



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 10, 2020 – 01:19 AM BST

PDB ID : 1YK0
Title : structure of natriuretic peptide receptor-C complexed with atrial natriuretic peptide
Authors : He, X.; Garcia, K.C.
Deposited on : 2005-01-16
Resolution : 2.40 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

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

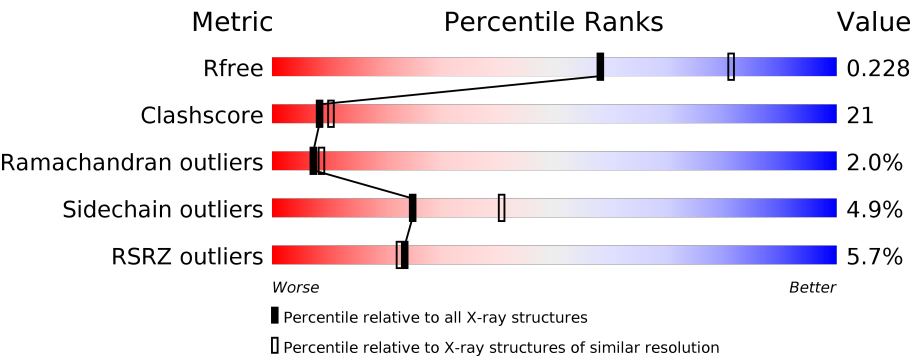
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 Å.

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



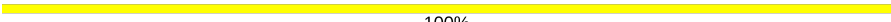
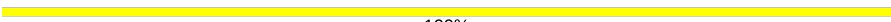
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	1-A	480	<div><div>2%</div><div><div></div><div>50%</div><div>29%</div><div>•</div><div>18%</div></div></div>
1	1-B	480	<div><div>4%</div><div><div></div><div>52%</div><div>28%</div><div>•</div><div>18%</div></div></div>
1	2-A	480	<div><div>2%</div><div><div></div><div>51%</div><div>29%</div><div>•</div><div>18%</div></div></div>
1	2-B	480	<div><div>4%</div><div><div></div><div>52%</div><div>29%</div><div>•</div><div>18%</div></div></div>
2	1-E	21	<div><div>100%</div><div><div>19%</div><div>52%</div><div>24%</div><div>5%</div></div></div>
2	2-E	21	<div><div>100%</div><div><div>10%</div><div>52%</div><div>29%</div><div>10%</div></div></div>

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Mol	Chain	Length	Quality of chain
3	1-C	2	 100%
3	2-C	2	 100%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	NAG	1-A	511	X	-	-	-
4	NAG	1-A	512	X	-	-	-
4	NAG	2-A	511	X	-	-	-
4	NAG	2-A	512	X	-	-	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 13526 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 Atrial natriuretic peptide clearance receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	1-A	394	Total	C	N	O	S	0	0	0
			3111	1972	532	591	16			
1	2-A	394	Total	C	N	O	S	0	0	0
			3111	1972	532	591	16			
1	1-B	394	Total	C	N	O	S	0	0	0
			3111	1972	532	591	16			
1	2-B	394	Total	C	N	O	S	0	0	0
			3111	1972	532	591	16			

- Molecule 2 is a protein called Atrial natriuretic factor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	1-E	21	Total	C	N	O	S	0	0	0
			149	88	29	29	3			
2	2-E	21	Total	C	N	O	S	0	0	0
			149	88	29	29	3			

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	1-C	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	2-C	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).



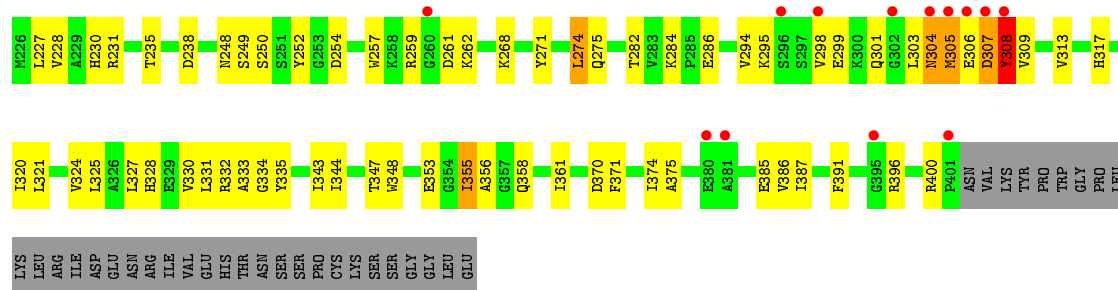
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	1-A	1	Total	C	N	O	0	0
			14	8	1	5		
4	2-A	1	Total	C	N	O	0	0
			14	8	1	5		
4	1-A	1	Total	C	N	O	0	0
			14	8	1	5		
4	2-A	1	Total	C	N	O	0	0
			14	8	1	5		
4	1-B	1	Total	C	N	O	0	0
			14	8	1	5		
4	2-B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

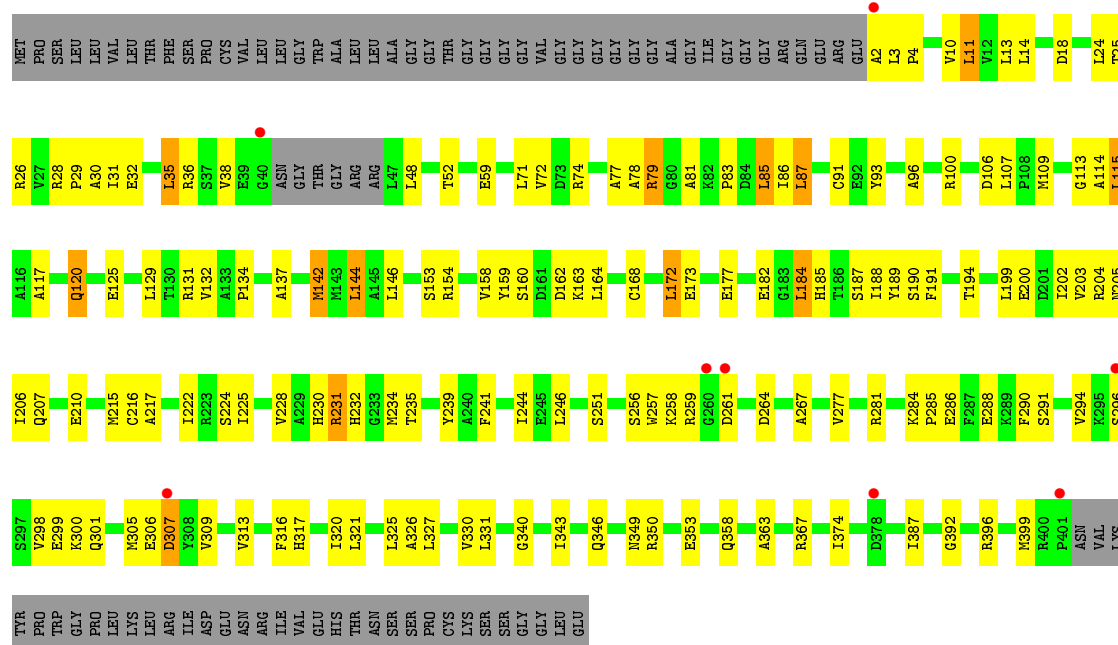
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	2-A	1	Total	Cl	0	0
			1	1		
5	1-B	1	Total	Cl	0	0
			1	1		
5	1-A	1	Total	Cl	0	0
			1	1		
5	2-B	1	Total	Cl	0	0
			1	1		

- Molecule 6 is water.

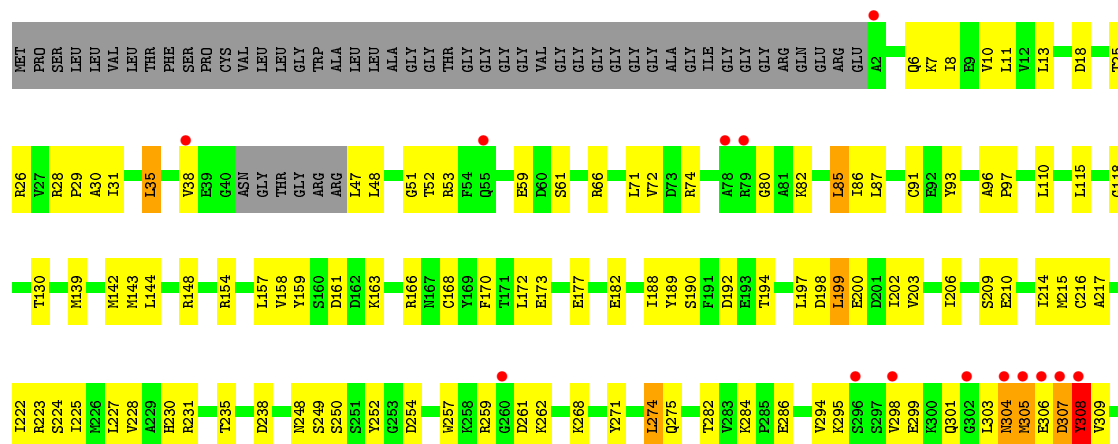
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	1-A	167	Total 167	O 167	0	0
6	2-A	168	Total 168	O 168	0	0
6	1-B	152	Total 152	O 152	0	0
6	2-B	151	Total 151	O 151	0	0
6	1-E	1	Total 1	O 1	0	0
6	2-E	1	Total 1	O 1	0	0

