



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:03 PM GMT

PDB ID : 3SQ9
Title : Crystal Structures of the Ligand Binding Domain of a Pentameric Alpha7 Nicotinic Receptor Chimera
Authors : Li, S.-X.; Huang, S.; Bren, N.; Noridomi, K.; Dellisanti, C.; Sine, S.; Chen, L.
Deposited on : 2011-07-05
Resolution : 3.10 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

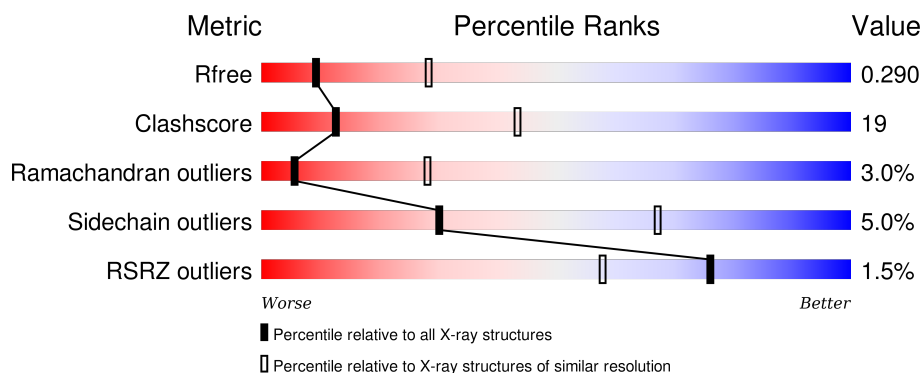
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	1114 (3.14-3.06)
Clashscore	102246	1222 (3.14-3.06)
Ramachandran outliers	100387	1174 (3.14-3.06)
Sidechain outliers	100360	1174 (3.14-3.06)
RSRZ outliers	91569	1119 (3.14-3.06)

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	204	 67% 27% 2% 4%
1	B	204	 63% 30% 5% 2% 1%
1	C	204	 2% 61% 35% 2% 1%
1	D	204	 2% 66% 29% 2% 1%
1	E	204	 2% 63% 32% 2% 1%

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Mol	Chain	Length	Quality of chain
1	F	204	<div><div><div></div><div></div><div></div></div><div><div>2%</div><div>68%</div><div>27%</div><div></div><div></div><div></div></div><div><div></div><div></div><div></div></div></div>
1	G	204	<div><div><div></div><div></div><div></div></div><div><div>2%</div><div>63%</div><div>31%</div><div></div><div></div><div></div></div><div><div></div><div></div><div></div></div></div>
1	H	204	<div><div><div></div><div></div><div></div></div><div><div>%</div><div>64%</div><div>30%</div><div></div><div></div><div></div></div><div><div></div><div></div><div></div></div></div>
1	I	204	<div><div><div></div><div></div><div></div></div><div><div>%</div><div>64%</div><div>30%</div><div></div><div></div><div></div></div><div><div></div><div></div><div></div></div></div>
1	J	204	<div><div><div></div><div></div><div></div></div><div><div>2%</div><div>63%</div><div>31%</div><div></div><div></div><div></div></div><div><div></div><div></div><div></div></div></div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 16750 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 Neuronal acetylcholine receptor subunit alpha-7, Acetylcholine-binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	202	Total	C	N	O	S	0	0	0
			1647	1055	276	309	7			
1	B	202	Total	C	N	O	S	0	0	0
			1647	1055	276	309	7			
1	C	202	Total	C	N	O	S	0	0	0
			1647	1055	276	309	7			
1	D	202	Total	C	N	O	S	0	0	0
			1647	1055	276	309	7			
1	E	202	Total	C	N	O	S	0	0	0
			1647	1055	276	309	7			
1	F	202	Total	C	N	O	S	0	0	0
			1647	1055	276	309	7			
1	G	202	Total	C	N	O	S	0	0	0
			1647	1055	276	309	7			
1	H	202	Total	C	N	O	S	0	0	0
			1647	1055	276	309	7			
1	I	202	Total	C	N	O	S	0	0	0
			1647	1055	276	309	7			
1	J	202	Total	C	N	O	S	0	0	0
			1647	1055	276	309	7			

- Molecule 2 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	D	1	Total	C	N	O	0	0
			14	8	1	5		
2	E	1	Total	C	N	O	0	0
			14	8	1	5		
2	E	1	Total	C	N	O	0	0
			14	8	1	5		
2	F	1	Total	C	N	O	0	0
			14	8	1	5		
2	G	1	Total	C	N	O	0	0
			14	8	1	5		
2	H	1	Total	C	N	O	0	0
			14	8	1	5		
2	I	1	Total	C	N	O	0	0
			14	8	1	5		
2	J	1	Total	C	N	O	0	0
			14	8	1	5		
2	J	1	Total	C	N	O	0	0
			14	8	1	5		

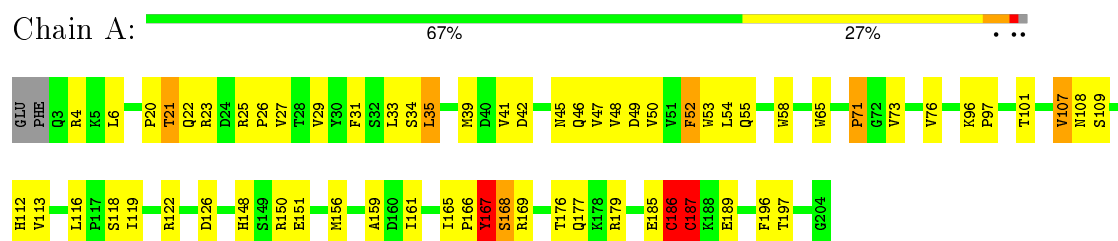
- Molecule 3 is a polymer of unknown type called SUGAR (2-MER).

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

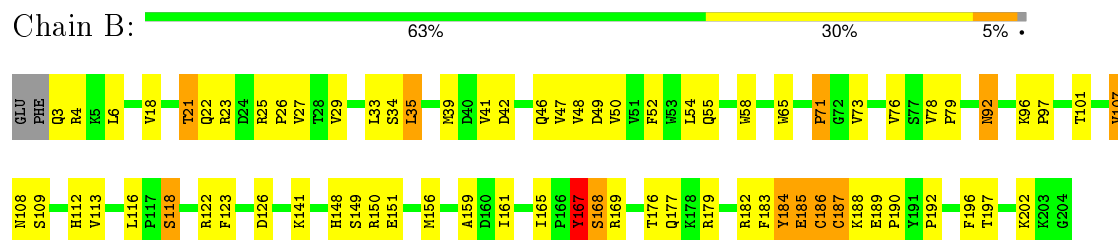
3 Residue-property plots

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.

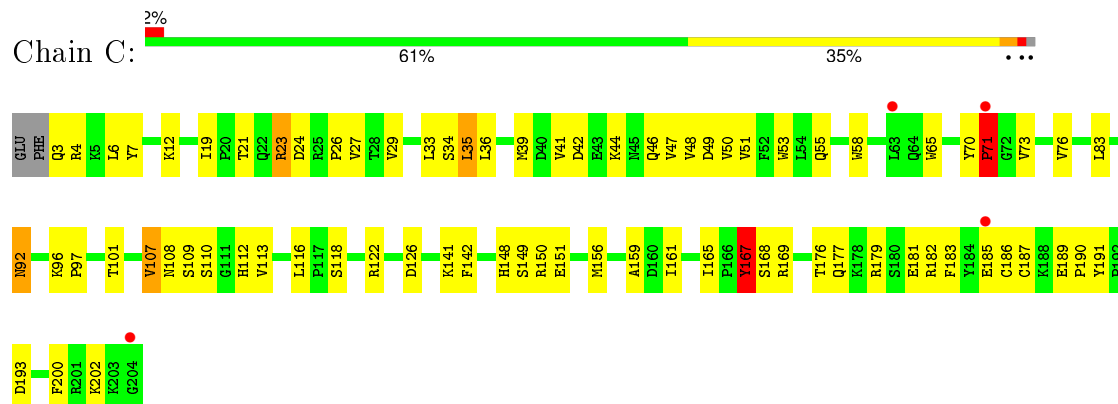
- Molecule 1: Neuronal acetylcholine receptor subunit alpha-7, Acetylcholine-binding protein



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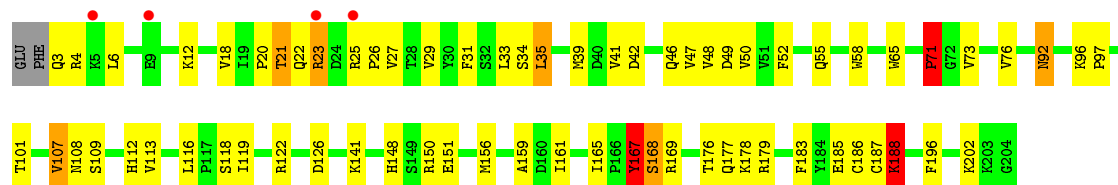


- Molecule 1: Neuronal acetylcholine receptor subunit alpha-7, Acetylcholine-binding protein

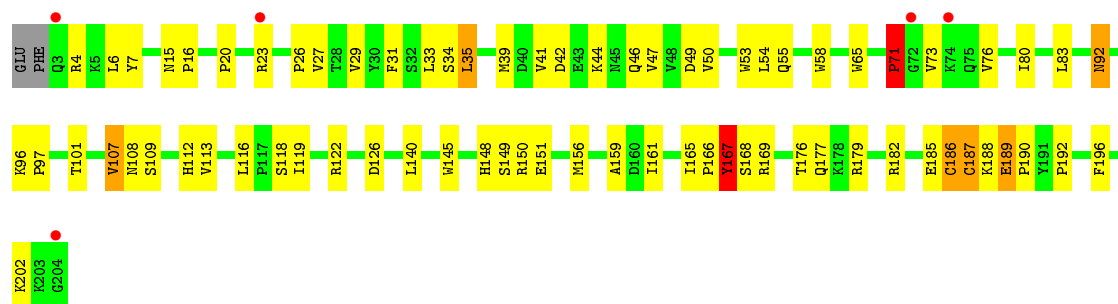


- Molecule 1: Neuronal acetylcholine receptor subunit alpha-7, Acetylcholine-binding protein

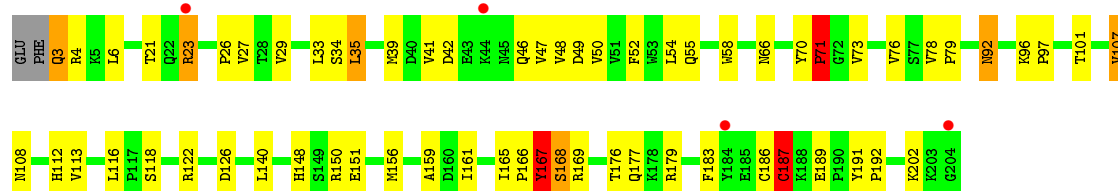




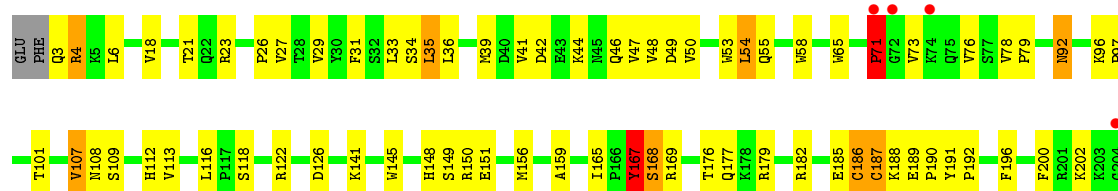
- Molecule 1: Neuronal acetylcholine receptor subunit alpha-7, Acetylcholine-binding protein



