:27:GLN:CD	2.82	0.48
3:M:83:MET:HB3	3:M:86:LEU:HD21	1.94	0.48
3:Q:91:THR:HG23	3:Q:119:THR:HA	1.94	0.48
3:H:64:VAL:HB	3:H:68:PHE:CD2	2.48	0.48
2:B:527:ILE:HG12	4:N:94:SER:HA	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:572:PHE:CE2	2:F:584:ILE:HG12	2.48	0.48
4:N:108:THR:O	4:N:139:TYR:CD2	2.66	0.48
3:Q:14:PRO:HD3	3:Q:122:SER:HB2	1.96	0.48
4:R:90:GLN:NE2	4:R:94:SER:O	2.47	0.48
4:N:10:THR:O	4:R:203:PRO:HD2	2.14	0.48
1:C:33:ILE:HB	2:D:588:LYS:HE3	1.95	0.48
3:Q:147:LEU:HD13	3:Q:220:VAL:HG21	1.94	0.48
6:I:3:BMA:H62	6:I:5:MAN:H2	1.49	0.47
1:C:99:TYR:HD2	1:C:101:ALA:O	1.97	0.47
3:Q:4:LEU:HD23	3:Q:24:ALA:HA	1.95	0.47
1:A:165:LEU:HG	2:D:577:THR:HG21	1.97	0.47
2:B:571:LEU:CD1	2:F:526:ALA:HB2	2.44	0.47
2:B:567:GLN:HA	2:F:531:TRP:CD2	2.49	0.47
2:B:560:GLN:HG2	3:H:103:TRP:CZ2	2.49	0.47
2:B:563:ASN:ND2	3:H:103:TRP:CZ3	2.82	0.47
1:A:130:ARG:HD3	1:A:163:ASP:OD2	2.14	0.47
3:Q:135:PRO:HG2	3:Q:222:PRO:HB3	1.95	0.47
2:B:551:GLN:HG2	2:B:554:LEU:CG	2.45	0.47
2:D:511:CYS:O	2:D:513:PRO:HD3	2.15	0.47
3:H:4:LEU:HA	3:H:23:ALA:O	2.15	0.47
1:E:98:ASN:HB3	2:F:582:PHE:CE2	2.50	0.47
3:H:40:ALA:HB3	3:H:43:LYS:HB2	1.96	0.47
2:D:531:TRP:CZ3	1:E:156:GLU:O	2.67	0.47
5:G:3:BMA:H62	5:G:6:MAN:H2	1.49	0.47
3:H:61:ALA:HB3	3:H:64:VAL:CG2	2.44	0.47
4:N:106:LYS:HD2	4:N:140:PRO:HA	1.97	0.47
3:Q:60:TYR:CZ	3:Q:70:ILE:HG22	2.49	0.47
1:E:89:ARG:HA	1:E:149:GLU:HG3	1.97	0.47
3:M:63:SER:O	3:M:67:ARG:NH1	2.47	0.47
4:L:200:LEU:HD13	4:L:204:VAL:HG23	1.97	0.46
3:M:131:PHE:HB3	4:N:120:SER:OG	2.15	0.46
4:N:118:PRO:HB3	4:N:208:PHE:CE2	2.51	0.46
4:N:78:LEU:HD12	4:N:82:ASP:OD2	2.15	0.46
1:C:51:LEU:HD21	2:D:596:ARG:HG2	1.98	0.46
3:H:202:THR:HB	3:H:219:LYS:HE3	1.96	0.46
3:M:101:ARG:CZ	6:I:3:BMA:H61	2.46	0.46
1:A:69:ASN:ND2	1:A:105:ALA:HB2	2.30	0.46
1:C:65:SER:HB3	2:D:585:LEU:HD21	1.96	0.46
2:D:554:LEU:HD23	2:D:554:LEU:O	2.16	0.46
1:E:57:LEU:CD1	1:E:62:GLN:NE2	2.45	0.46
2:B:570:GLN:HB2	2:F:531:TRP:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:101:ARG:NH1	6:I:3:BMA:C5	2.78	0.46
4:N:110:ALA:N	4:N:139:TYR:O	2.43	0.46
1:C:111:LEU:HD12	1:C:170:ILE:HG21	1.97	0.46
1:E:35:LEU:HD21	1:E:185:ILE:HD11	1.97	0.46
3:H:51:ILE:HD13	3:H:72:ARG:HG2	1.97	0.46
3:M:14:PRO:HD3	3:M:122:SER:CB	2.46	0.46
