



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:16 PM GMT

PDB ID : 3WJM
Title : Crystal structure of Bombyx mori Sp2/Sp3 heterohexamer
Authors : Yuan, Y.A.; Hou, Y.
Deposited on : 2013-10-11
Resolution : 2.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

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

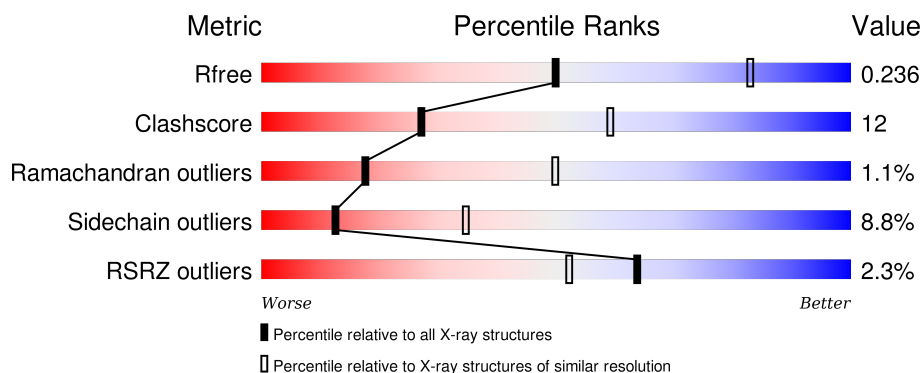
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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. 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	703	<div> <div>3%</div> <div>71% 22% 5%</div> </div>
1	E	703	<div> <div>3%</div> <div>72% 20% 5%</div> </div>
1	F	703	<div> <div>3%</div> <div>67% 24% 5%</div> </div>
2	B	696	<div> <div>2%</div> <div>67% 24% 5%</div> </div>
2	C	696	<div> <div>2%</div> <div>68% 23% 5%</div> </div>

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Mol	Chain	Length	Quality of chain
2	D	696	<div><div><div>%</div><div><div></div></div><div>69%</div><div>24%</div><div><div></div><div></div></div></div></div>

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 34590 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 Arylphorin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	670	Total	C	N	O	S	0	0	0
			5681	3734	892	1030	25			
1	E	669	Total	C	N	O	S	0	0	0
			5669	3725	891	1028	25			
1	F	669	Total	C	N	O	S	0	0	0
			5669	3725	891	1028	25			

- Molecule 2 is a protein called Silkworm storage protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	668	Total	C	N	O	S	0	0	0
			5669	3745	877	1021	26			
2	C	668	Total	C	N	O	S	0	0	0
			5669	3745	877	1021	26			
2	D	672	Total	C	N	O	S	0	0	0
			5703	3767	881	1029	26			

- Molecule 3 is a polymer of unknown type called SUGAR (5-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	5	Total	C	N	O	0	0
			61	34	2	25		
3	F	5	Total	C	N	O	0	0
			61	34	2	25		

- Molecule 4 is a polymer of unknown type called SUGAR (5-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	5	Total	C	N	O	0	0
			61	34	2	25		

- Molecule 5 is a polymer of unknown type called SUGAR (6-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	C	6	Total	C	N	O	0	0
			72	40	2	30		

- Molecule 6 is a polymer of unknown type called SUGAR (7-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	D	7	Total	C	N	O	0	0
			83	46	2	35		

- Molecule 7 is a polymer of unknown type called SUGAR (6-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	E	6	Total	C	N	O	0	0
			72	40	2	30		

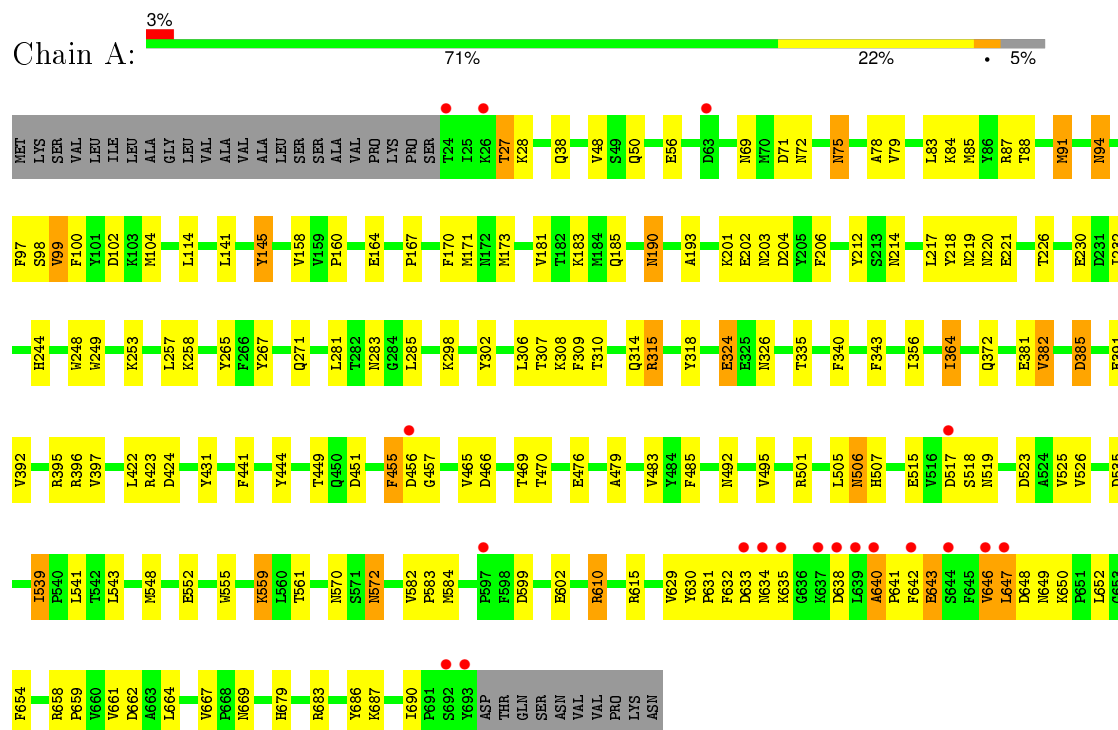
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	29	Total	O	0	0
			29	29		
8	B	14	Total	O	0	0
			14	14		
8	C	19	Total	O	0	0
			19	19		
8	D	27	Total	O	0	0
			27	27		
8	E	21	Total	O	0	0
			21	21		
8	F	10	Total	O	0	0
			10	10		

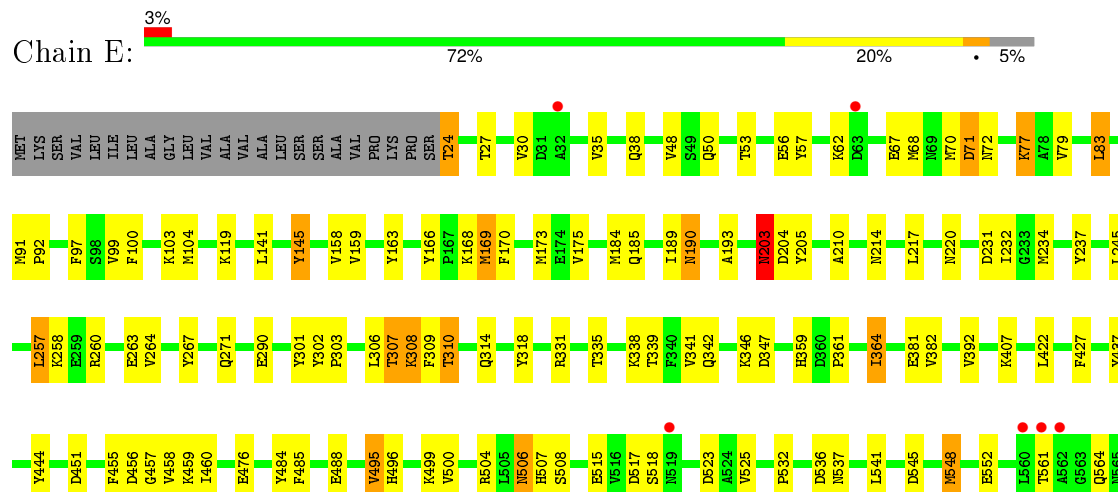
3 Residue-property plots

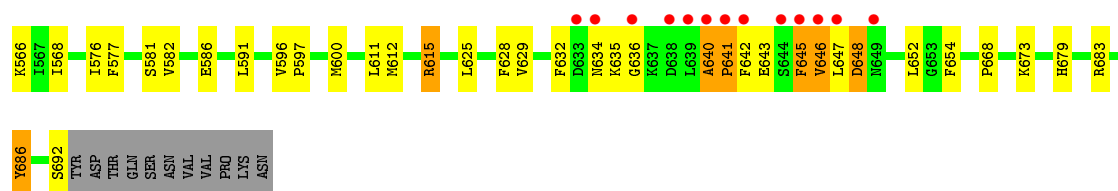
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

