



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 10, 2024 – 12:41 am GMT

PDB ID : 2X2J
Title : Crystal structure of the Gracilariopsis lemaneiformis alpha- 1,4-glucan lyase with deoxynojirimycin
Authors : Rozeboom, H.J.; Yu, S.; Madrid, S.; Kalk, K.H.; Dijkstra, B.W.
Deposited on : 2010-01-13
Resolution : 2.35 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

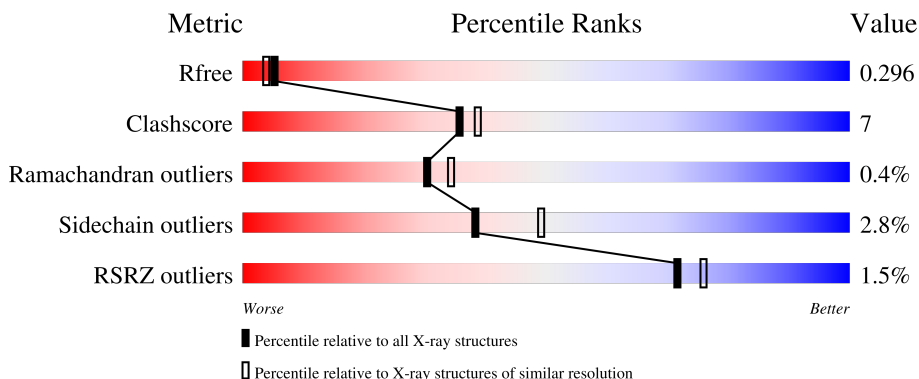
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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}	164625	1460 (2.36-2.36)
Clashscore	180529	1571 (2.36-2.36)
Ramachandran outliers	177936	1559 (2.36-2.36)
Sidechain outliers	177891	1559 (2.36-2.36)
RSRZ outliers	164620	1460 (2.36-2.36)

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

Mol	Chain	Length	Quality of chain
1	A	1027	<div> <div>2%</div> <div> <div></div> <div>81%</div> <div>18%</div> <div>.</div> </div> </div>
1	B	1027	<div> <div>%</div> <div> <div></div> <div>81%</div> <div>18%</div> <div>.</div> </div> </div>
1	C	1027	<div> <div>%</div> <div> <div></div> <div>80%</div> <div>19%</div> <div>.</div> </div> </div>
1	D	1027	<div> <div>2%</div> <div> <div></div> <div>85%</div> <div>14%</div> <div>.</div> </div> </div>

2 Entry composition [i](#)

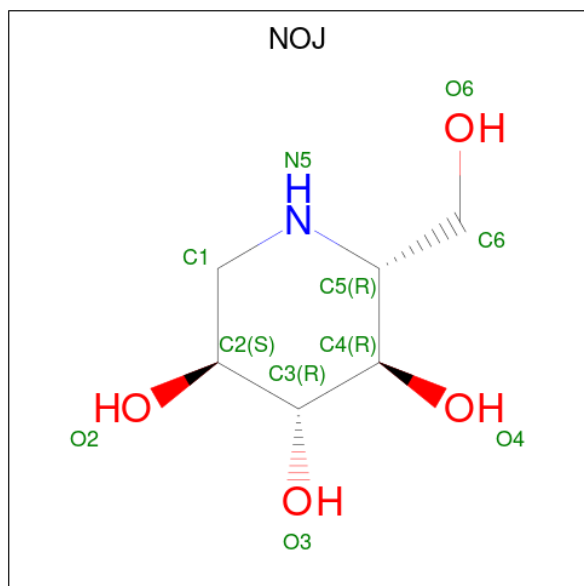
There are 5 unique types of molecules in this entry. The entry contains 34339 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 ALPHA-1,4-GLUCAN LYASE ISOZYME 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1025	Total	C	N	O	S	0	0	0
			8162	5135	1385	1595	47			
1	B	1025	Total	C	N	O	S	0	0	0
			8162	5135	1385	1595	47			
1	C	1025	Total	C	N	O	S	0	0	0
			8162	5135	1385	1595	47			
1	D	1025	Total	C	N	O	S	0	0	0
			8162	5135	1385	1595	47			

- Molecule 2 is 1-DEOXYNOJIRIMYCIN (three-letter code: NOJ) (formula: $C_6H_{13}NO_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			11	6	1	4		
2	B	1	Total	C	N	O	0	0
			11	6	1	4		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	C	1	Total	C	N	O	0	0
			11	6	1	4		
2	D	1	Total	C	N	O	0	0
			11	6	1	4		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	C	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Cl	0	0
			1	1		
4	B	1	Total	Cl	0	0
			1	1		
4	C	1	Total	Cl	0	0
			1	1		
4	D	1	Total	Cl	0	0
			1	1		

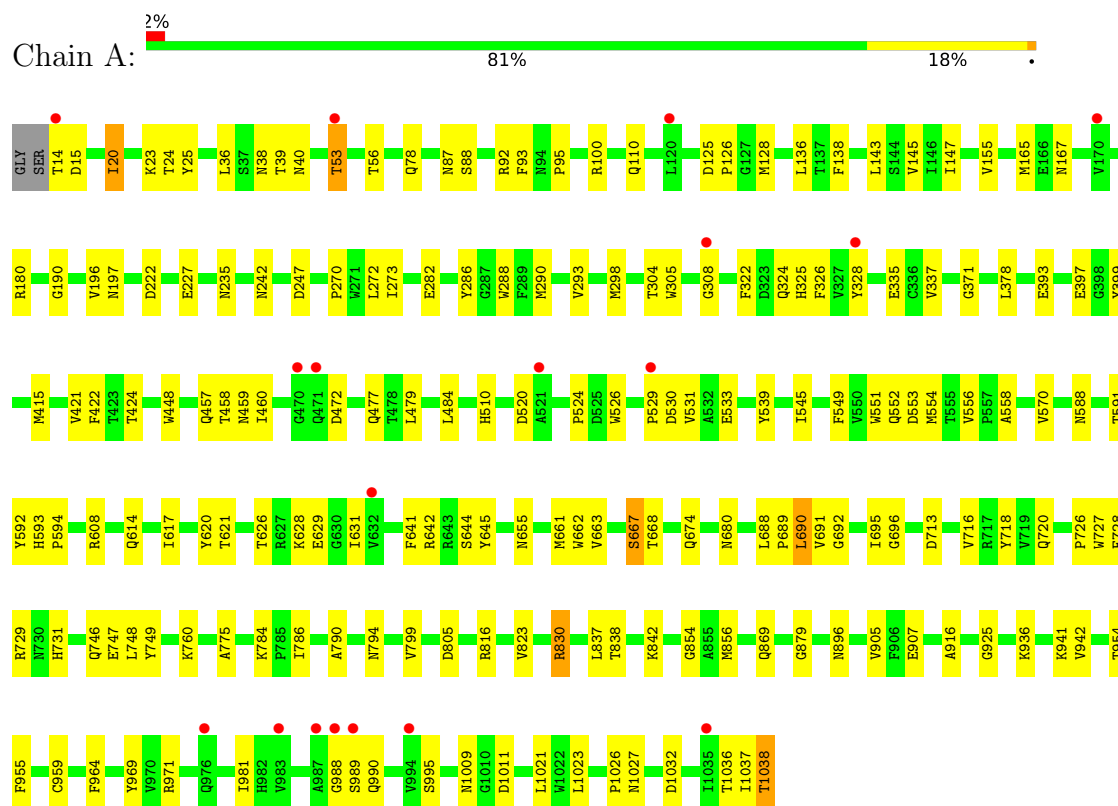
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	444	Total	O	0	0
			444	444		
5	B	362	Total	O	0	0
			362	362		
5	C	461	Total	O	0	0
			461	461		
5	D	310	Total	O	0	0
			310	310		