3:Q:29:PHE:CD2	3:Q:77:ASN:HA	2.51	0.46
4:R:48:ILE:HG13	4:R:54:LEU:HD23	1.96	0.46
4:N:33:LEU:CD2	4:N:71:PHE:CD1	2.93	0.46
2:B:572:PHE:O	2:B:576:THR:HG22	2.16	0.46
4:R:141:ARG:HB2	4:R:172:TYR:CE1	2.50	0.46
2:B:570:GLN:HG3	2:F:531:TRP:HE3	1.80	0.46
2:F:588:LYS:HA	2:F:588:LYS:HD3	1.74	0.46
3:H:128:PRO:HB2	3:H:151:VAL:HG13	1.98	0.46
1:E:162:TYR:HB2	1:E:165:LEU:O	2.15	0.46
3:H:91:THR:HG23	3:H:119:THR:HA	1.97	0.46
3:Q:67:ARG:HD2	3:Q:85:SER:HB2	1.97	0.46
1:A:70:LEU:N	1:A:178:GLU:O	2.44	0.46
2:B:528:GLY:C	2:B:531:TRP:HE1	2.19	0.46
4:L:109:VAL:HA	4:L:139:TYR:CB	2.46	0.46
1:E:113:ILE:CG2	1:E:121:CYS:HB2	2.44	0.45
1:C:182:ALA:HB2	2:D:562:ALA:CA	2.46	0.45
3:Q:14:PRO:HD3	3:Q:122:SER:CB	2.45	0.45
2:B:531:TRP:HB2	2:D:570:GLN:HB2	1.97	0.45
2:F:537:PRO:HG2	2:F:542:ILE:HG22	1.97	0.45
2:B:564:GLU:OE1	3:H:52:SER:HB2	2.17	0.45
3:Q:128:PRO:HB2	3:Q:151:VAL:HG13	1.99	0.45
3:Q:154:TYR:HB2	3:Q:209:HIS:CD2	2.52	0.45
1:E:34:PRO:HD2	2:F:565:THR:HG23	1.98	0.45
4:L:117:PHE:HA	4:L:118:PRO:HD3	1.72	0.45
4:N:4:LEU:HD13	4:N:23:CYS:SG	2.57	0.45
3:Q:164:ASN:HB3	3:Q:167:ALA:HB3	1.99	0.45
2:D:596:ARG:HD3	2:D:609:CYS:SG	2.57	0.45
3:H:164:ASN:HB3	3:H:167:ALA:HB3	1.98	0.45
3:M:10:THR:HB	3:M:18:LEU:HD21	1.99	0.45
4:N:106:LYS:O	4:N:106:LYS:HG3	2.17	0.45
4:N:33:LEU:HD12	4:N:89:GLN:O	2.17	0.45
3:Q:69:THR:O	3:Q:81:LEU:HD12	2.17	0.45
1:C:86:TRP:CD1	1:C:154:HIS:ND1	2.85	0.45
2:B:551:GLN:HG2	2:B:554:LEU:HB2	1.97	0.45
1:A:34:PRO:HB2	2:B:561:LEU:HD11	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:587:ARG:HG3	1:E:60:THR:HG21	1.99	0.45
1:C:49:ASP:OD1	1:C:50:LYS:N	2.50	0.45
3:H:94:TYR:HE1	3:H:118:VAL:HB	1.81	0.45
3:M:67:ARG:HD2	3:M:85:SER:O	2.17	0.45
1:C:70:LEU:HD12	1:C:178:GLU:OE1	2.17	0.45
3:M:128:PRO:HB2	3:M:151:VAL:HG13	1.98	0.45
3:M:178:VAL:HG22	3:M:186:SER:O	2.16	0.45
1:C:132:PHE:HB3	1:C:135:CYS:SG	2.57	0.45
2:D:531:TRP:CE2	2:D:532:ILE:HG23	2.51	0.45
1:A:133:PRO:HB3	2:B:543:TYR:CE2	2.52	0.44
3:M:2:VAL:N	3:M:26:GLY:HA3	2.32	0.44
4:R:13:ALA:O	4:R:105:ILE:HA	2.17	0.44
1:C:37:VAL:HG22	1:C:44:GLN:O	2.17	0.44
4:R:33:LEU:HD13	4:R:34:ALA:N	2.33	0.44
3:M:6:GLN:HE22	3:M:36:TRP:HZ3	1.66	0.44
4:N:166:ASP:HB2	4:N:169:ASP:OD1	2.16	0.44
3:M:160:THR:OG1	3:M:208:ASN:HB3	2.17	0.44