• Molecule 1: Arylphorin

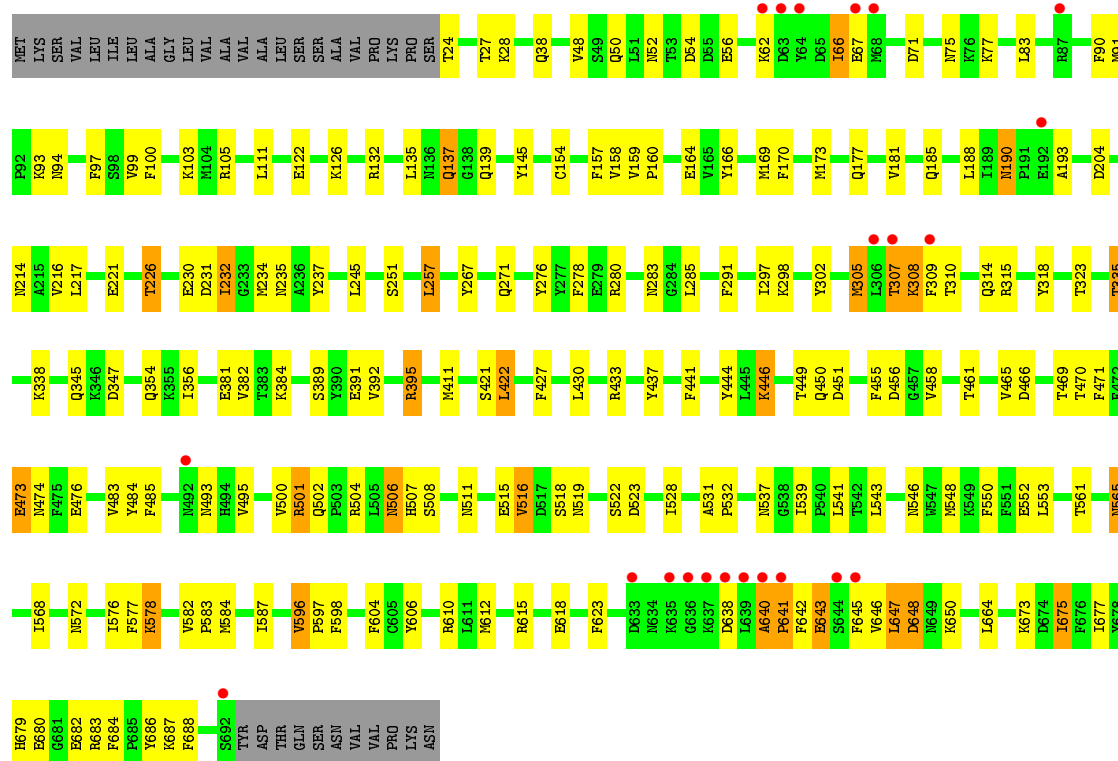


• Molecule 1: Arylphorin

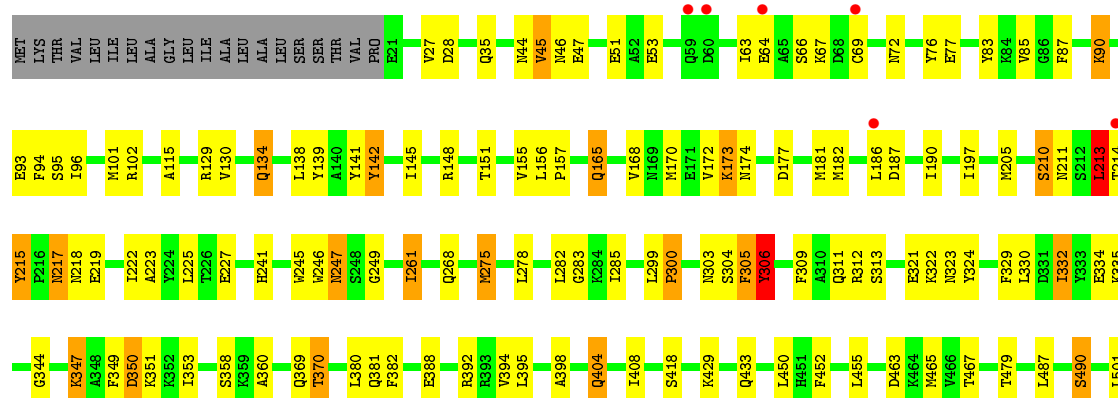


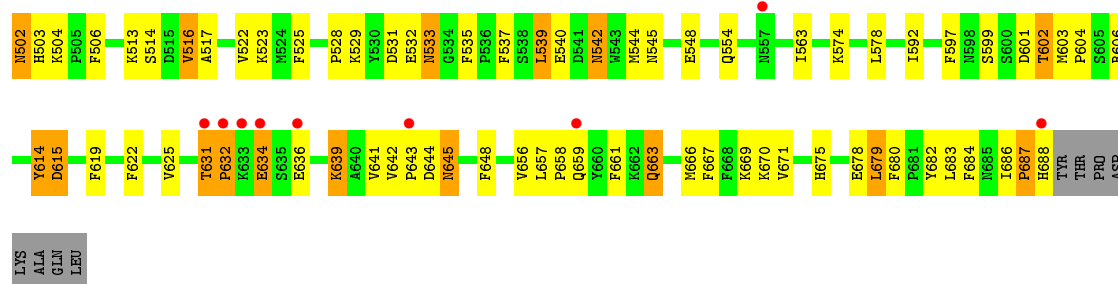


• Molecule 1: Arylphorin

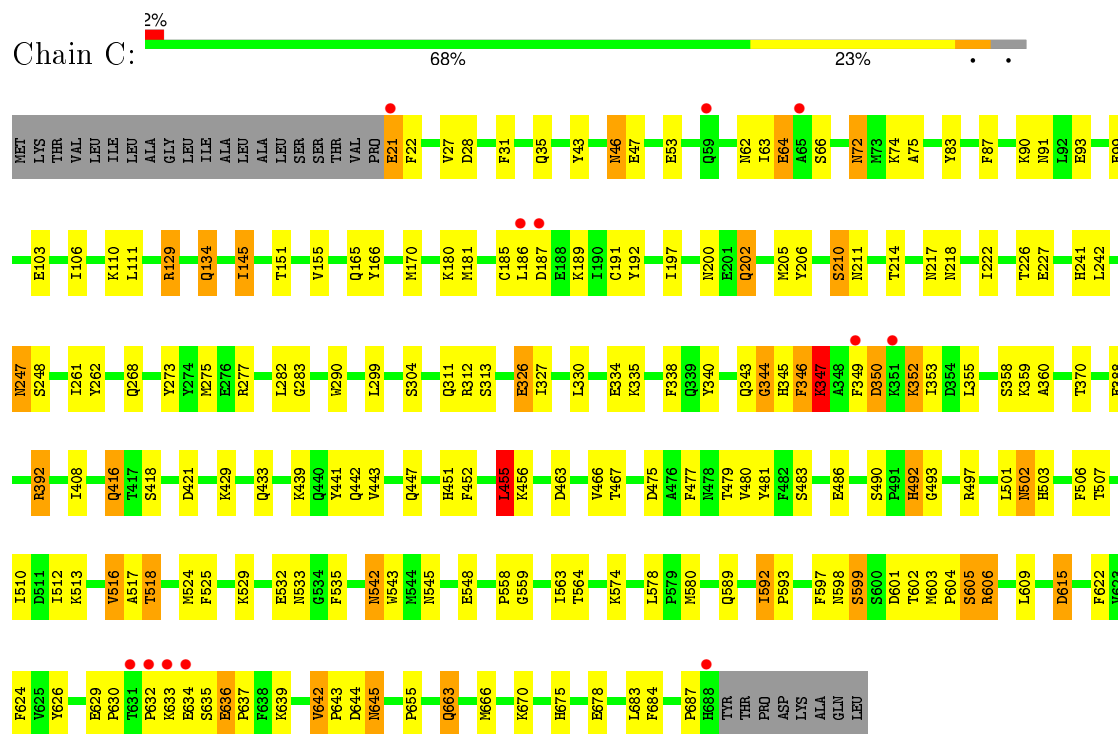


• Molecule 2: Silkworm storage protein

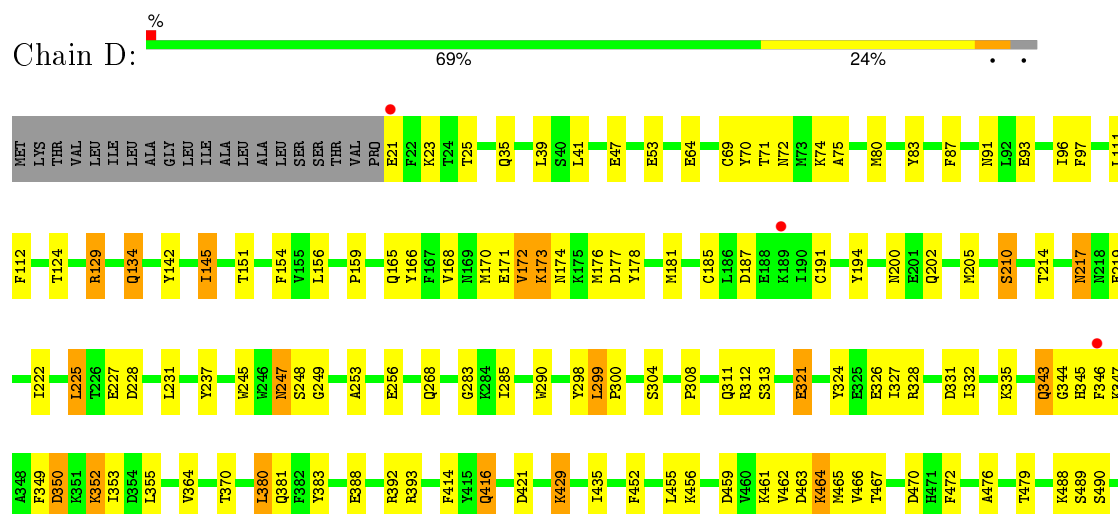


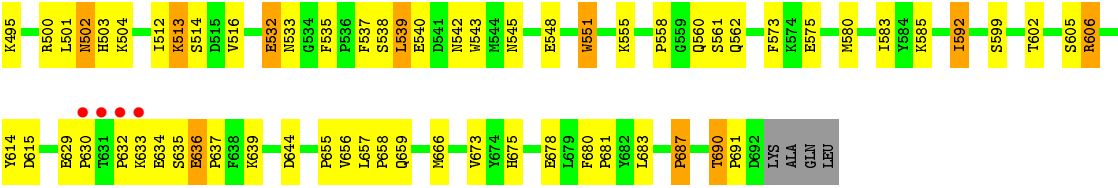


• Molecule 2: Silkworm storage protein



• Molecule 2: Silkworm storage protein





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	92.06Å 205.02Å 119.71Å 90.00° 103.00° 90.00°	Depositor
Resolution (Å)	48.37 – 2.80 48.37 – 2.80	Depositor EDS
% Data completeness (in resolution range)	96.5 (48.37-2.80) 96.5 (48.37-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.81 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.172 , 0.237 0.171 , 0.236	Depositor DCC
R_{free} test set	5121 reflections (5.27%)	DCC
Wilson B-factor (Å ²)	50.2	Xtriage
Anisotropy	0.238	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 43.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 102314 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	34590	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.42% 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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.62	0/5863	0.76	3/7934 (0.0%)
1	E	0.61	0/5850	0.74	1/7916 (0.0%)
1	F	0.58	0/5850	0.74	2/7916 (0.0%)
2	B	0.61	0/5865	0.76	1/7945 (0.0%)
2	C	0.64	0/5865	0.78	5/7945 (0.1%)
2	D	0.65	1/5901 (0.0%)	0.78	2/7996 (0.0%)
All	All	0.62	1/35194 (0.0%)	0.76	14/47652 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	171	GLU	CD-OE2	-5.18	1.20	1.25

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	213	LEU	CA-CB-CG	9.09	136.20	115.30
1	A	315	ARG	NE-CZ-NH2	-8.73	115.93	120.30
2	C	392	ARG	NE-CZ-NH2	-7.33	116.64	120.30
1	F	315	ARG	NE-CZ-NH2	-6.68	116.96	120.30
2	D	171	GLU	OE1-CD-OE2	-6.65	115.32	123.30
2	C	455	LEU	CA-CB-CG	6.56	130.40	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	392	ARG	NE-CZ-NH1	6.38	123.49	120.30
1	A	99	VAL	CB-CA-C	-6.05	99.90	111.40
1	E	541	LEU	CA-CB-CG	5.87	128.80	115.30
2	C	615	ASP	N-CA-CB	-5.80	100.15	110.60
2	D	470	ASP	CB-CG-OD1	5.65	123.39	118.30
1	F	395	ARG	NE-CZ-NH2	-5.64	117.48	120.30
1	A	395	ARG	NE-CZ-NH2	-5.61	117.50	120.30
2	C	187	ASP	CB-CG-OD2	5.04	122.84	118.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	246	TRP	Peptide
2	B	614	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	5681	0	5434	125	0
1	E	5669	0	5425	117	0
1	F	5669	0	5425	150	0
2	B	5669	0	5390	193	0
2	C	5669	0	5392	145	0
2	D	5703	0	5419	140	0
3	A	61	0	52	0	0
3	F	61	0	52	0	0
4	B	61	0	52	3	0
5	C	72	0	61	0	0
6	D	83	0	70	0	0
7	E	72	0	61	1	0
8	A	29	0	0	0	0
8	B	14	0	0	0	0
8	C	19	0	0	1	0
8	D	27	0	0	0	0
8	E	21	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	F	10	0	0	1	0
All	All	34590	0	32833	809	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 12.