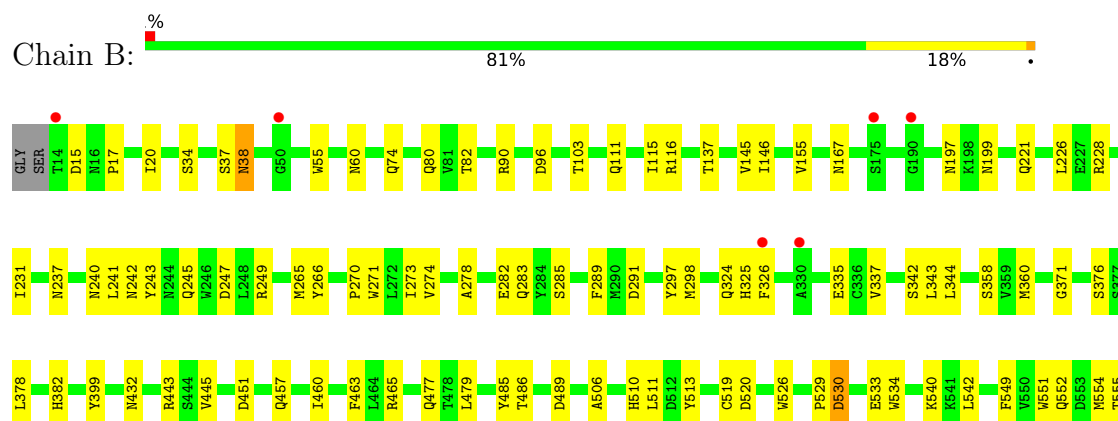
3 Residue-property plots

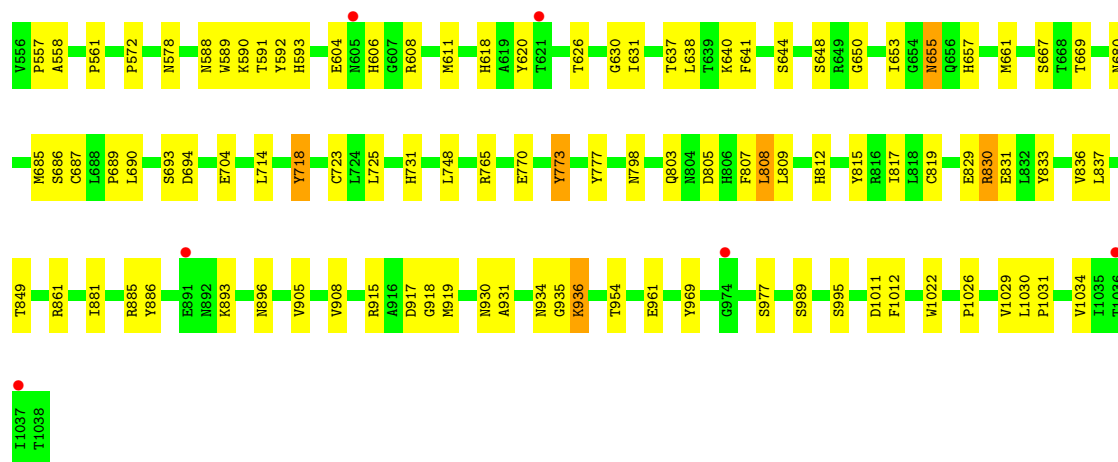
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: ALPHA-1,4-GLUCAN LYASE ISOZYME 1

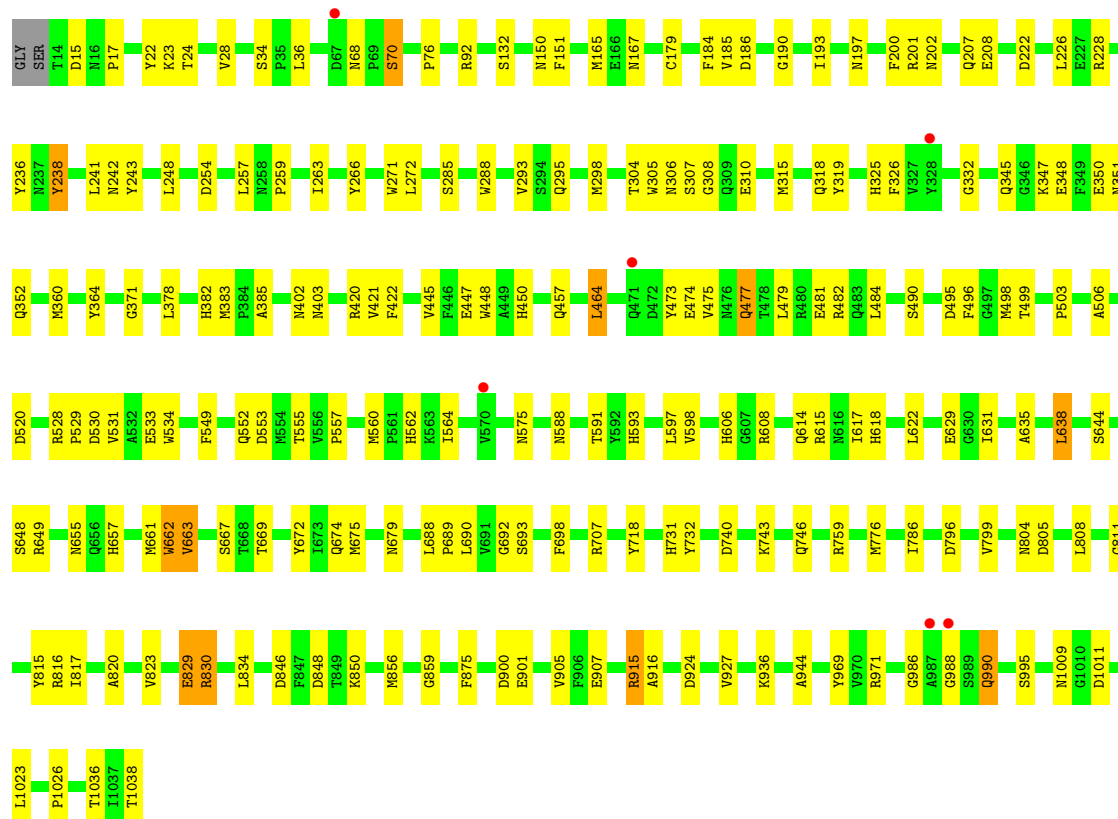
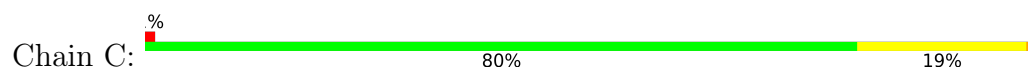


• Molecule 1: ALPHA-1,4-GLUCAN LYASE ISOZYME 1

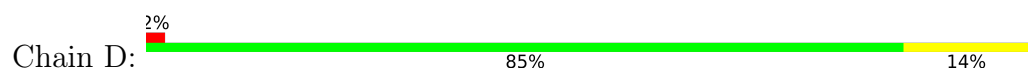


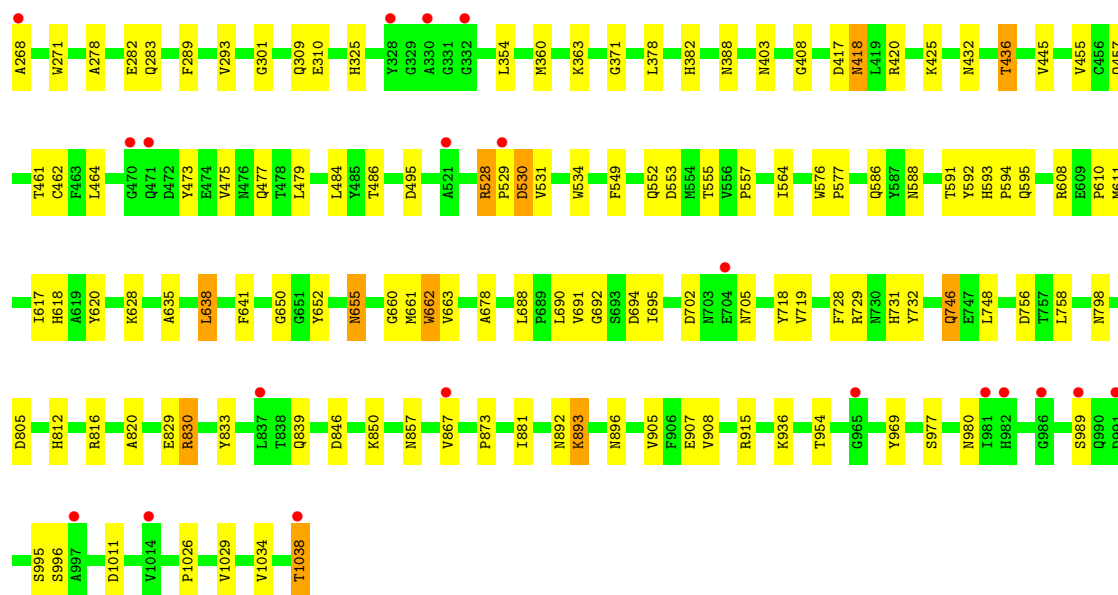


• Molecule 1: ALPHA-1,4-GLUCAN LYASE ISOZYME 1



• Molecule 1: ALPHA-1,4-GLUCAN LYASE ISOZYME 1





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	134.31Å 91.71Å 192.90Å 90.00° 99.33° 90.00°	Depositor
Resolution (Å)	33.19 – 2.35 33.19 – 2.35	Depositor EDS
% Data completeness (in resolution range)	91.0 (33.19-2.35) 90.9 (33.19-2.35)	Depositor EDS
R_{merge}	0.21	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.13 (at 2.34Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.234 , 0.291 0.236 , 0.296	Depositor DCC
R_{free} test set	8712 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	25.4	Xtriage
Anisotropy	0.461	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 54.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	34339	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 54.51 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.6127e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: GOL, CL, CSO, NOJ

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	0.54	0/8374	0.66	0/11389
1	B	0.51	0/8374	0.63	0/11389
1	C	0.61	0/8374	0.69	0/11389
1	D	0.46	0/8374	0.59	0/11389
All	All	0.53	0/33496	0.64	0/45556

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8162	0	7606	109	0
1	B	8162	0	7606	123	0
1	C	8162	0	7606	122	0
1	D	8162	0	7606	102	0
2	A	11	0	13	1	0
2	B	11	0	13	0	0
2	C	11	0	13	1	0
2	D	11	0	13	0	0
3	A	30	0	40	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	6	0	8	0	0
3	C	24	0	32	5	0
3	D	6	0	8	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	444	0	0	18	0
5	B	362	0	0	16	0
5	C	461	0	0	24	0
5	D	310	0	0	28	0
All	All	34339	0	30564	455	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 7.