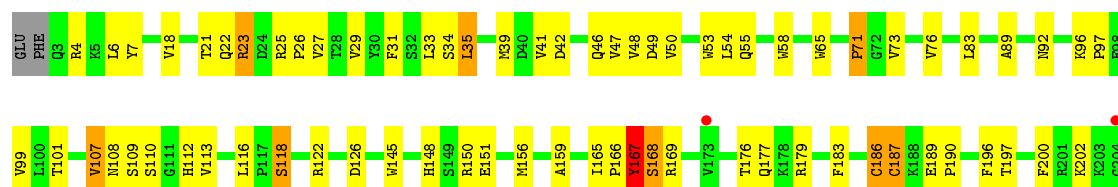
- Molecule 1: Neuronal acetylcholine receptor subunit alpha-7, Acetylcholine-binding protein



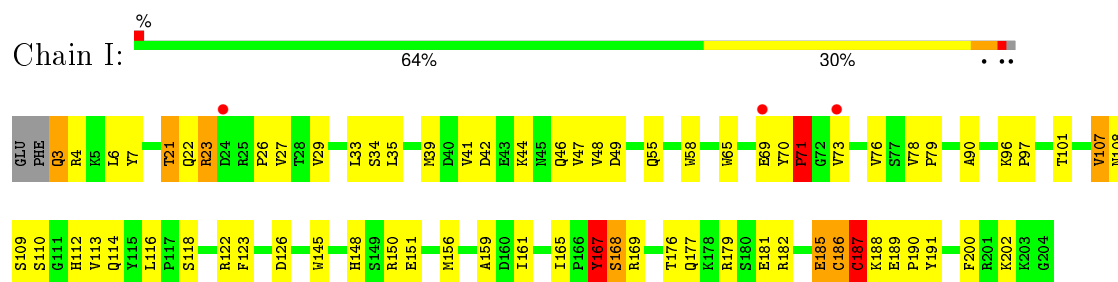
- Molecule 1: Neuronal acetylcholine receptor subunit alpha-7, Acetylcholine-binding protein



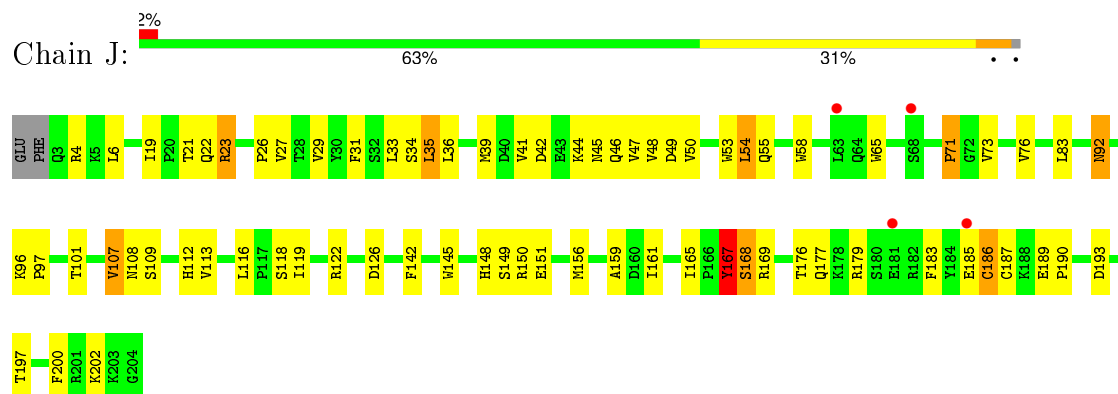
- Molecule 1: Neuronal acetylcholine receptor subunit alpha-7, Acetylcholine-binding protein



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4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	79.12Å 144.56Å 131.12Å 90.00° 102.46° 90.00°	Depositor
Resolution (Å)	46.45 – 3.10 46.44 – 3.10	Depositor EDS
% Data completeness (in resolution range)	90.4 (46.45-3.10) 90.5 (46.44-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.10 (at 3.12Å)	Xtriage
Refinement program	CNS 1.3	Depositor
R, R_{free}	0.262 , 0.289 0.264 , 0.290	Depositor DCC
R_{free} test set	4737 reflections (10.05%)	DCC
Wilson B-factor (Å ²)	79.5	Xtriage
Anisotropy	0.656	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 58.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 47134 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	16750	wwPDB-VP
Average B, all atoms (Å ²)	110.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.17% 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

5.1 Standard geometry

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

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	0.46	0/1691	0.64	0/2300
1	B	0.44	0/1691	0.63	0/2300
1	C	0.46	0/1691	0.64	0/2300
1	D	0.45	0/1691	0.64	0/2300
1	E	0.43	0/1691	0.65	0/2300
1	F	0.47	0/1691	0.64	0/2300
1	G	0.45	0/1691	0.64	0/2300
1	H	0.44	0/1691	0.64	0/2300
1	I	0.45	0/1691	0.64	0/2300
1	J	0.44	0/1691	0.65	0/2300
All	All	0.45	0/16910	0.64	0/23000

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

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	1647	0	1610	60	0
1	B	1647	0	1610	67	0
1	C	1647	0	1609	70	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	1647	0	1611	69	0
1	E	1647	0	1610	73	0
1	F	1647	0	1610	64	0
1	G	1647	0	1611	70	0
1	H	1647	0	1609	66	0
1	I	1647	0	1610	69	0
1	J	1647	0	1609	69	0
2	A	28	0	26	2	0
2	B	14	0	13	2	0
2	C	28	0	26	3	0
2	D	14	0	13	0	0
2	E	28	0	26	0	0
2	F	14	0	13	2	0
2	G	14	0	13	0	0
2	H	14	0	13	0	0
2	I	14	0	13	0	0
2	J	28	0	26	0	0
3	B	28	0	25	0	0
3	H	28	0	25	3	0
3	I	28	0	25	1	0
All	All	16750	0	16356	641	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 19.