All (809) 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)
2:B:631:THR:HB	2:B:632:PRO:CD	1.72	1.19
2:B:210:SER:HB2	2:B:214:THR:HG21	1.27	1.16
2:B:631:THR:CB	2:B:632:PRO:HD2	1.77	1.15
1:F:531:ALA:HB2	1:F:550:PHE:CD2	1.83	1.13
1:E:97:PHE:HA	1:E:104:MET:HE1	1.31	1.12
2:D:343:GLN:HE21	2:D:343:GLN:HA	1.15	1.11
2:B:95:SER:H	2:B:101:MET:CE	1.65	1.09
2:B:214:THR:HG23	2:B:215:TYR:HD2	1.14	1.08
1:F:531:ALA:HB2	1:F:550:PHE:CE2	1.95	1.01
2:B:631:THR:HB	2:B:632:PRO:HD2	1.01	1.00
2:B:332:ILE:HG12	2:C:335:LYS:HG2	1.42	1.00
1:F:640:ALA:N	1:F:641:PRO:HD3	1.77	1.00
1:A:314:GLN:HE22	2:D:311:GLN:H	1.08	1.00
2:D:134:GLN:HE21	2:D:134:GLN:H	1.04	0.99
1:F:232:ILE:HD13	1:F:232:ILE:H	1.26	0.98
2:B:615:ASP:H	2:D:615:ASP:HB3	1.28	0.98
1:E:640:ALA:H	1:E:641:PRO:HD3	1.30	0.97
2:C:340:TYR:HB3	2:C:346:PHE:HD2	1.31	0.95
1:F:531:ALA:CB	1:F:550:PHE:CE2	2.50	0.94
2:B:283:GLY:HA2	2:B:532:GLU:HG2	1.48	0.94
2:C:134:GLN:HE21	2:C:134:GLN:H	1.10	0.94
2:D:283:GLY:HA2	2:D:532:GLU:HG2	1.50	0.94
2:B:502:ASN:HD22	2:B:503:HIS:H	1.09	0.93
2:B:210:SER:HB2	2:B:214:THR:CG2	1.98	0.93
1:E:506:ASN:HD22	1:E:507:HIS:H	1.15	0.93
2:B:211:ASN:O	2:B:214:THR:HG22	1.67	0.93
2:C:72:ASN:HD22	2:C:75:ALA:H	1.12	0.93
1:F:99:VAL:HG22	1:F:105:ARG:HG3	1.49	0.92
2:B:663:GLN:HG2	2:B:666:MET:CE	1.98	0.92
1:F:66:ILE:HD12	1:F:66:ILE:H	1.35	0.92
2:B:134:GLN:H	2:B:134:GLN:NE2	1.68	0.92
2:D:134:GLN:NE2	2:D:134:GLN:H	1.67	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:50:GLN:HE22	1:E:485:PHE:H	1.19	0.91
2:C:165:GLN:HB3	2:C:479:THR:HG21	1.52	0.90
2:C:72:ASN:ND2	2:C:75:ALA:H	1.68	0.90
2:C:268:GLN:HE22	2:C:548:GLU:H	1.17	0.90
2:C:283:GLY:HA2	2:C:532:GLU:HG2	1.52	0.90
2:C:517:ALA:HB2	2:C:558:PRO:HD3	1.53	0.90
1:E:307:THR:HG22	1:E:310:THR:H	1.37	0.89
2:B:214:THR:HG23	2:B:215:TYR:CD2	2.06	0.89
2:B:134:GLN:H	2:B:134:GLN:HE21	0.89	0.88
2:B:247:ASN:ND2	2:B:249:GLY:H	1.72	0.88
2:B:210:SER:CB	2:B:214:THR:HG21	2.03	0.88
2:D:268:GLN:HE22	2:D:548:GLU:H	1.16	0.87
2:B:134:GLN:N	2:B:134:GLN:HE21	1.71	0.87
1:F:307:THR:HG22	1:F:310:THR:H	1.37	0.87
1:A:75:ASN:ND2	1:A:78:ALA:H	1.71	0.87
1:A:271:GLN:HE22	1:A:552:GLU:H	1.20	0.85
1:F:640:ALA:H	1:F:641:PRO:HD3	1.38	0.85
1:A:335:THR:OG1	2:B:335:LYS:HG2	1.75	0.85
2:C:615:ASP:OD1	1:F:618:GLU:HB3	1.75	0.85
2:C:134:GLN:HE21	2:C:134:GLN:N	1.75	0.84
1:F:190:ASN:HD22	1:F:193:ALA:H	1.24	0.84
1:A:212:TYR:HB3	1:A:226:THR:CG2	2.07	0.84
1:A:642:PHE:O	1:A:643:GLU:HG3	1.79	0.83
2:B:502:ASN:HD22	2:B:503:HIS:N	1.77	0.83
1:F:638:ASP:HB2	1:F:647:LEU:HA	1.59	0.82
2:B:663:GLN:HG2	2:B:666:MET:HE2	1.61	0.82
1:A:314:GLN:NE2	2:D:311:GLN:H	1.78	0.82
1:A:212:TYR:HB3	1:A:226:THR:HG21	1.60	0.82
1:E:97:PHE:HA	1:E:104:MET:CE	2.10	0.82
1:E:103:LYS:HG3	1:E:407:LYS:HB2	1.63	0.81
2:D:343:GLN:NE2	2:D:343:GLN:HA	1.93	0.80
2:B:35:GLN:HE22	2:B:155:VAL:H	1.26	0.80
1:A:298:LYS:HE2	1:E:318:TYR:OH	1.80	0.80
2:C:311:GLN:H	1:E:314:GLN:HE22	1.27	0.80
2:C:542:ASN:HD22	2:C:545:ASN:HD22	1.29	0.80
2:B:615:ASP:N	2:D:615:ASP:HB3	1.96	0.80
2:D:72:ASN:HD22	2:D:75:ALA:H	1.30	0.80
2:B:95:SER:N	2:B:101:MET:CE	2.45	0.80
2:D:573:PHE:HB3	2:D:605:SER:HB3	1.64	0.79
1:F:541:LEU:HD22	1:F:546:ASN:ND2	1.95	0.79
2:D:217:ASN:HD22	2:D:219:GLU:H	1.28	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:447:GLN:NE2	2:C:663:GLN:OE1	2.15	0.78
2:D:247:ASN:HD22	2:D:247:ASN:C	1.86	0.78
2:B:450:LEU:HB2	2:B:663:GLN:HE21	1.48	0.78
2:C:502:ASN:HD22	2:C:503:HIS:H	1.29	0.78
2:B:349:PHE:O	2:B:350:ASP:HB2	1.83	0.78
2:D:476:ALA:O	2:D:479:THR:HG22	1.84	0.78
2:B:311:GLN:H	1:F:314:GLN:HE22	1.29	0.78
1:E:271:GLN:HE22	1:E:552:GLU:H	1.29	0.78
2:C:134:GLN:NE2	2:C:134:GLN:H	1.82	0.78
2:C:211:ASN:HB3	8:C:919:HOH:O	1.84	0.78
2:B:663:GLN:HG2	2:B:666:MET:HE1	1.65	0.77
1:A:638:ASP:HB2	1:A:647:LEU:HA	1.66	0.77
1:F:450:GLN:HG2	1:F:664:LEU:HD23	1.66	0.77
2:C:166:TYR:CD1	2:C:416:GLN:HG3	2.20	0.76
2:B:165:GLN:HG3	2:B:479:THR:CG2	2.15	0.76
2:C:218:ASN:HB3	2:C:282:LEU:HD21	1.68	0.76
2:D:539:LEU:HG	2:D:656:VAL:HG11	1.66	0.76
2:B:275:MET:HE2	2:B:528:PRO:HD3	1.65	0.76
1:F:450:GLN:HG2	1:F:664:LEU:CD2	2.16	0.76
2:D:35:GLN:HE21	2:D:39:LEU:HG	1.51	0.75
2:C:542:ASN:ND2	2:C:545:ASN:HD22	1.84	0.75
2:B:268:GLN:HE22	2:B:548:GLU:H	1.31	0.75
2:B:95:SER:H	2:B:101:MET:HE2	1.52	0.75
2:C:599:SER:HB3	2:C:639:LYS:HD2	1.69	0.75
1:E:640:ALA:N	1:E:641:PRO:HD3	2.01	0.75
1:A:190:ASN:ND2	1:A:193:ALA:H	1.85	0.75
1:E:67:GLU:CG	1:E:83:LEU:HD21	2.17	0.75
2:B:222:ILE:HD11	2:B:282:LEU:HD12	1.69	0.74
2:D:25:THR:HB	2:D:592:ILE:HG22	1.68	0.74
1:F:231:ASP:O	1:F:235:ASN:ND2	2.19	0.74
1:F:307:THR:HG22	1:F:309:PHE:H	1.53	0.74
1:A:48:VAL:CG1	1:A:141:LEU:HD11	2.19	0.73
1:F:137:GLN:H	1:F:137:GLN:CD	1.91	0.73
1:F:640:ALA:N	1:F:641:PRO:CD	2.52	0.73
1:F:90:PHE:HD2	1:F:139:GLN:HE22	1.34	0.73
2:B:283:GLY:HA2	2:B:532:GLU:CG	2.19	0.73
2:B:615:ASP:OD1	2:D:614:TYR:HB2	1.88	0.72
1:E:307:THR:HG22	1:E:310:THR:N	2.03	0.72
1:A:75:ASN:HD22	1:A:78:ALA:H	1.36	0.72
1:F:474:ASN:HB3	1:F:501:ARG:HD3	1.69	0.72
1:A:298:LYS:HG2	1:A:318:TYR:CE2	2.24	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:507:THR:HG21	2:C:564:THR:CG2	2.21	0.71
2:C:202:GLN:HG3	2:C:493:GLY:HA2	1.72	0.71
1:E:460:ILE:HD11	1:E:629:VAL:HG23	1.73	0.71
2:B:311:GLN:H	1:F:314:GLN:NE2	1.88	0.71
1:E:525:VAL:HG23	1:E:632:PHE:HB2	1.71	0.71
1:A:48:VAL:HG11	1:A:141:LEU:HD11	1.72	0.71
1:F:232:ILE:HD13	1:F:232:ILE:N	2.06	0.70
2:C:507:THR:HG21	2:C:564:THR:HG23	1.72	0.70
1:F:506:ASN:HD22	1:F:507:HIS:H	1.37	0.70
2:D:23:LYS:HG2	2:D:575:GLU:OE1	1.90	0.70
2:C:340:TYR:HB3	2:C:346:PHE:CD2	2.22	0.70
2:C:202:GLN:HG3	2:C:493:GLY:CA	2.22	0.70
1:A:506:ASN:HD22	1:A:507:HIS:H	1.38	0.70
2:B:349:PHE:H	2:C:343:GLN:HE22	1.39	0.70
2:B:303:ASN:HB2	1:F:173:MET:HE1	1.73	0.70
1:E:506:ASN:ND2	1:E:507:HIS:H	1.88	0.69
2:C:507:THR:CG2	2:C:564:THR:HG23	2.22	0.69
2:C:502:ASN:ND2	2:C:503:HIS:H	1.90	0.69
2:B:283:GLY:CA	2:B:532:GLU:HG2	2.22	0.69
2:B:210:SER:OG	2:B:227:GLU:OE2	2.10	0.69
1:A:555:TRP:HH2	1:A:647:LEU:HD12	1.57	0.69
2:B:165:GLN:HG3	2:B:479:THR:HG22	1.73	0.69
2:C:202:GLN:CG	2:C:493:GLY:HA2	2.23	0.69
2:C:21:GLU:OE1	2:C:21:GLU:HA	1.92	0.69
2:C:512:ILE:HD12	2:C:563:ILE:HD12	1.75	0.69
1:A:470:THR:OG1	1:A:679:HIS:HD2	1.76	0.69
1:F:190:ASN:ND2	1:F:193:ALA:H	1.89	0.69
1:A:307:THR:O	1:A:309:PHE:N	2.26	0.69
2:D:72:ASN:ND2	2:D:75:ALA:H	1.90	0.68
1:F:298:LYS:HG2	1:F:318:TYR:CE2	2.28	0.68
2:B:632:PRO:HB2	2:B:634:GLU:OE2	1.93	0.68
1:A:314:GLN:H	2:D:311:GLN:HE22	1.41	0.68
1:E:100:PHE:HD1	1:E:392:VAL:HG22	1.57	0.68
1:E:35:VAL:HG22	1:E:591:LEU:HD23	1.74	0.68
2:D:299:LEU:HB3	2:D:311:GLN:HG2	1.76	0.68
2:B:467:THR:OG1	2:B:675:HIS:HD2	1.77	0.68
1:F:91:MET:HE1	1:F:97:PHE:HB2	1.75	0.68
1:F:271:GLN:HE22	1:F:552:GLU:H	1.38	0.68
1:A:91:MET:HE1	1:A:97:PHE:HD2	1.58	0.68
2:B:645:ASN:H	2:B:645:ASN:ND2	1.91	0.68
1:E:234:MET:HE1	1:E:611:LEU:HD13	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:476:GLU:HG2	1:F:501:ARG:HG2	1.75	0.67
1:F:232:ILE:CD1	1:F:232:ILE:H	1.94	0.67
1:F:465:VAL:HG21	1:F:675:ILE:HD11	1.76	0.67
2:B:615:ASP:H	2:D:615:ASP:CB	2.05	0.67
2:D:247:ASN:ND2	2:D:247:ASN:C	2.46	0.67
1:E:67:GLU:HG2	1:E:83:LEU:HD21	1.77	0.67
2:D:91:ASN:H	2:D:134:GLN:HE22	1.43	0.67
2:B:450:LEU:CB	2:B:663:GLN:HE21	2.08	0.67
1:A:98:SER:O	1:A:104:MET:HE3	1.93	0.67
2:D:349:PHE:O	2:D:350:ASP:HB2	1.94	0.67
1:E:640:ALA:H	1:E:641:PRO:CD	2.06	0.66
1:E:38:GLN:HE22	1:E:158:VAL:H	1.43	0.66
2:D:134:GLN:N	2:D:134:GLN:HE21	1.84	0.66
1:E:506:ASN:HD22	1:E:507:HIS:N	1.91	0.66
2:D:247:ASN:HD22	2:D:248:SER:N	1.94	0.66
2:C:467:THR:OG1	2:C:675:HIS:HD2	1.79	0.66
2:C:429:LYS:O	2:C:433:GLN:HG2	1.94	0.66
1:F:531:ALA:HB3	1:F:550:PHE:CE2	2.30	0.66
1:E:640:ALA:N	1:E:641:PRO:CD	2.59	0.66
2:C:35:GLN:HE21	2:C:592:ILE:HD11	1.60	0.66
1:E:361:PRO:O	1:E:364:ILE:HG13	1.95	0.66
1:F:66:ILE:HB	1:F:83:LEU:HD21	1.78	0.66
2:B:523:LYS:HE2	2:B:548:GLU:OE2	1.95	0.66
1:A:50:GLN:HE22	1:A:485:PHE:H	1.42	0.66
2:B:539:LEU:HD13	2:B:656:VAL:HG11	1.77	0.65
1:F:38:GLN:HE22	1:F:158:VAL:H	1.44	0.65
1:F:506:ASN:ND2	1:F:507:HIS:H	1.93	0.65
1:F:470:THR:OG1	1:F:679:HIS:HD2	1.78	0.65
2:C:516:VAL:CG1	2:C:518:THR:HG22	2.27	0.65
2:C:99:GLU:O	2:C:103:GLU:HG2	1.97	0.65
2:B:95:SER:H	2:B:101:MET:HE1	1.56	0.65
2:B:502:ASN:ND2	2:B:503:HIS:H	1.88	0.65
1:F:584:MET:HA	1:F:587:ILE:HD12	1.79	0.65
2:D:210:SER:OG	2:D:227:GLU:OE2	2.14	0.65
2:B:408:ILE:HG21	1:F:302:TYR:OH	1.97	0.65
2:D:166:TYR:CD1	2:D:416:GLN:HG3	2.32	0.64
2:D:185:CYS:HG	2:D:191:CYS:HG	1.46	0.64
2:D:346:PHE:HB3	2:D:353:ILE:HD11	1.79	0.64
2:C:516:VAL:HG12	2:C:518:THR:HG22	1.80	0.64
2:D:93:GLU:HG2	2:D:304:SER:HB2	1.78	0.64
1:E:628:PHE:HE1	1:E:654:PHE:CE2	2.15	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:181:MET:CE	1:E:484:TYR:H	2.09	0.64
1:A:526:VAL:HG22	1:A:629:VAL:HG22	1.80	0.64
2:B:96:ILE:HD13	2:B:139:TYR:CE2	2.33	0.64
2:C:529:LYS:NZ	2:C:670:LYS:HE3	2.12	0.64
2:C:347:LYS:HB3	2:C:352:LYS:HA	1.80	0.64
1:E:91:MET:SD	1:E:104:MET:CE	2.86	0.63
2:B:181:MET:CE	1:F:483:VAL:HG13	2.29	0.63
2:C:35:GLN:HE22	2:C:155:VAL:H	1.46	0.63
2:D:35:GLN:NE2	2:D:39:LEU:HG	2.14	0.63
1:F:307:THR:CG2	1:F:309:PHE:H	2.11	0.63
2:D:142:TYR:CD2	2:D:156:LEU:HD13	2.34	0.63
1:A:687:LYS:HA	1:A:690:ILE:CD1	2.29	0.62
1:E:163:TYR:CD1	1:E:232:ILE:HG23	2.35	0.62
2:B:66:SER:HB2	2:B:69:CYS:SG	2.40	0.62
1:A:314:GLN:H	2:D:311:GLN:NE2	1.96	0.62
1:F:469:THR:HG21	1:F:680:GLU:HG3	1.81	0.62
2:B:408:ILE:CG2	1:F:302:TYR:OH	2.47	0.62
2:C:344:GLY:HA2	2:C:355:LEU:HD12	1.81	0.62
1:F:221:GLU:HB3	1:F:285:LEU:HD21	1.82	0.62
1:E:457:GLY:O	1:E:518:SER:HA	2.00	0.62
1:F:307:THR:HG22	1:F:310:THR:N	2.14	0.62
1:A:640:ALA:H	1:A:641:PRO:CD	2.13	0.62
1:F:173:MET:O	1:F:177:GLN:HG2	2.00	0.61
2:B:305:PHE:CD2	2:B:305:PHE:N	2.68	0.61
1:A:314:GLN:HE22	2:D:311:GLN:N	1.90	0.61
2:D:225:LEU:HD22	2:D:231:LEU:HD22	1.80	0.61
1:A:535:ASP:HB3	1:A:541:LEU:HD21	1.83	0.61
1:F:245:LEU:HD21	1:F:251:SER:HB3	1.83	0.61
1:E:50:GLN:NE2	1:E:485:PHE:H	1.96	0.61
2:B:213:LEU:HG	8:F:904:HOH:O	2.00	0.61
2:C:346:PHE:HE1	2:C:353:ILE:HB	1.65	0.61
1:A:98:SER:H	1:A:104:MET:HE3	1.65	0.61
2:B:542:ASN:ND2	2:B:545:ASN:HD22	1.98	0.61
2:D:459:ASP:OD1	2:D:461:LYS:HE3	2.00	0.61
2:B:211:ASN:OD1	2:B:213:LEU:HB3	2.00	0.61
2:B:165:GLN:HG3	2:B:479:THR:HG21	1.83	0.61
2:D:542:ASN:HD22	2:D:545:ASN:HD22	1.49	0.61
2:C:516:VAL:HG12	2:C:518:THR:CG2	2.31	0.60
2:C:392:ARG:NH2	2:C:418:SER:OG	2.34	0.60
1:F:347:ASP:OD1	1:F:444:TYR:HE2	1.84	0.60
2:B:450:LEU:HB2	2:B:663:GLN:NE2	2.15	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:247:ASN:ND2	2:B:249:GLY:N	2.48	0.60
2:B:531:ASP:OD2	2:B:533:ASN:HB2	2.01	0.60
2:C:206:TYR:CE2	2:C:497:ARG:HD2	2.36	0.60
1:A:230:GLU:HG2	1:A:423:ARG:NH1	2.17	0.60
2:C:185:CYS:HG	2:C:191:CYS:HG	1.49	0.60
1:A:94:ASN:ND2	2:D:194:TYR:OH	2.35	0.60
2:B:173:LYS:HE2	2:B:177:ASP:OD2	2.02	0.60
2:D:465:MET:CE	2:D:673:VAL:HG22	2.32	0.60
2:B:93:GLU:HG2	2:B:304:SER:HB2	1.83	0.60
2:D:145:ILE:HG21	2:D:156:LEU:HD21	1.82	0.60
2:C:210:SER:OG	2:C:227:GLU:OE2	2.20	0.60
1:A:630:TYR:HB2	1:A:631:PRO:CD	2.32	0.60
2:C:181:MET:HE1	1:E:484:TYR:H	1.66	0.59
2:C:507:THR:CG2	2:C:564:THR:CG2	2.78	0.59
2:B:217:ASN:HD21	2:B:219:GLU:HB2	1.66	0.59
2:B:502:ASN:ND2	2:B:503:HIS:N	2.49	0.59
1:F:422:LEU:HD22	1:F:427:PHE:CE2	2.37	0.59
2:B:305:PHE:HA	1:F:177:GLN:HG3	1.85	0.59
2:B:392:ARG:NH2	2:B:418:SER:OG	2.35	0.59
2:C:247:ASN:HD22	2:C:247:ASN:N	1.99	0.59
1:A:190:ASN:HD22	1:A:190:ASN:C	2.06	0.59
1:E:257:LEU:HD11	1:E:264:VAL:HG21	1.84	0.59
1:E:260:ARG:HD3	1:E:263:GLU:OE1	2.03	0.59
1:F:446:LYS:HD3	1:F:446:LYS:H	1.68	0.59
1:E:307:THR:O	1:E:309:PHE:N	2.36	0.59
2:B:217:ASN:HD22	2:B:219:GLU:H	1.51	0.59
2:C:663:GLN:HB2	2:C:666:MET:CE	2.32	0.58
1:E:91:MET:SD	1:E:104:MET:HE3	2.44	0.58
2:B:531:ASP:CG	2:B:533:ASN:HB2	2.24	0.58
1:F:643:GLU:HB3	1:F:645:PHE:HB2	1.84	0.58
1:F:646:VAL:C	1:F:648:ASP:H	2.06	0.58
1:A:267:TYR:OH	1:A:552:GLU:OE1	2.19	0.58
1:E:91:MET:SD	1:E:104:MET:HE2	2.44	0.58
2:D:247:ASN:ND2	2:D:249:GLY:H	2.00	0.58
2:D:312:ARG:HH22	2:D:421:ASP:CG	2.07	0.58