All (455) 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:D:690:LEU:HB3	5:D:3199:HOH:O	1.29	1.28
1:A:941:LYS:HB3	5:A:3401:HOH:O	1.51	1.10
1:D:418:ASN:HB3	5:D:3119:HOH:O	1.62	0.98
1:A:995:SER:HB2	1:A:1011:ASP:HB3	1.43	0.97
1:B:15:ASP:HA	5:B:3221:HOH:O	1.65	0.96
1:B:529:PRO:O	1:B:530:ASP:HB2	1.73	0.87
1:A:959:CYS:HB3	5:A:3412:HOH:O	1.76	0.85
1:C:242:ASN:ND2	1:C:667:SER:HB2	1.92	0.85
1:A:1036:THR:HG23	5:A:3440:HOH:O	1.74	0.85
1:A:15:ASP:OD1	1:A:608:ARG:HD3	1.78	0.84
1:B:282:GLU:HG2	5:B:3104:HOH:O	1.76	0.83
1:C:382:HIS:HB3	5:C:3207:HOH:O	1.79	0.81
1:B:489:ASP:HB2	1:B:608:ARG:HH22	1.46	0.80
1:D:15:ASP:OD1	1:D:608:ARG:HD3	1.80	0.80
1:C:995:SER:HB2	1:C:1011:ASP:HB3	1.63	0.79
1:B:15:ASP:OD1	1:B:608:ARG:HD3	1.82	0.78
1:B:278:ALA:HA	1:B:283:GLN:HG3	1.65	0.78
1:D:805:ASP:CG	1:D:830:ARG:HH22	1.88	0.77
1:A:93:PHE:CE2	1:A:95:PRO:HG3	2.20	0.76
1:A:38:ASN:HD21	1:A:180:ARG:HH11	1.34	0.74
1:D:660:GLY:HA3	5:D:3199:HOH:O	1.88	0.74
1:D:529:PRO:O	1:D:530:ASP:HB2	1.87	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:705:ASN:HA	5:D:3223:HOH:O	1.89	0.71
1:A:588:ASN:HB3	1:A:593:HIS:CE1	2.26	0.70
1:B:360:MET:HE1	5:B:3274:HOH:O	1.90	0.70
1:B:995:SER:HB2	1:B:1011:ASP:HB3	1.72	0.70
1:C:325:HIS:HE1	5:C:3140:HOH:O	1.74	0.69
1:D:241:LEU:HB3	1:D:245:GLN:HE21	1.58	0.69
1:C:325:HIS:HD2	5:C:3037:HOH:O	1.76	0.68
1:D:254:ASP:HB2	5:D:3061:HOH:O	1.93	0.67
1:A:990:GLN:HB2	5:A:3423:HOH:O	1.94	0.67
1:D:325:HIS:HD2	5:D:3015:HOH:O	1.78	0.67
1:D:154:ARG:HD3	5:D:3032:HOH:O	1.94	0.67
1:A:393:GLU:HG2	1:A:397:GLU:OE2	1.94	0.66
1:A:964:PHE:O	1:A:1027:ASN:HB2	1.95	0.66
1:A:286:TYR:HB3	1:A:328:TYR:CD1	2.30	0.66
1:B:805:ASP:CG	1:B:830:ARG:HH22	1.99	0.65
1:C:307:SER:HB2	5:C:3014:HOH:O	1.96	0.65
1:D:56:THR:HG23	1:D:80:GLN:HB2	1.79	0.65
1:C:222:ASP:HB2	5:C:3105:HOH:O	1.97	0.64
1:C:588:ASN:HB3	1:C:593:HIS:CE1	2.32	0.64
1:D:325:HIS:HE1	5:D:3072:HOH:O	1.80	0.64
1:B:486:THR:HG21	1:B:592:TYR:CE1	2.32	0.64
1:D:528:ARG:HD3	5:D:3145:HOH:O	1.97	0.64
1:D:846:ASP:HB3	1:D:850:LYS:HE2	1.79	0.64
1:C:905:VAL:HG22	1:C:969:TYR:HB2	1.81	0.63
1:D:586:GLN:HG2	5:D:3179:HOH:O	1.99	0.63
1:B:460:ILE:HD11	1:B:542:LEU:HD11	1.81	0.63
1:B:561:PRO:HD3	1:B:590:LYS:HG2	1.80	0.63
1:C:662:TRP:HA	1:C:692:GLY:O	2.00	0.62
1:C:360:MET:CE	5:C:3353:HOH:O	2.48	0.62
1:C:907:GLU:HG3	1:C:971:ARG:HD3	1.82	0.61
1:A:533:GLU:HA	1:A:629:GLU:HG2	1.82	0.61
1:C:371:GLY:C	1:C:731:HIS:HD2	2.05	0.60
1:C:591:THR:HG21	1:C:615:ARG:NH1	2.16	0.60
1:D:457:GLN:HA	1:D:549:PHE:O	2.01	0.60
1:B:905:VAL:HG22	1:B:969:TYR:HB2	1.83	0.60
1:B:371:GLY:C	1:B:731:HIS:HD2	2.04	0.60
1:D:694:ASP:OD1	1:D:729:ARG:NH2	2.32	0.59
1:A:93:PHE:HE2	1:A:95:PRO:HG3	1.65	0.59
1:B:588:ASN:HB3	1:B:593:HIS:CE1	2.37	0.59
1:B:103:THR:HG21	1:B:604:GLU:HG2	1.85	0.59
1:D:954:THR:HG23	1:D:1034:VAL:HG22	1.85	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:773:TYR:O	5:B:3274:HOH:O	2.17	0.59
1:D:425:LYS:HE2	5:D:3117:HOH:O	2.03	0.59
1:D:594:PRO:HG3	5:D:3190:HOH:O	2.02	0.58
1:B:886:TYR:HB3	5:B:3314:HOH:O	2.02	0.58
1:A:335:GLU:OE2	1:A:784:LYS:HG2	2.03	0.58
1:C:304:THR:HG22	1:C:305:TRP:CD2	2.38	0.58
1:A:907:GLU:HG3	1:A:971:ARG:HD3	1.84	0.58
1:B:626:THR:O	1:B:630:GLY:HA3	2.04	0.58
1:C:242:ASN:HD22	1:C:667:SER:HB2	1.67	0.58
1:A:727:TRP:HZ2	1:A:729:ARG:HD3	1.69	0.58
1:B:631:ILE:HG12	1:B:644:SER:HB3	1.85	0.57
1:A:282:GLU:HB3	5:A:3134:HOH:O	2.04	0.57
1:D:484:LEU:HB3	1:D:531:VAL:HG22	1.86	0.57
1:A:905:VAL:HG22	1:A:969:TYR:HB2	1.86	0.57
1:A:989:SER:HB3	5:A:3421:HOH:O	2.03	0.57
1:D:620:TYR:HA	1:D:655:ASN:HD21	1.69	0.57
1:D:881:ILE:HG12	1:D:908:VAL:HG22	1.87	0.57
1:D:662:TRP:HA	1:D:692:GLY:O	2.05	0.57
1:D:893:LYS:HE3	5:D:3280:HOH:O	2.03	0.57
1:D:462:CYS:O	1:D:464:LEU:HD22	2.05	0.56
1:D:479:LEU:HD12	1:D:484:LEU:HB2	1.87	0.56
1:D:641:PHE:CZ	1:D:896:ASN:HB2	2.41	0.56
1:D:688:LEU:HD12	1:D:691:VAL:HB	1.86	0.56
1:C:257:LEU:HD11	1:C:263:ILE:HD11	1.87	0.56
1:A:713:ASP:OD1	1:A:869:GLN:HG3	2.05	0.56
1:D:678:ALA:HB2	5:D:3050:HOH:O	2.06	0.56
1:C:242:ASN:HD21	1:C:667:SER:HB2	1.71	0.56
1:C:562:HIS:HB3	1:C:588:ASN:ND2	2.21	0.56
1:D:378:LEU:HD13	1:D:445:VAL:HG23	1.87	0.55
1:B:640:LYS:HE2	5:B:3321:HOH:O	2.05	0.55
1:C:805:ASP:CG	1:C:830:ARG:HH22	2.10	0.55
1:C:238:TYR:CD2	1:C:248:LEU:HD11	2.42	0.54
1:A:242:ASN:ND2	1:A:667:SER:HB2	2.22	0.54
1:B:685:MET:N	5:B:3248:HOH:O	2.40	0.54
1:B:479:LEU:HD13	1:B:534:TRP:CH2	2.42	0.54
1:D:382:HIS:CD2	1:D:432:ASN:HB2	2.42	0.54
1:D:388:ASN:N	5:D:3107:HOH:O	2.33	0.54
1:D:408:GLY:HA3	1:D:455:VAL:O	2.07	0.54
1:B:360:MET:CE	5:B:3274:HOH:O	2.54	0.54
1:D:529:PRO:O	1:D:530:ASP:CB	2.55	0.54
1:A:661:MET:O	1:A:691:VAL:HA	2.08	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:539:TYR:CZ	1:A:626:THR:HG23	2.42	0.54
1:C:68:ASN:OD1	1:C:70:SER:OG	2.26	0.54
1:D:588:ASN:HB3	1:D:593:HIS:CE1	2.43	0.54
1:B:271:TRP:HE3	1:B:289:PHE:HB2	1.73	0.54
1:B:237:ASN:HA	1:B:265:MET:O	2.09	0.53
1:C:804:ASN:HB2	5:C:3369:HOH:O	2.07	0.53
1:B:242:ASN:O	1:B:243:TYR:HB2	2.07	0.53
1:C:479:LEU:HD13	1:C:534:TRP:CH2	2.43	0.53
1:B:60:ASN:HB3	1:B:74:GLN:NE2	2.24	0.53