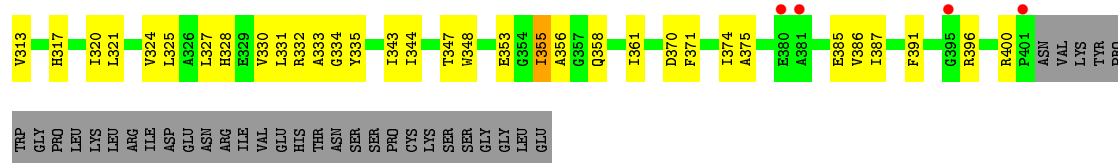


- Molecule 1: Atrial natriuretic peptide clearance receptor

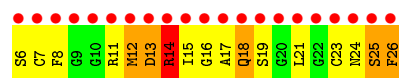
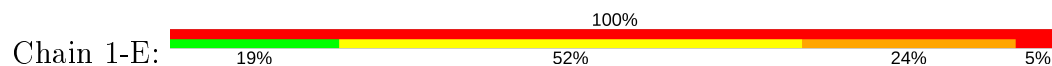


- Molecule 1: Atrial natriuretic peptide clearance receptor

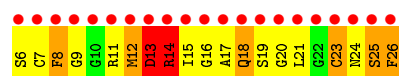
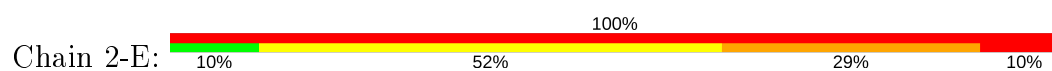




- Molecule 2: Atrial natriuretic factor



- Molecule 2: Atrial natriuretic factor



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	56.87Å 135.47Å 137.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.40 6.95 – 2.26	Depositor EDS
% Data completeness (in resolution range)	98.6 (50.00-2.40) 94.1 (6.95-2.26)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.81 (at 2.27Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.240 , 0.284 0.224 , 0.228	Depositor DCC
R_{free} test set	2321 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	53.0	Xtriage
Anisotropy	0.732	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	1.00 , 78.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.029 for -h,l,k	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	13526	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.43% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	1-A	0.37	0/3180	0.62	0/4297
1	1-B	0.38	0/3180	0.61	0/4297
1	2-A	0.37	0/3180	0.62	0/4297
1	2-B	0.38	0/3180	0.61	0/4297
2	1-E	0.57	0/150	0.90	0/195
2	2-E	0.59	0/150	0.88	0/195
All	All	0.38	0/13020	0.62	0/17578

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1-A	3111	0	3013	132	0
1	1-B	3111	0	3014	122	0
1	2-A	3111	0	3013	131	0
1	2-B	3111	0	3014	124	0
2	1-E	149	0	135	25	0
2	2-E	149	0	135	28	0
3	1-C	28	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	2-C	28	0	25	0	0
4	1-A	28	0	26	0	0
4	1-B	14	0	13	0	0
4	2-A	28	0	26	0	0
4	2-B	14	0	13	0	0
5	1-A	1	0	0	0	0
5	1-B	1	0	0	0	0
5	2-A	1	0	0	0	0
5	2-B	1	0	0	0	0
6	1-A	167	0	0	11	0
6	1-B	152	0	0	6	0
6	1-E	1	0	0	0	0
6	2-A	168	0	0	11	0
6	2-B	151	0	0	6	0
6	2-E	1	0	0	0	0
All	All	13526	0	12452	529	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 21.