3:Q:155:PHE:HA	3:Q:156:PRO:HA	1.76	0.44
4:R:63:SER:O	4:R:73:LEU:HD12	2.18	0.44
2:D:515:LEU:HB2	2:D:555:ILE:HD12	1.98	0.44
1:E:130:ARG:HH21	1:E:164:ARG:HH11	1.65	0.44
2:B:578:GLU:HG3	2:F:582:PHE:CE1	2.52	0.44
4:N:139:TYR:HA	4:N:140:PRO:C	2.38	0.44
4:N:33:LEU:HD23	4:N:71:PHE:CG	2.46	0.44
3:M:13:GLN:HB3	3:M:14:PRO:HD2	1.99	0.44
4:R:39:LYS:HG2	4:R:84:ALA:HB2	1.99	0.44
1:C:35:LEU:HD21	1:C:185:ILE:HD11	2.00	0.44
1:C:45:VAL:CG2	3:M:54:LEU:HG	2.46	0.44
4:N:123:GLN:O	4:N:126:SER:OG	2.27	0.44
1:A:191:LYS:HE2	3:M:65:LYS:NZ	2.32	0.44
2:B:539:ALA:O	2:B:542:ILE:HG12	2.17	0.44
2:B:567:GLN:HG3	2:F:531:TRP:CD1	2.53	0.44
3:Q:152:LYS:HG2	3:Q:153:ASP:OD1	2.17	0.44
1:C:94:PRO:CB	1:C:169:ILE:HD12	2.39	0.44
7:B:701:NAG:C8	2:F:531:TRP:HH2	2.30	0.44
4:L:166:ASP:HB2	4:L:169:ASP:OD1	2.17	0.44
3:Q:133:LEU:HD12	3:Q:148:GLY:HA3	2.00	0.44
3:Q:160:THR:HG23	3:Q:208:ASN:HB3	2.00	0.43
3:M:83:MET:HE1	3:M:118:VAL:HG21	2.00	0.43
3:Q:131:PHE:HB3	4:R:120:SER:OG	2.17	0.43
4:R:206:LYS:HA	4:R:206:LYS:HD3	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:98:LYS:O	3:Q:109:PHE:HA	2.19	0.43
1:C:99:TYR:CZ	1:C:161:LEU:HD22	2.53	0.43
4:N:80:PRO:HA	4:N:83:PHE:CE2	2.52	0.43
2:B:523:GLU:OE1	2:B:526:ALA:HB2	2.17	0.43
2:D:563:ASN:HD21	6:I:1:NAG:C1	2.32	0.43
4:L:61:ARG:HD2	4:L:77:SER:O	2.19	0.43
3:M:17:SER:HA	3:M:83:MET:O	2.19	0.43
2:B:527:ILE:HG13	4:N:95:PRO:HD3	2.00	0.43
1:C:77:THR:OG1	1:C:107:ASN:ND2	2.52	0.43
1:E:78:ASP:OD1	1:E:78:ASP:N	2.51	0.43
4:N:154:GLN:HB3	4:N:157:ASN:ND2	2.27	0.43
2:B:531:TRP:CD2	2:D:567:GLN:HA	2.54	0.43
3:H:155:PHE:HA	3:H:156:PRO:HA	1.72	0.43
3:Q:12:VAL:HG21	3:Q:120:VAL:HG22	2.00	0.43
2:F:527:ILE:HG13	4:L:93:SER:HA	2.01	0.43
1:A:68:LEU:HD11	2:B:558:LEU:HG	2.01	0.43
4:L:4:LEU:C	4:L:4:LEU:CD1	2.85	0.43
4:N:4:LEU:HD12	4:N:4:LEU:C	2.39	0.43
4:R:202:SER:HA	4:R:203:PRO:HD2	1.89	0.43
1:E:69:ASN:ND2	1:E:105:ALA:HB2	2.34	0.43
3:Q:31:SER:HG	3:Q:103:TRP:HE1	1.67	0.43
1:A:74:GLY:HA3	2:B:510:LYS:HB2	2.00	0.42
1:C:156:GLU:HG2	6:I:2:NAG:H61	2.01	0.42
2:D:521:GLN:HE21	2:D:524:GLY:HA3	1.82	0.42
1:E:33:ILE:HD11	2:F:572:PHE:CG	2.52	0.42
4:L:7:SER:OG	4:L:8:PRO:HD3	2.18	0.42
3:Q:68:PHE:CE1	3:Q:83:MET:HB3	2.53	0.42
2:B:517:TYR:CZ	2:B:546:GLY:HA3	2.54	0.42
2:B:592:PHE:CE2	2:B:596:ARG:NH1	2.79	0.42