1:C:848:ASP:HB2	5:C:3348:HOH:O	2.08	0.53
1:A:553:ASP:OD1	1:A:554:MET:N	2.41	0.53
1:C:266:TYR:HB3	1:C:649:ARG:O	2.09	0.53
1:C:553:ASP:OD2	2:C:1050:NOJ:H2	2.09	0.53
1:A:727:TRP:CZ2	1:A:729:ARG:HD3	2.43	0.53
1:A:529:PRO:O	1:A:530:ASP:HB2	2.09	0.53
1:A:1009:ASN:HB3	1:A:1026:PRO:HG3	1.91	0.53
1:B:533:GLU:HA	1:B:533:GLU:OE1	2.09	0.53
1:B:765:ARG:HG3	1:B:765:ARG:HH11	1.73	0.53
1:C:403:ASN:O	1:C:759:ARG:HD2	2.09	0.53
1:B:812:HIS:CD2	1:B:917:ASP:HB2	2.44	0.52
1:C:901:GLU:HG2	5:C:3415:HOH:O	2.10	0.52
1:A:645:TYR:CE2	1:A:690:LEU:HD13	2.44	0.52
1:A:145:VAL:HG22	1:A:155:VAL:HG22	1.90	0.52
1:A:642:ARG:NH2	5:A:3282:HOH:O	2.35	0.52
1:A:371:GLY:C	1:A:731:HIS:HD2	2.13	0.52
1:B:930:ASN:HB3	1:B:936:LYS:HD3	1.92	0.52
1:D:371:GLY:C	1:D:731:HIS:HD2	2.11	0.52
1:A:53:THR:HG21	5:A:3025:HOH:O	2.08	0.52
1:A:1038:THR:HB	5:A:3441:HOH:O	2.10	0.52
1:B:289:PHE:CZ	1:B:291:ASP:OD1	2.63	0.52
1:B:714:LEU:O	1:B:718:TYR:HB2	2.09	0.52
1:C:383:MET:HE1	5:C:3189:HOH:O	2.10	0.52
1:A:526:TRP:HB3	1:A:621:THR:HG21	1.92	0.52
1:A:661:MET:HG2	1:A:688:LEU:HD11	1.92	0.52
1:C:464:LEU:HD23	1:C:479:LEU:HD22	1.92	0.52
1:D:473:TYR:CZ	1:D:475:VAL:HB	2.45	0.52
1:C:325:HIS:CD2	5:C:3037:HOH:O	2.57	0.51
1:C:969:TYR:HA	1:C:1023:LEU:O	2.10	0.51
1:C:28:VAL:HG11	3:C:2039:GOL:O2	2.10	0.51
1:D:905:VAL:HG22	1:D:969:TYR:HB2	1.92	0.51
1:B:443:ARG:NH1	1:B:451:ASP:OD2	2.44	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:378:LEU:HD13	1:C:445:VAL:HG23	1.93	0.51
1:B:489:ASP:HB2	1:B:608:ARG:NH2	2.21	0.51
1:D:628:LYS:HD2	5:D:3053:HOH:O	2.10	0.51
1:D:278:ALA:HA	1:D:283:GLN:HG3	1.92	0.51
1:C:17:PRO:HG3	1:C:606:HIS:O	2.10	0.51
1:B:378:LEU:HD13	1:B:445:VAL:HG23	1.92	0.51
1:A:988:GLY:HA2	5:A:3420:HOH:O	2.11	0.51
1:B:17:PRO:HG3	1:B:606:HIS:O	2.10	0.51
1:B:680:ASN:ND2	1:B:725:LEU:HB3	2.26	0.51
1:C:669:THR:OG1	1:C:672:TYR:HD2	1.94	0.51
1:C:689:PRO:HB2	1:C:786:ILE:HG13	1.92	0.51
1:D:486:THR:HG21	1:D:592:TYR:CE1	2.46	0.51
1:C:360:MET:HE1	5:C:3353:HOH:O	2.09	0.51
1:C:533:GLU:HA	1:C:629:GLU:HG2	1.92	0.50
1:C:815:TYR:CZ	3:C:2042:GOL:H31	2.47	0.50
1:B:561:PRO:HB2	1:B:572:PRO:HD2	1.92	0.50
1:C:856:MET:HE3	1:C:875:PHE:CD1	2.47	0.50
1:D:241:LEU:HB3	1:D:245:GLN:NE2	2.26	0.50
1:B:611:MET:HE2	5:B:3216:HOH:O	2.11	0.50
1:C:575:ASN:HD22	1:D:989:SER:HB2	1.76	0.50
1:D:425:LYS:NZ	5:D:3102:HOH:O	2.44	0.50
1:B:382:HIS:CD2	1:B:432:ASN:HB2	2.47	0.50
1:A:545:ILE:HG23	5:A:3247:HOH:O	2.12	0.50
1:B:399:TYR:HE1	1:B:748:LEU:HB2	1.77	0.50
1:D:748:LEU:HB3	1:D:758:LEU:HD13	1.94	0.50
1:B:557:PRO:HG3	1:B:618:HIS:CE1	2.47	0.50
1:A:614:GLN:O	1:A:617:ILE:HG22	2.12	0.50
1:A:620:TYR:HA	1:A:655:ASN:ND2	2.26	0.50
1:B:324:GLN:HG2	1:B:326:PHE:CZ	2.47	0.50
1:B:540:LYS:HD3	1:B:637:THR:HG21	1.92	0.50
1:C:272:LEU:HG	1:C:315:MET:HE2	1.93	0.50
1:D:867:VAL:HG11	1:D:873:PRO:HD3	1.93	0.50
1:D:1026:PRO:O	1:D:1029:VAL:HG22	2.12	0.50
1:A:981:ILE:HG12	1:A:1037:ILE:HG12	1.93	0.49
1:B:954:THR:HG23	1:B:1034:VAL:HG22	1.93	0.49
1:C:1009:ASN:HB3	1:C:1026:PRO:HG3	1.94	0.49
1:D:661:MET:HB2	1:D:691:VAL:HG23	1.93	0.49
1:D:719:VAL:HG13	1:D:728:PHE:HZ	1.76	0.49
1:A:87:ASN:HB3	1:A:143:LEU:HD12	1.93	0.49
1:A:663:VAL:HG23	5:A:3297:HOH:O	2.12	0.49
1:A:620:TYR:HA	1:A:655:ASN:HD21	1.78	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:457:GLN:HA	1:C:549:PHE:O	2.12	0.49
1:C:477:GLN:O	1:C:481:GLU:HB2	2.13	0.49
1:C:663:VAL:HG11	1:C:679:ASN:OD1	2.12	0.49
1:A:421:VAL:O	1:A:422:PHE:HB2	2.13	0.49
1:B:881:ILE:HB	1:B:918:GLY:HA3	1.94	0.49
1:D:403:ASN:OD1	1:D:892:ASN:HB2	2.12	0.49
1:A:167:ASN:HA	1:A:197:ASN:HA	1.93	0.48
1:A:969:TYR:HA	1:A:1023:LEU:O	2.13	0.48
1:D:167:ASN:HA	1:D:197:ASN:HA	1.96	0.48
1:A:553:ASP:OD2	2:A:1050:NOJ:H2	2.13	0.48
1:C:811:GLY:HA3	1:C:816:ARG:HG3	1.96	0.48
1:A:663:VAL:CG2	5:A:3297:HOH:O	2.61	0.48
1:D:732:TYR:HB3	1:D:746:GLN:NE2	2.29	0.48
1:A:272:LEU:HD11	1:A:298:MET:HB3	1.96	0.48
1:B:486:THR:HG21	1:B:592:TYR:HE1	1.75	0.48
1:C:672:TYR:HA	1:C:675:MET:HE3	1.95	0.48
1:D:995:SER:HB2	1:D:1011:ASP:HB3	1.94	0.48
1:B:145:VAL:HG22	1:B:155:VAL:HG13	1.95	0.48
1:D:22:TYR:CZ	1:D:610:PRO:HD2	2.49	0.48
1:D:980:ASN:O	1:D:1038:THR:HG23	2.13	0.48
1:C:496:PHE:CE1	1:C:593:HIS:HB2	2.49	0.47
1:C:698:PHE:HA	1:C:732:TYR:HA	1.96	0.47
1:B:554:MET:HB3	1:B:558:ALA:HB3	1.96	0.47
1:A:879:GLY:HA2	1:A:916:ALA:HA	1.96	0.47
1:B:297:TYR:C	1:B:298:MET:HG3	2.34	0.47
1:C:834:LEU:O	1:C:859:GLY:N	2.39	0.47
1:B:693:SER:O	1:B:694:ASP:C	2.53	0.47
1:B:936:LYS:HA	1:B:961:GLU:HB3	1.96	0.47
1:C:347:LYS:HB2	1:C:352:GLN:HG3	1.95	0.47
1:C:829:GLU:HG2	5:C:3378:HOH:O	2.15	0.47
1:D:820:ALA:HB3	1:D:873:PRO:HB2	1.97	0.47
1:B:242:ASN:ND2	1:B:667:SER:HB2	2.30	0.47
1:B:641:PHE:CZ	1:B:896:ASN:HB2	2.48	0.47
1:B:931:ALA:O	1:B:935:GLY:HA2	2.15	0.47
1:C:529:PRO:O	1:C:530:ASP:HB2	2.14	0.47
1:A:680:ASN:HB2	5:A:3292:HOH:O	2.14	0.47
1:B:221:GLN:HA	1:B:221:GLN:NE2	2.29	0.47
1:C:808:LEU:HA	1:C:817:ILE:O	2.14	0.47
1:D:39:THR:O	1:D:40:ASN:HB2	2.15	0.47
1:D:93:PHE:CE2	1:D:95:PRO:HG3	2.50	0.47
1:D:576:TRP:CG	1:D:577:PRO:HA	2.50	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:399:TYR:HE1	1:A:748:LEU:HB2	1.79	0.47