All (529) 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:E:12:MET:HE3	2:E:15:ILE:HG12	1.14	1.12
1:B:130:THR:HG22	1:B:348:TRP:HE1	1.13	1.11
1:B:130:THR:HG22	1:B:348:TRP:HE1	1.13	1.11
2:E:12:MET:HE3	2:E:15:ILE:HG12	1.13	1.07
1:B:295:LYS:HG3	1:B:305:MET:HG3	1.49	0.94
1:B:295:LYS:HG3	1:B:305:MET:HG3	1.49	0.94
1:A:118:GLY:H	2:E:15:ILE:HD12	1.33	0.94
1:B:31:ILE:HG23	1:B:320:ILE:HD11	1.50	0.93
1:B:31:ILE:HG23	1:B:320:ILE:HD11	1.50	0.93
1:B:284:LYS:HE3	1:B:286:GLU:HB3	1.54	0.89
1:B:284:LYS:HE3	1:B:286:GLU:HB3	1.54	0.89
1:B:327:LEU:O	1:B:330:VAL:HG12	1.78	0.83
1:B:327:LEU:O	1:B:330:VAL:HG12	1.78	0.83
1:B:74:ARG:HD3	6:B:606:HOH:O	1.78	0.82
1:B:74:ARG:HD3	6:B:605:HOH:O	1.78	0.82
1:A:159:TYR:HB3	1:A:172:LEU:HD22	1.61	0.82
1:A:159:TYR:HB3	1:A:172:LEU:HD22	1.61	0.82
1:A:91:CYS:HB3	6:A:566:HOH:O	1.79	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:91:CYS:HB3	6:A:567:HOH:O	1.79	0.82
1:A:79:ARG:HH11	1:A:79:ARG:HB3	1.45	0.82
1:A:79:ARG:HH11	1:A:79:ARG:HB3	1.45	0.82
1:B:38:VAL:HG21	1:B:324:VAL:HG21	1.62	0.81
1:B:38:VAL:HG21	1:B:324:VAL:HG21	1.62	0.81
2:E:12:MET:CE	2:E:15:ILE:HG12	2.06	0.81
2:E:12:MET:CE	2:E:15:ILE:HG12	2.06	0.80
1:B:130:THR:HG22	1:B:348:TRP:NE1	1.95	0.79
1:B:96:ALA:HB3	1:B:97:PRO:HD3	1.65	0.79
1:B:130:THR:HG22	1:B:348:TRP:NE1	1.95	0.79
1:B:96:ALA:HB3	1:B:97:PRO:HD3	1.65	0.79
1:B:118:GLY:H	2:E:15:ILE:HD12	1.49	0.78
1:B:202:ILE:O	1:B:206:ILE:HG12	1.86	0.75
1:B:202:ILE:O	1:B:206:ILE:HG12	1.86	0.75
1:B:93:TYR:CD1	2:E:16:GLY:HA2	2.23	0.74
1:A:93:TYR:CD1	2:E:16:GLY:HA2	2.22	0.74
1:A:78:ALA:HB1	1:A:81:ALA:HB3	1.70	0.72
1:A:78:ALA:HB1	1:A:81:ALA:HB3	1.70	0.72
1:A:100:ARG:HD3	1:A:125:GLU:OE2	1.90	0.71
1:A:100:ARG:HD3	1:A:125:GLU:OE2	1.90	0.71
1:B:163:LYS:HA	1:B:166:ARG:HD3	1.73	0.71
1:B:330:VAL:HG22	1:B:335:TYR:HB2	1.71	0.71
1:B:163:LYS:HA	1:B:166:ARG:HD3	1.73	0.71
1:B:330:VAL:HG22	1:B:335:TYR:HB2	1.71	0.71
1:A:93:TYR:HD1	2:E:16:GLY:HA2	1.55	0.71
1:A:215:MET:HE1	1:A:225:ILE:HG21	1.73	0.71
1:A:215:MET:HE1	1:A:225:ILE:HG21	1.73	0.71
1:B:374:ILE:HG23	6:B:652:HOH:O	1.91	0.70
1:B:374:ILE:HG23	6:B:652:HOH:O	1.91	0.70
1:A:215:MET:CE	1:A:225:ILE:HG21	2.22	0.69
1:A:215:MET:CE	1:A:225:ILE:HG21	2.22	0.69
1:B:374:ILE:HG12	6:B:652:HOH:O	1.92	0.69
1:B:374:ILE:HG12	6:B:652:HOH:O	1.92	0.69
1:B:386:VAL:HB	1:B:400:ARG:NH1	2.07	0.69
1:B:386:VAL:HB	1:B:400:ARG:NH1	2.07	0.69
1:A:153:SER:HA	1:A:184:LEU:HD13	1.73	0.69
1:A:153:SER:HA	1:A:184:LEU:HD13	1.73	0.69
1:B:93:TYR:HD1	2:E:16:GLY:HA2	1.57	0.69
1:B:130:THR:HG23	1:B:344:ILE:HD12	1.74	0.68
1:B:31:ILE:HG23	1:B:320:ILE:CD1	2.23	0.68
1:B:130:THR:HG23	1:B:344:ILE:HD12	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:31:ILE:HG23	1:B:320:ILE:CD1	2.23	0.68
1:A:353:GLU:OE2	1:A:358:GLN:HG2	1.95	0.67
1:A:353:GLU:OE2	1:A:358:GLN:HG2	1.95	0.67
1:A:204:ARG:HH11	1:A:204:ARG:HG3	1.60	0.67
1:A:204:ARG:HG3	1:A:204:ARG:HH11	1.60	0.67
1:A:11:LEU:HD22	1:A:13:LEU:HG	1.77	0.66
1:B:249:SER:HA	1:B:252:TYR:CE2	2.31	0.66
1:B:52:THR:O	1:B:53:ARG:HD3	1.94	0.66
1:A:11:LEU:HD22	1:A:13:LEU:HG	1.77	0.66
1:B:249:SER:HA	1:B:252:TYR:CE2	2.31	0.66
1:B:52:THR:O	1:B:53:ARG:HD3	1.94	0.66
2:E:12:MET:O	2:E:14:ARG:N	2.30	0.65
2:E:12:MET:O	2:E:14:ARG:N	2.29	0.65
1:A:93:TYR:CD1	2:E:17:ALA:HB1	2.32	0.65
1:A:188:ILE:HD12	1:A:188:ILE:N	2.11	0.65
1:A:188:ILE:N	1:A:188:ILE:HD12	2.11	0.65
1:A:326:ALA:O	1:A:330:VAL:HG23	1.97	0.65
1:A:326:ALA:O	1:A:330:VAL:HG23	1.97	0.65
1:A:189:TYR:HE2	1:A:202:ILE:HD13	1.63	0.64
1:B:217:ALA:HB3	1:B:222:ILE:CD1	2.27	0.64
1:A:189:TYR:HE2	1:A:202:ILE:HD13	1.63	0.64
1:B:217:ALA:HB3	1:B:222:ILE:CD1	2.27	0.64
1:B:192:ASP:OD1	1:B:194:THR:HB	1.97	0.64
1:B:173:GLU:OE2	2:E:21:LEU:HB2	1.97	0.64
1:B:192:ASP:OD1	1:B:194:THR:HB	1.97	0.64
1:A:144:LEU:HD11	1:A:182:GLU:HG3	1.80	0.63
1:A:144:LEU:HD11	1:A:182:GLU:HG3	1.80	0.63
2:E:12:MET:HE3	2:E:15:ILE:CG1	2.08	0.63
1:B:130:THR:HG21	1:B:347:THR:OG1	1.99	0.63
1:B:130:THR:HG21	1:B:347:THR:OG1	1.99	0.63
1:B:148:ARG:HG3	1:B:148:ARG:HH21	1.62	0.63
1:B:148:ARG:HG3	1:B:148:ARG:HH21	1.62	0.63
1:B:118:GLY:N	2:E:15:ILE:HD12	2.13	0.63
1:A:35:LEU:O	1:A:38:VAL:HG22	1.98	0.62
1:A:35:LEU:O	1:A:38:VAL:HG22	1.98	0.62
1:A:284:LYS:HD2	1:A:286:GLU:HB2	1.82	0.62
1:B:189:TYR:HE2	1:B:202:ILE:HG12	1.64	0.62
1:A:284:LYS:HD2	1:A:286:GLU:HB2	1.82	0.62
1:B:189:TYR:HE2	1:B:202:ILE:HG12	1.64	0.62
1:A:18:ASP:OD2	1:A:25:THR:HB	1.99	0.62
1:A:18:ASP:OD2	1:A:25:THR:HB	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2:ALA:O	1:A:3:LEU:HD23	2.00	0.61
1:A:2:ALA:O	1:A:3:LEU:HD23	2.00	0.61
1:B:6:GLN:O	1:B:52:THR:HA	2.00	0.61
1:B:80:GLY:O	1:B:82:LYS:HE3	2.00	0.61
1:B:93:TYR:CD1	2:E:17:ALA:HB1	2.35	0.61
1:B:6:GLN:O	1:B:52:THR:HA	2.00	0.61
1:B:80:GLY:O	1:B:82:LYS:HE3	2.00	0.61
1:A:173:GLU:OE1	2:E:21:LEU:HB2	2.01	0.61
1:A:298:VAL:O	1:A:301:GLN:HB3	2.00	0.61
1:A:298:VAL:O	1:A:301:GLN:HB3	2.00	0.61
1:B:170:PHE:CE1	2:E:15:ILE:HG23	2.36	0.60
1:B:215:MET:CE	1:B:225:ILE:HG21	2.31	0.60
1:B:215:MET:CE	1:B:225:ILE:HG21	2.31	0.60
1:A:217:ALA:HB3	1:A:222:ILE:HD12	1.82	0.60
1:A:217:ALA:HB3	1:A:222:ILE:HD12	1.82	0.60
1:A:203:VAL:O	1:A:207:GLN:HG2	2.01	0.60
1:A:203:VAL:O	1:A:207:GLN:HG2	2.01	0.60
1:A:85:LEU:HD22	1:A:86:ILE:N	2.16	0.59
1:A:85:LEU:HD22	1:A:86:ILE:N	2.16	0.59
1:B:51:GLY:O	1:B:53:ARG:HG2	2.02	0.59
1:B:13:LEU:HD23	1:B:59:GLU:HB3	1.85	0.59
1:B:51:GLY:O	1:B:53:ARG:HG2	2.02	0.59
1:B:13:LEU:HD23	1:B:59:GLU:HB3	1.85	0.59
1:A:117:ALA:O	1:A:120:GLN:HB2	2.02	0.59
1:A:117:ALA:O	1:A:120:GLN:HB2	2.02	0.59
1:A:31:ILE:HG23	1:A:320:ILE:HD11	1.85	0.58
1:B:148:ARG:HH11	1:B:182:GLU:CG	2.16	0.58
1:A:31:ILE:HG23	1:A:320:ILE:HD11	1.85	0.58
1:B:148:ARG:HH11	1:B:182:GLU:CG	2.16	0.58
1:A:170:PHE:CE1	2:E:15:ILE:HG23	2.38	0.58
1:A:106:ASP:O	1:A:340:GLY:HA3	2.04	0.57
1:A:106:ASP:O	1:A:340:GLY:HA3	2.04	0.57
1:A:158:VAL:HG21	1:A:206:ILE:CD1	2.34	0.57
1:A:173:GLU:O	1:A:177:GLU:HG2	2.03	0.57
1:A:158:VAL:HG21	1:A:206:ILE:CD1	2.34	0.57
1:A:173:GLU:O	1:A:177:GLU:HG2	2.03	0.57
1:A:325:LEU:HD13	6:A:621:HOH:O	2.03	0.57
1:A:163:LYS:HZ1	2:E:9:GLY:HA3	1.69	0.57
1:A:325:LEU:HD13	6:A:623:HOH:O	2.03	0.57
1:B:30:ALA:HB2	1:B:313:VAL:HG13	1.87	0.57
1:B:30:ALA:HB2	1:B:313:VAL:HG13	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:198:ASP:C	1:B:200:GLU:H	2.09	0.56
1:A:132:VAL:HG12	1:A:132:VAL:O	2.04	0.56
1:B:198:ASP:C	1:B:200:GLU:H	2.09	0.56
1:A:132:VAL:O	1:A:132:VAL:HG12	2.04	0.56
1:B:321:LEU:O	1:B:325:LEU:HD13	2.05	0.56
1:B:321:LEU:O	1:B:325:LEU:HD13	2.05	0.56
1:A:159:TYR:HB3	1:A:172:LEU:CD2	2.33	0.56
1:A:187:SER:C	1:A:188:ILE:HD12	2.25	0.56
1:A:159:TYR:HB3	1:A:172:LEU:CD2	2.33	0.56
1:A:187:SER:C	1:A:188:ILE:HD12	2.25	0.56
1:B:294:VAL:O	1:B:298:VAL:HG23	2.06	0.56
1:B:294:VAL:O	1:B:298:VAL:HG23	2.06	0.56
1:B:148:ARG:HG3	1:B:148:ARG:NH2	2.21	0.56
1:B:148:ARG:HG3	1:B:148:ARG:NH2	2.21	0.56
1:B:161:ASP:OD2	1:B:166:ARG:HD2	2.06	0.56
1:B:161:ASP:OD2	1:B:166:ARG:HD2	2.06	0.56
1:A:158:VAL:HG21	1:A:206:ILE:HD11	1.88	0.56
1:B:110:LEU:HG	1:B:130:THR:OG1	2.06	0.56
1:A:158:VAL:HG21	1:A:206:ILE:HD11	1.88	0.56
1:B:110:LEU:HG	1:B:130:THR:OG1	2.06	0.56
1:A:163:LYS:NZ	2:E:9:GLY:HA3	2.21	0.56
1:A:217:ALA:HB3	1:A:222:ILE:CD1	2.35	0.56
1:A:217:ALA:HB3	1:A:222:ILE:CD1	2.35	0.56
1:A:251:SER:HB3	1:A:256:SER:HA	1.87	0.55
1:A:309:VAL:HG22	6:A:647:HOH:O	2.05	0.55
1:B:189:TYR:HE1	2:E:26:PHE:O	1.90	0.55
1:A:251:SER:HB3	1:A:256:SER:HA	1.87	0.55
1:A:309:VAL:HG22	6:A:649:HOH:O	2.05	0.55
1:A:330:VAL:HG21	1:A:343:ILE:HG12	1.88	0.55
1:A:330:VAL:HG21	1:A:343:ILE:HG12	1.88	0.55
1:A:199:LEU:HD11	1:A:224:SER:HB3	1.88	0.55
1:B:227:LEU:O	1:B:230:HIS:HB3	2.07	0.55
1:B:203:VAL:HG21	1:B:228:VAL:CG1	2.36	0.55
1:A:199:LEU:HD11	1:A:224:SER:HB3	1.88	0.55
1:B:227:LEU:O	1:B:230:HIS:HB3	2.07	0.55
1:B:203:VAL:HG21	1:B:228:VAL:CG1	2.36	0.55
1:B:159:TYR:HB3	1:B:172:LEU:HD12	1.87	0.55