1:C:108:CYS:HB3	1:C:175:THR:CG2	2.50	0.42
1:C:88:PHE:CB	1:C:149:GLU:HB2	2.47	0.42
3:Q:163:TRP:O	3:Q:164:ASN:C	2.55	0.42
2:B:577:THR:HG21	1:E:164:ARG:O	2.19	0.42
1:E:49:ASP:OD1	1:E:50:LYS:N	2.52	0.42
3:H:36:TRP:CZ2	3:H:79:LEU:HG	2.55	0.42
3:Q:36:TRP:CE2	3:Q:81:LEU:HB2	2.54	0.42
1:A:39:HIS:CB	1:A:44:GLN:HE22	2.32	0.42
4:N:61:ARG:HD2	4:N:77:SER:O	2.20	0.42
2:F:532:ILE:HA	2:F:533:PRO:HD3	1.86	0.42
3:H:157:GLU:HB3	3:H:158:PRO:HA	2.01	0.42
3:Q:61:ALA:HB3	3:Q:64:VAL:HG22	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:91:THR:HG23	3:Q:118:VAL:O	2.20	0.42
3:M:12:VAL:CG2	3:M:18:LEU:HD22	2.50	0.42
3:Q:140:THR:HB	3:Q:195:SER:CB	2.50	0.42
3:Q:60:TYR:OH	3:Q:70:ILE:HG22	2.20	0.42
1:A:33:ILE:HA	1:A:34:PRO:HD3	1.75	0.42
1:A:39:HIS:HB2	1:A:44:GLN:HE22	1.85	0.42
1:E:132:PHE:HA	1:E:133:PRO:HD3	1.91	0.42
3:H:147:LEU:HD13	3:H:220:VAL:HG21	2.01	0.42
3:M:29:PHE:HE1	3:M:72:ARG:NH1	2.18	0.42
1:A:89:ARG:HB3	1:A:153:PHE:CD1	2.55	0.42
1:C:114:LYS:HE3	1:C:120:GLU:OE2	2.20	0.42
1:C:90:ALA:N	1:C:149:GLU:HG2	2.35	0.42
1:E:147:CYS:N	1:E:148:PRO:CD	2.82	0.42
1:E:151:TYR:CB	1:E:169:ILE:HD13	2.50	0.42
1:A:45:VAL:CG2	3:H:56:GLY:HA3	2.50	0.42
4:N:106:LYS:NZ	4:N:140:PRO:HB3	2.35	0.42
4:R:139:TYR:CE1	4:R:171:THR:HG22	2.55	0.42
1:A:51:LEU:HD11	2:B:596:ARG:CG	2.50	0.41
1:C:165:LEU:HD21	2:F:577:THR:OG1	2.20	0.41
1:C:69:ASN:OD1	1:C:69:ASN:N	2.53	0.41
2:D:561:LEU:HD13	3:M:54:LEU:CD2	2.50	0.41
4:L:139:TYR:CZ	4:L:171:THR:HG22	2.55	0.41
4:L:4:LEU:HD21	4:L:88:CYS:O	2.19	0.41
2:B:525:ALA:HB1	2:B:527:ILE:HD13	2.02	0.41
1:C:156:GLU:OE2	6:I:1:NAG:O3	2.38	0.41
2:D:530:ALA:HB1	2:D:537:PRO:HD3	2.02	0.41
3:H:161:VAL:HG11	3:H:189:SER:CB	2.51	0.41
4:N:78:LEU:HD11	4:N:82:ASP:HB2	2.02	0.41
1:C:45:VAL:HG11	3:M:56:GLY:CA	2.51	0.41
3:M:2:VAL:HG22	3:M:2:VAL:O	2.19	0.41
1:C:33:ILE:HA	1:C:34:PRO:HD3	1.87	0.41
1:C:45:VAL:HG11	3:M:56:GLY:HA3	2.02	0.41
1:E:182:ALA:HB2	2:F:562:ALA:CB	2.50	0.41
5:G:5:NAG:O7	5:G:5:NAG:H3	2.20	0.41
3:H:30:SER:HA	3:H:72:ARG:NH2	2.36	0.41
2:B:531:TRP:HB2	2:D:570:GLN:CB	2.49	0.41
2:B:551:GLN:CG	2:B:554:LEU:HB2	2.50	0.41
1:E:151:TYR:HB3	1:E:169:ILE:HD13	2.02	0.41
3:H:86:LEU:CB	3:H:120:VAL:HG11	2.51	0.41
4:N:61:ARG:CZ	4:N:79:GLN:HG3	2.51	0.41