2:D:268:GLN:NE2	2:D:548:GLU:H	1.96	0.58
2:B:217:ASN:ND2	2:B:219:GLU:H	2.00	0.58
2:B:463:ASP:HB2	2:B:506:PHE:HB2	1.85	0.58
2:C:502:ASN:HD22	2:C:503:HIS:N	1.97	0.58
2:B:145:ILE:HG23	2:B:151:THR:CG2	2.33	0.58
1:E:566:LYS:HD3	1:E:568:ILE:HD11	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:582:VAL:HG12	1:E:586:GLU:HB3	1.85	0.58
1:A:642:PHE:O	1:A:643:GLU:CG	2.51	0.57
1:F:50:GLN:HE22	1:F:485:PHE:H	1.52	0.57
2:C:290:TRP:HB3	2:C:327:ILE:HG12	1.86	0.57
2:C:93:GLU:HG2	2:C:304:SER:HB2	1.85	0.57
2:D:599:SER:HB3	2:D:639:LYS:HE3	1.86	0.57
2:B:332:ILE:CG1	2:C:335:LYS:HG2	2.27	0.57
2:B:388:GLU:O	2:B:392:ARG:HG3	2.05	0.57
2:C:525:PHE:CE2	2:C:548:GLU:HG3	2.39	0.57
1:F:283:ASN:OD1	1:F:615:ARG:NH2	2.38	0.57
1:E:67:GLU:HG3	1:E:83:LEU:HD21	1.87	0.57
1:F:267:TYR:OH	1:F:552:GLU:OE1	2.23	0.57
2:D:283:GLY:HA2	2:D:532:GLU:CG	2.31	0.57
2:B:661:PHE:HA	2:B:666:MET:HE1	1.86	0.57
2:D:503:HIS:HD2	2:D:504:LYS:O	1.88	0.57
1:E:495:VAL:HG23	1:E:496:HIS:CD2	2.40	0.56
1:A:687:LYS:HA	1:A:690:ILE:HD12	1.87	0.56
2:B:429:LYS:O	2:B:433:GLN:HG2	2.06	0.56
2:D:344:GLY:HA2	2:D:355:LEU:HD12	1.85	0.56
1:F:170:PHE:HB3	1:F:232:ILE:HG22	1.86	0.56
2:D:388:GLU:O	2:D:392:ARG:HG3	2.05	0.56
1:A:160:PRO:HB3	1:A:584:MET:HG3	1.86	0.56
1:F:24:THR:HG22	1:F:24:THR:O	2.05	0.56
1:A:257:LEU:O	1:A:257:LEU:HG	2.04	0.56
1:E:347:ASP:OD1	1:E:444:TYR:HE2	1.89	0.56
2:C:145:ILE:HG23	2:C:151:THR:HG22	1.85	0.56
1:E:615:ARG:HG2	1:E:679:HIS:CD2	2.41	0.56
2:B:358:SER:C	2:B:360:ALA:H	2.08	0.56
1:E:205:TYR:CE2	1:E:499:LYS:HE3	2.40	0.56
1:E:245:LEU:HB2	1:E:642:PHE:HE1	1.70	0.56
2:D:177:ASP:O	2:D:181:MET:HG3	2.05	0.56
2:C:603:MET:HG2	2:C:604:PRO:HD2	1.88	0.56
2:D:331:ASP:OD2	1:E:338:LYS:HE2	2.04	0.56
2:B:261:ILE:HG12	2:B:648:PHE:CE1	2.41	0.56
2:D:346:PHE:O	2:D:353:ILE:HG13	2.06	0.56
1:A:221:GLU:HB3	1:A:285:LEU:HD21	1.87	0.56
1:E:168:LYS:NZ	1:E:308:LYS:HE3	2.21	0.56
1:A:271:GLN:HE22	1:A:552:GLU:N	1.98	0.56
2:B:141:TYR:O	2:B:145:ILE:HD12	2.05	0.56
2:B:358:SER:C	2:B:360:ALA:N	2.59	0.56
1:A:570:ASN:OD1	1:A:572:ASN:HB2	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:638:ASP:HB2	1:F:647:LEU:HD22	1.87	0.55
2:D:222:ILE:CG2	2:D:222:ILE:O	2.54	0.55
2:C:222:ILE:HG22	2:C:226:THR:HG23	1.88	0.55
2:C:349:PHE:O	2:C:350:ASP:HB2	2.05	0.55
1:A:98:SER:H	1:A:104:MET:CE	2.19	0.55
1:E:628:PHE:HE1	1:E:654:PHE:HE2	1.52	0.55
1:A:212:TYR:HB3	1:A:226:THR:HG22	1.86	0.55
1:A:244:HIS:HD2	1:A:642:PHE:CE1	2.25	0.55
1:A:283:ASN:OD1	1:A:615:ARG:NH2	2.39	0.55
2:C:480:VAL:HA	1:E:184:MET:HE1	1.88	0.55
2:B:663:GLN:CG	2:B:666:MET:HE2	2.33	0.55
2:B:522:VAL:HG22	2:B:625:VAL:HG22	1.89	0.55
1:F:686:TYR:CE2	1:F:687:LYS:HD2	2.41	0.55
1:A:145:TYR:OH	1:A:160:PRO:O	2.24	0.55
2:D:551:TRP:C	2:D:551:TRP:CD1	2.80	0.55
2:C:268:GLN:HE22	2:C:548:GLU:N	1.95	0.55
2:B:667:PHE:HE2	2:B:669:LYS:HG3	1.72	0.55
1:F:541:LEU:HD13	1:F:546:ASN:HB3	1.88	0.55
1:F:422:LEU:N	1:F:422:LEU:HD23	2.22	0.55
1:E:581:SER:HB2	1:E:600:MET:SD	2.47	0.55
2:D:551:TRP:CH2	2:D:644:ASP:HB2	2.42	0.54
2:B:217:ASN:HD22	2:B:217:ASN:C	2.10	0.54
2:D:513:LYS:NZ	2:D:560:GLN:HE21	2.06	0.54
1:F:111:LEU:HD22	1:F:135:LEU:HD12	1.89	0.54
1:A:642:PHE:C	1:A:643:GLU:HG3	2.27	0.54
2:D:678:GLU:HG3	2:D:691:PRO:HB3	1.89	0.54
1:F:291:PHE:HB2	1:F:297:ILE:HG22	1.90	0.54
2:B:661:PHE:HA	2:B:666:MET:CE	2.37	0.54
1:F:395:ARG:NH2	1:F:421:SER:OG	2.41	0.54
2:D:145:ILE:HG23	2:D:151:THR:HG22	1.90	0.54
2:D:285:ILE:HD12	2:D:429:LYS:HG2	1.89	0.54
1:E:185:GLN:NE2	1:E:189:ILE:HD12	2.23	0.54
2:D:462:VAL:HG12	2:D:463:ASP:O	2.08	0.54
1:A:265:TYR:CE1	1:A:372:GLN:HB2	2.43	0.54
2:C:275:MET:CE	2:C:545:ASN:O	2.56	0.54
1:E:190:ASN:HB3	1:E:193:ALA:HB3	1.90	0.53
2:D:83:TYR:HA	2:D:87:PHE:CE1	2.43	0.53
1:A:75:ASN:ND2	1:A:78:ALA:N	2.50	0.53
1:A:173:MET:HE2	1:A:306:LEU:HD21	1.89	0.53
1:F:166:TYR:HB3	1:F:169:MET:HG3	1.89	0.53
2:B:67:LYS:HG2	2:B:76:TYR:CE2	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:47:GLU:O	2:D:129:ARG:NH2	2.41	0.53
2:D:636:GLU:H	2:D:636:GLU:CD	2.12	0.53
1:E:35:VAL:HG22	1:E:591:LEU:CD2	2.37	0.53
1:A:525:VAL:HG23	1:A:632:PHE:HB2	1.90	0.53
1:E:301:TYR:CD2	1:E:303:PRO:HD3	2.43	0.53
2:C:346:PHE:CE1	2:C:353:ILE:HB	2.43	0.53
1:F:465:VAL:HG21	1:F:675:ILE:CD1	2.39	0.53
1:E:335:THR:OG1	1:F:338:LYS:HG2	2.08	0.53
2:B:218:ASN:HB3	2:B:282:LEU:HD21	1.91	0.52
1:E:234:MET:CE	1:E:611:LEU:HD13	2.39	0.52
1:F:307:THR:HG22	1:F:309:PHE:N	2.23	0.52
2:B:94:PHE:HA	2:B:101:MET:HE3	1.91	0.52
2:C:624:PHE:CE1	2:C:626:TYR:CD2	2.98	0.52
1:F:214:ASN:HA	1:F:217:LEU:O	2.08	0.52
2:C:510:ILE:HD11	2:C:524:MET:CE	2.39	0.52
2:B:174:ASN:ND2	1:F:308:LYS:HA	2.25	0.52
2:D:464:LYS:HD3	2:D:466:VAL:CG2	2.39	0.52
1:A:190:ASN:HD22	1:A:193:ALA:H	1.55	0.52
2:C:83:TYR:HA	2:C:87:PHE:HE1	1.74	0.52
2:C:502:ASN:ND2	2:C:503:HIS:N	2.58	0.52
1:A:470:THR:OG1	1:A:679:HIS:CD2	2.61	0.52
1:A:476:GLU:HG2	1:A:501:ARG:HG3	1.91	0.52
2:B:303:ASN:HB2	1:F:173:MET:CE	2.39	0.52
2:B:304:SER:O	2:B:305:PHE:C	2.47	0.52
1:F:100:PHE:HD1	1:F:392:VAL:HG22	1.74	0.52
1:F:506:ASN:HD22	1:F:507:HIS:N	2.06	0.52
2:B:531:ASP:OD1	2:B:533:ASN:HB2	2.10	0.52
2:B:533:ASN:HB3	2:B:535:PHE:HB2	1.91	0.52
1:E:646:VAL:C	1:E:648:ASP:H	2.13	0.52
1:E:459:LYS:HG3	1:E:668:PRO:HB3	1.92	0.52
1:F:93:LYS:O	1:F:94:ASN:HB2	2.09	0.52
2:C:145:ILE:HG23	2:C:151:THR:CG2	2.40	0.51
1:F:278:PHE:CE1	1:F:532:PRO:HG3	2.44	0.51
1:E:70:MET:HG3	1:E:79:VAL:HG11	1.92	0.51
2:D:455:LEU:C	2:D:455:LEU:HD23	2.31	0.51
1:A:505:LEU:O	1:A:610:ARG:HD3	2.10	0.51
2:D:91:ASN:H	2:D:134:GLN:NE2	2.08	0.51
1:F:495:VAL:HG12	1:F:495:VAL:O	2.10	0.51
2:D:465:MET:HE3	2:D:673:VAL:HG22	1.91	0.51
2:D:222:ILE:HG22	2:D:222:ILE:O	2.09	0.51
1:A:164:GLU:OE2	1:A:583:PRO:HA	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:343:GLN:NE2	2:D:343:GLN:CA	2.68	0.51
2:D:290:TRP:HB3	2:D:327:ILE:HG12	1.92	0.51
4:B:802:NAG:H61	4:B:803:BMA:C1	2.41	0.51
2:B:615:ASP:HB2	2:D:615:ASP:HB3	1.92	0.51
1:E:686:TYR:CD2	1:E:686:TYR:C	2.84	0.51
2:D:214:THR:HB	2:D:299:LEU:O	2.11	0.51
1:A:444:TYR:HD1	1:A:444:TYR:N	2.09	0.51
2:B:645:ASN:N	2:B:645:ASN:ND2	2.56	0.51
2:D:349:PHE:O	2:D:350:ASP:CB	2.59	0.51
2:C:312:ARG:NH2	2:C:421:ASP:OD2	2.43	0.51
2:B:275:MET:HG2	2:B:619:PHE:CE1	2.45	0.51
1:F:94:ASN:H	1:F:137:GLN:HE22	1.58	0.51
1:A:640:ALA:H	1:A:641:PRO:HD2	1.75	0.51
2:B:217:ASN:HD22	2:B:219:GLU:N	2.09	0.50
2:B:245:TRP:HA	2:B:380:LEU:HG	1.93	0.50
2:C:533:ASN:HD21	1:F:214:ASN:HD22	1.58	0.50
2:C:578:LEU:HD12	2:C:593:PRO:HG3	1.94	0.50
2:C:330:LEU:O	2:C:334:GLU:HG3	2.10	0.50
2:C:47:GLU:O	2:C:129:ARG:NH2	2.44	0.50
1:F:190:ASN:ND2	1:F:193:ALA:N	2.60	0.50
2:C:475:ASP:OD1	2:C:477:PHE:HB3	2.10	0.50
1:E:615:ARG:HG2	1:E:679:HIS:HD2	1.74	0.50
1:A:181:VAL:O	1:A:185:GLN:HG3	2.12	0.50
1:A:217:LEU:HD21	1:A:302:TYR:HB3	1.93	0.50
2:B:663:GLN:H	2:B:666:MET:CE	2.25	0.50
2:B:222:ILE:HD11	2:B:282:LEU:CD1	2.39	0.50
1:E:234:MET:O	1:E:237:TYR:HB3	2.11	0.50
2:C:480:VAL:HG12	1:E:184:MET:HE1	1.93	0.50
1:F:278:PHE:HE1	1:F:532:PRO:HG3	1.76	0.49
2:D:533:ASN:OD1	2:D:535:PHE:HD1	1.95	0.49
2:B:44:ASN:HD22	2:B:487:LEU:HD21	1.76	0.49
2:C:529:LYS:HZ2	2:C:670:LYS:HE3	1.77	0.49
2:C:180:LYS:HE3	2:C:481:TYR:O	2.12	0.49
2:D:173:LYS:HA	2:D:176:MET:HE2	1.93	0.49
2:D:502:ASN:HD22	2:D:503:HIS:H	1.59	0.49
2:B:321:GLU:HA	2:B:324:TYR:CE1	2.47	0.49
2:B:631:THR:HG21	2:B:645:ASN:OD1	2.13	0.49
2:B:94:PHE:HA	2:B:101:MET:CE	2.42	0.49
2:D:332:ILE:HG21	1:E:341:VAL:HB	1.95	0.49
2:C:678:GLU:OE1	2:C:683:LEU:HD13	2.12	0.49
1:F:458:VAL:HG22	1:F:518:SER:HB2	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:299:LEU:HD23	1:F:411:MET:SD	2.53	0.49
1:E:485:PHE:CD1	1:E:495:VAL:HG12	2.47	0.49
1:E:552:GLU:HG2	1:E:576:ILE:HD13	1.95	0.49
1:F:450:GLN:H	1:F:664:LEU:HD22	1.77	0.49
2:C:636:GLU:HB3	2:C:637:PRO:HD2	1.94	0.49
1:E:307:THR:HG23	1:E:309:PHE:H	1.76	0.49
2:D:217:ASN:ND2	2:D:219:GLU:H	2.04	0.49
1:A:100:PHE:HD1	1:A:392:VAL:HG22	1.77	0.49
1:A:559:LYS:N	1:A:559:LYS:HD3	2.28	0.49
2:C:31:PHE:CE2	2:C:592:ILE:HD12	2.48	0.49
1:A:444:TYR:N	1:A:444:TYR:CD1	2.80	0.49
2:B:631:THR:O	2:B:632:PRO:O	2.29	0.49
2:B:210:SER:HB2	2:B:214:THR:CB	2.43	0.49
1:E:267:TYR:OH	1:E:552:GLU:OE1	2.29	0.49
2:C:678:GLU:HB2	2:C:684:PHE:CE1	2.47	0.49
1:F:159:VAL:CG1	1:F:160:PRO:HD2	2.43	0.49
1:A:646:VAL:C	1:A:648:ASP:H	2.16	0.49
1:A:202:GLU:O	1:A:203:ASN:HB2	2.12	0.49
2:C:214:THR:HB	2:C:299:LEU:O	2.13	0.49
1:F:469:THR:CG2	1:F:680:GLU:HG3	2.43	0.49
1:A:84:LYS:HG3	1:A:87:ARG:NH2	2.28	0.49
2:B:145:ILE:HG23	2:B:151:THR:HG22	1.95	0.48
2:B:151:THR:O	2:B:151:THR:HG22	2.13	0.48
1:F:52:ASN:OD1	1:F:54:ASP:HB2	2.13	0.48
2:B:465:MET:HE3	2:B:671:VAL:HB	1.94	0.48
2:B:332:ILE:HD11	2:C:338:PHE:CD1	2.48	0.48
2:C:222:ILE:O	2:C:222:ILE:HG22	2.13	0.48
1:F:430:LEU:O	1:F:433:ARG:HB3	2.14	0.48
1:F:577:PHE:CZ	1:F:612:MET:HG3	2.47	0.48
1:F:67:GLU:HG2	1:F:83:LEU:HD13	1.95	0.48
2:C:663:GLN:HB2	2:C:666:MET:HE2	1.94	0.48
2:C:241:HIS:CE1	2:C:601:ASP:HB3	2.48	0.48
2:D:328:ARG:HD2	1:E:437:TYR:OH	2.13	0.48
1:E:91:MET:HE3	1:E:97:PHE:HB2	1.96	0.48
2:C:344:GLY:HA2	2:C:355:LEU:CD1	2.42	0.48
1:A:214:ASN:O	1:E:537:ASN:ND2	2.36	0.48
2:B:168:VAL:HG13	2:B:172:VAL:HB	1.96	0.48
1:E:190:ASN:HD22	1:E:190:ASN:C	2.17	0.48
1:E:231:ASP:OD2	1:E:504:ARG:NH1	2.46	0.48
2:B:615:ASP:CA	2:D:615:ASP:HB3	2.43	0.48
2:D:151:THR:HA	2:D:154:PHE:HD2	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:529:LYS:HE2	2:B:670:LYS:HG2	1.96	0.48
1:A:48:VAL:HG13	1:A:141:LEU:HD11	1.92	0.48
2:D:145:ILE:CG1	2:D:151:THR:HG21	2.44	0.48
2:B:142:TYR:OH	2:B:157:PRO:O	2.26	0.48
2:C:192:TYR:HD1	2:C:197:ILE:CG2	2.26	0.48
2:B:404:GLN:HE21	2:B:404:GLN:HA	1.78	0.48
2:B:304:SER:O	2:B:306:TYR:HB2	2.13	0.48
2:B:181:MET:HE1	1:F:483:VAL:HA	1.96	0.48
1:F:159:VAL:HG12	1:F:160:PRO:HD2	1.96	0.48
2:C:326:GLU:O	2:C:330:LEU:HG	2.14	0.48
1:F:234:MET:O	1:F:237:TYR:HB3	2.13	0.48
1:A:506:ASN:HD22	1:A:507:HIS:N	2.08	0.47
1:F:643:GLU:HG3	1:F:645:PHE:HD1	1.79	0.47
2:B:304:SER:O	2:B:306:TYR:N	2.46	0.47
2:D:513:LYS:HZ2	2:D:560:GLN:HG2	1.79	0.47
1:A:326:ASN:ND2	1:A:397:VAL:HG13	2.29	0.47
1:A:167:PRO:HB2	1:A:171:MET:CE	2.44	0.47
1:F:638:ASP:CB	1:F:647:LEU:HA	2.39	0.47
2:B:408:ILE:HG21	1:F:302:TYR:CZ	2.49	0.47
2:D:542:ASN:ND2	2:D:545:ASN:HD22	2.13	0.47
2:B:141:TYR:CZ	2:B:145:ILE:HD11	2.50	0.47
1:E:517:ASP:OD1	1:E:564:GLN:HG2	2.14	0.47
2:B:614:TYR:HE1	2:B:679:LEU:HD12	1.79	0.47
2:C:46:ASN:OD1	2:C:46:ASN:N	2.40	0.47
1:E:173:MET:CG	1:E:306:LEU:HG	2.44	0.47
2:C:483:SER:OG	2:C:486:GLU:HG3	2.14	0.47
1:A:492:ASN:N	1:A:492:ASN:HD22	2.11	0.47
2:B:285:ILE:HD12	2:B:429:LYS:HG3	1.97	0.47
2:D:298:TYR:CE2	2:D:300:PRO:HG3	2.49	0.47
2:D:335:LYS:HB3	1:F:335:THR:HG23	1.96	0.47
1:F:154:CYS:HA	1:F:157:PHE:HD1	1.78	0.47
2:B:503:HIS:HD2	2:B:504:LYS:O	1.98	0.47
1:F:38:GLN:HE22	1:F:158:VAL:N	2.10	0.47
1:A:457:GLY:O	1:A:518:SER:HA	2.15	0.47
1:A:667:VAL:HG13	1:A:669:ASN:OD1	2.15	0.47
2:D:168:VAL:CG1	2:D:172:VAL:HB	2.45	0.47
1:F:623:PHE:CD2	1:F:677:ILE:HD12	2.49	0.47
2:B:657:LEU:HB3	2:B:659:GLN:HE22	1.79	0.47
2:C:451:HIS:ND1	2:C:663:GLN:NE2	2.61	0.47
1:E:57:TYR:CD1	1:E:57:TYR:C	2.88	0.47
1:F:305:MET:HB3	1:F:305:MET:HE3	1.63	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:218:TYR:OH	1:E:536:ASP:HB3	2.15	0.47
2:B:680:PHE:HB2	2:B:683:LEU:HD12	1.96	0.47
1:E:38:GLN:HE22	1:E:158:VAL:N	2.09	0.47
2:B:96:ILE:HD11	2:B:102:ARG:HG3	1.96	0.47
2:B:96:ILE:HG13	2:B:96:ILE:O	2.15	0.47
2:D:151:THR:HA	2:D:154:PHE:CD2	2.50	0.47
2:D:636:GLU:CB	2:D:637:PRO:CD	2.92	0.47
2:B:174:ASN:HD22	1:F:308:LYS:C	2.19	0.47
1:A:171:MET:HE1	1:A:479:ALA:HB1	1.97	0.47
1:A:658:ARG:HB2	1:A:659:PRO:HD2	1.97	0.47
2:C:642:VAL:O	2:C:644:ASP:N	2.47	0.47
2:C:451:HIS:HA	2:C:663:GLN:HG3	1.97	0.47
2:D:346:PHE:CB	2:D:353:ILE:HD11	2.45	0.47
1:E:646:VAL:HG21	1:E:652:LEU:HD21	1.96	0.47
2:B:182:MET:HE2	2:B:186:LEU:HG	1.97	0.47
2:D:41:LEU:HD22	2:D:129:ARG:HG2	1.97	0.46
1:E:217:LEU:HD21	1:E:302:TYR:HB3	1.98	0.46
1:F:648:ASP:C	1:F:650:LYS:H	2.19	0.46
1:A:79:VAL:O	1:A:83:LEU:HG	2.14	0.46
1:A:219:ASN:O	1:A:220:ASN:HB3	2.15	0.46