1:B:159:TYR:HB3	1:B:172:LEU:HD12	1.87	0.55
1:A:3:LEU:HB3	1:A:4:PRO:HD2	1.88	0.55
1:B:173:GLU:O	1:B:177:GLU:HG2	2.07	0.55
1:A:3:LEU:HB3	1:A:4:PRO:HD2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:173:GLU:O	1:B:177:GLU:HG2	2.07	0.55
1:A:291:SER:HB2	6:A:647:HOH:O	2.06	0.54
1:A:291:SER:HB2	6:A:649:HOH:O	2.06	0.54
1:A:194:THR:HG21	6:A:537:HOH:O	2.07	0.54
1:A:228:VAL:O	1:A:232:HIS:HD2	1.90	0.54
1:A:194:THR:HG21	6:A:538:HOH:O	2.07	0.54
1:A:228:VAL:O	1:A:232:HIS:HD2	1.90	0.54
1:B:157:LEU:HD12	1:B:188:ILE:CD1	2.38	0.54
1:B:157:LEU:HD12	1:B:188:ILE:CD1	2.38	0.54
1:A:305:MET:CE	1:A:309:VAL:HG12	2.37	0.54
1:A:305:MET:CE	1:A:309:VAL:HG12	2.37	0.54
1:B:223:ARG:HA	1:B:271:TYR:OH	2.08	0.53
1:B:223:ARG:HA	1:B:271:TYR:OH	2.08	0.53
1:B:7:LYS:HE2	1:B:53:ARG:HG2	1.91	0.53
1:B:7:LYS:HE2	1:B:53:ARG:HG2	1.91	0.53
1:A:93:TYR:CE2	2:E:14:ARG:HG3	2.42	0.53
1:B:282:THR:O	1:B:356:ALA:HB1	2.08	0.53
1:B:91:CYS:HB3	6:B:631:HOH:O	2.09	0.53
1:B:282:THR:O	1:B:356:ALA:HB1	2.08	0.53
1:B:91:CYS:HB3	6:B:629:HOH:O	2.09	0.53
1:B:35:LEU:HA	1:B:38:VAL:HG12	1.90	0.53
1:B:35:LEU:HA	1:B:38:VAL:HG12	1.90	0.53
1:A:327:LEU:O	1:A:331:LEU:HD13	2.07	0.53
1:A:327:LEU:O	1:A:331:LEU:HD13	2.07	0.53
1:B:200:GLU:OE1	1:B:231:ARG:NH2	2.42	0.53
1:B:200:GLU:OE1	1:B:231:ARG:NH2	2.42	0.53
1:B:257:TRP:CE3	1:B:268:LYS:HB2	2.44	0.52
1:B:303:LEU:HD23	1:B:303:LEU:C	2.29	0.52
1:B:257:TRP:CE3	1:B:268:LYS:HB2	2.44	0.52
1:B:303:LEU:HD23	1:B:303:LEU:C	2.29	0.52
1:A:160:SER:HA	1:A:191:PHE:O	2.09	0.52
1:A:160:SER:HA	1:A:191:PHE:O	2.09	0.52
1:B:215:MET:HE1	1:B:225:ILE:HG21	1.90	0.52
1:B:215:MET:HE1	1:B:225:ILE:HG21	1.90	0.52
1:A:284:LYS:HG2	1:A:285:PRO:HD2	1.90	0.52
1:B:7:LYS:HD3	1:B:53:ARG:H	1.74	0.52
1:A:284:LYS:HG2	1:A:285:PRO:HD2	1.90	0.52
1:B:7:LYS:HD3	1:B:53:ARG:H	1.74	0.52
1:A:48:LEU:HD23	1:A:52:THR:HG21	1.91	0.52
1:B:317:HIS:CE1	1:B:355:ILE:HG23	2.45	0.52
1:A:48:LEU:HD23	1:A:52:THR:HG21	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:317:HIS:CE1	1:B:355:ILE:HG23	2.45	0.52
1:B:385:GLU:C	6:B:652:HOH:O	2.48	0.52
1:B:385:GLU:C	6:B:652:HOH:O	2.48	0.52
1:B:197:LEU:HB3	1:B:199:LEU:HG	1.91	0.51
1:B:197:LEU:HB3	1:B:199:LEU:HG	1.91	0.51
1:A:162:ASP:O	1:A:163:LYS:HB2	2.10	0.51
1:A:162:ASP:O	1:A:163:LYS:HB2	2.10	0.51
1:A:158:VAL:O	1:A:215:MET:HA	2.10	0.51
1:A:158:VAL:O	1:A:215:MET:HA	2.10	0.51
1:B:48:LEU:HD13	1:B:52:THR:HG21	1.92	0.51
1:B:48:LEU:HD13	1:B:52:THR:HG21	1.92	0.51
1:A:118:GLY:N	2:E:15:ILE:HD12	2.14	0.51
1:A:93:TYR:HD1	2:E:17:ALA:HB1	1.75	0.51
1:A:392:GLY:HA3	6:A:605:HOH:O	2.11	0.50
1:A:392:GLY:HA3	6:A:607:HOH:O	2.11	0.50
1:B:309:VAL:O	1:B:309:VAL:HG23	2.11	0.50
1:B:309:VAL:O	1:B:309:VAL:HG23	2.11	0.50
1:A:146:LEU:HG	6:A:666:HOH:O	2.11	0.50
1:A:146:LEU:HG	6:A:666:HOH:O	2.11	0.50
1:B:157:LEU:HD12	1:B:188:ILE:HD11	1.93	0.50
1:B:157:LEU:HD12	1:B:188:ILE:HD11	1.93	0.50
1:B:35:LEU:HA	1:B:38:VAL:CG1	2.42	0.50
1:B:35:LEU:HA	1:B:38:VAL:CG1	2.42	0.50
1:A:93:TYR:CD2	2:E:14:ARG:HG3	2.47	0.49
1:A:83:PRO:HD3	6:A:675:HOH:O	2.11	0.49
1:A:83:PRO:HD3	6:A:676:HOH:O	2.11	0.49
1:B:142:MET:HG3	1:B:371:PHE:HB2	1.94	0.49
1:B:217:ALA:HB3	1:B:222:ILE:HD12	1.93	0.49
1:B:334:GLY:HA2	6:B:571:HOH:O	2.11	0.49
1:B:142:MET:HG3	1:B:371:PHE:HB2	1.94	0.49
1:B:217:ALA:HB3	1:B:222:ILE:HD12	1.93	0.49
1:B:334:GLY:HA2	6:B:571:HOH:O	2.11	0.49
1:A:85:LEU:HD11	1:A:87:LEU:HD13	1.95	0.49
1:A:85:LEU:HD11	1:A:87:LEU:HD13	1.95	0.49
1:A:199:LEU:CD1	1:A:224:SER:HB3	2.43	0.49
1:A:31:ILE:HD11	1:A:316:PHE:HB3	1.94	0.49
1:A:199:LEU:CD1	1:A:224:SER:HB3	2.43	0.49
1:A:31:ILE:HD11	1:A:316:PHE:HB3	1.94	0.49
1:A:25:THR:HG23	1:A:301:GLN:HG2	1.94	0.49
1:A:25:THR:HG23	1:A:301:GLN:HG2	1.94	0.49
1:A:28:ARG:HB3	1:A:29:PRO:HD3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:370:ASP:OD1	1:B:391:PHE:HA	2.13	0.49
1:A:28:ARG:HB3	1:A:29:PRO:HD3	1.94	0.49
1:B:370:ASP:OD1	1:B:391:PHE:HA	2.13	0.49
1:B:35:LEU:C	1:B:38:VAL:HG12	2.34	0.48
1:B:35:LEU:C	1:B:38:VAL:HG12	2.34	0.48
1:A:215:MET:HE3	1:A:225:ILE:HG21	1.95	0.48
1:B:307:ASP:O	1:B:308:TYR:HB3	2.12	0.48
1:A:215:MET:HE3	1:A:225:ILE:HG21	1.95	0.48
1:B:307:ASP:O	1:B:308:TYR:HB3	2.12	0.48
1:A:203:VAL:HG21	1:A:228:VAL:CG1	2.43	0.48
1:A:204:ARG:HG3	1:A:204:ARG:NH1	2.27	0.48
1:A:374:ILE:HD13	6:A:660:HOH:O	2.12	0.48
1:A:203:VAL:HG21	1:A:228:VAL:CG1	2.43	0.48
1:A:204:ARG:HG3	1:A:204:ARG:NH1	2.27	0.48
1:A:374:ILE:HD13	6:A:660:HOH:O	2.12	0.48
1:A:306:GLU:O	1:A:307:ASP:C	2.51	0.48
1:A:85:LEU:CD1	1:A:87:LEU:HD13	2.43	0.48
1:A:306:GLU:O	1:A:307:ASP:C	2.51	0.48
1:A:85:LEU:CD1	1:A:87:LEU:HD13	2.43	0.48
1:A:96:ALA:O	1:A:100:ARG:HG3	2.14	0.48
1:A:96:ALA:O	1:A:100:ARG:HG3	2.14	0.48
1:A:32:GLU:O	1:A:36:ARG:HG3	2.13	0.48
1:A:32:GLU:O	1:A:36:ARG:HG3	2.13	0.48
1:A:203:VAL:CG1	1:A:234:MET:SD	3.01	0.48
1:A:203:VAL:CG1	1:A:234:MET:SD	3.01	0.48
1:B:188:ILE:HD12	2:E:8:PHE:HE2	1.78	0.48
1:A:142:MET:HE3	1:A:277:VAL:HG13	1.96	0.48
1:B:158:VAL:HG21	1:B:206:ILE:HD11	1.96	0.48
1:A:142:MET:HE3	1:A:277:VAL:HG13	1.96	0.48
1:B:158:VAL:HG21	1:B:206:ILE:HD11	1.96	0.48
1:A:203:VAL:HG21	1:A:228:VAL:HG12	1.96	0.47
1:A:203:VAL:HG21	1:A:228:VAL:HG12	1.96	0.47
1:B:192:ASP:C	1:B:194:THR:H	2.17	0.47
1:B:192:ASP:C	1:B:194:THR:H	2.17	0.47
1:B:215:MET:HE2	1:B:225:ILE:HG21	1.95	0.47
1:B:215:MET:HE2	1:B:225:ILE:HG21	1.95	0.47
1:A:116:ALA:HB1	2:E:15:ILE:HD13	1.95	0.47
1:A:284:LYS:HG2	1:A:285:PRO:CD	2.45	0.47
1:A:346:GLN:O	1:A:350:ARG:HD2	2.14	0.47
1:B:261:ASP:CG	1:B:262:LYS:H	2.16	0.47
1:B:330:VAL:HG11	1:B:343:ILE:HD13	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:284:LYS:HG2	1:A:285:PRO:CD	2.45	0.47
1:A:346:GLN:O	1:A:350:ARG:HD2	2.14	0.47
1:B:261:ASP:CG	1:B:262:LYS:H	2.16	0.47
1:B:330:VAL:HG11	1:B:343:ILE:HD13	1.96	0.47
1:B:93:TYR:HD1	2:E:17:ALA:HB1	1.79	0.47
1:A:231:ARG:NH2	1:A:232:HIS:CE1	2.82	0.47
1:A:257:TRP:HB2	1:A:267:ALA:HB1	1.97	0.47
1:A:18:ASP:HB3	1:A:26:ARG:HH22	1.80	0.47
1:A:231:ARG:NH2	1:A:232:HIS:CE1	2.82	0.47
1:A:257:TRP:HB2	1:A:267:ALA:HB1	1.97	0.47
1:A:18:ASP:HB3	1:A:26:ARG:HH22	1.80	0.47
1:B:8:ILE:HG22	1:B:10:VAL:HG23	1.97	0.47
1:B:8:ILE:HG22	1:B:10:VAL:HG23	1.97	0.47
1:A:114:ALA:O	1:A:131:ARG:HD3	2.15	0.47
1:A:299:GLU:C	1:A:301:GLN:H	2.17	0.47
1:A:114:ALA:O	1:A:131:ARG:HD3	2.15	0.47
1:A:299:GLU:C	1:A:301:GLN:H	2.17	0.47
1:A:159:TYR:CZ	1:A:190:SER:HB3	2.51	0.46
1:A:159:TYR:CZ	1:A:190:SER:HB3	2.51	0.46
1:A:168:CYS:SG	1:A:216:CYS:C	2.93	0.46
1:B:299:GLU:HG2	1:B:305:MET:HB2	1.96	0.46
1:A:168:CYS:SG	1:A:216:CYS:C	2.93	0.46
1:B:299:GLU:HG2	1:B:305:MET:HB2	1.96	0.46
1:A:163:LYS:O	1:A:164:LEU:HD12	2.15	0.46
1:A:163:LYS:O	1:A:164:LEU:HD12	2.15	0.46
1:B:158:VAL:HG21	1:B:206:ILE:CD1	2.46	0.46
1:B:274:LEU:HD23	1:B:275:GLN:N	2.29	0.46
1:B:158:VAL:HG21	1:B:206:ILE:CD1	2.46	0.46
1:B:274:LEU:HD23	1:B:275:GLN:N	2.29	0.46
1:A:189:TYR:CE1	1:A:205:ASN:ND2	2.83	0.46
1:B:249:SER:HA	1:B:252:TYR:CZ	2.51	0.46
1:B:303:LEU:HD23	1:B:304:ASN:C	2.36	0.46
1:A:189:TYR:CE1	1:A:205:ASN:ND2	2.83	0.46
1:B:249:SER:HA	1:B:252:TYR:CZ	2.51	0.46
1:B:303:LEU:HD23	1:B:304:ASN:C	2.36	0.46
1:A:285:PRO:O	1:A:288:GLU:HB2	2.16	0.46
1:B:143:MET:HE2	1:B:214:ILE:HD12	1.97	0.46
1:A:285:PRO:O	1:A:288:GLU:HB2	2.16	0.46
1:B:143:MET:HE2	1:B:214:ILE:HD12	1.97	0.46
1:A:173:GLU:OE2	2:E:15:ILE:HD11	2.16	0.46
1:B:189:TYR:CE1	2:E:26:PHE:O	2.69	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:387:ILE:O	1:B:400:ARG:N	2.49	0.46
1:B:387:ILE:O	1:B:400:ARG:N	2.49	0.46
1:B:199:LEU:O	1:B:203:VAL:HG23	2.16	0.46
1:B:199:LEU:O	1:B:203:VAL:HG23	2.16	0.46
2:E:6:SER:O	2:E:25:SER:HA	2.16	0.46
1:B:177:GLU:OE1	2:E:11:ARG:NH1	2.49	0.46
2:E:23:CYS:HB3	2:E:24:ASN:H	1.49	0.46
1:B:194:THR:O	1:B:194:THR:HG22	2.15	0.45
1:B:194:THR:O	1:B:194:THR:HG22	2.15	0.45
1:B:61:SER:O	1:B:66:ARG:HB3	2.16	0.45
1:B:61:SER:O	1:B:66:ARG:HB3	2.16	0.45
1:A:120:GLN:HE22	1:A:137:ALA:CB	2.30	0.45