1:A:147:CYS:N	1:A:148:PRO:CD	2.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:89:ARG:NE	1:E:90:ALA:O	2.53	0.41
3:H:14:PRO:HD3	3:H:122:SER:HB2	2.03	0.41
3:M:134:ALA:HA	3:M:135:PRO:HD3	1.75	0.41
1:A:96:VAL:HB	2:B:580:ARG:HG2	2.02	0.41
2:D:532:ILE:HD12	2:D:535:PHE:CD2	2.52	0.41
2:D:554:LEU:CD2	2:D:554:LEU:C	2.85	0.41
3:H:208:ASN:OD1	3:H:215:LYS:HG2	2.21	0.41
2:F:527:ILE:CG1	4:L:93:SER:HA	2.51	0.41
1:E:95:LYS:NZ	2:F:574:ARG:HA	2.36	0.41
1:E:33:ILE:HB	2:F:588:LYS:HE3	2.01	0.41
4:L:114:VAL:HG22	4:L:195:VAL:HG21	2.03	0.41
3:M:12:VAL:HG23	3:M:18:LEU:HD22	2.02	0.41
4:R:82:ASP:N	4:R:82:ASP:OD1	2.53	0.41
1:E:125:ALA:HA	1:E:126:PRO:HD3	1.84	0.41
4:L:33:LEU:HD21	4:L:88:CYS:HB2	2.02	0.41
4:N:78:LEU:CD1	4:N:82:ASP:HB2	2.50	0.41
3:Q:45:LEU:HB2	4:R:97:PHE:CG	2.56	0.41
1:C:57:LEU:HD12	1:C:62:GLN:OE1	2.21	0.41
3:H:12:VAL:CG1	3:H:13:GLN:N	2.43	0.41
4:L:4:LEU:HD22	4:L:23:CYS:SG	2.61	0.41
4:L:37:GLN:HB2	4:L:86:TYR:HE1	1.86	0.41
3:M:12:VAL:HG12	3:M:13:GLN:O	2.21	0.41
3:Q:102:VAL:HG21	3:Q:106:GLY:CA	2.51	0.41
3:Q:64:VAL:HB	3:Q:68:PHE:CD2	2.56	0.41
2:B:527:ILE:HG12	4:N:94:SER:CA	2.51	0.40
1:C:72:GLY:HA3	2:D:559:ARG:HH22	1.79	0.40
1:C:94:PRO:O	1:C:95:LYS:HD3	2.21	0.40
4:L:202:SER:HA	4:L:203:PRO:HD2	1.89	0.40
4:N:106:LYS:HZ2	4:N:140:PRO:HB3	1.86	0.40
4:N:39:LYS:HG2	4:N:84:ALA:HB2	2.03	0.40
2:B:512:ASN:HA	2:B:513:PRO:HD3	1.87	0.40
1:C:148:PRO:HB2	1:C:149:GLU:OE1	2.20	0.40
1:C:161:LEU:HD23	1:C:161:LEU:HA	1.92	0.40
1:C:56:LYS:HG2	2:F:599:GLY:HA2	2.03	0.40
2:F:529:LEU:HD21	3:H:106:GLY:HA2	2.04	0.40
3:M:29:PHE:CE1	3:M:72:ARG:HD2	2.56	0.40
1:C:95:LYS:HB3	2:D:573:LEU:HB3	2.04	0.40
3:M:101:ARG:CZ	6:I:3:BMA:C6	2.99	0.40
3:Q:36:TRP:CZ2	3:Q:79:LEU:HG	2.56	0.40
1:A:194:PHE:CE1	2:B:519:THR:HG21	2.57	0.40
2:D:537:PRO:HD2	2:F:574:ARG:NH2	2.37	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:52:VAL:HB	1:E:55:ASP:OD2	2.21	0.40
3:H:6:GLN:HE22	3:H:95:TYR:HA	1.87	0.40
4:L:154:GLN:HB3	4:L:157:ASN:HD21	1.86	0.40
3:Q:71:SER:O	3:Q:79:LEU:HD12	2.22	0.40
1:C:183:PHE:O	1:C:184:LEU:HD12	2.21	0.40
2:B:531:TRP:CE3	2:D:570:GLN:HG3	2.56	0.40
1:E:149:GLU:HA	1:E:149:GLU:OE1	2.22	0.40
3:M:128:PRO:HB3	3:M:154:TYR:HB3	2.03	0.40