All (641) 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:J:92:ASN:H	1:J:92:ASN:HD22	1.07	0.99
1:D:92:ASN:HD22	1:D:92:ASN:H	1.03	0.97
1:F:92:ASN:HD22	1:F:92:ASN:H	0.96	0.93
1:C:92:ASN:H	1:C:92:ASN:HD22	1.17	0.89
1:A:185:GLU:O	1:A:186:CYS:HB3	1.71	0.88
1:J:31:PHE:CE1	1:J:54:LEU:HD21	2.08	0.88
1:J:21:THR:HG22	1:J:27:VAL:HG23	1.56	0.88
1:F:92:ASN:HD22	1:F:92:ASN:N	1.71	0.87
1:D:21:THR:HG23	1:D:27:VAL:HG23	1.57	0.86
1:A:186:CYS:SG	1:A:187:CYS:N	2.49	0.85
1:E:185:GLU:O	1:E:186:CYS:HB3	1.76	0.85
1:D:92:ASN:ND2	1:D:92:ASN:H	1.75	0.83
1:D:101:THR:HG23	1:D:118:SER:HB2	1.60	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:55:GLN:HG3	1:D:116:LEU:HD11	1.59	0.82
1:J:31:PHE:HE1	1:J:54:LEU:HD21	1.43	0.82
1:F:92:ASN:H	1:F:92:ASN:ND2	1.75	0.81
1:J:101:THR:HG23	1:J:118:SER:HB2	1.62	0.81
1:G:31:PHE:HE1	1:G:54:LEU:HD11	1.43	0.81
1:G:101:THR:HG23	1:G:118:SER:HB2	1.61	0.81
1:H:159:ALA:HB2	1:H:177:GLN:OE1	1.82	0.80
1:F:101:THR:HG23	1:F:118:SER:HB2	1.64	0.80
1:F:55:GLN:HG3	1:F:116:LEU:HD11	1.62	0.80
1:B:101:THR:HG23	1:B:118:SER:HB2	1.63	0.80
1:A:101:THR:HG23	1:A:118:SER:HB2	1.62	0.80
1:E:108:ASN:HD22	1:E:112:HIS:HB3	1.46	0.80
1:E:101:THR:HG23	1:E:118:SER:HB2	1.62	0.79
1:E:149:SER:HB2	1:E:190:PRO:HG2	1.61	0.79
1:D:26:PRO:HB3	1:D:150:ARG:O	1.83	0.78
1:I:159:ALA:HB2	1:I:177:GLN:OE1	1.84	0.78
1:C:26:PRO:HB3	1:C:150:ARG:O	1.84	0.78
1:I:101:THR:HG23	1:I:118:SER:HB2	1.65	0.78
1:G:55:GLN:HG3	1:G:116:LEU:HD11	1.66	0.78
1:H:101:THR:HG23	1:H:118:SER:HB2	1.65	0.77
1:B:159:ALA:HB2	1:B:177:GLN:OE1	1.85	0.77
1:F:108:ASN:HD22	1:F:112:HIS:HB3	1.49	0.77
1:G:149:SER:HB2	1:G:190:PRO:HG2	1.66	0.77
1:E:55:GLN:HG3	1:E:116:LEU:HD11	1.65	0.76
1:F:66:ASN:HB2	2:F:801:NAG:H2	1.67	0.76
1:A:55:GLN:HG3	1:A:116:LEU:HD11	1.68	0.76
1:I:181:GLU:HG2	1:I:190:PRO:HB2	1.67	0.76
1:D:92:ASN:HD22	1:D:92:ASN:N	1.84	0.76
1:H:148:HIS:CG	1:H:189:GLU:HG2	2.21	0.75
1:C:55:GLN:HG3	1:C:116:LEU:HD11	1.67	0.75
1:G:31:PHE:CE1	1:G:54:LEU:HD11	2.21	0.75
1:H:21:THR:HG22	1:H:27:VAL:HG23	1.68	0.75
1:A:159:ALA:HB2	1:A:177:GLN:OE1	1.84	0.75
1:F:159:ALA:HB2	1:F:177:GLN:OE1	1.87	0.75
1:J:92:ASN:N	1:J:92:ASN:HD22	1.84	0.74
1:H:55:GLN:HG3	1:H:116:LEU:HD11	1.69	0.74
1:J:55:GLN:HG3	1:J:116:LEU:HD11	1.69	0.74
1:C:101:THR:HG23	1:C:118:SER:HB2	1.68	0.74
1:D:108:ASN:HD22	1:D:112:HIS:HB3	1.51	0.74
1:J:26:PRO:HB3	1:J:150:ARG:O	1.87	0.73
1:D:55:GLN:HA	1:D:116:LEU:HD13	1.71	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:185:GLU:O	1:G:186:CYS:HB3	1.88	0.73
1:A:26:PRO:HB3	1:A:150:ARG:O	1.89	0.73
1:C:159:ALA:HB2	1:C:177:GLN:OE1	1.88	0.73
1:B:26:PRO:HB3	1:B:150:ARG:O	1.87	0.72
1:I:21:THR:HG23	1:I:27:VAL:HG23	1.71	0.72
1:B:108:ASN:HD22	1:B:112:HIS:HB3	1.55	0.72
1:F:26:PRO:HB3	1:F:150:ARG:O	1.90	0.72
1:D:159:ALA:HB2	1:D:177:GLN:OE1	1.89	0.72
1:B:55:GLN:HG3	1:B:116:LEU:HD11	1.72	0.72
1:I:26:PRO:HB3	1:I:150:ARG:O	1.91	0.71
1:H:26:PRO:HB3	1:H:150:ARG:O	1.88	0.71
1:G:159:ALA:HB2	1:G:177:GLN:OE1	1.91	0.70
1:E:26:PRO:HB3	1:E:150:ARG:O	1.91	0.70
1:J:159:ALA:HB2	1:J:177:GLN:OE1	1.91	0.70
1:I:55:GLN:HG3	1:I:116:LEU:HD11	1.73	0.69
1:F:39:MET:HB2	1:F:49:ASP:HB3	1.74	0.69
1:E:176:THR:O	1:E:177:GLN:HB3	1.92	0.69
1:C:176:THR:O	1:C:177:GLN:HB3	1.92	0.69
1:E:159:ALA:HB2	1:E:177:GLN:OE1	1.92	0.69
3:H:901:NAG:H4	3:H:902:NAG:N2	2.07	0.69
1:F:55:GLN:HA	1:F:116:LEU:HD13	1.74	0.69
1:I:182:ARG:HG3	1:I:182:ARG:HH11	1.58	0.69
1:E:54:LEU:HD12	1:E:119:ILE:HD12	1.75	0.68
1:I:185:GLU:O	1:I:186:CYS:HB3	1.94	0.68
1:A:55:GLN:HA	1:A:116:LEU:HD13	1.74	0.68
1:G:182:ARG:O	1:G:190:PRO:HA	1.93	0.68
1:I:55:GLN:HA	1:I:116:LEU:HD13	1.76	0.67
1:E:39:MET:HB2	1:E:49:ASP:HB3	1.76	0.67
1:B:183:PHE:O	1:B:184:TYR:O	2.13	0.67
1:J:39:MET:HB2	1:J:49:ASP:HB3	1.76	0.67
1:E:55:GLN:HA	1:E:116:LEU:HD13	1.76	0.67
1:J:176:THR:O	1:J:177:GLN:HB3	1.92	0.67
1:G:26:PRO:HB3	1:G:150:ARG:O	1.93	0.67
1:J:186:CYS:SG	1:J:187:CYS:N	2.64	0.67
1:I:176:THR:O	1:I:177:GLN:HB3	1.93	0.67
1:B:39:MET:HB2	1:B:49:ASP:HB3	1.75	0.67
1:F:165:ILE:HG22	1:F:168:SER:HB2	1.77	0.67
1:J:92:ASN:H	1:J:92:ASN:ND2	1.88	0.67
1:H:21:THR:CG2	1:H:27:VAL:HG23	2.25	0.67
1:G:39:MET:HB2	1:G:49:ASP:HB3	1.76	0.66
1:J:21:THR:CG2	1:J:27:VAL:HG23	2.23	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:MET:HB2	1:A:49:ASP:HB3	1.77	0.66
1:F:186:CYS:C	1:F:187:CYS:SG	2.74	0.66
1:A:176:THR:O	1:A:177:GLN:HB3	1.96	0.66
1:I:39:MET:HB2	1:I:49:ASP:HB3	1.76	0.66
1:H:176:THR:O	1:H:177:GLN:HB3	1.95	0.65
1:D:39:MET:HB2	1:D:49:ASP:HB3	1.77	0.65
1:D:23:ARG:O	1:D:25:ARG:HG2	1.96	0.65
1:D:176:THR:O	1:D:177:GLN:HB3	1.96	0.65
1:I:150:ARG:NH1	1:I:190:PRO:HD2	2.11	0.65
1:C:39:MET:HB2	1:C:49:ASP:HB3	1.79	0.65
1:D:165:ILE:HG22	1:D:168:SER:HB2	1.79	0.65
1:A:116:LEU:O	1:E:145:TRP:HZ2	1.80	0.65
1:A:108:ASN:HD22	1:A:112:HIS:HB3	1.62	0.65
1:A:165:ILE:HG22	1:A:168:SER:HB2	1.79	0.64
1:G:55:GLN:HA	1:G:116:LEU:HD13	1.79	0.64
1:I:181:GLU:OE2	1:I:190:PRO:HG3	1.97	0.64
1:B:176:THR:O	1:B:177:GLN:HB3	1.97	0.64
1:F:176:THR:O	1:F:177:GLN:HB3	1.95	0.64
1:G:176:THR:O	1:G:177:GLN:HB3	1.96	0.64
1:F:42:ASP:HB3	1:F:47:VAL:HG22	1.79	0.64
1:A:46:GLN:OE1	1:A:126:ASP:HA	1.97	0.64
1:A:21:THR:HG23	1:A:27:VAL:HG23	1.80	0.64
1:I:3:GLN:OE1	1:I:3:GLN:N	2.31	0.64
1:I:169:ARG:HD2	1:I:202:LYS:HE3	1.80	0.64
1:B:55:GLN:HA	1:B:116:LEU:HD13	1.79	0.63
1:B:141:LYS:NZ	1:B:182:ARG:HH22	1.96	0.63
1:J:42:ASP:HB3	1:J:47:VAL:HG22	1.80	0.63
1:H:165:ILE:HG22	1:H:168:SER:HB2	1.80	0.63
1:D:21:THR:CG2	1:D:27:VAL:HG23	2.27	0.63
1:C:55:GLN:HA	1:C:116:LEU:HD13	1.79	0.63
1:D:29:VAL:HG12	1:D:58:TRP:HB3	1.81	0.63
1:C:3:GLN:HA	1:C:3:GLN:HE21	1.62	0.63
1:D:42:ASP:HB3	1:D:47:VAL:HG22	1.80	0.62
1:E:108:ASN:HB2	1:E:112:HIS:H	1.64	0.62
1:H:55:GLN:HA	1:H:116:LEU:HD13	1.80	0.62
1:B:108:ASN:HB2	1:B:112:HIS:H	1.64	0.62
1:C:46:GLN:OE1	1:C:126:ASP:HA	1.99	0.62
1:B:42:ASP:HB3	1:B:47:VAL:HG22	1.79	0.62
1:I:46:GLN:OE1	1:I:126:ASP:HA	1.98	0.62
1:C:169:ARG:HD2	1:C:202:LYS:HE3	1.81	0.62
1:E:165:ILE:HG22	1:E:168:SER:HB2	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:46:GLN:OE1	1:H:126:ASP:HA	1.98	0.62
1:J:6:LEU:HD23	1:J:73:VAL:HG11	1.81	0.62
1:D:96:LYS:HG3	1:D:97:PRO:HD2	1.82	0.61
1:G:42:ASP:HB3	1:G:47:VAL:HG22	1.81	0.61
1:B:141:LYS:HZ2	1:B:182:ARG:HH22	1.48	0.61
1:F:23:ARG:HH11	1:G:71:PRO:HB3	1.65	0.61
1:I:181:GLU:OE2	1:I:190:PRO:CG	2.48	0.61
1:G:149:SER:OG	1:G:192:PRO:HD3	2.01	0.61
1:A:42:ASP:HB3	1:A:47:VAL:HG22	1.81	0.61
1:J:108:ASN:HB2	1:J:112:HIS:H	1.66	0.61
1:F:29:VAL:HG12	1:F:58:TRP:HB3	1.83	0.61
1:A:107:VAL:HG12	1:A:113:VAL:HG22	1.83	0.61
1:J:55:GLN:HA	1:J:116:LEU:HD13	1.80	0.61
1:B:22:GLN:HG3	1:B:25:ARG:HB2	1.83	0.61
1:B:6:LEU:HD23	1:B:73:VAL:HG11	1.83	0.61
1:C:108:ASN:HB2	1:C:112:HIS:H	1.65	0.61
1:H:42:ASP:HB3	1:H:47:VAL:HG22	1.83	0.61
1:J:165:ILE:HG22	1:J:168:SER:HB2	1.82	0.60
1:D:108:ASN:HB2	1:D:112:HIS:H	1.65	0.60
1:F:39:MET:HE1	1:J:47:VAL:HG11	1.83	0.60
1:E:107:VAL:HG12	1:E:113:VAL:HG22	1.82	0.60
1:A:108:ASN:HB2	1:A:112:HIS:H	1.66	0.60
1:H:39:MET:HB2	1:H:49:ASP:HB3	1.84	0.60
1:B:46:GLN:OE1	1:B:126:ASP:HA	2.01	0.60
1:B:185:GLU:O	1:B:186:CYS:HB3	2.01	0.60
1:G:165:ILE:HG22	1:G:168:SER:HB2	1.81	0.60
1:H:6:LEU:HD23	1:H:73:VAL:HG11	1.83	0.60
1:F:6:LEU:HD23	1:F:73:VAL:HG11	1.83	0.60
1:D:6:LEU:HD23	1:D:73:VAL:HG11	1.83	0.60
1:G:107:VAL:HG12	1:G:113:VAL:HG22	1.84	0.59
1:H:108:ASN:HB2	1:H:112:HIS:H	1.65	0.59
1:A:6:LEU:HD23	1:A:73:VAL:HG11	1.84	0.59
1:G:108:ASN:HB2	1:G:112:HIS:H	1.67	0.59
1:I:42:ASP:HB3	1:I:47:VAL:HG22	1.84	0.59
1:I:165:ILE:HG22	1:I:168:SER:HB2	1.83	0.59
1:C:165:ILE:HG22	1:C:168:SER:HB2	1.84	0.59
1:G:6:LEU:HD23	1:G:73:VAL:HG11	1.84	0.59
1:D:107:VAL:HG12	1:D:113:VAL:HG22	1.84	0.59
1:F:169:ARG:HD2	1:F:202:LYS:HE3	1.85	0.59
1:A:148:HIS:HB2	1:A:189:GLU:HB3	1.83	0.59
2:B:901:NAG:H3	2:B:901:NAG:C8	2.33	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:46:GLN:OE1	1:D:126:ASP:HA	2.02	0.59
1:F:108:ASN:HB2	1:F:112:HIS:H	1.65	0.59
1:C:141:LYS:HZ2	1:C:182:ARG:NH1	2.01	0.59
1:C:6:LEU:HD23	1:C:73:VAL:HG11	1.83	0.59
1:F:150:ARG:HD3	1:F:189:GLU:CG	2.33	0.59
1:J:96:LYS:HG3	1:J:97:PRO:HD2	1.85	0.59
1:F:46:GLN:OE1	1:F:126:ASP:HA	2.02	0.59
1:H:22:GLN:O	1:H:23:ARG:O	2.21	0.58
1:F:96:LYS:HG3	1:F:97:PRO:HD2	1.85	0.58
1:E:187:CYS:HB3	1:E:189:GLU:HB2	1.85	0.58
1:J:46:GLN:OE1	1:J:126:ASP:HA	2.03	0.58
1:C:21:THR:HG22	1:C:27:VAL:HG23	1.84	0.58
1:D:185:GLU:O	1:D:186:CYS:SG	2.62	0.58
1:I:108:ASN:HB2	1:I:112:HIS:H	1.67	0.58
1:G:92:ASN:HD21	1:G:141:LYS:H	1.50	0.58
1:B:165:ILE:HG22	1:B:168:SER:HB2	1.85	0.58
1:F:107:VAL:HG12	1:F:113:VAL:HG22	1.85	0.58
1:E:46:GLN:OE1	1:E:126:ASP:HA	2.03	0.58
1:B:169:ARG:HD2	1:B:202:LYS:HE3	1.85	0.58
1:G:3:GLN:O	1:G:4:ARG:HD3	2.03	0.58
1:E:42:ASP:HB3	1:E:47:VAL:HG22	1.86	0.58
1:I:6:LEU:HD23	1:I:73:VAL:HG11	1.85	0.58
1:C:3:GLN:HA	1:C:3:GLN:NE2	2.19	0.57
1:B:29:VAL:HG12	1:B:58:TRP:HB3	1.86	0.57
1:C:23:ARG:HH11	1:D:71:PRO:HB3	1.69	0.57
1:I:29:VAL:HG12	1:I:58:TRP:HB3	1.86	0.57
1:I:96:LYS:HG3	1:I:97:PRO:HD2	1.86	0.57
1:G:29:VAL:HG12	1:G:58:TRP:HB3	1.87	0.57
1:C:42:ASP:HB3	1:C:47:VAL:HG22	1.87	0.57
1:G:92:ASN:N	1:G:92:ASN:HD22	2.02	0.56
1:E:148:HIS:CD2	1:E:189:GLU:HG2	2.39	0.56
1:G:108:ASN:HD22	1:G:112:HIS:HB3	1.70	0.56
1:G:46:GLN:OE1	1:G:126:ASP:HA	2.04	0.56
1:J:22:GLN:O	1:J:23:ARG:O	2.23	0.56
1:E:6:LEU:HD23	1:E:73:VAL:HG11	1.87	0.56
1:H:23:ARG:O	1:H:25:ARG:HG2	2.06	0.56
1:J:149:SER:HB2	1:J:190:PRO:HG2	1.88	0.56
1:A:29:VAL:HG12	1:A:58:TRP:HB3	1.87	0.56
1:C:107:VAL:HG12	1:C:113:VAL:HG22	1.87	0.56
1:E:187:CYS:C	1:E:189:GLU:N	2.58	0.56