1:A:294:VAL:O	1:A:298:VAL:HG23	2.16	0.45
1:A:120:GLN:HE22	1:A:137:ALA:CB	2.30	0.45
1:A:294:VAL:O	1:A:298:VAL:HG23	2.16	0.45
2:E:7:CYS:O	2:E:7:CYS:SG	2.74	0.45
1:A:188:ILE:CD1	1:A:188:ILE:N	2.80	0.45
1:B:159:TYR:CZ	1:B:190:SER:HB3	2.51	0.45
1:A:188:ILE:CD1	1:A:188:ILE:N	2.80	0.45
1:B:159:TYR:CZ	1:B:190:SER:HB3	2.51	0.45
1:B:274:LEU:HD23	1:B:275:GLN:H	1.81	0.45
1:B:274:LEU:HD23	1:B:275:GLN:H	1.81	0.45
1:A:109:MET:CE	1:A:129:LEU:HD13	2.47	0.45
2:E:7:CYS:SG	2:E:7:CYS:O	2.74	0.45
1:A:109:MET:CE	1:A:129:LEU:HD13	2.47	0.45
1:B:330:VAL:HG11	1:B:343:ILE:CD1	2.47	0.44
2:E:24:ASN:O	2:E:25:SER:CB	2.65	0.44
1:B:330:VAL:HG11	1:B:343:ILE:CD1	2.47	0.44
2:E:24:ASN:O	2:E:25:SER:CB	2.65	0.44
1:B:148:ARG:HH11	1:B:182:GLU:HG2	1.80	0.44
1:B:148:ARG:HH11	1:B:182:GLU:HG2	1.80	0.44
1:B:198:ASP:O	1:B:200:GLU:N	2.50	0.44
1:B:298:VAL:CG1	1:B:303:LEU:HD22	2.48	0.44
1:B:198:ASP:O	1:B:200:GLU:N	2.50	0.44
1:B:298:VAL:CG1	1:B:303:LEU:HD22	2.48	0.44
1:B:223:ARG:NE	1:B:259:ARG:HG3	2.33	0.44
1:B:223:ARG:NE	1:B:259:ARG:HG3	2.33	0.44
1:A:349:ASN:HB2	1:A:363:ALA:HA	2.00	0.44
1:A:349:ASN:HB2	1:A:363:ALA:HA	2.00	0.44
1:A:13:LEU:HD23	1:A:59:GLU:HB3	2.00	0.43
1:B:47:LEU:O	1:B:328:HIS:ND1	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:13:LEU:HD23	1:A:59:GLU:HB3	2.00	0.43
1:B:47:LEU:O	1:B:328:HIS:ND1	2.51	0.43
1:A:259:ARG:C	1:A:261:ASP:N	2.71	0.43
1:A:72:VAL:HG13	1:B:72:VAL:HG13	2.00	0.43
1:B:361:ILE:N	1:B:361:ILE:HD12	2.33	0.43
1:A:259:ARG:C	1:A:261:ASP:N	2.71	0.43
1:A:72:VAL:HG13	1:B:72:VAL:HG13	2.00	0.43
1:B:361:ILE:N	1:B:361:ILE:HD12	2.33	0.43
1:B:330:VAL:HG22	1:B:335:TYR:CB	2.46	0.43
2:E:6:SER:N	2:E:26:PHE:H	2.16	0.43
1:B:330:VAL:HG22	1:B:335:TYR:CB	2.46	0.43
1:B:25:THR:HG23	1:B:301:GLN:HG2	2.01	0.43
1:B:85:LEU:HD22	1:B:86:ILE:N	2.34	0.43
1:B:25:THR:HG23	1:B:301:GLN:HG2	2.01	0.43
1:B:85:LEU:HD22	1:B:86:ILE:N	2.34	0.43
1:A:113:GLY:C	1:A:115:LEU:HD13	2.39	0.43
1:A:113:GLY:C	1:A:115:LEU:HD13	2.39	0.43
1:A:107:LEU:HD22	6:A:646:HOH:O	2.19	0.43
1:A:200:GLU:HA	1:A:200:GLU:OE1	2.19	0.43
1:A:107:LEU:HD22	6:A:648:HOH:O	2.19	0.43
1:A:200:GLU:HA	1:A:200:GLU:OE1	2.19	0.43
1:B:198:ASP:C	1:B:200:GLU:N	2.72	0.43
1:B:28:ARG:HB3	1:B:29:PRO:HD3	2.00	0.43
1:B:198:ASP:C	1:B:200:GLU:N	2.72	0.43
1:B:28:ARG:HB3	1:B:29:PRO:HD3	2.00	0.43
1:B:375:ALA:HB3	1:B:387:ILE:HG13	2.01	0.43
1:B:375:ALA:HB3	1:B:387:ILE:HG13	2.01	0.43
1:A:31:ILE:HG22	1:A:35:LEU:HD22	2.00	0.43
1:A:396:ARG:HG3	1:A:396:ARG:O	2.19	0.43
1:A:74:ARG:HH11	1:A:74:ARG:HB3	1.84	0.43
1:A:31:ILE:HG22	1:A:35:LEU:HD22	2.00	0.43
1:A:396:ARG:O	1:A:396:ARG:HG3	2.19	0.43
1:A:74:ARG:HH11	1:A:74:ARG:HB3	1.84	0.43
1:A:203:VAL:HG13	1:A:234:MET:SD	2.59	0.42
1:A:77:ALA:C	1:A:79:ARG:H	2.22	0.42
1:B:317:HIS:C	1:B:317:HIS:ND1	2.73	0.42
1:A:203:VAL:HG13	1:A:234:MET:SD	2.59	0.42
1:A:77:ALA:C	1:A:79:ARG:H	2.22	0.42
1:B:317:HIS:ND1	1:B:317:HIS:C	2.73	0.42
1:A:202:ILE:O	1:A:206:ILE:HG12	2.19	0.42
1:A:244:ILE:CG2	1:A:246:LEU:HG	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:ARG:HH11	1:A:79:ARG:CB	2.22	0.42
1:B:224:SER:HA	1:B:227:LEU:HD12	2.01	0.42
1:A:202:ILE:O	1:A:206:ILE:HG12	2.19	0.42
1:A:244:ILE:CG2	1:A:246:LEU:HG	2.48	0.42
1:A:79:ARG:HH11	1:A:79:ARG:CB	2.22	0.42
1:B:224:SER:HA	1:B:227:LEU:HD12	2.01	0.42
1:A:281:ARG:NH1	1:A:309:VAL:O	2.51	0.42
1:A:132:VAL:O	1:A:367:ARG:HD3	2.18	0.42
1:B:259:ARG:HH21	1:B:259:ARG:HG2	1.84	0.42
1:A:281:ARG:NH1	1:A:309:VAL:O	2.51	0.42
1:A:132:VAL:O	1:A:367:ARG:HD3	2.18	0.42
1:B:259:ARG:HH21	1:B:259:ARG:HG2	1.84	0.42
1:A:134:PRO:HD2	6:A:603:HOH:O	2.19	0.42
1:A:14:LEU:HB2	1:A:24:LEU:CD2	2.50	0.42
1:B:168:CYS:SG	1:B:216:CYS:C	2.97	0.42
1:B:35:LEU:HA	1:B:35:LEU:HD12	1.90	0.42
1:A:134:PRO:HD2	6:A:605:HOH:O	2.19	0.42
1:A:14:LEU:HB2	1:A:24:LEU:CD2	2.50	0.42
1:B:168:CYS:SG	1:B:216:CYS:C	2.97	0.42
1:B:35:LEU:HD12	1:B:35:LEU:HA	1.90	0.42
1:A:258:LYS:HG3	1:A:264:ASP:OD2	2.18	0.42
1:A:317:HIS:HE1	1:A:321:LEU:HD11	1.83	0.42
1:A:258:LYS:HG3	1:A:264:ASP:OD2	2.18	0.42
1:A:317:HIS:HE1	1:A:321:LEU:HD11	1.83	0.42
2:E:12:MET:HE3	2:E:15:ILE:CG1	2.09	0.42
1:A:239:TYR:HB2	1:A:241:PHE:CE1	2.54	0.42
2:E:17:ALA:O	2:E:18:GLN:HB2	2.19	0.42
1:A:239:TYR:HB2	1:A:241:PHE:CE1	2.54	0.42
1:A:162:ASP:HB3	1:A:164:LEU:HB2	2.00	0.42
1:A:162:ASP:HB3	1:A:164:LEU:HB2	2.00	0.42
2:E:17:ALA:O	2:E:18:GLN:HB2	2.20	0.42
1:A:188:ILE:CD1	2:E:6:SER:HB2	2.50	0.42
2:E:6:SER:N	2:E:26:PHE:H	2.17	0.42
1:A:154:ARG:HG2	1:A:185:HIS:HB3	2.01	0.42
1:A:228:VAL:O	1:A:232:HIS:CD2	2.72	0.42
1:A:154:ARG:HG2	1:A:185:HIS:HB3	2.01	0.42
1:A:228:VAL:O	1:A:232:HIS:CD2	2.72	0.42
1:A:93:TYR:CD1	2:E:14:ARG:HD2	2.54	0.42
1:A:290:PHE:O	1:A:294:VAL:HG23	2.19	0.42
2:E:6:SER:O	2:E:25:SER:HA	2.18	0.42
1:A:290:PHE:O	1:A:294:VAL:HG23	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:18:ASP:O	1:A:26:ARG:NH2	2.54	0.41
1:B:284:LYS:HE3	1:B:286:GLU:CB	2.37	0.41
1:A:18:ASP:O	1:A:26:ARG:NH2	2.54	0.41
1:B:284:LYS:HE3	1:B:286:GLU:CB	2.37	0.41
1:A:30:ALA:HB2	1:A:313:VAL:HG13	2.02	0.41
1:A:169:TYR:HE1	2:E:12:MET:HE1	1.83	0.41
1:A:30:ALA:HB2	1:A:313:VAL:HG13	2.02	0.41
1:B:139:MET:O	1:B:142:MET:HB3	2.20	0.41
1:B:154:ARG:HD3	1:B:210:GLU:OE2	2.21	0.41
1:B:8:ILE:N	1:B:8:ILE:HD12	2.35	0.41
1:B:139:MET:O	1:B:142:MET:HB3	2.20	0.41
1:B:154:ARG:HD3	1:B:210:GLU:OE2	2.21	0.41
1:B:8:ILE:N	1:B:8:ILE:HD12	2.35	0.41
1:B:35:LEU:CA	1:B:38:VAL:HG12	2.51	0.41
1:B:163:LYS:HD2	2:E:20:GLY:O	2.21	0.41
1:B:35:LEU:CA	1:B:38:VAL:HG12	2.51	0.41
1:A:142:MET:CE	1:A:277:VAL:HG13	2.50	0.41
1:A:346:GLN:O	1:A:350:ARG:NH1	2.51	0.41
1:A:142:MET:CE	1:A:277:VAL:HG13	2.50	0.41
1:A:346:GLN:O	1:A:350:ARG:NH1	2.51	0.41
1:B:223:ARG:NH1	1:B:259:ARG:HB2	2.36	0.41
1:B:223:ARG:NH1	1:B:259:ARG:HB2	2.36	0.41
1:A:85:LEU:HD11	1:A:87:LEU:CD1	2.50	0.41
1:B:157:LEU:HB2	1:B:188:ILE:HD13	2.03	0.41
1:B:18:ASP:O	1:B:26:ARG:NH2	2.34	0.41
1:B:203:VAL:HG21	1:B:228:VAL:HB	2.01	0.41
1:A:85:LEU:HD11	1:A:87:LEU:CD1	2.50	0.41
1:B:157:LEU:HB2	1:B:188:ILE:HD13	2.03	0.41
1:B:18:ASP:O	1:B:26:ARG:NH2	2.34	0.41
1:B:203:VAL:HG21	1:B:228:VAL:HB	2.01	0.41
1:A:207:GLN:HA	1:A:239:TYR:OH	2.20	0.41
1:B:396:ARG:CB	1:B:396:ARG:NH1	2.84	0.41
1:A:207:GLN:HA	1:A:239:TYR:OH	2.20	0.41
1:B:396:ARG:NH1	1:B:396:ARG:CB	2.84	0.41
1:A:230:HIS:HA	1:A:235:THR:HG23	2.02	0.41
1:A:301:GLN:HA	1:A:301:GLN:OE1	2.20	0.41
1:A:296:SER:O	1:A:300:LYS:HG2	2.21	0.41
1:A:230:HIS:HA	1:A:235:THR:HG23	2.02	0.41
1:A:301:GLN:HA	1:A:301:GLN:OE1	2.20	0.41
1:A:296:SER:O	1:A:300:LYS:HG2	2.21	0.41
1:B:396:ARG:HH11	1:B:396:ARG:HB3	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:396:ARG:HH11	1:B:396:ARG:HB3	1.86	0.41
1:B:332:ARG:C	1:B:334:GLY:H	2.24	0.40
1:B:332:ARG:C	1:B:334:GLY:H	2.24	0.40
2:E:12:MET:O	2:E:13:ASP:C	2.60	0.40
1:A:284:LYS:HG2	1:A:285:PRO:N	2.36	0.40
2:E:11:ARG:HB3	2:E:12:MET:H	1.59	0.40
1:B:189:TYR:OH	2:E:26:PHE:CE2	2.67	0.40
1:A:284:LYS:HG2	1:A:285:PRO:N	2.36	0.40
1:A:244:ILE:HD12	1:A:244:ILE:N	2.36	0.40
1:B:248:ASN:OD1	1:B:250:SER:HB2	2.21	0.40
1:B:353:GLU:OE2	1:B:358:GLN:NE2	2.54	0.40
1:A:244:ILE:HD12	1:A:244:ILE:N	2.36	0.40
1:B:248:ASN:OD1	1:B:250:SER:HB2	2.21	0.40
1:B:353:GLU:OE2	1:B:358:GLN:NE2	2.54	0.40
2:E:11:ARG:HB3	2:E:12:MET:H	1.59	0.40
1:A:35:LEU:HA	1:A:35:LEU:HD12	1.91	0.40
1:A:387:ILE:HD12	1:A:399:MET:CE	2.52	0.40
1:A:35:LEU:HD12	1:A:35:LEU:HA	1.91	0.40
1:A:387:ILE:HD12	1:A:399:MET:CE	2.52	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	1-A	390/480 (81%)	363 (93%)	26 (7%)	1 (0%)	41	55
1	1-B	390/480 (81%)	359 (92%)	24 (6%)	7 (2%)	8	10
1	2-A	390/480 (81%)	363 (93%)	26 (7%)	1 (0%)	41	55
1	2-B	390/480 (81%)	359 (92%)	24 (6%)	7 (2%)	8	10
2	1-E	19/21 (90%)	8 (42%)	3 (16%)	8 (42%)	0	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	2-E	19/21 (90%)	8 (42%)	3 (16%)	8 (42%)	0	0
All	All	1598/1962 (81%)	1460 (91%)	106 (7%)	32 (2%)	7	9