4:N:185:TYR:CZ	4:N:210:ARG:HG3	2.57	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:527:ILE:CB	4:R:93:SER:O[2_565]	1.99	0.21

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	160/162 (99%)	156 (98%)	4 (2%)	0	100	100
1	C	156/162 (96%)	152 (97%)	4 (3%)	0	100	100
1	E	153/162 (94%)	147 (96%)	6 (4%)	0	100	100
2	B	102/111 (92%)	96 (94%)	6 (6%)	0	100	100
2	D	102/111 (92%)	98 (96%)	4 (4%)	0	100	100
2	F	101/111 (91%)	97 (96%)	4 (4%)	0	100	100
3	H	209/233 (90%)	204 (98%)	5 (2%)	0	100	100
3	M	213/233 (91%)	206 (97%)	7 (3%)	0	100	100
3	Q	220/233 (94%)	214 (97%)	6 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	L	206/213 (97%)	198 (96%)	8 (4%)	0	100	100
4	N	210/213 (99%)	201 (96%)	9 (4%)	0	100	100
4	R	209/213 (98%)	205 (98%)	4 (2%)	0	100	100
All	All	2041/2157 (95%)	1974 (97%)	67 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	135/135 (100%)	135 (100%)	0	100	100
1	C	130/135 (96%)	130 (100%)	0	100	100
1	E	128/135 (95%)	128 (100%)	0	100	100
2	B	84/91 (92%)	83 (99%)	1 (1%)	71	84
2	D	84/91 (92%)	83 (99%)	1 (1%)	71	84
2	F	84/91 (92%)	83 (99%)	1 (1%)	71	84
3	H	176/194 (91%)	176 (100%)	0	100	100
3	M	180/194 (93%)	180 (100%)	0	100	100
3	Q	183/194 (94%)	183 (100%)	0	100	100
4	L	184/187 (98%)	184 (100%)	0	100	100
4	N	186/187 (100%)	186 (100%)	0	100	100
4	R	185/187 (99%)	185 (100%)	0	100	100
All	All	1739/1821 (96%)	1736 (100%)	3 (0%)	93	96

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	601	CYS
2	D	601	CYS

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Mol	Chain	Res	Type
2	F	601	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	521	GLN
1	C	62	GLN
1	C	107	ASN
2	D	521	GLN
1	E	62	GLN
3	H	6	GLN
4	L	37	GLN
3	Q	77	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 ⓘ

11 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	$\# Z > 2$
5	NAG	G	1	5	14,14,15	0.38	0	17,19,21	0.45	0
5	NAG	G	2	5	14,14,15	0.32	0	17,19,21	0.51	0
5	BMA	G	3	5	11,11,12	0.64	0	15,15,17	0.93	1 (6%)
5	MAN	G	4	5	11,11,12	0.74	0	15,15,17	1.21	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	G	5	5	14,14,15	0.31	0	17,19,21	1.01	1 (5%)
5	MAN	G	6	5	11,11,12	0.96	1 (9%)	15,15,17	1.13	2 (13%)
6	NAG	I	1	6	14,14,15	0.39	0	17,19,21	0.44	0
6	NAG	I	2	6	14,14,15	0.33	0	17,19,21	0.51	0
6	BMA	I	3	6	11,11,12	0.64	0	15,15,17	0.93	1 (6%)