2:B:222:ILE:O	2:B:222:ILE:HG22	2.15	0.46
1:F:347:ASP:OD1	1:F:444:TYR:CE2	2.66	0.46
1:A:315:ARG:HH22	1:A:424:ASP:CG	2.17	0.46
1:F:596:VAL:HG12	1:F:597:PRO:HD2	1.98	0.46
2:C:206:TYR:CZ	2:C:497:ARG:HD2	2.51	0.46
2:C:83:TYR:HA	2:C:87:PHE:CE1	2.51	0.46
2:B:83:TYR:HB2	2:B:87:PHE:HE1	1.81	0.46
2:B:501:LEU:HG	2:B:502:ASN:N	2.30	0.46
2:B:181:MET:HE2	1:F:484:TYR:H	1.81	0.46
1:F:231:ASP:OD1	1:F:504:ARG:HD2	2.14	0.46
1:A:50:GLN:NE2	1:A:485:PHE:H	2.12	0.46
2:D:185:CYS:SG	2:D:191:CYS:SG	3.02	0.46
2:B:542:ASN:HD22	2:B:545:ASN:HD22	1.62	0.46
2:C:262:TYR:OH	2:C:388:GLU:OE1	2.26	0.46
1:E:339:THR:HG21	1:F:345:GLN:HE22	1.81	0.46
1:F:682:GLU:HB2	1:F:688:PHE:CE1	2.51	0.46
2:B:44:ASN:O	2:B:46:ASN:N	2.49	0.46
2:B:182:MET:CE	2:B:186:LEU:HG	2.46	0.46
1:A:465:VAL:HG12	1:A:466:ASP:O	2.16	0.46
1:A:615:ARG:HG3	1:A:679:HIS:CD2	2.51	0.46
2:B:145:ILE:HG23	2:B:151:THR:HG21	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:678:GLU:OE1	2:D:683:LEU:HD13	2.16	0.46
2:B:93:GLU:CG	2:B:304:SER:HB2	2.46	0.45
1:A:535:ASP:OD1	1:A:539:ILE:HD12	2.16	0.45
2:C:62:ASN:OD1	2:C:64:GLU:HG3	2.15	0.45
2:B:599:SER:HA	2:B:639:LYS:HD3	1.98	0.45
1:F:232:ILE:HD12	1:F:502:GLN:OE1	2.17	0.45
1:F:476:GLU:HA	1:F:500:VAL:O	2.15	0.45
1:A:667:VAL:CG1	1:A:669:ASN:OD1	2.64	0.45
1:F:578:LYS:HG2	1:F:606:TYR:HB2	1.98	0.45
1:A:102:ASP:HB3	1:A:385:ASP:OD2	2.16	0.45
2:C:72:ASN:HD21	2:C:74:LYS:HB3	1.81	0.45
2:C:35:GLN:NE2	2:C:155:VAL:HB	2.31	0.45
2:C:349:PHE:O	2:C:350:ASP:CB	2.64	0.45
1:E:643:GLU:HB3	1:E:645:PHE:HB2	1.97	0.45
1:E:568:ILE:N	1:E:568:ILE:HD12	2.31	0.45
2:D:690:THR:HA	2:D:691:PRO:HD3	1.63	0.45
4:B:802:NAG:C6	4:B:803:BMA:C1	2.94	0.45
2:C:283:GLY:HA2	2:C:532:GLU:CG	2.34	0.45
2:C:542:ASN:HD22	2:C:545:ASN:ND2	2.05	0.45
2:C:273:TYR:CE1	2:C:277:ARG:HD2	2.52	0.45
1:F:181:VAL:O	1:F:185:GLN:HG3	2.16	0.45
2:C:513:LYS:HA	2:C:559:GLY:O	2.17	0.45
1:E:507:HIS:HD2	1:E:508:SER:O	2.00	0.45
2:D:247:ASN:HD22	2:D:249:GLY:H	1.63	0.45
1:A:91:MET:HE1	1:A:97:PHE:CD2	2.44	0.45
2:C:529:LYS:HZ3	2:C:670:LYS:HE3	1.78	0.45
2:B:603:MET:HG2	2:B:604:PRO:HD2	1.99	0.45
2:B:347:LYS:HA	2:B:351:LYS:O	2.16	0.45
2:B:467:THR:OG1	2:B:675:HIS:CD2	2.65	0.45
1:A:582:VAL:HG12	1:A:583:PRO:HD2	1.98	0.45
1:E:331:ARG:HD2	1:F:437:TYR:OH	2.16	0.45
2:D:657:LEU:HB3	2:D:659:GLN:NE2	2.32	0.45
2:B:27:VAL:HG21	2:B:592:ILE:HG12	1.98	0.45
2:D:253:ALA:O	2:D:256:GLU:HG2	2.16	0.45
1:E:77:LYS:N	1:E:77:LYS:HD2	2.31	0.45
2:D:636:GLU:HB3	2:D:637:PRO:HD3	1.99	0.45
1:A:38:GLN:NE2	1:A:158:VAL:HB	2.32	0.45
1:E:476:GLU:HA	1:E:500:VAL:O	2.17	0.45
2:C:480:VAL:HG12	1:E:184:MET:CE	2.47	0.45
2:D:467:THR:OG1	2:D:675:HIS:HD2	1.99	0.45
1:E:72:ASN:HA	1:E:119:LYS:HE2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:636:GLU:CD	2:C:636:GLU:H	2.19	0.44
1:A:27:THR:HG23	1:A:28:LYS:N	2.32	0.44
1:A:391:GLU:OE2	1:A:431:TYR:OH	2.31	0.44
2:C:455:LEU:HD12	2:C:456:LYS:N	2.32	0.44
2:B:35:GLN:HE22	2:B:155:VAL:N	2.03	0.44
2:B:311:GLN:NE2	1:F:314:GLN:H	2.14	0.44
1:E:234:MET:HB2	1:E:234:MET:HE2	1.78	0.44
1:A:632:PHE:O	1:A:632:PHE:CG	2.71	0.44
2:C:408:ILE:HG21	1:E:302:TYR:OH	2.17	0.44
2:D:202:GLN:OE1	2:D:495:LYS:HE3	2.18	0.44
2:D:343:GLN:HE21	2:D:343:GLN:CA	2.03	0.44
1:F:541:LEU:HD13	1:F:546:ASN:CB	2.47	0.44
2:C:180:LYS:HG2	1:E:184:MET:HE2	1.98	0.44
1:E:141:LEU:O	1:E:145:TYR:HB2	2.17	0.44
1:F:576:ILE:HG22	1:F:576:ILE:O	2.17	0.44
2:C:512:ILE:HD12	2:C:563:ILE:CD1	2.44	0.44
2:D:332:ILE:HG12	1:E:342:GLN:HG3	1.99	0.44
1:F:391:GLU:O	1:F:395:ARG:HG3	2.16	0.44
2:B:525:PHE:HB2	2:B:622:PHE:HB3	1.99	0.44
2:B:540:GLU:HG3	2:B:658:PRO:HD3	1.98	0.44
2:B:213:LEU:CD2	1:F:411:MET:HB2	2.48	0.44
2:B:299:LEU:HD23	1:F:411:MET:HE3	1.99	0.44
1:A:244:HIS:HD2	1:A:642:PHE:CZ	2.36	0.44
1:E:458:VAL:HA	1:E:517:ASP:O	2.18	0.44
1:E:173:MET:HG2	1:E:306:LEU:HG	1.99	0.44
2:D:512:ILE:HD11	2:D:561:SER:OG	2.17	0.44
2:B:312:ARG:HD3	2:B:395:LEU:O	2.18	0.44
1:A:648:ASP:C	1:A:650:LYS:H	2.21	0.44
2:D:112:PHE:HE1	2:D:124:THR:HG22	1.82	0.44
2:D:347:LYS:HE3	2:D:352:LYS:HE3	1.99	0.44
2:B:311:GLN:HE22	1:F:314:GLN:H	1.66	0.44
2:D:174:ASN:O	2:D:178:TYR:CD1	2.71	0.44
1:A:75:ASN:HD21	1:A:78:ALA:H	1.61	0.44
1:F:679:HIS:HE1	1:F:682:GLU:O	2.01	0.44
2:B:686:ILE:HA	2:B:687:PRO:HD2	1.70	0.44
1:E:203:ASN:HD22	1:E:204:ASP:H	1.66	0.44
1:F:226:THR:O	1:F:230:GLU:HB2	2.18	0.44
1:F:122:GLU:O	1:F:126:LYS:HG3	2.18	0.44
2:C:106:ILE:HG22	2:C:110:LYS:HE3	1.99	0.44
2:D:93:GLU:CG	2:D:304:SER:HB2	2.45	0.44
2:C:151:THR:O	2:C:151:THR:HG22	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:253:LYS:HG2	1:A:253:LYS:O	2.16	0.44
2:B:329:PHE:HA	2:B:332:ILE:CD1	2.48	0.43
1:A:364:ILE:O	1:A:364:ILE:HD13	2.17	0.43
2:B:211:ASN:C	2:B:213:LEU:H	2.22	0.43
1:A:214:ASN:HA	1:A:217:LEU:O	2.18	0.43
1:A:340:PHE:O	1:A:343:PHE:HB2	2.17	0.43
1:E:24:THR:HG23	1:E:24:THR:O	2.17	0.43
1:F:640:ALA:H	1:F:641:PRO:CD	2.18	0.43
2:B:35:GLN:NE2	2:B:155:VAL:H	2.04	0.43
2:D:321:GLU:HA	2:D:324:TYR:CE1	2.53	0.43
2:B:322:LYS:NZ	2:B:398:ALA:O	2.50	0.43
2:C:525:PHE:HB2	2:C:622:PHE:HB3	2.01	0.43
2:C:666:MET:HB2	2:C:666:MET:HE2	1.36	0.43
2:C:35:GLN:HE22	2:C:155:VAL:HB	1.83	0.43
2:D:455:LEU:HD23	2:D:456:LYS:N	2.34	0.43
2:D:364:VAL:HG11	2:D:435:ILE:HG23	2.00	0.43
2:B:678:GLU:HB2	2:B:684:PHE:CE1	2.53	0.43
2:B:278:LEU:CD2	2:B:532:GLU:HG3	2.49	0.43
1:E:170:PHE:O	1:E:232:ILE:HD11	2.18	0.43
1:F:458:VAL:HG22	1:F:518:SER:CB	2.48	0.43
2:B:241:HIS:CE1	2:B:601:ASP:HB3	2.54	0.43
1:F:466:ASP:OD2	1:F:511:ASN:HB2	2.19	0.43
2:D:159:PRO:HD3	2:D:237:TYR:OH	2.19	0.43
2:C:629:GLU:HA	2:C:630:PRO:HD3	1.87	0.43
1:A:173:MET:HE2	1:A:306:LEU:CD2	2.48	0.43
1:F:28:LYS:HD2	1:F:598:PHE:HD1	1.84	0.43
1:F:276:TYR:CE1	1:F:280:ARG:HD2	2.54	0.43
2:B:531:ASP:OD1	2:B:533:ASN:CB	2.66	0.43
1:F:528:ILE:HG22	1:F:553:LEU:HD12	2.00	0.43
2:D:383:TYR:CZ	1:E:359:HIS:HE1	2.36	0.43
2:C:21:GLU:CA	2:C:21:GLU:OE1	2.66	0.43
1:A:455:PHE:CD2	1:A:630:TYR:HA	2.53	0.43
1:A:173:MET:CE	2:D:308:PRO:HD3	2.48	0.43
2:C:501:LEU:O	2:C:606:ARG:HB2	2.19	0.43
1:A:183:LYS:HG2	1:A:483:VAL:HG13	2.01	0.43
1:E:577:PHE:CZ	1:E:612:MET:HG3	2.53	0.43
2:B:323:ASN:ND2	2:B:394:VAL:HG13	2.33	0.43
2:B:115:ALA:HB3	2:B:148:ARG:NH1	2.34	0.43
2:C:247:ASN:ND2	2:C:247:ASN:N	2.66	0.43
1:F:543:LEU:HD23	1:F:543:LEU:HA	1.68	0.43
1:E:71:ASP:N	1:E:71:ASP:OD1	2.40	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:83:TYR:HB2	2:B:87:PHE:CE1	2.53	0.43
2:B:682:TYR:CD2	4:B:801:NAG:H62	2.53	0.43
1:F:164:GLU:OE2	1:F:583:PRO:HA	2.19	0.43
1:A:69:ASN:HB3	1:A:72:ASN:HD22	1.84	0.43
2:C:574:LYS:O	2:C:605:SER:HB2	2.18	0.43
2:B:329:PHE:O	2:B:332:ILE:HD12	2.19	0.42
1:A:298:LYS:HG2	1:A:318:TYR:HE2	1.78	0.42
2:D:543:TRP:CZ2	2:D:655:PRO:HD3	2.54	0.42
2:D:501:LEU:O	2:D:606:ARG:HB2	2.19	0.42
1:A:100:PHE:O	1:A:396:ARG:NH2	2.51	0.42
1:F:28:LYS:HZ2	1:F:598:PHE:HE1	1.66	0.42
1:F:516:VAL:HB	1:F:565:ASN:HD21	1.84	0.42
1:A:640:ALA:N	1:A:641:PRO:CD	2.82	0.42
1:A:630:TYR:HB2	1:A:631:PRO:HD2	2.01	0.42
2:D:636:GLU:HB3	2:D:637:PRO:CD	2.49	0.42
2:C:64:GLU:HG2	2:C:64:GLU:H	1.24	0.42
2:D:174:ASN:HB3	2:D:178:TYR:CE1	2.54	0.42
2:D:64:GLU:HA	2:D:80:MET:HE1	2.01	0.42
2:C:439:LYS:HD2	2:C:442:GLN:OE1	2.18	0.42
2:C:492:HIS:HB2	2:C:493:GLY:H	1.65	0.42
2:D:533:ASN:OD1	2:D:535:PHE:CD1	2.72	0.42
2:D:245:TRP:HA	2:D:380:LEU:HB2	2.02	0.42
2:D:228:ASP:OD2	2:D:500:ARG:NH1	2.52	0.42
2:C:43:TYR:CE1	2:C:580:MET:HE1	2.55	0.42
2:C:355:LEU:HD13	2:C:441:TYR:CD2	2.55	0.42
2:B:554:GLN:HG2	2:B:563:ILE:HD11	2.00	0.42
2:C:645:ASN:ND2	2:C:645:ASN:H	2.16	0.42
2:B:96:ILE:HD12	2:B:102:ARG:HA	2.02	0.42
2:D:580:MET:HA	2:D:583:ILE:HD12	2.00	0.42
2:B:329:PHE:HA	2:B:332:ILE:HD11	2.01	0.42
1:A:686:TYR:CD2	1:A:686:TYR:C	2.92	0.42
1:A:315:ARG:NH2	1:A:424:ASP:OD2	2.53	0.42
2:C:463:ASP:HB2	2:C:506:PHE:HB2	2.02	0.42
1:A:85:MET:O	1:A:88:THR:HB	2.20	0.42
2:B:332:ILE:HG12	2:C:335:LYS:CG	2.30	0.41
1:F:111:LEU:HD22	1:F:135:LEU:CD1	2.49	0.41
1:F:354:GLN:HB2	1:F:356:ILE:CD1	2.50	0.41
2:D:69:CYS:HB2	2:D:70:TYR:CE2	2.55	0.41
2:C:543:TRP:CZ2	2:C:655:PRO:HD3	2.55	0.41
1:A:541:LEU:HA	1:A:541:LEU:HD23	1.80	0.41
2:C:312:ARG:HH22	2:C:421:ASP:CG	2.22	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:352:LYS:NZ	2:D:352:LYS:HB2	2.34	0.41
2:D:472:PHE:HB3	2:D:500:ARG:HG3	2.01	0.41
1:F:170:PHE:HD2	1:F:232:ILE:HG22	1.84	0.41
2:B:181:MET:HE3	1:F:483:VAL:HG13	2.02	0.41
2:D:344:GLY:O	2:D:355:LEU:HG	2.20	0.41
2:D:332:ILE:HD13	1:E:338:LYS:HB3	2.02	0.41
2:C:510:ILE:HD11	2:C:524:MET:HE2	2.01	0.41
2:B:90:LYS:HE3	2:B:130:VAL:O	2.20	0.41
2:B:223:ALA:O	2:B:227:GLU:HG3	2.21	0.41
2:B:349:PHE:O	2:B:350:ASP:CB	2.62	0.41
1:F:471:PHE:HE1	1:F:473:GLU:HB3	1.85	0.41
2:D:666:MET:HE3	2:D:666:MET:HB3	1.69	0.41
2:D:629:GLU:HA	2:D:630:PRO:HD2	1.93	0.41
2:B:170:MET:HE2	2:B:170:MET:HB3	1.96	0.41
2:C:261:ILE:HD13	2:C:261:ILE:HA	1.88	0.41
2:B:278:LEU:HD21	2:B:532:GLU:HG3	2.03	0.41
1:E:67:GLU:HG2	1:E:83:LEU:CD2	2.48	0.41
2:C:510:ILE:HD11	2:C:524:MET:HE1	2.02	0.41
1:A:650:LYS:HD2	1:A:654:PHE:CE2	2.55	0.41
2:C:242:LEU:HD21	2:C:248:SER:HB3	2.02	0.41
1:A:248:TRP:O	1:A:382:VAL:HA	2.21	0.41
2:B:642:VAL:O	2:B:644:ASP:N	2.54	0.41
1:A:114:LEU:HD23	1:A:114:LEU:HA	1.82	0.41
2:B:300:PRO:HG2	2:B:309:PHE:HB3	2.02	0.41
1:F:507:HIS:HD2	1:F:508:SER:O	2.03	0.41
1:F:278:PHE:HE1	1:F:532:PRO:CG	2.34	0.41
2:D:540:GLU:OE2	2:D:658:PRO:HG2	2.20	0.41
2:D:97:PHE:O	2:D:393:ARG:NH2	2.54	0.41
2:C:90:LYS:O	2:C:91:ASN:HB2	2.21	0.41
2:D:680:PHE:HA	2:D:681:PRO:HD3	1.85	0.41
2:D:514:SER:O	2:D:558:PRO:HA	2.21	0.41
2:B:661:PHE:C	2:B:666:MET:HE3	2.40	0.41
1:A:214:ASN:HB2	1:E:537:ASN:OD1	2.21	0.41
1:E:634:ASN:HB3	1:E:635:LYS:H	1.78	0.41
1:E:596:VAL:HA	1:E:597:PRO:HD3	1.95	0.41
1:F:137:GLN:H	1:F:137:GLN:NE2	2.19	0.41
2:B:639:LYS:N	2:B:639:LYS:HD2	2.36	0.41
2:C:455:LEU:HD12	2:C:455:LEU:C	2.40	0.41
1:E:545:ASP:O	1:E:548:MET:CE	2.69	0.41
1:A:634:ASN:HB3	1:A:635:LYS:H	1.76	0.41
2:B:574:LYS:HG2	2:B:602:THR:HG22	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:358:SER:C	2:C:360:ALA:N	2.73	0.41
1:A:201:LYS:HG3	1:A:206:PHE:CE2	2.55	0.41
1:E:91:MET:HA	1:E:92:PRO:HD3	1.92	0.41
2:B:528:PRO:HA	2:B:619:PHE:HD1	1.85	0.41
2:C:145:ILE:HG13	2:C:151:THR:HG21	2.03	0.41
1:E:168:LYS:HE3	1:E:308:LYS:HE3	2.03	0.41
1:A:646:VAL:CG2	1:A:652:LEU:HD21	2.51	0.41
1:A:646:VAL:HG22	1:A:652:LEU:HD21	2.03	0.41
1:F:623:PHE:CE2	1:F:677:ILE:HD12	2.55	0.41
1:F:537:ASN:HB3	1:F:539:ILE:HD13	2.03	0.41
2:B:138:LEU:HA	2:B:138:LEU:HD23	1.92	0.41
2:B:516:VAL:HG12	2:B:517:ALA:H	1.86	0.41
1:F:257:LEU:HG	1:F:257:LEU:O	2.20	0.41
1:F:170:PHE:CD2	1:F:232:ILE:HG22	2.55	0.41
2:B:155:VAL:CG1	2:B:156:LEU:N	2.84	0.41
1:F:267:TYR:O	1:F:271:GLN:HG2	2.20	0.41
2:C:181:MET:HE2	1:E:484:TYR:H	1.82	0.41
2:B:44:ASN:C	2:B:46:ASN:H	2.24	0.41
1:E:214:ASN:HA	1:E:217:LEU:O	2.21	0.41
7:E:804:BMA:O2	7:E:805:BMA:C1	2.69	0.41
2:B:95:SER:N	2:B:101:MET:HE3	2.32	0.40
1:E:307:THR:C	1:E:309:PHE:H	2.25	0.40
1:A:190:ASN:ND2	1:A:190:ASN:C	2.74	0.40
1:F:217:LEU:HD21	1:F:302:TYR:HB3	2.04	0.40
2:C:222:ILE:CG2	2:C:222:ILE:O	2.69	0.40
1:A:248:TRP:CE3	1:A:249:TRP:HB2	2.56	0.40
2:B:330:LEU:O	2:B:334:GLU:HG3	2.20	0.40
2:D:145:ILE:HG23	2:D:151:THR:CG2	2.52	0.40
2:D:675:HIS:HE1	2:D:678:GLU:O	2.04	0.40
2:D:170:MET:CE	2:D:174:ASN:HD21	2.34	0.40
2:B:45:VAL:HG11	2:B:138:LEU:HD11	2.03	0.40
2:D:222:ILE:HD13	2:D:222:ILE:HG21	1.42	0.40
1:F:684:PHE:O	1:F:687:LYS:HB2	2.21	0.40
1:A:218:TYR:CZ	1:E:536:ASP:HB3	2.56	0.40
1:E:422:LEU:HD22	1:E:427:PHE:CE2	2.56	0.40
1:A:170:PHE:HB3	1:A:232:ILE:HG22	2.03	0.40
1:E:175:VAL:HG21	1:E:210:ALA:HB2	2.04	0.40
2:B:369:GLN:O	2:B:370:THR:C	2.60	0.40
1:E:166:TYR:HB3	1:E:169:MET:HG3	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	668/703 (95%)	629 (94%)	33 (5%)	6 (1%)	21	55
1	E	667/703 (95%)	628 (94%)	32 (5%)	7 (1%)	19	52
1	F	667/703 (95%)	630 (94%)	34 (5%)	3 (0%)	39	74
2	B	666/696 (96%)	619 (93%)	33 (5%)	14 (2%)	9	29
2	C	666/696 (96%)	633 (95%)	24 (4%)	9 (1%)	14	42
2	D	670/696 (96%)	637 (95%)	27 (4%)	6 (1%)	21	55
All	All	4004/4197 (95%)	3776 (94%)	183 (5%)	45 (1%)	17	50