1:D:55:GLN:HG3	1:D:116:LEU:CD1	2.34	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:29:VAL:HG12	1:E:58:TRP:HB3	1.88	0.56
1:I:150:ARG:NH1	1:I:189:GLU:HA	2.21	0.55
1:B:96:LYS:HG3	1:B:97:PRO:HD2	1.87	0.55
1:E:149:SER:CB	1:E:190:PRO:HG2	2.34	0.55
1:G:185:GLU:O	1:G:186:CYS:CB	2.55	0.55
1:H:29:VAL:HG12	1:H:58:TRP:HB3	1.88	0.55
1:B:107:VAL:HG12	1:B:113:VAL:HG22	1.87	0.55
1:H:49:ASP:HA	1:H:122:ARG:HG3	1.89	0.55
1:F:107:VAL:CG1	1:F:113:VAL:HG22	2.37	0.55
1:G:169:ARG:HD2	1:G:202:LYS:HE3	1.89	0.55
1:G:189:GLU:HA	1:G:189:GLU:OE2	2.05	0.55
1:A:101:THR:HG21	1:E:145:TRP:CH2	2.42	0.55
1:A:39:MET:HE1	1:E:47:VAL:HG11	1.89	0.55
1:D:169:ARG:HD2	1:D:202:LYS:HE3	1.88	0.55
1:C:108:ASN:CG	2:C:901:NAG:HN2	2.10	0.55
1:J:167:TYR:O	1:J:168:SER:HB3	2.07	0.55
1:H:108:ASN:ND2	1:H:112:HIS:HB3	2.21	0.55
1:C:167:TYR:O	1:C:168:SER:HB3	2.07	0.55
1:I:107:VAL:HG12	1:I:113:VAL:HG22	1.89	0.55
1:F:3:GLN:HE22	1:J:23:ARG:NE	2.05	0.54
1:J:169:ARG:HD2	1:J:202:LYS:HE3	1.89	0.54
1:G:96:LYS:HG3	1:G:97:PRO:HD2	1.89	0.54
1:D:107:VAL:CG1	1:D:113:VAL:HG22	2.37	0.54
1:C:96:LYS:HG3	1:C:97:PRO:HD2	1.88	0.54
1:E:96:LYS:HG3	1:E:97:PRO:HD2	1.88	0.54
1:H:189:GLU:HG3	1:H:190:PRO:HD2	1.89	0.54
1:E:92:ASN:HD21	1:E:140:LEU:HA	1.72	0.54
1:A:52:PHE:N	1:A:52:PHE:CD1	2.75	0.54
1:J:29:VAL:HG12	1:J:58:TRP:HB3	1.87	0.54
1:B:148:HIS:CE1	1:B:189:GLU:HG2	2.43	0.54
1:C:110:SER:HB3	2:C:901:NAG:C8	2.38	0.54
1:H:107:VAL:HG12	1:H:113:VAL:HG22	1.89	0.54
1:D:76:VAL:HG23	1:D:107:VAL:HG23	1.88	0.54
1:I:108:ASN:HD22	1:I:112:HIS:HB3	1.72	0.54
1:J:107:VAL:HG12	1:J:113:VAL:HG22	1.89	0.54
1:A:156:MET:CE	1:A:177:GLN:HE21	2.21	0.54
1:I:49:ASP:HA	1:I:122:ARG:HG3	1.90	0.54
1:A:167:TYR:O	1:A:168:SER:HB3	2.08	0.54
1:G:187:CYS:O	1:G:189:GLU:HG2	2.07	0.54
1:A:96:LYS:HG3	1:A:97:PRO:HD2	1.88	0.53
1:G:47:VAL:HG11	1:H:39:MET:HE1	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:167:TYR:O	1:D:168:SER:HB3	2.08	0.53
1:A:107:VAL:CG1	1:A:113:VAL:HG22	2.38	0.53
1:G:34:SER:HB3	1:G:53:TRP:HB3	1.90	0.53
1:C:49:ASP:HA	1:C:122:ARG:HG3	1.91	0.53
1:E:107:VAL:CG1	1:E:113:VAL:HG22	2.39	0.53
1:B:76:VAL:HG23	1:B:107:VAL:HG23	1.91	0.53
1:C:189:GLU:OE2	1:C:190:PRO:HD2	2.08	0.53
1:H:186:CYS:SG	1:H:187:CYS:N	2.81	0.53
1:G:107:VAL:CG1	1:G:113:VAL:HG22	2.37	0.53
1:H:22:GLN:HG3	1:H:25:ARG:HG3	1.91	0.52
1:F:21:THR:HG22	1:F:27:VAL:HG23	1.90	0.52
1:H:110:SER:HB3	3:H:901:NAG:H82	1.91	0.52
1:G:150:ARG:NH1	1:G:190:PRO:HG3	2.24	0.52
1:A:49:ASP:HA	1:A:122:ARG:HG3	1.92	0.52
1:B:107:VAL:CG1	1:B:113:VAL:HG22	2.39	0.52
1:I:110:SER:OG	3:I:901:NAG:H61	2.08	0.52
1:G:55:GLN:HG3	1:G:116:LEU:CD1	2.38	0.52
1:C:47:VAL:HG11	1:D:39:MET:HE1	1.90	0.52
1:F:76:VAL:HG23	1:F:107:VAL:HG23	1.91	0.52
1:H:96:LYS:HG3	1:H:97:PRO:HD2	1.91	0.52
1:B:141:LYS:NZ	1:B:182:ARG:NH2	2.57	0.52
1:C:21:THR:CG2	1:C:27:VAL:HG23	2.40	0.52
1:H:33:LEU:HD23	1:H:34:SER:N	2.25	0.52
1:I:156:MET:CE	1:I:177:GLN:HE21	2.22	0.52
1:E:167:TYR:O	1:E:168:SER:HB3	2.10	0.52
1:G:21:THR:HG22	1:G:27:VAL:HG23	1.90	0.52
1:D:188:LYS:HD3	1:D:188:LYS:O	2.10	0.52
1:D:3:GLN:HA	1:D:3:GLN:NE2	2.24	0.52
1:G:156:MET:CE	1:G:177:GLN:HE21	2.23	0.52
1:I:185:GLU:O	1:I:186:CYS:CB	2.58	0.52
1:I:167:TYR:O	1:I:168:SER:HB3	2.10	0.51
1:G:186:CYS:O	1:G:188:LYS:N	2.39	0.51
1:A:45:ASN:ND2	1:B:39:MET:O	2.43	0.51
1:H:165:ILE:CG2	1:H:168:SER:HB2	2.41	0.51
1:C:29:VAL:HG12	1:C:58:TRP:HB3	1.93	0.51
1:E:49:ASP:HA	1:E:122:ARG:HG3	1.92	0.51
1:B:49:ASP:HA	1:B:122:ARG:HG3	1.91	0.51
1:F:167:TYR:O	1:F:168:SER:HB3	2.10	0.51
1:E:186:CYS:O	1:E:188:LYS:N	2.40	0.51
1:F:66:ASN:HB2	2:F:801:NAG:C2	2.40	0.51
1:D:165:ILE:CG2	1:D:168:SER:HB2	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:107:VAL:CG1	1:I:113:VAL:HG22	2.41	0.51
1:J:34:SER:HB3	1:J:53:TRP:HB3	1.92	0.51
1:D:3:GLN:HA	1:D:3:GLN:HE21	1.76	0.51
1:B:101:THR:CG2	1:B:118:SER:HB2	2.39	0.51
1:I:186:CYS:SG	1:I:187:CYS:N	2.83	0.51
1:A:76:VAL:HG23	1:A:107:VAL:HG23	1.92	0.51
1:I:145:TRP:CH2	1:J:101:THR:HG21	2.45	0.51
1:E:101:THR:CG2	1:E:118:SER:HB2	2.39	0.51
1:A:20:PRO:O	1:A:27:VAL:HG22	2.11	0.51
1:B:3:GLN:NE2	1:B:3:GLN:HA	2.25	0.51
1:H:34:SER:HB3	1:H:53:TRP:HB3	1.91	0.51
1:H:18:VAL:HG22	1:I:7:TYR:CD2	2.46	0.51
1:H:49:ASP:OD2	1:H:122:ARG:HD2	2.11	0.50
1:J:107:VAL:CG1	1:J:113:VAL:HG22	2.41	0.50
1:F:165:ILE:CG2	1:F:168:SER:HB2	2.40	0.50
1:J:49:ASP:HA	1:J:122:ARG:HG3	1.93	0.50
1:C:148:HIS:HA	1:C:191:TYR:CD2	2.46	0.50
1:E:156:MET:CE	1:E:177:GLN:HE21	2.24	0.50
1:F:186:CYS:SG	1:F:187:CYS:N	2.84	0.50
1:A:165:ILE:CG2	1:A:168:SER:HB2	2.42	0.50
1:C:107:VAL:CG1	1:C:113:VAL:HG22	2.41	0.50
1:C:161:ILE:O	1:C:161:ILE:HG12	2.11	0.50
1:D:49:ASP:HA	1:D:122:ARG:HG3	1.93	0.50
1:B:22:GLN:HG3	1:B:25:ARG:CB	2.42	0.50
1:F:55:GLN:HG3	1:F:116:LEU:CD1	2.36	0.49
1:E:54:LEU:HD12	1:E:119:ILE:CD1	2.42	0.49
1:F:169:ARG:HH12	1:J:44:LYS:HD3	1.77	0.49
1:A:169:ARG:NH1	1:E:44:LYS:HD3	2.27	0.49
1:E:31:PHE:CE1	1:E:54:LEU:HD22	2.47	0.49
1:D:23:ARG:NH1	1:E:71:PRO:HB3	2.27	0.49
1:F:23:ARG:NH1	1:G:71:PRO:HB3	2.26	0.49
1:J:165:ILE:CG2	1:J:168:SER:HB2	2.42	0.49
1:G:101:THR:CG2	1:G:118:SER:HB2	2.38	0.49
1:B:150:ARG:NH1	1:B:190:PRO:CD	2.75	0.49
1:F:21:THR:CG2	1:F:27:VAL:HG23	2.42	0.49
1:B:92:ASN:HD22	1:B:123:PHE:HD2	1.60	0.49
1:G:145:TRP:CH2	1:H:101:THR:HG21	2.47	0.49
1:H:55:GLN:HG3	1:H:116:LEU:CD1	2.42	0.49
1:B:186:CYS:SG	1:B:187:CYS:N	2.84	0.49
1:B:167:TYR:O	1:B:168:SER:HB3	2.13	0.49
1:C:44:LYS:HD3	1:D:169:ARG:HH12	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:52:PHE:CE2	1:F:54:LEU:HG	2.48	0.49
1:J:142:PHE:O	1:J:193:ASP:HB2	2.13	0.49
1:H:148:HIS:CE1	1:H:151:GLU:HG3	2.47	0.49
1:E:165:ILE:CG2	1:E:168:SER:HB2	2.42	0.49
1:C:76:VAL:HG23	1:C:107:VAL:HG23	1.94	0.49
1:D:92:ASN:HD21	1:D:141:LYS:H	1.58	0.49
1:B:150:ARG:HD3	1:B:189:GLU:HG3	1.95	0.49
1:H:107:VAL:CG1	1:H:113:VAL:HG22	2.43	0.49
1:A:31:PHE:HE2	1:A:196:PHE:HE1	1.59	0.49
1:E:187:CYS:O	1:E:188:LYS:HB2	2.13	0.49
1:G:165:ILE:CG2	1:G:168:SER:HB2	2.43	0.49
1:H:76:VAL:HG23	1:H:107:VAL:HG23	1.94	0.49
1:B:156:MET:CE	1:B:177:GLN:HE21	2.26	0.49
1:G:49:ASP:HA	1:G:122:ARG:HG3	1.94	0.49
1:D:12:LYS:HE3	1:I:69:GLU:OE1	2.13	0.49
1:I:41:VAL:HG12	1:I:48:VAL:HG12	1.94	0.49
1:D:156:MET:CE	1:D:177:GLN:HE21	2.26	0.48
1:E:150:ARG:NH1	1:E:190:PRO:CD	2.76	0.48
1:I:21:THR:CG2	1:I:27:VAL:HG23	2.41	0.48
1:F:49:ASP:HA	1:F:122:ARG:HG3	1.95	0.48
1:G:76:VAL:HG23	1:G:107:VAL:HG23	1.94	0.48
1:F:3:GLN:HA	1:F:3:GLN:HE21	1.78	0.48
1:C:92:ASN:ND2	1:C:92:ASN:H	1.97	0.48
1:E:55:GLN:HG3	1:E:116:LEU:CD1	2.38	0.48
1:F:92:ASN:N	1:F:92:ASN:ND2	2.39	0.48
1:E:167:TYR:CD1	1:E:167:TYR:N	2.81	0.48
1:J:149:SER:CB	1:J:190:PRO:HG2	2.44	0.48
1:J:76:VAL:HG23	1:J:107:VAL:HG23	1.94	0.48
1:D:65:TRP:CE2	1:D:109:SER:HA	2.49	0.48
1:C:92:ASN:HD22	1:C:92:ASN:N	1.95	0.48
1:D:20:PRO:O	1:D:27:VAL:HG22	2.14	0.48
1:F:33:LEU:HD23	1:F:34:SER:N	2.28	0.48
1:F:161:ILE:HG12	1:F:161:ILE:O	2.13	0.48
1:F:101:THR:HG21	1:J:145:TRP:CZ2	2.48	0.48
1:D:76:VAL:CG2	1:D:107:VAL:HG23	2.44	0.48
1:H:33:LEU:C	1:H:33:LEU:HD23	2.34	0.48
1:I:148:HIS:HB3	1:I:191:TYR:CZ	2.47	0.48
1:A:49:ASP:OD2	1:A:122:ARG:HD2	2.13	0.48
1:E:169:ARG:HD2	1:E:202:LYS:HE3	1.95	0.48
1:F:156:MET:CE	1:F:177:GLN:HE21	2.26	0.48
1:I:165:ILE:CG2	1:I:168:SER:HB2	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:33:LEU:HD23	1:G:34:SER:N	2.29	0.48
1:J:36:LEU:CD2	1:J:53:TRP:HB2	2.43	0.48
1:J:41:VAL:HG12	1:J:48:VAL:HG12	1.96	0.48
1:H:156:MET:CE	1:H:177:GLN:HE21	2.28	0.47
1:A:169:ARG:HH12	1:E:44:LYS:HD3	1.79	0.47
1:A:33:LEU:HD23	1:A:34:SER:N	2.29	0.47
1:J:161:ILE:HG12	1:J:161:ILE:O	2.13	0.47
1:C:165:ILE:CG2	1:C:168:SER:HB2	2.43	0.47
1:H:35:LEU:HD21	1:H:50:VAL:HG13	1.95	0.47
1:I:76:VAL:HG23	1:I:107:VAL:HG23	1.96	0.47
1:B:150:ARG:NH1	1:B:190:PRO:HD3	2.28	0.47
1:B:149:SER:OG	1:B:192:PRO:HD3	2.14	0.47
1:C:110:SER:HB3	2:C:901:NAG:H82	1.95	0.47
1:E:33:LEU:HD23	1:E:34:SER:N	2.28	0.47
1:A:101:THR:CG2	1:A:118:SER:HB2	2.39	0.47
1:F:156:MET:HE1	1:F:177:GLN:HE21	1.79	0.47
1:J:76:VAL:CG2	1:J:107:VAL:HG23	2.45	0.47
1:G:148:HIS:CE1	1:G:151:GLU:HG3	2.49	0.47
1:B:148:HIS:CE1	1:B:151:GLU:HG3	2.50	0.47
1:A:112:HIS:HD2	2:A:901:NAG:C8	2.28	0.47
1:G:92:ASN:N	1:G:92:ASN:ND2	2.61	0.47
1:J:36:LEU:HD21	1:J:53:TRP:HB2	1.96	0.47
1:F:101:THR:HG21	1:J:145:TRP:CH2	2.49	0.46
1:H:101:THR:CG2	1:H:118:SER:HB2	2.41	0.46
1:D:101:THR:CG2	1:D:118:SER:HB2	2.38	0.46
1:H:23:ARG:NH1	1:I:71:PRO:HB3	2.30	0.46
1:F:169:ARG:NH1	1:J:44:LYS:HD3	2.30	0.46
1:G:44:LYS:HD3	1:H:169:ARG:NH1	2.30	0.46
1:E:148:HIS:CE1	1:E:151:GLU:HG3	2.50	0.46
1:B:49:ASP:OD2	1:B:122:ARG:HD2	2.15	0.46
1:J:33:LEU:HD23	1:J:34:SER:N	2.30	0.46
1:F:148:HIS:CE1	1:F:151:GLU:HG3	2.51	0.46
1:A:55:GLN:HG3	1:A:116:LEU:CD1	2.43	0.46
1:A:76:VAL:CG2	1:A:107:VAL:HG23	2.45	0.46
1:C:76:VAL:CG2	1:C:107:VAL:HG23	2.45	0.46
1:B:21:THR:HG23	1:B:27:VAL:HG23	1.98	0.46
1:D:33:LEU:HD23	1:D:34:SER:N	2.30	0.46
1:E:20:PRO:HG2	1:E:27:VAL:HG21	1.96	0.46
1:D:41:VAL:HG12	1:D:48:VAL:HG12	1.96	0.46
1:E:150:ARG:HH11	1:E:190:PRO:CD	2.29	0.46
1:E:76:VAL:HG23	1:E:107:VAL:HG23	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:76:VAL:HG23	1:D:107:VAL:CG2	2.45	0.46
1:G:44:LYS:HD3	1:H:169:ARG:HH12	1.79	0.46
1:G:18:VAL:HG22	1:H:7:TYR:CD2	2.51	0.46
1:B:189:GLU:HA	1:B:190:PRO:HD3	1.83	0.46
1:C:148:HIS:CE1	1:C:151:GLU:HG3	2.51	0.46
1:C:41:VAL:HG12	1:C:48:VAL:HG12	1.98	0.46
1:J:187:CYS:HB3	1:J:189:GLU:OE1	2.16	0.46
1:G:167:TYR:O	1:G:168:SER:HB3	2.15	0.46
1:B:76:VAL:CG2	1:B:107:VAL:HG23	2.46	0.46
1:I:148:HIS:CE1	1:I:151:GLU:HG3	2.51	0.46