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1-B	209	SER
2	1-E	13	ASP
2	1-E	18	GLN
2	1-E	19	SER
1	2-B	209	SER
2	2-E	13	ASP
2	2-E	18	GLN
2	2-E	19	SER
1	1-B	199	LEU
1	1-B	306	GLU
2	1-E	12	MET
2	1-E	23	CYS
2	1-E	25	SER
1	2-B	199	LEU
1	2-B	306	GLU
2	2-E	12	MET
2	2-E	23	CYS
2	2-E	25	SER
1	1-A	307	ASP
1	1-B	308	TYR
1	1-B	333	ALA
2	1-E	14	ARG
1	2-A	307	ASP
1	2-B	308	TYR
1	2-B	333	ALA
2	2-E	14	ARG
1	1-B	304	ASN
2	1-E	8	PHE
1	2-B	304	ASN
2	2-E	8	PHE
1	1-B	254	ASP
1	2-B	254	ASP

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1-A	329/390 (84%)	314 (95%)	15 (5%)	27	43
1	1-B	329/390 (84%)	314 (95%)	15 (5%)	27	43
1	2-A	329/390 (84%)	314 (95%)	15 (5%)	27	43
1	2-B	329/390 (84%)	314 (95%)	15 (5%)	27	43
2	1-E	15/15 (100%)	12 (80%)	3 (20%)	1	1
2	2-E	15/15 (100%)	12 (80%)	3 (20%)	1	1
All	All	1346/1590 (85%)	1280 (95%)	66 (5%)	25	40