All (45) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	308	LYS
2	B	247	ASN
2	B	632	PRO
2	B	636	GLU
2	B	687	PRO
2	C	347	LYS
2	C	350	ASP
2	C	632	PRO
2	C	687	PRO
2	D	350	ASP
2	D	632	PRO
2	D	687	PRO
1	E	308	LYS
2	B	45	VAL
2	B	350	ASP
2	B	382	PHE
2	B	615	ASP
2	C	344	GLY
2	D	488	LYS
1	E	203	ASN

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Mol	Chain	Res	Type
1	F	308	LYS
1	F	641	PRO
1	A	94	ASN
1	A	647	LEU
2	D	635	SER
1	A	324	GLU
1	A	640	ALA
2	B	306	TYR
2	C	635	SER
1	E	640	ALA
2	B	344	GLY
2	C	186	LEU
2	C	599	SER
2	D	321	GLU
1	E	220	ASN
1	E	636	GLY
1	E	641	PRO
1	E	647	LEU
1	F	640	ALA
2	B	631	THR
2	B	85	VAL
2	B	490	SER
2	C	643	PRO
1	A	495	VAL
2	B	643	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	610/638 (96%)	563 (92%)	47 (8%)	16	41
1	E	609/638 (96%)	563 (92%)	46 (8%)	16	42
1	F	609/638 (96%)	548 (90%)	61 (10%)	9	27
2	B	606/629 (96%)	548 (90%)	58 (10%)	10	29
2	C	606/629 (96%)	550 (91%)	56 (9%)	11	32