1:E:33:LEU:C	1:E:33:LEU:HD23	2.37	0.46
1:A:54:LEU:HD12	1:A:119:ILE:HD12	1.98	0.46
1:H:76:VAL:CG2	1:H:107:VAL:HG23	2.46	0.45
1:D:148:HIS:CE1	1:D:151:GLU:HG3	2.50	0.45
1:I:33:LEU:HD23	1:I:34:SER:N	2.31	0.45
1:H:167:TYR:O	1:H:168:SER:HB3	2.17	0.45
1:D:185:GLU:OE1	1:D:185:GLU:HA	2.16	0.45
1:C:23:ARG:NH1	1:D:71:PRO:HB3	2.30	0.45
1:H:169:ARG:HD2	1:H:202:LYS:HE3	1.99	0.45
1:D:33:LEU:C	1:D:33:LEU:HD23	2.37	0.45
1:A:35:LEU:HD21	1:A:50:VAL:HG13	1.97	0.45
1:J:156:MET:CE	1:J:177:GLN:HE21	2.29	0.45
1:I:47:VAL:HG11	1:J:39:MET:HE1	1.98	0.45
1:B:167:TYR:N	1:B:167:TYR:CD1	2.84	0.45
1:G:33:LEU:HB3	1:G:196:PHE:CE2	2.51	0.45
1:H:54:LEU:HD23	1:H:54:LEU:HA	1.67	0.45
1:J:54:LEU:HD12	1:J:119:ILE:HD12	1.99	0.45
1:F:76:VAL:CG2	1:F:107:VAL:HG23	2.46	0.45
1:I:167:TYR:N	1:I:167:TYR:CD1	2.83	0.45
1:J:41:VAL:O	1:J:41:VAL:HG23	2.17	0.45
1:E:34:SER:HB3	1:E:53:TRP:HB3	1.97	0.45
1:G:76:VAL:CG2	1:G:107:VAL:HG23	2.47	0.45
1:F:76:VAL:HG23	1:F:107:VAL:CG2	2.47	0.45
1:A:33:LEU:HD23	1:A:33:LEU:C	2.36	0.45
1:G:41:VAL:O	1:G:41:VAL:HG23	2.16	0.45
1:A:41:VAL:HG12	1:A:48:VAL:HG12	1.99	0.45
1:B:52:PHE:CE2	1:B:54:LEU:HG	2.51	0.45
1:F:150:ARG:HD3	1:F:189:GLU:HG2	1.97	0.45
1:E:76:VAL:CG2	1:E:107:VAL:HG23	2.46	0.45
1:A:148:HIS:CE1	1:A:151:GLU:HG3	2.51	0.45
1:C:29:VAL:O	1:C:29:VAL:HG23	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:22:GLN:HG3	1:A:25:ARG:HB2	1.98	0.45
1:H:167:TYR:CD1	1:H:167:TYR:N	2.82	0.45
1:I:101:THR:CG2	1:I:118:SER:HB2	2.43	0.45
1:G:149:SER:CB	1:G:190:PRO:HG2	2.43	0.45
1:B:165:ILE:CG2	1:B:168:SER:HB2	2.46	0.45
1:J:183:PHE:CE1	1:J:190:PRO:HB3	2.52	0.45
1:F:41:VAL:HG12	1:F:48:VAL:HG12	1.99	0.45
1:D:161:ILE:O	1:D:161:ILE:HG12	2.17	0.45
1:A:21:THR:CG2	1:A:27:VAL:HG23	2.47	0.45
1:H:22:GLN:HG3	1:H:25:ARG:CB	2.47	0.45
1:A:176:THR:OG1	1:A:197:THR:HB	2.17	0.44
1:D:35:LEU:HD21	1:D:50:VAL:HG13	1.99	0.44
1:B:76:VAL:HG23	1:B:107:VAL:CG2	2.47	0.44
1:C:34:SER:HB3	1:C:53:TRP:HB3	1.99	0.44
1:J:148:HIS:CE1	1:J:151:GLU:HG3	2.52	0.44
1:E:41:VAL:HG23	1:E:41:VAL:O	2.17	0.44
1:A:156:MET:HE1	1:A:177:GLN:HE21	1.81	0.44
1:B:33:LEU:HD23	1:B:34:SER:N	2.33	0.44
1:G:191:TYR:HA	1:G:192:PRO:HD2	1.84	0.44
2:B:901:NAG:H83	2:B:901:NAG:H3	1.99	0.44
1:B:156:MET:HE1	1:B:177:GLN:HE21	1.83	0.44
1:I:182:ARG:NH1	1:I:182:ARG:HG3	2.30	0.44
1:I:22:GLN:O	1:I:23:ARG:O	2.35	0.44
1:E:187:CYS:CB	1:E:189:GLU:HB2	2.46	0.44
1:C:55:GLN:HG3	1:C:116:LEU:CD1	2.41	0.44
1:G:156:MET:HE1	1:G:177:GLN:HE21	1.83	0.44
1:H:165:ILE:HA	1:H:166:PRO:HD3	1.89	0.44
1:D:178:LYS:O	1:D:178:LYS:HG3	2.18	0.44
1:J:65:TRP:CE2	1:J:109:SER:HA	2.53	0.44
1:J:49:ASP:OD2	1:J:122:ARG:HD2	2.18	0.44
1:A:76:VAL:HG23	1:A:107:VAL:CG2	2.48	0.44
1:C:148:HIS:CG	1:C:189:GLU:HG2	2.53	0.44
1:B:52:PHE:CD1	1:B:52:PHE:N	2.86	0.44
1:B:35:LEU:HD21	1:B:50:VAL:HG13	1.99	0.44
1:I:90:ALA:HB1	1:I:123:PHE:HE2	1.83	0.44
1:F:108:ASN:ND2	1:F:112:HIS:HB3	2.26	0.43
1:D:167:TYR:CD1	1:D:167:TYR:N	2.84	0.43
1:D:42:ASP:CB	1:D:47:VAL:HG22	2.48	0.43
1:F:42:ASP:CB	1:F:47:VAL:HG22	2.47	0.43
1:F:78:VAL:HA	1:F:79:PRO:HD3	1.83	0.43
1:B:41:VAL:HG12	1:B:48:VAL:HG12	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:156:MET:CE	1:C:177:GLN:HE21	2.31	0.43
1:C:19:ILE:HG12	1:C:21:THR:HG23	1.99	0.43
1:E:29:VAL:O	1:E:29:VAL:HG23	2.19	0.43
1:C:41:VAL:O	1:C:41:VAL:HG23	2.17	0.43
1:D:52:PHE:CE2	1:D:119:ILE:HB	2.52	0.43
1:B:22:GLN:HG3	1:B:25:ARG:HG3	2.00	0.43
1:C:83:LEU:HD23	1:C:83:LEU:H	1.83	0.43
1:E:83:LEU:HD23	1:E:83:LEU:H	1.83	0.43
1:E:108:ASN:ND2	1:E:112:HIS:HB3	2.24	0.43
1:H:89:ALA:HB3	1:H:145:TRP:CE3	2.53	0.43
1:E:156:MET:HE1	1:E:177:GLN:HE21	1.83	0.43
3:H:901:NAG:C4	3:H:902:NAG:N2	2.81	0.43
1:C:49:ASP:OD2	1:C:122:ARG:HD2	2.18	0.43
1:C:108:ASN:ND2	1:C:112:HIS:HB3	2.34	0.43
1:B:176:THR:OG1	1:B:197:THR:HB	2.19	0.43
1:C:167:TYR:CD1	1:C:167:TYR:N	2.82	0.43
1:C:181:GLU:HG2	1:C:190:PRO:HB2	2.01	0.43
1:H:41:VAL:HG23	1:H:41:VAL:O	2.19	0.43
1:J:167:TYR:N	1:J:167:TYR:CD1	2.82	0.43
1:G:76:VAL:HG23	1:G:107:VAL:CG2	2.49	0.43
1:G:36:LEU:CD2	1:G:53:TRP:HB2	2.49	0.43
1:I:189:GLU:CD	1:I:189:GLU:H	2.22	0.43
1:E:165:ILE:HA	1:E:166:PRO:HD3	1.93	0.43
1:F:191:TYR:HA	1:F:192:PRO:HD2	1.90	0.43
1:I:200:PHE:N	1:I:200:PHE:CD1	2.87	0.43
1:D:55:GLN:CG	1:D:116:LEU:HD11	2.41	0.42
1:D:41:VAL:HG23	1:D:41:VAL:O	2.19	0.42
1:B:65:TRP:CE2	1:B:109:SER:HA	2.54	0.42
1:J:19:ILE:HG12	1:J:21:THR:HG23	2.01	0.42
1:D:22:GLN:O	1:D:23:ARG:O	2.37	0.42
1:C:36:LEU:HB2	1:C:51:VAL:O	2.19	0.42
1:B:55:GLN:HG3	1:B:116:LEU:CD1	2.46	0.42
1:I:49:ASP:OD2	1:I:122:ARG:HD2	2.19	0.42
1:H:29:VAL:O	1:H:29:VAL:HG23	2.18	0.42
1:C:200:PHE:CD1	1:C:200:PHE:N	2.88	0.42
1:J:83:LEU:H	1:J:83:LEU:HD23	1.84	0.42
1:A:31:PHE:CE2	1:A:196:PHE:HE1	2.37	0.42
1:F:33:LEU:HD23	1:F:33:LEU:C	2.40	0.42
1:B:33:LEU:HB3	1:B:196:PHE:CE2	2.53	0.42
1:I:65:TRP:CE2	1:I:109:SER:HA	2.54	0.42
1:I:156:MET:HE1	1:I:177:GLN:HE21	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:55:GLN:HG3	1:J:116:LEU:CD1	2.43	0.42
1:E:33:LEU:HB3	1:E:196:PHE:CE2	2.55	0.42
1:G:65:TRP:CE2	1:G:109:SER:HA	2.53	0.42
1:J:35:LEU:HD21	1:J:50:VAL:HG13	2.01	0.42
1:B:141:LYS:HZ1	1:B:182:ARG:NH2	2.16	0.42
1:C:33:LEU:HD23	1:C:34:SER:N	2.34	0.42
1:E:83:LEU:N	1:E:83:LEU:HD23	2.35	0.42
1:E:149:SER:OG	1:E:192:PRO:HD3	2.20	0.42
1:J:42:ASP:CB	1:J:47:VAL:HG22	2.49	0.42
1:D:49:ASP:OD2	1:D:122:ARG:HD2	2.20	0.42
1:F:186:CYS:O	1:F:187:CYS:O	2.38	0.42
1:A:165:ILE:HA	1:A:166:PRO:HD3	1.91	0.42
1:B:22:GLN:CG	1:B:25:ARG:HB2	2.50	0.42
1:I:44:LYS:HD3	1:J:169:ARG:HH12	1.85	0.42
1:J:76:VAL:HG23	1:J:107:VAL:CG2	2.50	0.42
1:E:35:LEU:HD21	1:E:50:VAL:HG13	2.02	0.42
1:E:185:GLU:O	1:E:186:CYS:CB	2.54	0.42
1:G:49:ASP:OD2	1:G:122:ARG:HD2	2.19	0.42
1:E:65:TRP:CE2	1:E:109:SER:HA	2.55	0.42
1:G:35:LEU:HD21	1:G:50:VAL:HG13	2.02	0.42
1:I:161:ILE:HG12	1:I:161:ILE:O	2.20	0.42
1:D:108:ASN:ND2	1:D:112:HIS:HB3	2.27	0.42
1:A:42:ASP:CB	1:A:47:VAL:HG22	2.50	0.42
1:D:31:PHE:HE2	1:D:196:PHE:HE1	1.68	0.42
1:J:176:THR:OG1	1:J:197:THR:HB	2.20	0.41
1:I:3:GLN:HB3	1:I:71:PRO:HG2	2.00	0.41
1:A:148:HIS:CB	1:A:189:GLU:HB3	2.48	0.41
1:H:76:VAL:HG23	1:H:107:VAL:CG2	2.49	0.41
1:G:33:LEU:HD23	1:G:33:LEU:C	2.39	0.41
1:I:33:LEU:C	1:I:33:LEU:HD23	2.41	0.41
1:C:148:HIS:HA	1:C:191:TYR:HD2	1.84	0.41
1:B:33:LEU:HD23	1:B:33:LEU:C	2.41	0.41
1:G:200:PHE:N	1:G:200:PHE:CD1	2.89	0.41
1:B:29:VAL:HG23	1:B:29:VAL:O	2.19	0.41
1:I:29:VAL:O	1:I:29:VAL:HG23	2.19	0.41
1:C:44:LYS:CG	1:D:169:ARG:NH1	2.84	0.41
1:I:76:VAL:CG2	1:I:107:VAL:HG23	2.50	0.41
1:A:161:ILE:O	1:A:161:ILE:HG12	2.19	0.41
1:B:47:VAL:HG11	1:C:39:MET:HE1	2.02	0.41
1:C:44:LYS:HD3	1:D:169:ARG:NH1	2.34	0.41
1:H:31:PHE:HE2	1:H:196:PHE:HE1	1.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:78:VAL:HA	1:I:79:PRO:HD3	1.82	0.41
1:H:176:THR:OG1	1:H:197:THR:HB	2.20	0.41
1:A:65:TRP:CE2	1:A:109:SER:HA	2.56	0.41
1:D:18:VAL:HG22	1:E:7:TYR:CE2	2.56	0.41
1:C:65:TRP:CE2	1:C:109:SER:HA	2.55	0.41
1:E:187:CYS:C	1:E:189:GLU:H	2.19	0.41
1:I:156:MET:HE3	1:I:177:GLN:HE21	1.86	0.41
1:E:49:ASP:OD2	1:E:122:ARG:HD2	2.20	0.41
1:C:76:VAL:HG23	1:C:107:VAL:CG2	2.50	0.41
1:G:187:CYS:C	1:G:189:GLU:N	2.72	0.41
1:I:182:ARG:CG	1:I:182:ARG:HH11	2.29	0.41
1:D:23:ARG:C	1:D:25:ARG:N	2.73	0.41
1:E:76:VAL:HG23	1:E:107:VAL:CG2	2.51	0.41
1:G:41:VAL:HG12	1:G:48:VAL:HG12	2.02	0.41
1:J:200:PHE:N	1:J:200:PHE:CD1	2.88	0.41
1:B:150:ARG:HH12	1:B:190:PRO:HD3	1.86	0.41
1:C:83:LEU:N	1:C:83:LEU:HD23	2.36	0.41
1:C:142:PHE:O	1:C:193:ASP:HB2	2.20	0.41
1:F:35:LEU:HD21	1:F:50:VAL:HG13	2.02	0.41
1:B:78:VAL:HA	1:B:79:PRO:HD3	1.82	0.41
1:G:145:TRP:HZ2	1:H:116:LEU:O	2.04	0.41
1:A:112:HIS:HD2	2:A:901:NAG:H82	1.85	0.41
1:J:108:ASN:ND2	1:J:112:HIS:HB3	2.35	0.41
1:C:149:SER:HB2	1:C:190:PRO:HG2	2.02	0.41
1:H:41:VAL:HG12	1:H:48:VAL:HG12	2.02	0.41
1:F:70:TYR:O	1:F:71:PRO:O	2.39	0.41
1:H:145:TRP:CZ2	1:I:101:THR:HG21	2.55	0.41
1:A:41:VAL:HG23	1:A:41:VAL:O	2.21	0.41
1:H:65:TRP:CE2	1:H:109:SER:HA	2.56	0.41
1:C:12:LYS:HE2	1:H:23:ARG:HH22	1.85	0.40
1:G:96:LYS:HD3	1:H:99:VAL:O	2.20	0.40
1:D:3:GLN:HE21	1:D:3:GLN:CA	2.32	0.40
1:J:83:LEU:N	1:J:83:LEU:HD23	2.35	0.40
1:E:80:ILE:C	1:E:80:ILE:HD12	2.41	0.40
1:E:15:ASN:HA	1:E:16:PRO:HD2	1.93	0.40
1:C:35:LEU:HD21	1:C:50:VAL:HG13	2.03	0.40
1:C:70:TYR:O	1:C:71:PRO:O	2.39	0.40
1:I:150:ARG:HH11	1:I:190:PRO:HD2	1.85	0.40
1:H:200:PHE:N	1:H:200:PHE:CD1	2.89	0.40
1:H:83:LEU:HD23	1:H:83:LEU:H	1.87	0.40
1:B:161:ILE:HG12	1:B:161:ILE:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:182:ARG:O	1:E:190:PRO:HA	2.21	0.40
1:D:65:TRP:CZ2	1:D:109:SER:HA	2.56	0.40
1:B:18:VAL:HG22	1:C:7:TYR:CD2	2.56	0.40
1:I:70:TYR:O	1:I:71:PRO:O	2.40	0.40
1:G:29:VAL:O	1:G:29:VAL:HG23	2.21	0.40
1:I:113:VAL:HG12	1:I:114:GLN:N	2.36	0.40
1:F:39:MET:O	1:J:45:ASN:ND2	2.55	0.40
1:F:165:ILE:HA	1:F:166:PRO:HD3	1.89	0.40
1:A:29:VAL:O	1:A:29:VAL:HG23	2.21	0.40
1:I:41:VAL:O	1:I:41:VAL:HG23	2.21	0.40
1:G:78:VAL:HA	1:G:79:PRO:HD3	1.85	0.40
1:F:140:LEU:HD12	1:F:140:LEU:N	2.37	0.40
1:E:161:ILE:O	1:E:161:ILE:HG12	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	200/204 (98%)	173 (86%)	21 (10%)	6 (3%)	5	28
1	B	200/204 (98%)	168 (84%)	23 (12%)	9 (4%)	3	17
1	C	200/204 (98%)	171 (86%)	26 (13%)	3 (2%)	13	46
1	D	200/204 (98%)	171 (86%)	22 (11%)	7 (4%)	4	24
1	E	200/204 (98%)	171 (86%)	24 (12%)	5 (2%)	7	32
1	F	200/204 (98%)	173 (86%)	22 (11%)	5 (2%)	7	32
1	G	200/204 (98%)	169 (84%)	25 (12%)	6 (3%)	5	28
1	H	200/204 (98%)	173 (86%)	22 (11%)	5 (2%)	7	32
1	I	200/204 (98%)	168 (84%)	24 (12%)	8 (4%)	4	21
1	J	200/204 (98%)	172 (86%)	22 (11%)	6 (3%)	5	28