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1-A	10	VAL
1	1-A	11	LEU
1	1-A	35	LEU
1	1-A	71	LEU
1	1-A	79	ARG
1	1-A	85	LEU
1	1-A	87	LEU
1	1-A	115	LEU
1	1-A	120	GLN
1	1-A	142	MET
1	1-A	144	LEU
1	1-A	172	LEU
1	1-A	184	LEU
1	1-A	210	GLU
1	1-A	231	ARG
1	1-B	11	LEU
1	1-B	35	LEU
1	1-B	71	LEU
1	1-B	85	LEU
1	1-B	87	LEU
1	1-B	115	LEU
1	1-B	144	LEU

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Mol	Chain	Res	Type
1	1-B	235	THR
1	1-B	238	ASP
1	1-B	274	LEU
1	1-B	305	MET
1	1-B	307	ASP
1	1-B	308	TYR
1	1-B	331	LEU
1	1-B	355	ILE
2	1-E	13	ASP
2	1-E	14	ARG
2	1-E	26	PHE
1	2-A	10	VAL
1	2-A	11	LEU
1	2-A	35	LEU
1	2-A	71	LEU
1	2-A	79	ARG
1	2-A	85	LEU
1	2-A	87	LEU
1	2-A	115	LEU
1	2-A	120	GLN
1	2-A	142	MET
1	2-A	144	LEU
1	2-A	172	LEU
1	2-A	184	LEU
1	2-A	210	GLU
1	2-A	231	ARG
1	2-B	11	LEU
1	2-B	35	LEU
1	2-B	71	LEU
1	2-B	85	LEU
1	2-B	87	LEU
1	2-B	115	LEU
1	2-B	144	LEU
1	2-B	235	THR
1	2-B	238	ASP
1	2-B	274	LEU
1	2-B	305	MET
1	2-B	307	ASP
1	2-B	308	TYR
1	2-B	331	LEU
1	2-B	355	ILE
2	2-E	13	ASP

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Mol	Chain	Res	Type
2	2-E	14	ARG
2	2-E	26	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	1-A	205	ASN
1	1-A	232	HIS
1	1-B	55	GLN
1	1-B	205	ASN
1	1-B	230	HIS
1	1-B	345	GLN
1	2-A	205	ASN
1	2-A	232	HIS
1	2-B	55	GLN
1	2-B	205	ASN
1	2-B	230	HIS
1	2-B	345	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 ⓘ

4 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	1-C	1	1,3	14,14,15	0.55	0	17,19,21	0.72	1 (5%)
3	NAG	1-C	2	3	14,14,15	0.46	0	17,19,21	0.84	1 (5%)
3	NAG	2-C	1	1,3	14,14,15	0.55	0	17,19,21	0.72	1 (5%)
3	NAG	2-C	2	3	14,14,15	0.46	0	17,19,21	0.84	1 (5%)

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	1-C	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	1-C	2	3	-	4/6/23/26	0/1/1/1
3	NAG	2-C	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	2-C	2	3	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	2-C	2	NAG	C2-N2-C7	-2.76	118.98	122.90
3	1-C	2	NAG	C2-N2-C7	-2.76	118.98	122.90
3	2-C	1	NAG	C2-N2-C7	-2.26	119.68	122.90
3	1-C	1	NAG	C2-N2-C7	-2.26	119.68	122.90