1:B:137:THR:HB	5:B:3048:HOH:O	2.15	0.47
1:D:201:ARG:HH12	1:D:310:GLU:HG2	1.80	0.47
1:A:87:ASN:O	1:A:328:TYR:HD2	1.98	0.47
1:B:273:ILE:HG23	1:B:337:VAL:HG11	1.96	0.47
1:B:680:ASN:HD22	1:B:725:LEU:HD13	1.80	0.47
1:B:289:PHE:HZ	1:B:291:ASP:OD1	1.98	0.47
1:B:555:THR:OG1	1:B:650:GLY:HA3	2.15	0.47
1:C:661:MET:HG2	1:C:688:LEU:HD11	1.97	0.47
1:B:20:ILE:CD1	1:B:96:ASP:HB3	2.45	0.46
1:B:830:ARG:NH1	1:B:831:GLU:O	2.48	0.46
1:A:510:HIS:ND1	1:A:520:ASP:OD1	2.47	0.46
1:C:402:ASN:O	1:C:759:ARG:NH1	2.43	0.46
1:D:101:ASP:HA	5:D:3021:HOH:O	2.15	0.46
1:A:747:GLU:HB3	1:A:749:TYR:CE1	2.51	0.46
1:A:842:LYS:HB2	1:A:856:MET:HE1	1.97	0.46
1:A:128:MET:HG2	1:A:138:PHE:CB	2.45	0.46
1:B:37:SER:O	1:B:38:ASN:HB2	2.16	0.46
1:B:228:ARG:HB3	1:B:231:ILE:HD11	1.98	0.46
1:D:301:GLY:HA2	1:D:309:GLN:O	2.16	0.46
1:D:479:LEU:HB2	1:D:534:TRP:CZ2	2.50	0.46
1:A:716:VAL:O	1:A:720:GLN:HG3	2.15	0.46
1:D:268:ALA:HB3	1:D:652:TYR:HD1	1.81	0.46
1:D:378:LEU:HB3	5:D:3127:HOH:O	2.15	0.46
1:D:881:ILE:HA	1:D:907:GLU:O	2.16	0.46
1:A:270:PRO:HB2	1:A:290:MET:O	2.15	0.46
1:A:689:PRO:O	1:A:726:PRO:HG2	2.16	0.46
1:B:240:ASN:HA	1:B:245:GLN:HG2	1.97	0.46
1:B:798:ASN:HD22	1:B:861:ARG:NH2	2.14	0.46
1:C:271:TRP:HA	1:C:288:TRP:O	2.16	0.46
1:A:136:LEU:HD23	1:A:147:ILE:HD12	1.97	0.46
1:A:293:VAL:O	1:A:614:GLN:HA	2.15	0.46
1:B:249:ARG:NH2	1:B:578:ASN:HB3	2.31	0.46
1:C:167:ASN:HA	1:C:197:ASN:HA	1.98	0.46
1:D:695:ILE:HG13	1:D:728:PHE:CE1	2.51	0.46
1:C:495:ASP:O	1:C:564:ILE:HD12	2.16	0.46
1:B:221:GLN:HA	1:B:221:GLN:HE21	1.80	0.45
1:B:526:TRP:HE1	1:B:618:HIS:CE1	2.34	0.45
1:B:680:ASN:ND2	1:B:725:LEU:HD13	2.31	0.45
1:B:723:CYS:O	1:B:765:ARG:HG3	2.16	0.45
1:A:674:GLN:HG3	1:A:823:VAL:HB	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:881:ILE:HG12	1:B:908:VAL:HG13	1.98	0.45
1:B:1012:PHE:HA	1:B:1022:TRP:O	2.17	0.45
1:C:150:ASN:O	1:C:179:CYS:HB2	2.16	0.45
1:C:378:LEU:HD11	1:C:448:TRP:CE3	2.52	0.45
1:D:662:TRP:CD1	1:D:729:ARG:NH2	2.85	0.45
1:A:128:MET:HG2	1:A:138:PHE:HB3	1.98	0.45
1:B:199:ASN:OD1	1:B:199:ASN:C	2.54	0.45
1:B:485:TYR:CE2	1:B:506:ALA:HB2	2.51	0.45
1:B:849:THR:HG23	5:B:3299:HOH:O	2.16	0.45
1:C:528:ARG:HB2	1:C:531:VAL:HG23	1.97	0.45
1:C:648:SER:O	1:C:661:MET:HA	2.16	0.45
1:C:856:MET:CE	1:C:875:PHE:CD1	3.00	0.45
1:A:591:THR:OG1	1:A:592:TYR:N	2.50	0.45
1:A:760:LYS:NZ	5:A:3325:HOH:O	2.49	0.45
1:C:332:GLY:HA3	5:C:3155:HOH:O	2.17	0.45
1:C:635:ALA:HA	1:C:638:LEU:HD12	1.97	0.45
1:C:655:ASN:HB3	5:C:3293:HOH:O	2.16	0.45
1:C:846:ASP:HB3	1:C:850:LYS:HE2	1.99	0.45
1:D:661:MET:O	1:D:691:VAL:HA	2.17	0.45
1:A:526:TRP:HA	1:A:531:VAL:HG11	1.98	0.45
1:A:837:LEU:O	1:A:838:THR:HB	2.16	0.45
1:C:490:SER:HA	1:C:597:LEU:HG	1.98	0.45
1:D:77:VAL:HA	1:D:93:PHE:HB3	1.98	0.45
1:B:510:HIS:ND1	1:B:520:ASP:OD1	2.49	0.45
1:C:345:GLN:O	1:C:657:HIS:CE1	2.70	0.45
1:C:557:PRO:HG3	1:C:618:HIS:CE1	2.51	0.45
1:D:555:THR:OG1	1:D:650:GLY:HA3	2.17	0.45
1:A:981:ILE:HD11	1:A:1021:LEU:HD21	1.99	0.45
1:C:403:ASN:O	1:C:759:ARG:CD	2.65	0.45
1:A:36:LEU:HD12	1:A:308:GLY:HA2	1.98	0.45
1:A:378:LEU:HD11	1:A:448:TRP:CE3	2.52	0.45
1:B:226:LEU:HB3	1:B:803:GLN:HG3	1.99	0.45
1:B:511:LEU:HD11	1:B:513:TYR:CZ	2.52	0.45
1:A:691:VAL:HG22	1:A:692:GLY:N	2.31	0.45
1:C:201:ARG:HD3	1:C:310:GLU:O	2.17	0.45
1:C:503:PRO:HG2	1:C:506:ALA:HB2	1.99	0.45
1:A:458:THR:O	1:A:551:TRP:HB3	2.17	0.44
1:C:185:VAL:HG12	1:C:186:ASP:O	2.16	0.44
1:C:598:VAL:O	1:C:608:ARG:HB3	2.17	0.44
1:A:38:ASN:ND2	1:A:180:ARG:HH11	2.10	0.44
1:A:524:PRO:HG2	1:A:526:TRP:CZ2	2.52	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:641:PHE:CZ	1:A:896:ASN:HB2	2.52	0.44
1:D:839:GLN:OE1	1:D:857:ASN:HA	2.17	0.44
1:D:816:ARG:HG3	5:D:3284:HOH:O	2.17	0.44
1:B:686:SER:O	1:B:687:CYS:HB2	2.18	0.44
1:B:20:ILE:HD11	1:B:96:ASP:HB3	1.99	0.44
1:C:22:TYR:HD1	1:C:319:TYR:CE1	2.35	0.44
1:D:271:TRP:HE3	1:D:289:PHE:HB2	1.82	0.44
1:D:325:HIS:CE1	5:D:3072:HOH:O	2.64	0.44
1:A:325:HIS:HD2	5:A:3040:HOH:O	2.00	0.44
1:B:325:HIS:HD2	5:B:3018:HOH:O	2.00	0.44
1:C:165:MET:HE2	1:C:326:PHE:CE1	2.53	0.44
1:B:777:TYR:CE2	1:B:919:MET:CE	3.01	0.44
1:C:243:TYR:HB2	1:C:259:PRO:HB3	2.00	0.44
1:C:528:ARG:HB2	1:C:531:VAL:CG2	2.47	0.44
1:D:420:ARG:HB3	1:D:473:TYR:CE1	2.53	0.44
1:B:463:PHE:CD1	1:B:511:LEU:HB2	2.52	0.44
1:D:436:THR:HB	5:D:3129:HOH:O	2.18	0.44
1:D:936:LYS:HG2	5:D:3298:HOH:O	2.17	0.44
1:C:318:GLN:HE22	3:C:2039:GOL:H11	1.83	0.43
1:D:557:PRO:HG3	1:D:618:HIS:CE1	2.53	0.43
1:B:685:MET:HB3	5:B:3248:HOH:O	2.17	0.43
1:C:23:LYS:HG3	1:C:190:GLY:HA2	1.99	0.43
1:C:915:ARG:HG3	1:C:916:ALA:N	2.33	0.43
1:D:417:ASP:O	1:D:418:ASN:C	2.55	0.43
1:B:457:GLN:HA	1:B:549:PHE:O	2.18	0.43
1:A:661:MET:CG	1:A:688:LEU:HD11	2.49	0.43
1:C:208:GLU:OE2	5:C:3099:HOH:O	2.21	0.43
1:C:421:VAL:O	1:C:422:PHE:HB2	2.19	0.43
1:D:461:THR:HG22	1:D:553:ASP:O	2.18	0.43
1:B:55:TRP:CE3	1:B:116:ARG:HG3	2.53	0.43
1:B:271:TRP:CE3	1:B:289:PHE:HB2	2.52	0.43
1:C:241:LEU:O	1:C:242:ASN:HB2	2.18	0.43
1:A:273:ILE:HG23	1:A:337:VAL:HG11	2.01	0.43
1:B:765:ARG:HG3	1:B:765:ARG:NH1	2.33	0.43