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	2000/2040 (98%)	1709 (86%)	231 (12%)	60 (3%)	5	28

All (60) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	71	PRO
1	A	187	CYS
1	B	23	ARG
1	B	71	PRO
1	B	184	TYR
1	B	186	CYS
1	B	187	CYS
1	C	23	ARG
1	C	71	PRO
1	D	23	ARG
1	D	71	PRO
1	D	187	CYS
1	E	23	ARG
1	E	71	PRO
1	E	186	CYS
1	E	187	CYS
1	F	23	ARG
1	F	71	PRO
1	F	187	CYS
1	G	23	ARG
1	G	71	PRO
1	G	186	CYS
1	H	23	ARG
1	H	71	PRO
1	I	23	ARG
1	I	71	PRO
1	I	186	CYS
1	J	23	ARG
1	J	71	PRO
1	J	186	CYS
1	A	23	ARG
1	A	167	TYR
1	B	185	GLU
1	C	167	TYR
1	D	167	TYR
1	D	188	LYS
1	E	167	TYR

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Mol	Chain	Res	Type
1	F	167	TYR
1	G	167	TYR
1	H	167	TYR
1	I	185	GLU
1	I	187	CYS
1	J	167	TYR
1	A	186	CYS
1	B	167	TYR
1	B	188	LYS
1	D	183	PHE
1	G	187	CYS
1	I	167	TYR
1	J	185	GLU
1	I	188	LYS
1	B	168	SER
1	H	168	SER
1	H	186	CYS
1	I	168	SER
1	A	168	SER
1	D	168	SER
1	F	168	SER
1	G	168	SER
1	J	168	SER