6	MAN	I	4	6	11,11,12	0.73	0	15,15,17	1.21	2 (13%)
6	MAN	I	5	6	11,11,12	0.96	1 (9%)	15,15,17	1.13	2 (13%)

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	G	1	5	-	0/6/23/26	0/1/1/1
5	NAG	G	2	5	-	1/6/23/26	0/1/1/1
5	BMA	G	3	5	-	2/2/19/22	0/1/1/1
5	MAN	G	4	5	-	1/2/19/22	0/1/1/1
5	NAG	G	5	5	-	3/6/23/26	0/1/1/1
5	MAN	G	6	5	-	0/2/19/22	0/1/1/1
6	NAG	I	1	6	-	0/6/23/26	0/1/1/1
6	NAG	I	2	6	-	1/6/23/26	0/1/1/1
6	BMA	I	3	6	-	2/2/19/22	0/1/1/1
6	MAN	I	4	6	-	1/2/19/22	0/1/1/1
6	MAN	I	5	6	-	0/2/19/22	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	G	6	MAN	C1-C2	2.75	1.58	1.52
6	I	5	MAN	C1-C2	2.70	1.58	1.52

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	G	5	NAG	C2-N2-C7	3.43	127.79	122.90
5	G	4	MAN	C1-O5-C5	3.23	116.57	112.19
6	I	4	MAN	C1-O5-C5	3.22	116.56	112.19
5	G	3	BMA	C1-O5-C5	2.52	115.60	112.19
5	G	4	MAN	O2-C2-C3	-2.49	105.14	110.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	I	3	BMA	C1-O5-C5	2.49	115.56	112.19
6	I	4	MAN	O2-C2-C3	-2.48	105.16	110.14
6	I	5	MAN	O2-C2-C3	-2.33	105.47	110.14
5	G	6	MAN	O2-C2-C3	-2.32	105.50	110.14
5	G	6	MAN	C1-O5-C5	2.27	115.26	112.19
6	I	5	MAN	C1-O5-C5	2.26	115.26	112.19

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	G	5	NAG	C3-C2-N2-C7
6	I	3	BMA	C4-C5-C6-O6
5	G	3	BMA	C4-C5-C6-O6
6	I	3	BMA	O5-C5-C6-O6
5	G	3	BMA	O5-C5-C6-O6
5	G	5	NAG	O5-C5-C6-O6
5	G	4	MAN	O5-C5-C6-O6
6	I	4	MAN	O5-C5-C6-O6
5	G	2	NAG	O5-C5-C6-O6
6	I	2	NAG	O5-C5-C6-O6
5	G	5	NAG	C4-C5-C6-O6

There are no ring outliers.

9 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	I	5	MAN	1	0
6	I	3	BMA	7	0
5	G	2	NAG	1	0
6	I	1	NAG	3	0
5	G	1	NAG	8	0
5	G	6	MAN	1	0
5	G	3	BMA	1	0
5	G	5	NAG	1	0
6	I	2	NAG	1	0

5.6 Ligand geometry

2 ligands 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	$\# Z > 2$
7	NAG	B	701	-	14,14,15	0.38	0	17,19,21	0.48	0
7	NAG	A	201	1	14,14,15	0.40	0	17,19,21	0.45	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
7	NAG	B	701	-	-	2/6/23/26	0/1/1/1
7	NAG	A	201	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	B	701	NAG	O5-C5-C6-O6
7	B	701	NAG	C4-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	701	NAG	4	0
7	A	201	NAG	6	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.