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	D	610/629 (97%)	556 (91%)	54 (9%)	12	34
All	All	3650/3801 (96%)	3328 (91%)	322 (9%)	12	35

All (322) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	THR
1	A	56	GLU
1	A	71	ASP
1	A	75	ASN
1	A	91	MET
1	A	99	VAL
1	A	145	TYR
1	A	190	ASN
1	A	204	ASP
1	A	258	LYS
1	A	281	LEU
1	A	310	THR
1	A	324	GLU
1	A	356	ILE
1	A	364	ILE
1	A	381	GLU
1	A	382	VAL
1	A	385	ASP
1	A	422	LEU
1	A	441	PHE
1	A	449	THR
1	A	451	ASP
1	A	455	PHE
1	A	456	ASP
1	A	469	THR
1	A	506	ASN
1	A	515	GLU
1	A	517	ASP
1	A	519	ASN
1	A	523	ASP
1	A	539	ILE
1	A	543	LEU
1	A	548	MET
1	A	559	LYS
1	A	561	THR
1	A	572	ASN

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Mol	Chain	Res	Type
1	A	599	ASP
1	A	602	GLU
1	A	610	ARG
1	A	633	ASP
1	A	643	GLU
1	A	646	VAL
1	A	649	ASN
1	A	661	VAL
1	A	662	ASP
1	A	664	LEU
1	A	683	ARG
2	B	28	ASP
2	B	47	GLU
2	B	51	GLU
2	B	53	GLU
2	B	63	ILE
2	B	64	GLU
2	B	72	ASN
2	B	77	GLU
2	B	90	LYS
2	B	129	ARG
2	B	134	GLN
2	B	142	TYR
2	B	165	GLN
2	B	173	LYS
2	B	187	ASP
2	B	190	ILE
2	B	197	ILE
2	B	205	MET
2	B	210	SER
2	B	213	LEU
2	B	215	TYR
2	B	217	ASN
2	B	225	LEU
2	B	261	ILE
2	B	275	MET
2	B	300	PRO
2	B	305	PHE
2	B	306	TYR
2	B	313	SER
2	B	332	ILE
2	B	347	LYS

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Mol	Chain	Res	Type
2	B	353	ILE
2	B	370	THR
2	B	381	GLN
2	B	404	GLN
2	B	452	PHE
2	B	455	LEU
2	B	490	SER
2	B	502	ASN
2	B	513	LYS
2	B	514	SER
2	B	516	VAL
2	B	533	ASN
2	B	537	PHE
2	B	539	LEU
2	B	542	ASN
2	B	544	MET
2	B	578	LEU
2	B	597	PHE
2	B	602	THR
2	B	606	ARG
2	B	634	GLU
2	B	639	LYS
2	B	641	VAL
2	B	645	ASN
2	B	663	GLN
2	B	679	LEU
2	B	688	HIS
2	C	21	GLU
2	C	22	PHE
2	C	27	VAL
2	C	28	ASP
2	C	46	ASN
2	C	53	GLU
2	C	63	ILE
2	C	64	GLU
2	C	66	SER
2	C	72	ASN
2	C	111	LEU
2	C	129	ARG
2	C	134	GLN
2	C	145	ILE
2	C	170	MET

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Mol	Chain	Res	Type
2	C	189	LYS
2	C	200	ASN
2	C	202	GLN
2	C	205	MET
2	C	210	SER
2	C	217	ASN
2	C	247	ASN
2	C	313	SER
2	C	326	GLU
2	C	345	HIS
2	C	346	PHE
2	C	347	LYS
2	C	352	LYS
2	C	359	LYS
2	C	370	THR
2	C	416	GLN
2	C	443	VAL
2	C	452	PHE
2	C	455	LEU
2	C	466	VAL
2	C	490	SER
2	C	492	HIS
2	C	502	ASN
2	C	516	VAL
2	C	518	THR
2	C	535	PHE
2	C	542	ASN
2	C	589	GLN
2	C	592	ILE
2	C	597	PHE
2	C	598	ASN
2	C	602	THR
2	C	605	SER
2	C	606	ARG
2	C	609	LEU
2	C	633	LYS
2	C	634	GLU
2	C	636	GLU
2	C	642	VAL
2	C	645	ASN
2	C	663	GLN
2	D	21	GLU

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Mol	Chain	Res	Type
2	D	53	GLU
2	D	71	THR
2	D	74	LYS
2	D	96	ILE
2	D	111	LEU
2	D	129	ARG
2	D	134	GLN
2	D	145	ILE
2	D	165	GLN
2	D	172	VAL
2	D	173	LYS
2	D	187	ASP
2	D	200	ASN
2	D	205	MET
2	D	210	SER
2	D	217	ASN
2	D	225	LEU
2	D	247	ASN
2	D	299	LEU
2	D	313	SER
2	D	326	GLU
2	D	343	GLN
2	D	345	HIS
2	D	352	LYS
2	D	370	THR
2	D	380	LEU
2	D	381	GLN
2	D	414	PHE
2	D	416	GLN
2	D	429	LYS
2	D	452	PHE
2	D	464	LYS
2	D	489	SER
2	D	490	SER
2	D	502	ASN
2	D	513	LYS
2	D	516	VAL
2	D	532	GLU
2	D	537	PHE
2	D	538	SER
2	D	539	LEU
2	D	551	TRP

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Mol	Chain	Res	Type
2	D	555	LYS
2	D	562	GLN
2	D	585	LYS
2	D	592	ILE
2	D	602	THR
2	D	606	ARG
2	D	633	LYS
2	D	634	GLU
2	D	636	GLU
2	D	687	PRO
2	D	690	THR
1	E	24	THR
1	E	27	THR
1	E	30	VAL
1	E	48	VAL
1	E	53	THR
1	E	56	GLU
1	E	62	LYS
1	E	68	MET
1	E	71	ASP
1	E	77	LYS
1	E	83	LEU
1	E	99	VAL
1	E	145	TYR
1	E	159	VAL
1	E	169	MET
1	E	190	ASN
1	E	203	ASN
1	E	257	LEU
1	E	258	LYS
1	E	290	GLU
1	E	307	THR
1	E	310	THR
1	E	346	LYS
1	E	364	ILE
1	E	381	GLU
1	E	382	VAL
1	E	451	ASP
1	E	455	PHE
1	E	456	ASP
1	E	488	GLU
1	E	495	VAL

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Mol	Chain	Res	Type
1	E	506	ASN
1	E	515	GLU
1	E	523	ASP
1	E	532	PRO
1	E	548	MET
1	E	561	THR
1	E	615	ARG
1	E	625	LEU
1	E	645	PHE
1	E	646	VAL
1	E	648	ASP
1	E	673	LYS
1	E	683	ARG
1	E	686	TYR
1	E	692	SER
1	F	27	THR
1	F	48	VAL
1	F	56	GLU
1	F	62	LYS
1	F	66	ILE
1	F	71	ASP
1	F	75	ASN
1	F	77	LYS
1	F	103	LYS
1	F	132	ARG
1	F	137	GLN
1	F	145	TYR
1	F	188	LEU
1	F	190	ASN
1	F	204	ASP
1	F	216	VAL
1	F	226	THR
1	F	232	ILE
1	F	257	LEU
1	F	305	MET
1	F	307	THR
1	F	323	THR
1	F	335	THR
1	F	381	GLU
1	F	382	VAL
1	F	384	LYS
1	F	389	SER

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Mol	Chain	Res	Type
1	F	422	LEU
1	F	441	PHE
1	F	446	LYS
1	F	449	THR
1	F	451	ASP
1	F	455	PHE
1	F	456	ASP
1	F	461	THR
1	F	473	GLU
1	F	493	ASN
1	F	501	ARG
1	F	506	ASN
1	F	515	GLU
1	F	516	VAL
1	F	519	ASN
1	F	522	SER
1	F	523	ASP
1	F	548	MET
1	F	561	THR
1	F	565	ASN
1	F	568	ILE
1	F	572	ASN
1	F	578	LYS
1	F	582	VAL
1	F	596	VAL
1	F	604	PHE
1	F	610	ARG
1	F	642	PHE
1	F	643	GLU
1	F	647	LEU
1	F	648	ASP
1	F	673	LYS
1	F	675	ILE
1	F	683	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (103) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	GLN
1	A	50	GLN
1	A	69	ASN
1	A	72	ASN

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Mol	Chain	Res	Type
1	A	75	ASN
1	A	94	ASN
1	A	190	ASN
1	A	244	HIS
1	A	271	GLN
1	A	314	GLN
1	A	359	HIS
1	A	492	ASN
1	A	494	HIS
1	A	506	ASN
1	A	507	HIS
1	A	513	ASN
1	A	546	ASN
1	A	679	HIS
2	B	35	GLN
2	B	44	ASN
2	B	59	GLN
2	B	134	GLN
2	B	217	ASN
2	B	232	ASN
2	B	247	ASN
2	B	268	GLN
2	B	303	ASN
2	B	311	GLN
2	B	404	GLN
2	B	433	GLN
2	B	502	ASN
2	B	503	HIS
2	B	542	ASN
2	B	645	ASN
2	B	663	GLN
2	B	675	HIS
2	C	35	GLN
2	C	72	ASN
2	C	134	GLN
2	C	217	ASN
2	C	232	ASN
2	C	247	ASN
2	C	268	GLN
2	C	311	GLN
2	C	343	GLN
2	C	447	GLN

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Mol	Chain	Res	Type
2	C	471	HIS
2	C	502	ASN
2	C	503	HIS
2	C	533	ASN
2	C	542	ASN
2	C	645	ASN
2	C	663	GLN
2	C	675	HIS
2	C	688	HIS
2	D	72	ASN
2	D	134	GLN
2	D	174	ASN
2	D	217	ASN
2	D	232	ASN
2	D	247	ASN
2	D	268	GLN
2	D	311	GLN
2	D	343	GLN
2	D	447	GLN
2	D	502	ASN
2	D	503	HIS
2	D	542	ASN
2	D	560	GLN
2	D	663	GLN
2	D	675	HIS
1	E	38	GLN
1	E	50	GLN
1	E	139	GLN
1	E	177	GLN
1	E	190	ASN
1	E	203	ASN
1	E	235	ASN
1	E	244	HIS
1	E	271	GLN
1	E	314	GLN
1	E	359	HIS
1	E	506	ASN
1	E	507	HIS
1	E	513	ASN
1	E	679	HIS
1	F	38	GLN
1	F	50	GLN

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Mol	Chain	Res	Type
1	F	137	GLN
1	F	139	GLN
1	F	190	ASN
1	F	271	GLN
1	F	314	GLN
1	F	345	GLN
1	F	359	HIS
1	F	493	ASN
1	F	506	ASN
1	F	507	HIS
1	F	519	ASN
1	F	546	ASN
1	F	565	ASN
1	F	649	ASN
1	F	679	HIS

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 ⓘ

34 carbohydrates are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	NAG	A	801	1,3	14,14,15	0.97	1 (7%)	15,19,21	2.01	4 (26%)
3	NAG	A	802	3	14,14,15	0.83	1 (7%)	15,19,21	2.01	5 (33%)
3	BMA	A	803	3	11,11,12	0.81	0	14,15,17	2.34	4 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	MAN	A	804	3	11,11,12	0.71	0	14,15,17	1.23	1 (7%)
3	BMA	A	805	3	11,11,12	1.07	1 (9%)	14,15,17	3.50	4 (28%)
4	NAG	B	801	2,4	14,14,15	0.73	1 (7%)	15,19,21	1.68	2 (13%)
4	NAG	B	802	4	14,14,15	0.62	0	15,19,21	1.49	2 (13%)
4	BMA	B	803	4	11,11,12	1.28	1 (9%)	14,15,17	1.56	3 (21%)
4	BMA	B	804	4	11,11,12	0.62	0	14,15,17	1.27	1 (7%)
4	MAN	B	805	4	11,11,12	0.70	0	14,15,17	1.24	1 (7%)
5	NAG	C	801	2,5	14,14,15	0.59	0	15,19,21	1.80	2 (13%)
5	NAG	C	802	5	14,14,15	0.75	1 (7%)	15,19,21	1.53	1 (6%)
5	BMA	C	803	5	11,11,12	0.68	0	14,15,17	2.36	5 (35%)
5	MAN	C	804	5	11,11,12	0.77	0	14,15,17	2.03	3 (21%)
5	MAN	C	805	5	11,11,12	0.93	1 (9%)	14,15,17	2.22	4 (28%)
5	MAN	C	806	5	11,11,12	0.66	0	14,15,17	2.72	5 (35%)
6	NAG	D	801	2,6	14,14,15	0.55	0	15,19,21	1.29	1 (6%)
6	NAG	D	802	6	14,14,15	0.87	1 (7%)	15,19,21	1.53	2 (13%)
6	BMA	D	803	6	11,11,12	0.47	0	14,15,17	1.96	3 (21%)
6	MAN	D	804	6	11,11,12	0.55	0	14,15,17	1.48	1 (7%)
6	MAN	D	805	6	11,11,12	0.82	0	14,15,17	1.33	2 (14%)
6	MAN	D	807	6	11,11,12	0.65	0	14,15,17	1.20	2 (14%)
6	MAN	D	808	6	11,11,12	0.66	0	14,15,17	2.74	4 (28%)
7	NAG	E	801	1,7	14,14,15	0.69	0	15,19,21	1.31	2 (13%)
7	NAG	E	802	7	14,14,15	0.53	0	15,19,21	1.10	0
7	BMA	E	803	7	11,11,12	0.62	0	14,15,17	2.31	4 (28%)
7	BMA	E	804	7	11,11,12	0.69	0	14,15,17	2.29	3 (21%)
7	BMA	E	805	7	11,11,12	0.94	1 (9%)	14,15,17	2.54	3 (21%)
7	MAN	E	806	7	11,11,12	0.82	0	14,15,17	1.78	2 (14%)
3	NAG	F	801	1,3	14,14,15	0.52	0	15,19,21	1.83	4 (26%)
3	NAG	F	802	3	14,14,15	0.54	0	15,19,21	1.27	1 (6%)
3	BMA	F	803	3	11,11,12	0.45	0	14,15,17	1.31	3 (21%)
3	MAN	F	804	3	11,11,12	0.84	1 (9%)	14,15,17	1.66	3 (21%)
3	BMA	F	805	3	11,11,12	0.71	0	14,15,17	2.64	3 (21%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	A	801	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	802	3	-	0/6/23/26	0/1/1/1
3	BMA	A	803	3	-	0/2/19/22	0/1/1/1
3	MAN	A	804	3	-	0/2/19/22	0/1/1/1
3	BMA	A	805	3	-	0/2/19/22	0/1/1/1
4	NAG	B	801	2,4	-	0/6/23/26	0/1/1/1
4	NAG	B	802	4	-	0/6/23/26	0/1/1/1
4	BMA	B	803	4	-	0/2/19/22	0/1/1/1
4	BMA	B	804	4	-	0/2/19/22	0/1/1/1
4	MAN	B	805	4	-	0/2/19/22	0/1/1/1
5	NAG	C	801	2,5	-	0/6/23/26	0/1/1/1
5	NAG	C	802	5	-	0/6/23/26	0/1/1/1
5	BMA	C	803	5	-	0/2/19/22	0/1/1/1
5	MAN	C	804	5	-	0/2/19/22	0/1/1/1
5	MAN	C	805	5	-	0/2/19/22	0/1/1/1
5	MAN	C	806	5	-	0/2/19/22	0/1/1/1
6	NAG	D	801	2,6	-	0/6/23/26	0/1/1/1
6	NAG	D	802	6	-	0/6/23/26	0/1/1/1
6	BMA	D	803	6	-	0/2/19/22	0/1/1/1
6	MAN	D	804	6	-	0/2/19/22	0/1/1/1
6	MAN	D	805	6	-	0/2/19/22	0/1/1/1
6	MAN	D	807	6	-	0/2/19/22	0/1/1/1
6	MAN	D	808	6	-	0/2/19/22	0/1/1/1
7	NAG	E	801	1,7	-	0/6/23/26	0/1/1/1
7	NAG	E	802	7	-	0/6/23/26	0/1/1/1
7	BMA	E	803	7	-	0/2/19/22	0/1/1/1
7	BMA	E	804	7	-	0/2/19/22	0/1/1/1
7	BMA	E	805	7	-	0/2/19/22	0/1/1/1
7	MAN	E	806	7	-	0/2/19/22	0/1/1/1
3	NAG	F	801	1,3	-	0/6/23/26	0/1/1/1
3	NAG	F	802	3	-	0/6/23/26	0/1/1/1
3	BMA	F	803	3	-	0/2/19/22	0/1/1/1
3	MAN	F	804	3	-	0/2/19/22	0/1/1/1
3	BMA	F	805	3	-	0/2/19/22	0/1/1/1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	803	BMA	O5-C1	-3.75	1.37	1.43
3	A	801	NAG	O5-C1	-2.62	1.39	1.43
6	D	802	NAG	O5-C1	-2.27	1.39	1.43
4	B	801	NAG	O5-C1	-2.23	1.40	1.43
5	C	802	NAG	O5-C1	-2.15	1.40	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	802	NAG	O3-C3	-2.13	1.37	1.43
7	E	805	BMA	C2-C3	2.22	1.55	1.52
5	C	805	MAN	C2-C3	2.36	1.55	1.52
3	F	804	MAN	C2-C3	2.38	1.55	1.52
3	A	805	BMA	C2-C3	2.77	1.56	1.52