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	188/190 (99%)	177 (94%)	11 (6%)	24	60
1	B	188/190 (99%)	179 (95%)	9 (5%)	31	69
1	C	188/190 (99%)	176 (94%)	12 (6%)	22	57
1	D	188/190 (99%)	179 (95%)	9 (5%)	31	69
1	E	188/190 (99%)	180 (96%)	8 (4%)	35	72
1	F	188/190 (99%)	178 (95%)	10 (5%)	28	64

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	188/190 (99%)	180 (96%)	8 (4%)	35	72
1	H	188/190 (99%)	178 (95%)	10 (5%)	28	64
1	I	188/190 (99%)	179 (95%)	9 (5%)	31	69
1	J	188/190 (99%)	180 (96%)	8 (4%)	35	72
All	All	1880/1900 (99%)	1786 (95%)	94 (5%)	30	67

All (94) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ARG
1	A	21	THR
1	A	35	LEU
1	A	52	PHE
1	A	53	TRP
1	A	71	PRO
1	A	107	VAL
1	A	167	TYR
1	A	179	ARG
1	A	186	CYS
1	A	187	CYS
1	B	4	ARG
1	B	21	THR
1	B	35	LEU
1	B	71	PRO
1	B	92	ASN
1	B	107	VAL
1	B	118	SER
1	B	167	TYR
1	B	179	ARG
1	C	4	ARG
1	C	24	ASP
1	C	35	LEU
1	C	71	PRO
1	C	92	ASN
1	C	107	VAL
1	C	167	TYR
1	C	179	ARG
1	C	183	PHE
1	C	185	GLU
1	C	186	CYS
1	C	187	CYS

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Mol	Chain	Res	Type
1	D	4	ARG
1	D	21	THR
1	D	35	LEU
1	D	71	PRO
1	D	92	ASN
1	D	107	VAL
1	D	167	TYR
1	D	179	ARG
1	D	188	LYS
1	E	4	ARG
1	E	35	LEU
1	E	71	PRO
1	E	92	ASN
1	E	107	VAL
1	E	167	TYR
1	E	179	ARG
1	E	189	GLU
1	F	3	GLN
1	F	4	ARG
1	F	35	LEU
1	F	71	PRO
1	F	92	ASN
1	F	107	VAL
1	F	167	TYR
1	F	179	ARG
1	F	183	PHE
1	F	187	CYS
1	G	4	ARG
1	G	35	LEU
1	G	54	LEU
1	G	71	PRO
1	G	92	ASN
1	G	107	VAL
1	G	167	TYR
1	G	179	ARG
1	H	4	ARG
1	H	35	LEU
1	H	71	PRO
1	H	92	ASN
1	H	107	VAL
1	H	118	SER
1	H	167	TYR