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	2-C	2	NAG	C8-C7-N2-C2
3	2-C	2	NAG	O7-C7-N2-C2
3	1-C	2	NAG	C8-C7-N2-C2
3	1-C	2	NAG	O7-C7-N2-C2
3	2-C	2	NAG	O5-C5-C6-O6
3	1-C	2	NAG	O5-C5-C6-O6
3	2-C	2	NAG	C4-C5-C6-O6
3	1-C	2	NAG	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

5.6 Ligand geometry

Of 10 ligands modelled in this entry, 4 are monoatomic - leaving 6 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	NAG	1-A	512	1	14,14,15	0.53	0	17,19,21	0.65	0
4	NAG	1-A	511	1	14,14,15	0.66	0	17,19,21	0.65	0
4	NAG	2-A	512	1	14,14,15	0.53	0	17,19,21	0.65	0
4	NAG	1-B	511	1	14,14,15	0.54	0	17,19,21	0.70	1 (5%)
4	NAG	2-A	511	1	14,14,15	0.66	0	17,19,21	0.65	0
4	NAG	2-B	511	1	14,14,15	0.54	0	17,19,21	0.70	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	1-A	512	1	1/1/5/7	6/6/23/26	0/1/1/1
4	NAG	1-A	511	1	1/1/5/7	2/6/23/26	0/1/1/1
4	NAG	2-A	512	1	1/1/5/7	6/6/23/26	0/1/1/1
4	NAG	1-B	511	1	-	2/6/23/26	0/1/1/1
4	NAG	2-A	511	1	1/1/5/7	2/6/23/26	0/1/1/1
4	NAG	2-B	511	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	1-B	511	NAG	C2-N2-C7	-2.24	119.71	122.90
4	2-B	511	NAG	C2-N2-C7	-2.24	119.71	122.90

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	1-A	512	NAG	C1
4	1-A	511	NAG	C1
4	2-A	512	NAG	C1
4	2-A	511	NAG	C1

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	1-A	512	NAG	C8-C7-N2-C2
4	1-A	512	NAG	O7-C7-N2-C2
4	1-A	511	NAG	C8-C7-N2-C2
4	1-A	511	NAG	O7-C7-N2-C2
4	2-A	512	NAG	C8-C7-N2-C2
4	2-A	512	NAG	O7-C7-N2-C2
4	1-B	511	NAG	C8-C7-N2-C2
4	1-B	511	NAG	O7-C7-N2-C2
4	2-A	511	NAG	C8-C7-N2-C2
4	2-A	511	NAG	O7-C7-N2-C2
4	2-B	511	NAG	C8-C7-N2-C2
4	2-B	511	NAG	O7-C7-N2-C2
4	1-A	512	NAG	C4-C5-C6-O6
4	2-A	512	NAG	C4-C5-C6-O6
4	1-A	512	NAG	O5-C5-C6-O6
4	2-A	512	NAG	O5-C5-C6-O6
4	1-A	512	NAG	C1-C2-N2-C7
4	2-A	512	NAG	C1-C2-N2-C7
4	1-A	512	NAG	C3-C2-N2-C7
4	2-A	512	NAG	C3-C2-N2-C7

There are no ring outliers.

No monomer is involved in short contacts.

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	1-A	394/480 (82%)	-0.29	8 (2%) 65 63	26, 47, 83, 96	0
1	1-B	394/480 (82%)	-0.15	18 (4%) 32 31	28, 51, 87, 98	0
1	2-A	394/480 (82%)	-0.29	8 (2%) 65 63	26, 47, 83, 96	0
1	2-B	394/480 (82%)	-0.15	18 (4%) 32 31	28, 51, 87, 98	0
2	1-E	21/21 (100%)	5.62	21 (100%) 0 0	58, 91, 98, 98	21 (100%)
2	2-E	21/21 (100%)	5.62	21 (100%) 0 0	58, 91, 98, 98	21 (100%)
All	All	1618/1962 (82%)	-0.07	94 (5%) 23 22	26, 50, 89, 98	42 (2%)

All (94) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	1-E	25	SER	7.8
2	2-E	25	SER	7.8
2	1-E	19	SER	7.6
2	2-E	19	SER	7.6
2	1-E	21	LEU	7.3
2	2-E	21	LEU	7.3
2	1-E	14	ARG	6.9
2	2-E	14	ARG	6.9
2	1-E	12	MET	6.8
2	2-E	12	MET	6.8
2	1-E	9	GLY	6.8
2	2-E	9	GLY	6.8
2	1-E	7	CYS	6.7
2	2-E	7	CYS	6.7
2	1-E	22	GLY	6.3
2	2-E	22	GLY	6.3
2	1-E	20	GLY	6.1
2	2-E	20	GLY	6.1
2	1-E	16	GLY	6.0

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Mol	Chain	Res	Type	RSRZ
2	2-E	16	GLY	6.0
2	1-E	23	CYS	5.9
2	2-E	23	CYS	5.9
2	1-E	11	ARG	5.7
2	2-E	11	ARG	5.7
2	1-E	15	ILE	5.6
2	2-E	15	ILE	5.6
2	1-E	6	SER	5.5
2	2-E	6	SER	5.5
2	1-E	8	PHE	5.5
2	2-E	8	PHE	5.5
1	1-B	304	ASN	5.2
1	2-B	304	ASN	5.2
1	1-A	296	SER	4.4
1	2-A	296	SER	4.4
2	1-E	17	ALA	4.4
2	2-E	17	ALA	4.4
1	1-A	401	PRO	4.0
1	2-A	401	PRO	4.0
2	1-E	26	PHE	3.9
2	2-E	26	PHE	3.9
2	1-E	24	ASN	3.7
2	2-E	24	ASN	3.7
2	1-E	13	ASP	3.5
2	2-E	13	ASP	3.5
2	1-E	10	GLY	3.2
2	2-E	10	GLY	3.2
1	1-B	55	GLN	3.2
1	2-B	55	GLN	3.2
1	1-A	2	ALA	3.2
1	2-A	2	ALA	3.2
1	1-B	78	ALA	3.1
1	2-B	78	ALA	3.1
1	1-B	381	ALA	3.1
1	2-B	381	ALA	3.1
1	1-B	302	GLY	3.0
1	2-B	302	GLY	3.0
1	1-B	296	SER	2.9
1	2-B	296	SER	2.9
1	1-B	260	GLY	2.9
1	2-B	260	GLY	2.9
1	1-A	261	ASP	2.9

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Mol	Chain	Res	Type	RSRZ
1	2-A	261	ASP	2.9
1	1-B	380	GLU	2.9
1	2-B	380	GLU	2.9
1	1-B	2	ALA	2.9
1	2-B	2	ALA	2.9
2	1-E	18	GLN	2.8
2	2-E	18	GLN	2.8
1	1-B	306	GLU	2.7
1	2-B	306	GLU	2.7
1	1-A	307	ASP	2.7
1	2-A	307	ASP	2.7
1	1-B	305	MET	2.7
1	2-B	305	MET	2.7
1	1-B	298	VAL	2.6
1	2-B	298	VAL	2.6
1	1-A	378	ASP	2.6
1	2-A	378	ASP	2.6
1	1-B	401	PRO	2.4
1	2-B	401	PRO	2.4
1	1-A	260	GLY	2.4
1	2-A	260	GLY	2.4
1	1-A	40	GLY	2.4
1	2-A	40	GLY	2.4
1	1-B	308	TYR	2.3
1	2-B	308	TYR	2.3
1	1-B	395	GLY	2.2
1	2-B	395	GLY	2.2
1	1-B	38	VAL	2.1
1	2-B	38	VAL	2.1
1	1-B	307	ASP	2.1
1	2-B	307	ASP	2.1
1	1-B	79	ARG	2.0
1	2-B	79	ARG	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 [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	NAG	2-C	2	14/15	0.78	0.22	76,79,81,81	0
3	NAG	1-C	2	14/15	0.78	0.22	76,79,81,81	0
3	NAG	2-C	1	14/15	0.86	0.17	57,61,65,71	0
3	NAG	1-C	1	14/15	0.86	0.17	57,61,65,71	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. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	NAG	1-B	511	14/15	0.38	0.39	94,98,98,98	0
4	NAG	2-B	511	14/15	0.38	0.39	94,98,98,98	0
4	NAG	1-A	512	14/15	0.77	0.32	89,96,97,97	0
4	NAG	2-A	512	14/15	0.77	0.32	89,96,97,97	0
4	NAG	2-A	511	14/15	0.79	0.32	91,96,98,98	0
4	NAG	1-A	511	14/15	0.79	0.32	91,96,98,98	0
5	CL	1-B	512	1/1	0.98	0.04	35,35,35,35	0
5	CL	2-B	512	1/1	0.98	0.04	35,35,35,35	0
5	CL	1-A	513	1/1	0.99	0.04	36,36,36,36	0
5	CL	2-A	513	1/1	0.99	0.04	36,36,36,36	0

6.5 Other polymers [i](#)

There are no such residues in this entry.