1:B:807:PHE:CE2	1:B:819:CYS:HB2	2.54	0.43
1:C:631:ILE:CG2	1:C:644:SER:HB3	2.48	0.43
1:D:25:TYR:CE1	1:D:595:GLN:HA	2.54	0.43
1:B:589:TRP:O	1:B:591:THR:HG22	2.18	0.43
1:B:808:LEU:HA	1:B:817:ILE:O	2.18	0.43
1:A:556:VAL:CG1	1:A:591:THR:HB	2.49	0.43
1:B:240:ASN:HA	1:B:245:GLN:CG	2.49	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:555:THR:HG22	1:C:622:LEU:HD23	2.00	0.43
1:B:648:SER:O	1:B:661:MET:HA	2.19	0.43
1:B:798:ASN:HB2	1:B:833:TYR:CZ	2.54	0.43
1:C:900:ASP:OD1	3:C:2040:GOL:O1	2.37	0.43
1:A:235:ASN:ND2	1:A:298:MET:CE	2.81	0.42
1:C:499:THR:HG21	1:C:520:ASP:OD2	2.19	0.42
1:C:560:MET:HA	5:C:3252:HOH:O	2.19	0.42
1:A:56:THR:CG2	1:A:78:GLN:HG2	2.49	0.42
1:B:457:GLN:HG3	1:B:551:TRP:HB2	2.02	0.42
1:C:924:ASP:O	1:C:927:VAL:HG23	2.18	0.42
1:D:729:ARG:HB2	5:D:3231:HOH:O	2.18	0.42
1:B:274:VAL:O	1:B:285:SER:HA	2.19	0.42
1:D:201:ARG:NH1	1:D:301:GLY:O	2.52	0.42
1:D:812:HIS:HE1	5:D:3257:HOH:O	2.02	0.42
1:A:794:ASN:H	3:A:2039:GOL:H12	1.84	0.42
1:C:76:PRO:HD2	5:C:3043:HOH:O	2.19	0.42
1:C:776:MET:SD	1:C:786:ILE:HD11	2.59	0.42
1:A:247:ASP:OD1	1:A:247:ASP:N	2.53	0.42
1:B:241:LEU:HB3	1:B:245:GLN:NE2	2.34	0.42
1:C:916:ALA:HB3	1:C:944:ALA:HB3	2.02	0.42
1:D:39:THR:HG22	1:D:67:ASP:HB3	2.01	0.42
1:A:695:ILE:HG13	1:A:728:PHE:CE1	2.54	0.42
1:C:707:ARG:HA	1:C:743:LYS:HA	2.01	0.42
1:B:620:TYR:HA	1:B:655:ASN:HD21	1.84	0.42
1:B:1026:PRO:O	1:B:1029:VAL:HG22	2.19	0.42
1:A:631:ILE:HG23	1:A:644:SER:HB3	2.02	0.42
1:C:385:ALA:HA	5:C:3184:HOH:O	2.18	0.42
1:C:473:TYR:CZ	1:C:475:VAL:HB	2.55	0.42
1:C:805:ASP:O	1:C:820:ALA:HA	2.20	0.42
1:A:36:LEU:HD21	1:A:196:VAL:HG11	2.02	0.42
1:A:88:SER:HA	1:A:326:PHE:O	2.20	0.42
1:B:82:THR:HB	1:B:344:LEU:CD2	2.49	0.42
1:B:278:ALA:HA	1:B:283:GLN:CG	2.41	0.42
1:D:293:VAL:HG11	1:D:617:ILE:HB	2.01	0.42
1:D:702:ASP:HB3	1:D:705:ASN:O	2.20	0.42
1:C:293:VAL:HG11	1:C:617:ILE:HD12	2.01	0.42
1:A:668:THR:HG23	1:A:696:GLY:O	2.20	0.41
1:B:335:GLU:OE1	1:B:815:TYR:OH	2.28	0.41
1:A:288:TRP:HE1	1:A:324:GLN:CD	2.20	0.41
1:A:790:ALA:HB1	1:A:799:VAL:HB	2.00	0.41
1:B:146:ILE:HG22	5:B:3049:HOH:O	2.19	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:200:PHE:HB2	1:C:208:GLU:HG3	2.03	0.41
1:C:740:ASP:HB2	5:C:3330:HOH:O	2.20	0.41
1:A:39:THR:O	1:A:40:ASN:HB2	2.20	0.41
1:B:247:ASP:OD1	1:B:247:ASP:N	2.53	0.41
1:B:265:MET:HB3	1:B:266:TYR:H	1.65	0.41
1:B:669:THR:HA	5:B:3244:HOH:O	2.20	0.41
1:C:226:LEU:O	1:C:228:ARG:NH1	2.53	0.41
1:C:236:TYR:HD1	1:C:295:GLN:HB2	1.86	0.41
1:D:237:ASN:HB3	5:D:3065:HOH:O	2.20	0.41
1:A:20:ILE:H	1:A:20:ILE:HG12	1.55	0.41
1:A:23:LYS:HG3	1:A:190:GLY:HA2	2.02	0.41
1:A:288:TRP:NE1	1:A:324:GLN:OE1	2.34	0.41
1:A:942:VAL:HA	1:A:954:THR:O	2.20	0.41
1:B:807:PHE:CZ	1:B:819:CYS:HB2	2.56	0.41
1:D:371:GLY:O	1:D:731:HIS:HA	2.21	0.41
1:A:304:THR:HG22	1:A:305:TRP:CD2	2.55	0.41
1:C:17:PRO:HB2	5:C:3002:HOH:O	2.20	0.41
1:D:635:ALA:HA	1:D:638:LEU:HD12	2.01	0.41
1:A:805:ASP:CG	1:A:830:ARG:HH22	2.24	0.41
1:A:955:PHE:O	1:A:1032:ASP:HA	2.20	0.41
1:B:680:ASN:HD21	1:B:725:LEU:HB3	1.85	0.41
1:C:674:GLN:HG3	1:C:823:VAL:HB	2.03	0.41
1:C:990:GLN:HE21	1:C:990:GLN:HB3	1.62	0.41
1:B:270:PRO:HA	1:B:298:MET:SD	2.61	0.41
1:B:460:ILE:HD11	1:B:542:LEU:CD1	2.47	0.41
1:B:770:GLU:HG2	1:B:885:ARG:HG2	2.02	0.41
1:B:1030:LEU:N	1:B:1031:PRO:CD	2.84	0.41
1:C:202:ASN:HA	5:C:3093:HOH:O	2.21	0.41
1:C:420:ARG:HG2	1:C:473:TYR:CG	2.56	0.41
1:C:447:GLU:O	1:C:450:HIS:HB2	2.21	0.41
1:D:420:ARG:NH1	5:D:3119:HOH:O	2.52	0.41
1:A:25:TYR:HB3	1:A:594:PRO:HB2	2.03	0.41
1:A:227:GLU:HB2	5:A:3113:HOH:O	2.20	0.41
1:A:570:VAL:HA	5:A:3253:HOH:O	2.20	0.41
1:B:111:GLN:O	1:B:115:ILE:HG13	2.21	0.41
1:B:657:HIS:HD2	5:B:3137:HOH:O	2.03	0.41
1:B:836:VAL:HG22	1:B:837:LEU:N	2.36	0.41
1:C:36:LEU:HD12	1:C:308:GLY:HA2	2.02	0.41
1:C:796:ASP:CG	1:C:799:VAL:HG13	2.41	0.41
1:D:354:LEU:HD21	1:D:360:MET:HG3	2.03	0.41
1:C:815:TYR:CE2	3:C:2042:GOL:H31	2.56	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:325:HIS:CD2	5:D:3015:HOH:O	2.62	0.41
1:A:415:MET:SD	1:A:424:THR:HG22	2.61	0.40
1:A:925:GLY:CA	3:A:2041:GOL:H11	2.51	0.40
1:B:638:LEU:HD23	1:B:638:LEU:HA	1.89	0.40
1:D:60:ASN:HB3	1:D:74:GLN:NE2	2.36	0.40
1:D:403:ASN:O	1:D:403:ASN:CG	2.60	0.40
1:D:588:ASN:HB2	1:D:591:THR:O	2.21	0.40
1:C:350:GLU:O	1:C:351:ASN:HB2	2.21	0.40
1:A:459:ASN:O	1:A:460:ILE:HD13	2.21	0.40
1:A:479:LEU:HD12	1:A:484:LEU:HB2	2.02	0.40
1:A:775:ALA:HB1	1:A:786:ILE:HG23	2.04	0.40
1:B:465:ARG:HG3	1:B:519:CYS:SG	2.61	0.40
1:C:184:PHE:HA	1:C:193:ILE:HA	2.04	0.40
1:A:125:ASP:HA	1:A:126:PRO:HD2	1.93	0.40
1:B:80:GLN:O	1:B:90:ARG:N	2.53	0.40
1:B:167:ASN:HA	1:B:197:ASN:HA	2.03	0.40
1:C:207:GLN:HG2	5:C:3094:HOH:O	2.21	0.40
1:C:482:ARG:O	1:C:484:LEU:HG	2.22	0.40
1:C:597:LEU:HD23	1:C:597:LEU:HA	1.75	0.40
1:D:495:ASP:O	1:D:564:ILE:HG23	2.21	0.40
1:C:971:ARG:HD2	5:C:3407:HOH:O	2.20	0.40
1:D:224:TYR:HE2	1:D:259:PRO:O	2.04	0.40
1:D:798:ASN:HB2	1:D:833:TYR:CZ	2.57	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	1022/1027 (100%)	969 (95%)	50 (5%)	3 (0%)	37 43
1	B	1022/1027 (100%)	957 (94%)	60 (6%)	5 (0%)	25 28