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Mol	Chain	Res	Type
1	H	179	ARG
1	H	183	PHE
1	H	187	CYS
1	I	3	GLN
1	I	4	ARG
1	I	21	THR
1	I	35	LEU
1	I	71	PRO
1	I	107	VAL
1	I	167	TYR
1	I	179	ARG
1	I	187	CYS
1	J	4	ARG
1	J	35	LEU
1	J	54	LEU
1	J	71	PRO
1	J	92	ASN
1	J	107	VAL
1	J	167	TYR
1	J	179	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (60) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	37	GLN
1	A	45	ASN
1	A	112	HIS
1	A	157	GLN
1	A	177	GLN
1	B	3	GLN
1	B	37	GLN
1	B	45	ASN
1	B	92	ASN
1	B	157	GLN
1	B	177	GLN
1	C	3	GLN
1	C	37	GLN
1	C	45	ASN
1	C	92	ASN
1	C	157	GLN
1	C	177	GLN
1	D	3	GLN

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Mol	Chain	Res	Type
1	D	37	GLN
1	D	45	ASN
1	D	92	ASN
1	D	108	ASN
1	D	157	GLN
1	D	177	GLN
1	E	3	GLN
1	E	37	GLN
1	E	45	ASN
1	E	112	HIS
1	E	157	GLN
1	E	177	GLN
1	F	3	GLN
1	F	37	GLN
1	F	45	ASN
1	F	92	ASN
1	F	108	ASN
1	F	157	GLN
1	F	177	GLN
1	G	3	GLN
1	G	37	GLN
1	G	45	ASN
1	G	92	ASN
1	G	157	GLN
1	G	177	GLN
1	H	37	GLN
1	H	45	ASN
1	H	121	GLN
1	H	157	GLN
1	H	177	GLN
1	I	3	GLN
1	I	37	GLN
1	I	45	ASN
1	I	157	GLN
1	I	177	GLN
1	J	3	GLN
1	J	37	GLN
1	J	45	ASN
1	J	92	ASN
1	J	112	HIS
1	J	157	GLN
1	J	177	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

6 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	B	801	1,3	14,14,15	0.89	1 (7%)	15,19,21	0.66	0
3	NAG	B	802	3	14,14,15	0.93	1 (7%)	15,19,21	0.99	1 (6%)
3	NAG	H	901	1,3	14,14,15	1.11	2 (14%)	15,19,21	1.14	2 (13%)
3	NAG	H	902	3	14,14,15	1.09	1 (7%)	15,19,21	0.69	0
3	NAG	I	901	1,3	14,14,15	0.85	0	15,19,21	0.93	1 (6%)
3	NAG	I	902	3	14,14,15	0.94	1 (7%)	15,19,21	1.02	1 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	B	801	1,3	-	0/6/23/26	0/1/1/1
3	NAG	B	802	3	-	0/6/23/26	0/1/1/1
3	NAG	H	901	1,3	-	0/6/23/26	0/1/1/1
3	NAG	H	902	3	-	0/6/23/26	0/1/1/1
3	NAG	I	901	1,3	-	0/6/23/26	0/1/1/1
3	NAG	I	902	3	-	0/6/23/26	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	801	NAG	C1-C2	2.10	1.55	1.52
3	I	902	NAG	C1-C2	2.22	1.55	1.52
3	H	901	NAG	C3-C2	2.32	1.57	1.52
3	H	901	NAG	C4-C3	2.33	1.58	1.52
3	B	802	NAG	C1-C2	2.40	1.55	1.52
3	H	902	NAG	C1-C2	2.98	1.56	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	901	NAG	C3-C4-C5	2.19	114.02	110.20
3	B	802	NAG	C1-O5-C5	2.37	115.26	112.25
3	H	901	NAG	C4-C3-C2	2.79	115.57	111.23
3	I	901	NAG	C1-O5-C5	2.83	115.84	112.25
3	I	902	NAG	C1-O5-C5	3.20	116.31	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	H	901	NAG	3	0
3	H	902	NAG	2	0
3	I	901	NAG	1	0

5.6 Ligand geometry ⓘ

14 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	$\# Z > 2$
2	NAG	A	801	1	14,14,15	1.00	2 (14%)	15,19,21	1.15	1 (6%)
2	NAG	A	901	1	14,14,15	0.73	0	15,19,21	0.71	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	B	901	1	14,14,15	1.05	1 (7%)	15,19,21	1.23	1 (6%)
2	NAG	C	801	1	14,14,15	0.83	1 (7%)	15,19,21	0.83	1 (6%)
2	NAG	C	901	1	14,14,15	0.93	1 (7%)	15,19,21	0.48	0
2	NAG	D	801	1	14,14,15	0.70	0	15,19,21	0.97	1 (6%)
2	NAG	E	801	1	14,14,15	0.63	0	15,19,21	0.56	0
2	NAG	E	901	1	14,14,15	0.76	0	15,19,21	0.86	0
2	NAG	F	801	1	14,14,15	0.93	1 (7%)	15,19,21	1.06	1 (6%)
2	NAG	G	901	1	14,14,15	0.91	0	15,19,21	1.38	2 (13%)
2	NAG	H	801	1	14,14,15	0.77	0	15,19,21	0.75	0
2	NAG	I	801	1	14,14,15	0.79	0	15,19,21	0.77	0
2	NAG	J	801	1	14,14,15	0.90	1 (7%)	15,19,21	0.61	0
2	NAG	J	901	1	14,14,15	0.76	0	15,19,21	0.78	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
2	NAG	A	801	1	-	0/6/23/26	0/1/1/1
2	NAG	A	901	1	-	0/6/23/26	0/1/1/1
2	NAG	B	901	1	-	0/6/23/26	0/1/1/1
2	NAG	C	801	1	-	0/6/23/26	0/1/1/1
2	NAG	C	901	1	-	0/6/23/26	0/1/1/1
2	NAG	D	801	1	-	0/6/23/26	0/1/1/1
2	NAG	E	801	1	-	0/6/23/26	0/1/1/1
2	NAG	E	901	1	-	0/6/23/26	0/1/1/1
2	NAG	F	801	1	-	0/6/23/26	0/1/1/1
2	NAG	G	901	1	-	2/6/23/26	0/1/1/1
2	NAG	H	801	1	-	0/6/23/26	0/1/1/1
2	NAG	I	801	1	-	0/6/23/26	0/1/1/1
2	NAG	J	801	1	-	0/6/23/26	0/1/1/1
2	NAG	J	901	1	-	0/6/23/26	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	NAG	C1-C2	2.30	1.55	1.52
2	A	801	NAG	C3-C2	2.31	1.57	1.52
2	C	801	NAG	C1-C2	2.35	1.55	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	801	NAG	C1-C2	2.44	1.55	1.52
2	J	801	NAG	C1-C2	2.49	1.55	1.52
2	C	901	NAG	C1-C2	2.54	1.56	1.52
2	B	901	NAG	C1-C2	2.75	1.56	1.52

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	801	NAG	C2-N2-C7	-2.34	120.04	123.04
2	C	801	NAG	C4-C3-C2	2.01	114.35	111.23
2	G	901	NAG	C3-C4-C5	2.15	113.94	110.20
2	F	801	NAG	C1-O5-C5	2.98	116.03	112.25
2	B	901	NAG	C4-C3-C2	3.20	116.21	111.23
2	A	801	NAG	C4-C3-C2	3.49	116.66	111.23
2	G	901	NAG	C4-C3-C2	4.18	117.73	111.23

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	G	901	NAG	C8-C7-N2-C2
2	G	901	NAG	O7-C7-N2-C2

There are no ring outliers.

4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	901	NAG	2	0
2	B	901	NAG	2	0
2	C	901	NAG	3	0
2	F	801	NAG	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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	202/204 (99%)	0.08	0 100 100	72, 108, 139, 150	0
1	B	202/204 (99%)	0.16	0 100 100	74, 110, 137, 154	0
1	C	202/204 (99%)	0.24	4 (1%) 68 46	70, 108, 138, 158	0
1	D	202/204 (99%)	0.24	4 (1%) 68 46	74, 108, 138, 156	0
1	E	202/204 (99%)	0.24	5 (2%) 61 37	75, 107, 136, 148	0
1	F	202/204 (99%)	0.31	4 (1%) 68 46	73, 112, 140, 161	0
1	G	202/204 (99%)	0.21	4 (1%) 68 46	75, 108, 138, 148	0
1	H	202/204 (99%)	0.22	2 (0%) 84 69	70, 107, 140, 153	0
1	I	202/204 (99%)	0.17	3 (1%) 76 58	76, 108, 138, 154	0
1	J	202/204 (99%)	0.19	4 (1%) 68 46	76, 110, 140, 155	0
All	All	2020/2040 (99%)	0.21	30 (1%) 76 58	70, 109, 140, 161	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	204	GLY	4.6
1	F	204	GLY	4.4
1	E	204	GLY	3.4
1	F	23	ARG	3.4
1	H	173	VAL	3.2
1	D	5	LYS	3.1
1	E	23	ARG	2.9
1	G	74	LYS	2.8
1	G	72	GLY	2.8
1	G	204	GLY	2.7
1	E	72	GLY	2.7
1	C	185	GLU	2.6
1	D	23	ARG	2.6

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Mol	Chain	Res	Type	RSRZ
1	J	185	GLU	2.5
1	I	73	VAL	2.4
1	G	71	PRO	2.4
1	F	44	LYS	2.3
1	J	63	LEU	2.3
1	D	25	ARG	2.3
1	I	24	ASP	2.2
1	C	63	LEU	2.2
1	C	71	PRO	2.2
1	D	9	GLU	2.1
1	H	204	GLY	2.1
1	J	181	GLU	2.1
1	I	69	GLU	2.1
1	J	68	SER	2.1
1	E	74	LYS	2.1
1	E	3	GLN	2.1
1	F	184	TYR	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	I	901	14/15	0.76	0.27	1.23	145,151,153,154	0
3	NAG	I	902	14/15	0.71	0.34	-	133,149,156,157	0
3	NAG	B	802	14/15	0.76	0.36	-	145,164,167,167	0
3	NAG	H	902	14/15	0.64	0.34	-	129,145,155,157	0
3	NAG	B	801	14/15	0.86	0.45	-	148,161,165,167	0
3	NAG	H	901	14/15	0.86	0.40	-	138,149,154,156	0

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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
2	NAG	E	901	14/15	0.72	0.33	1.30	127,145,147,150	0
2	NAG	B	901	14/15	0.72	0.21	1.15	115,127,130,132	0
2	NAG	G	901	14/15	0.70	0.38	-	145,151,155,155	0
2	NAG	A	801	14/15	0.77	0.38	-	132,144,152,152	0
2	NAG	C	801	14/15	0.64	0.50	-	139,159,162,163	0
2	NAG	J	801	14/15	0.60	0.55	-	147,161,162,163	0
2	NAG	H	801	14/15	0.76	0.36	-	129,149,155,155	0
2	NAG	E	801	14/15	0.78	0.51	-	138,161,166,167	0
2	NAG	F	801	14/15	0.69	0.50	-	141,162,164,165	0
2	NAG	D	801	14/15	0.72	0.69	-	160,170,171,173	0
2	NAG	C	901	14/15	0.75	0.28	-	125,139,146,148	0
2	NAG	I	801	14/15	0.74	0.29	-	133,151,155,156	0
2	NAG	A	901	14/15	0.71	0.37	-	140,149,153,156	0
2	NAG	J	901	14/15	0.73	0.34	-	142,153,156,158	0

6.5 Other polymers [i](#)

There are no such residues in this entry.