All (90) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	805	BMA	C1-O5-C5	-9.69	99.95	112.25
3	A	801	NAG	C2-N2-C7	-5.62	115.82	123.04
3	A	802	NAG	C3-C4-C5	-4.78	101.87	110.20
3	A	805	BMA	C3-C4-C5	-4.57	102.24	110.20
6	D	802	NAG	C2-N2-C7	-4.38	117.41	123.04
3	A	802	NAG	O3-C3-C2	-3.85	101.48	109.11
4	B	801	NAG	C3-C2-N2	-3.59	101.95	110.56
3	A	801	NAG	O6-C6-C5	-2.52	103.01	111.33
3	A	801	NAG	C3-C4-C5	-2.42	105.98	110.20
3	F	803	BMA	O2-C2-C1	-2.34	104.52	109.21
3	F	801	NAG	O7-C7-C8	-2.29	117.86	122.06
4	B	803	BMA	C1-O5-C5	-2.23	109.42	112.25
7	E	801	NAG	C3-C4-C5	-2.23	106.31	110.20
6	D	801	NAG	C3-C4-C5	-2.20	106.36	110.20
3	A	802	NAG	C1-O5-C5	-2.20	109.46	112.25
7	E	803	BMA	C1-C2-C3	-2.20	106.94	109.54
6	D	808	MAN	C3-C4-C5	-2.18	106.39	110.20
5	C	801	NAG	O4-C4-C5	-2.15	103.53	109.24
4	B	802	NAG	C3-C4-C5	-2.10	106.53	110.20
3	A	803	BMA	O4-C4-C3	-2.08	105.66	110.34
5	C	806	MAN	O5-C1-C2	2.02	114.13	110.86
3	A	802	NAG	C6-C5-C4	2.06	118.09	113.02
6	D	802	NAG	C1-O5-C5	2.09	114.91	112.25
3	F	803	BMA	C3-C4-C5	2.11	113.88	110.20
3	F	802	NAG	O3-C3-C2	2.11	113.30	109.11
6	D	805	MAN	C1-O5-C5	2.17	115.01	112.25
7	E	803	BMA	O3-C3-C4	2.18	115.25	110.34
3	F	801	NAG	O7-C7-N2	2.21	126.37	121.86
5	C	805	MAN	C2-C3-C4	2.32	114.98	111.04
5	C	803	BMA	C2-C3-C4	2.34	115.01	111.04
3	A	801	NAG	C1-O5-C5	2.35	115.24	112.25
5	C	805	MAN	O5-C1-C2	2.36	114.68	110.86
5	C	804	MAN	C2-C3-C4	2.47	115.24	111.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	805	BMA	C6-C5-C4	2.48	119.12	113.02
3	F	803	BMA	C1-C2-C3	2.54	112.55	109.54
6	D	807	MAN	O5-C5-C6	2.56	112.90	107.35
3	F	804	MAN	C2-C3-C4	2.59	115.45	111.04
4	B	804	BMA	C3-C4-C5	2.65	114.82	110.20
3	F	804	MAN	C1-O5-C5	2.68	115.65	112.25
7	E	805	BMA	O5-C1-C2	2.74	115.30	110.86
3	A	802	NAG	O5-C5-C6	2.81	113.44	107.35
7	E	804	BMA	O3-C3-C2	2.83	115.11	110.00
6	D	808	MAN	O5-C1-C2	2.90	115.56	110.86
4	B	803	BMA	O3-C3-C2	2.90	115.24	110.00
6	D	808	MAN	C1-C2-C3	2.93	113.01	109.54
6	D	807	MAN	C1-O5-C5	2.94	115.98	112.25
5	C	806	MAN	C2-C3-C4	2.96	116.07	111.04
3	A	803	BMA	C1-C2-C3	2.99	113.08	109.54
5	C	803	BMA	C1-O5-C5	3.01	116.07	112.25
4	B	803	BMA	C3-C4-C5	3.02	115.46	110.20
6	D	805	MAN	C1-C2-C3	3.02	113.12	109.54
5	C	803	BMA	O5-C1-C2	3.10	115.89	110.86
4	B	805	MAN	C1-O5-C5	3.16	116.26	112.25
3	F	801	NAG	C2-N2-C7	3.18	127.13	123.04
5	C	803	BMA	C3-C4-C5	3.22	115.81	110.20
3	F	805	BMA	O5-C1-C2	3.25	116.14	110.86
3	A	803	BMA	O6-C6-C5	3.27	122.13	111.33
3	F	804	MAN	C1-C2-C3	3.28	113.42	109.54
5	C	805	MAN	C1-O5-C5	3.42	116.59	112.25
6	D	803	BMA	O5-C1-C2	3.46	116.46	110.86
5	C	806	MAN	C3-C4-C5	3.48	116.26	110.20
3	A	804	MAN	C3-C4-C5	3.51	116.31	110.20
6	D	803	BMA	C1-O5-C5	3.54	116.74	112.25
7	E	806	MAN	C1-O5-C5	3.61	116.83	112.25
7	E	804	BMA	C3-C4-C5	3.61	116.49	110.20
7	E	801	NAG	C1-O5-C5	3.70	116.95	112.25
3	F	805	BMA	C1-C2-C3	3.88	114.13	109.54
7	E	803	BMA	O3-C3-C2	3.94	117.11	110.00
7	E	806	MAN	C1-C2-C3	4.10	114.40	109.54
3	F	801	NAG	C1-O5-C5	4.35	117.77	112.25
5	C	804	MAN	C1-C2-C3	4.43	114.78	109.54
4	B	802	NAG	C1-O5-C5	4.44	117.88	112.25
6	D	803	BMA	C1-C2-C3	4.47	114.83	109.54
4	B	801	NAG	C1-O5-C5	4.48	117.93	112.25
7	E	805	BMA	C1-O5-C5	4.69	118.20	112.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	802	NAG	C1-O5-C5	4.79	118.33	112.25
6	D	804	MAN	C1-O5-C5	4.91	118.47	112.25
5	C	804	MAN	C1-O5-C5	5.15	118.79	112.25
5	C	806	MAN	C1-C2-C3	5.50	116.05	109.54
5	C	801	NAG	C1-O5-C5	5.79	119.60	112.25
7	E	803	BMA	C1-O5-C5	5.93	119.78	112.25
5	C	803	BMA	C1-C2-C3	6.04	116.69	109.54
3	A	805	BMA	O5-C5-C6	6.25	120.87	107.35
3	A	803	BMA	O5-C5-C6	6.27	120.93	107.35
5	C	805	MAN	C1-C2-C3	6.29	116.98	109.54
5	C	806	MAN	C1-O5-C5	6.43	120.41	112.25
7	E	804	BMA	C1-O5-C5	6.57	120.58	112.25
7	E	805	BMA	C1-C2-C3	7.13	117.98	109.54
3	F	805	BMA	C1-O5-C5	7.88	122.25	112.25
6	D	808	MAN	C1-O5-C5	8.52	123.06	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	801	NAG	1	0
4	B	802	NAG	2	0
4	B	803	BMA	2	0
7	E	804	BMA	1	0
7	E	805	BMA	1	0

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	670/703 (95%)	-0.51	19 (2%) 56 44	20, 43, 85, 213	0
1	E	669/703 (95%)	-0.37	19 (2%) 56 44	24, 50, 91, 234	0
1	F	669/703 (95%)	-0.22	22 (3%) 50 38	27, 59, 102, 206	0
2	B	668/696 (95%)	-0.34	15 (2%) 65 54	25, 54, 92, 167	0
2	C	668/696 (95%)	-0.46	12 (1%) 71 61	24, 46, 86, 142	0
2	D	672/696 (96%)	-0.51	7 (1%) 84 77	20, 42, 82, 159	0
All	All	4016/4197 (95%)	-0.40	94 (2%) 64 52	20, 49, 92, 234	0

All (94) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	21	GLU	7.2
1	E	641	PRO	7.2
1	A	638	ASP	6.7
1	F	640	ALA	6.7
1	A	644	SER	6.3
2	D	633	LYS	6.2
1	F	641	PRO	5.9
1	E	642	PHE	5.5
2	D	346	PHE	5.4
1	A	637	LYS	5.4
1	F	636	GLY	5.3
1	E	645	PHE	5.3
1	E	646	VAL	5.1
1	A	639	LEU	5.1
1	E	639	LEU	4.9
2	B	633	LYS	4.9
1	F	637	LYS	4.8
1	F	638	ASP	4.7
1	E	638	ASP	4.5

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Mol	Chain	Res	Type	RSRZ
1	E	640	ALA	4.2
1	F	492	ASN	4.0
1	F	644	SER	3.6
2	C	632	PRO	3.5
1	E	649	ASN	3.4
2	C	633	LYS	3.3
1	F	67	GLU	3.3
1	E	647	LEU	3.2
2	C	349	PHE	3.2
2	B	60	ASP	3.1
1	F	639	LEU	3.0
2	B	688	HIS	3.0
2	B	186	LEU	3.0
1	A	640	ALA	3.0
1	A	635	LYS	3.0
2	C	187	ASP	2.9
2	B	557	ASN	2.9
1	A	646	VAL	2.9
2	C	351	LYS	2.8
2	C	688	HIS	2.8
1	E	634	ASN	2.8
1	E	32	ALA	2.8
2	C	631	THR	2.7
1	F	87	ARG	2.7
2	B	634	GLU	2.7
1	F	68	MET	2.7
1	F	63	ASP	2.7
1	E	644	SER	2.7
1	E	633	ASP	2.6
2	D	632	PRO	2.6
1	E	636	GLY	2.5
1	A	642	PHE	2.5
1	F	692	SER	2.5
1	F	645	PHE	2.5
2	D	189	LYS	2.5
1	E	560	LEU	2.5
2	B	59	GLN	2.4
2	B	631	THR	2.4
1	A	693	TYR	2.4
2	C	634	GLU	2.4
1	E	561	THR	2.4
1	F	62	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	E	63	ASP	2.4
2	C	59	GLN	2.4
2	C	21	GLU	2.3
1	A	692	SER	2.3
1	A	63	ASP	2.3
1	A	647	LEU	2.3
1	E	562	ALA	2.3
1	F	306	LEU	2.3
1	A	26	LYS	2.3
2	C	65	ALA	2.3
2	D	631	THR	2.3
1	E	519	ASN	2.3
2	B	64	GLU	2.3
2	B	659	GLN	2.3
1	F	307	THR	2.2
2	B	214	THR	2.2
2	D	630	PRO	2.2
1	A	633	ASP	2.2
1	A	597	PRO	2.2
2	B	632	PRO	2.2
2	B	69	CYS	2.2
1	A	517	ASP	2.2
1	F	633	ASP	2.2
1	F	192	GLU	2.2
1	F	309	PHE	2.1
1	F	635	LYS	2.1
2	C	186	LEU	2.1
2	B	643	PRO	2.1
2	B	636	GLU	2.1
1	A	24	THR	2.1
1	F	64	TYR	2.1
1	A	456	ASP	2.0
1	A	634	ASN	2.0

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

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

6.3 Carbohydrates ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	LLDF	B-factors(Å ²)	Q<0.9
3	NAG	A	801	14/15	0.98	0.11	-0.53	27,30,32,36	0
3	NAG	F	802	14/15	0.96	0.15	-0.59	55,60,65,68	0
4	NAG	B	801	14/15	0.96	0.14	-0.61	48,51,58,59	0
5	NAG	C	802	14/15	0.94	0.15	-0.79	51,57,63,70	0
7	NAG	E	801	14/15	0.98	0.10	-0.86	36,38,42,43	0
3	NAG	A	802	14/15	0.97	0.12	-0.90	37,42,49,49	0
6	NAG	D	802	14/15	0.96	0.13	-0.93	44,47,53,60	0
5	NAG	C	801	14/15	0.97	0.11	-0.95	40,43,46,49	0
3	NAG	F	801	14/15	0.96	0.11	-1.02	47,51,56,56	0
6	NAG	D	801	14/15	0.97	0.10	-1.09	36,37,39,43	0
7	NAG	E	802	14/15	0.96	0.11	-1.20	45,48,55,56	0
4	NAG	B	802	14/15	0.94	0.13	-1.48	58,66,76,83	0
5	MAN	C	805	11/12	0.83	0.18	-	92,96,101,105	0
6	BMA	D	803	11/12	0.90	0.18	-	66,77,88,89	0
6	MAN	D	808	11/12	0.76	0.35	-	98,111,114,115	0
3	MAN	A	804	11/12	0.85	0.17	-	66,67,72,74	0
4	BMA	B	803	11/12	0.90	0.16	-	89,95,100,101	0
7	BMA	E	803	11/12	0.92	0.13	-	57,65,73,74	0
5	MAN	C	806	11/12	0.66	0.34	-	102,112,115,115	0
5	BMA	C	803	11/12	0.89	0.16	-	72,82,88,93	0
3	BMA	F	805	11/12	0.69	0.32	-	110,121,124,125	0
3	BMA	A	805	11/12	0.80	0.20	-	82,89,96,102	0
7	BMA	E	805	11/12	0.70	0.25	-	103,108,112,114	0
5	MAN	C	804	11/12	0.69	0.28	-	88,94,97,98	0
3	BMA	F	803	11/12	0.89	0.14	-	71,74,79,87	0
4	BMA	B	804	11/12	0.88	0.21	-	104,108,110,110	0
6	MAN	D	807	11/12	0.75	0.20	-	98,100,105,111	0
7	BMA	E	804	11/12	0.85	0.17	-	78,88,92,99	0
4	MAN	B	805	11/12	0.77	0.17	-	91,97,100,100	0
6	MAN	D	804	11/12	0.92	0.22	-	89,94,100,106	0
3	MAN	F	804	11/12	0.86	0.18	-	95,97,104,108	0
3	BMA	A	803	11/12	0.93	0.14	-	50,59,65,72	0
6	MAN	D	805	11/12	0.72	0.30	-	95,110,118,122	0
7	MAN	E	806	11/12	0.85	0.16	-	69,73,76,77	0

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.