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	1022/1027 (100%)	957 (94%)	60 (6%)	5 (0%)	25	28
1	D	1022/1027 (100%)	966 (94%)	51 (5%)	5 (0%)	25	28
All	All	4088/4108 (100%)	3849 (94%)	221 (5%)	18 (0%)	30	34

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	746	GLN
1	C	663	VAL
1	C	746	GLN
1	D	530	ASP
1	D	746	GLN
1	A	854	GLY
1	D	221	GLN
1	D	418	ASN
1	B	38	ASN
1	B	358	SER
1	B	530	ASP
1	C	348	GLU
1	C	986	GLY
1	A	558	ALA
1	C	988	GLY
1	D	663	VAL
1	B	653	ILE
1	B	689	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	877/878 (100%)	853 (97%)	24 (3%)	40	50
1	B	877/878 (100%)	856 (98%)	21 (2%)	44	55
1	C	877/878 (100%)	846 (96%)	31 (4%)	31	40
1	D	877/878 (100%)	855 (98%)	22 (2%)	42	53

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	3508/3512 (100%)	3410 (97%)	98 (3%)	38 49

All (98) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	THR
1	A	20	ILE
1	A	24	THR
1	A	53	THR
1	A	92	ARG
1	A	100	ARG
1	A	110	GLN
1	A	165	MET
1	A	222	ASP
1	A	322	PHE
1	A	457	GLN
1	A	472	ASP
1	A	477	GLN
1	A	549	PHE
1	A	552	GLN
1	A	628	LYS
1	A	662	TRP
1	A	667	SER
1	A	690	LEU
1	A	718	TYR
1	A	816	ARG
1	A	830	ARG
1	A	936	LYS
1	A	1038	THR
1	B	34	SER
1	B	342	SER
1	B	343	LEU
1	B	376	SER
1	B	477	GLN
1	B	552	GLN
1	B	655	ASN
1	B	690	LEU
1	B	704	GLU
1	B	718	TYR
1	B	773	TYR
1	B	808	LEU
1	B	809	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	829	GLU
1	B	830	ARG
1	B	893	LYS
1	B	915	ARG
1	B	934	ASN
1	B	936	LYS
1	B	977	SER
1	B	989	SER
1	C	15	ASP
1	C	24	THR
1	C	34	SER
1	C	70	SER
1	C	92	ARG
1	C	132	SER
1	C	151	PHE
1	C	238	TYR
1	C	254	ASP
1	C	285	SER
1	C	298	MET
1	C	306	ASN
1	C	364	TYR
1	C	464	LEU
1	C	474	GLU
1	C	477	GLN
1	C	498	MET
1	C	552	GLN
1	C	614	GLN
1	C	638	LEU
1	C	662	TRP
1	C	690	LEU
1	C	693	SER
1	C	718	TYR
1	C	829	GLU
1	C	830	ARG
1	C	915	ARG
1	C	936	LYS
1	C	990	GLN
1	C	1036	THR
1	C	1038	THR
1	D	92	ARG
1	D	151	PHE
1	D	221	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	282	GLU
1	D	363	LYS
1	D	436	THR
1	D	477	GLN
1	D	528	ARG
1	D	552	GLN
1	D	611	MET
1	D	638	LEU
1	D	655	ASN
1	D	662	TRP
1	D	718	TYR
1	D	756	ASP
1	D	829	GLU
1	D	830	ARG
1	D	893	LYS
1	D	915	ARG
1	D	977	SER
1	D	996	SER
1	D	1038	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (59) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	ASN
1	A	177	ASN
1	A	221	GLN
1	A	242	ASN
1	A	309	GLN
1	A	325	HIS
1	A	471	GLN
1	A	552	GLN
1	A	586	GLN
1	A	605	ASN
1	A	655	ASN
1	A	657	HIS
1	A	671	ASN
1	A	731	HIS
1	A	798	ASN
1	A	812	HIS
1	B	74	GLN
1	B	177	ASN
1	B	221	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	235	ASN
1	B	242	ASN
1	B	552	GLN
1	B	605	ASN
1	B	657	HIS
1	B	671	ASN
1	B	731	HIS
1	B	794	ASN
1	B	798	ASN
1	B	930	ASN
1	C	177	ASN
1	C	217	ASN
1	C	242	ASN
1	C	325	HIS
1	C	477	GLN
1	C	552	GLN
1	C	586	GLN
1	C	605	ASN
1	C	657	HIS
1	C	671	ASN
1	C	731	HIS
1	C	798	ASN
1	C	812	HIS
1	C	930	ASN
1	C	934	ASN
1	C	990	GLN
1	D	74	GLN
1	D	177	ASN
1	D	217	ASN
1	D	221	GLN
1	D	242	ASN
1	D	245	GLN
1	D	605	ASN
1	D	655	ASN
1	D	657	HIS
1	D	671	ASN
1	D	679	ASN
1	D	731	HIS
1	D	798	ASN
1	D	930	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
1	CSO	D	336	1	3,6,7	0.58	0	0,6,8	-	-
1	CSO	C	336	1	3,6,7	0.67	0	0,6,8	-	-
1	CSO	B	336	1	3,6,7	0.60	0	0,6,8	-	-
1	CSO	A	336	1	3,6,7	0.66	0	0,6,8	-	-

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
1	CSO	D	336	1	-	0/1/5/7	-
1	CSO	C	336	1	-	0/1/5/7	-
1	CSO	B	336	1	-	0/1/5/7	-
1	CSO	A	336	1	-	0/1/5/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 19 ligands modelled in this entry, 4 are monoatomic - leaving 15 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
3	GOL	C	2040	-	5,5,5	0.38	0	5,5,5	0.61	0
3	GOL	C	2041	-	5,5,5	0.30	0	5,5,5	0.31	0
3	GOL	A	2042	-	5,5,5	0.48	0	5,5,5	0.23	0
3	GOL	C	2039	-	5,5,5	0.41	0	5,5,5	0.48	0
3	GOL	B	2039	-	5,5,5	0.31	0	5,5,5	0.90	0
3	GOL	D	2039	-	5,5,5	0.46	0	5,5,5	0.50	0
2	NOJ	D	1050	-	11,11,11	0.76	0	13,15,15	1.43	1 (7%)
2	NOJ	B	1050	-	11,11,11	0.50	0	13,15,15	1.55	1 (7%)
3	GOL	A	2039	-	5,5,5	0.36	0	5,5,5	0.53	0
3	GOL	A	2043	-	5,5,5	0.31	0	5,5,5	0.30	0
2	NOJ	C	1050	-	11,11,11	0.68	0	13,15,15	1.41	1 (7%)
3	GOL	C	2042	-	5,5,5	0.53	0	5,5,5	0.37	0
3	GOL	A	2040	-	5,5,5	0.30	0	5,5,5	0.29	0
2	NOJ	A	1050	-	11,11,11	0.77	0	13,15,15	1.27	1 (7%)
3	GOL	A	2041	-	5,5,5	0.51	0	5,5,5	0.52	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
3	GOL	C	2040	-	-	0/4/4/4	-
3	GOL	C	2041	-	-	0/4/4/4	-
3	GOL	A	2042	-	-	4/4/4/4	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	C	2039	-	-	2/4/4/4	-
3	GOL	B	2039	-	-	4/4/4/4	-
3	GOL	D	2039	-	-	4/4/4/4	-
2	NOJ	D	1050	-	-	1/2/19/19	0/1/1/1
2	NOJ	B	1050	-	-	0/2/19/19	0/1/1/1
3	GOL	A	2039	-	-	3/4/4/4	-
3	GOL	A	2043	-	-	2/4/4/4	-
2	NOJ	C	1050	-	-	0/2/19/19	0/1/1/1
3	GOL	C	2042	-	-	2/4/4/4	-
3	GOL	A	2040	-	-	0/4/4/4	-
2	NOJ	A	1050	-	-	0/2/19/19	0/1/1/1
3	GOL	A	2041	-	-	4/4/4/4	-

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1050	NOJ	C1-N5-C5	5.20	120.86	109.61
2	C	1050	NOJ	C1-N5-C5	4.57	119.49	109.61
2	D	1050	NOJ	C1-N5-C5	4.45	119.24	109.61
2	A	1050	NOJ	C1-N5-C5	4.06	118.39	109.61

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	2039	GOL	C1-C2-C3-O3
3	A	2039	GOL	O2-C2-C3-O3
3	A	2041	GOL	O1-C1-C2-C3
3	A	2041	GOL	C1-C2-C3-O3
3	A	2042	GOL	O1-C1-C2-O2
3	A	2042	GOL	O1-C1-C2-C3
3	A	2042	GOL	C1-C2-C3-O3
3	A	2043	GOL	C1-C2-C3-O3
3	B	2039	GOL	O1-C1-C2-C3
3	C	2042	GOL	O1-C1-C2-C3
3	D	2039	GOL	O1-C1-C2-C3
3	D	2039	GOL	C1-C2-C3-O3
3	D	2039	GOL	O2-C2-C3-O3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	A	2041	GOL	O2-C2-C3-O3
3	C	2039	GOL	C1-C2-C3-O3
3	A	2041	GOL	O1-C1-C2-O2
3	A	2042	GOL	O2-C2-C3-O3
3	B	2039	GOL	O1-C1-C2-O2
3	C	2039	GOL	O2-C2-C3-O3
3	C	2042	GOL	O1-C1-C2-O2
3	D	2039	GOL	O1-C1-C2-O2
2	D	1050	NOJ	N5-C5-C6-O6
3	A	2043	GOL	O2-C2-C3-O3
3	B	2039	GOL	O2-C2-C3-O3
3	A	2039	GOL	O1-C1-C2-C3
3	B	2039	GOL	C1-C2-C3-O3

There are no ring outliers.

7 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	2040	GOL	1	0
3	C	2039	GOL	2	0
3	A	2039	GOL	1	0
2	C	1050	NOJ	1	0
3	C	2042	GOL	2	0
2	A	1050	NOJ	1	0
3	A	2041	GOL	1	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	1024/1027 (99%)	0.44	18 (1%) 67 72	35, 42, 53, 79	0
1	B	1024/1027 (99%)	0.53	12 (1%) 76 80	36, 47, 63, 79	0
1	C	1024/1027 (99%)	0.25	6 (0%) 85 88	31, 39, 51, 73	0
1	D	1024/1027 (99%)	0.71	24 (2%) 61 66	39, 53, 72, 91	0
All	All	4096/4108 (99%)	0.48	60 (1%) 71 76	31, 44, 64, 91	0

All (60) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	987	ALA	5.7
1	C	987	ALA	4.4
1	A	988	GLY	3.8
1	C	988	GLY	3.7
1	D	174	SER	3.4
1	D	521	ALA	3.2
1	A	529	PRO	3.1
1	A	471	GLN	3.0
1	D	989	SER	2.9
1	A	328	TYR	2.9
1	D	997	ALA	2.8
1	B	891	GLU	2.7
1	D	1014	VAL	2.7
1	D	330	ALA	2.6
1	D	14	THR	2.6
1	D	982	HIS	2.6
1	D	328	TYR	2.6
1	C	328	TYR	2.5
1	A	632	VAL	2.5
1	B	330	ALA	2.4
1	D	332	GLY	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	605	ASN	2.4
1	D	867	VAL	2.4
1	D	1038	THR	2.4
1	D	704	GLU	2.3
1	B	974	GLY	2.3
1	B	14	THR	2.3
1	D	991	ASP	2.3
1	D	173	ALA	2.3
1	B	1036	THR	2.3
1	A	308	GLY	2.3
1	C	471	GLN	2.3
1	A	470	GLY	2.3
1	A	983	VAL	2.2
1	A	994	VAL	2.2
1	B	50	GLY	2.2
1	D	965	GLY	2.2
1	D	529	PRO	2.2
1	D	268	ALA	2.2
1	B	326	PHE	2.2
1	D	981	ILE	2.1
1	D	471	GLN	2.1
1	A	14	THR	2.1
1	C	570	VAL	2.1
1	C	67	ASP	2.1
1	A	989	SER	2.1
1	B	175	SER	2.1
1	D	470	GLY	2.1
1	A	1035	ILE	2.1
1	A	120	LEU	2.1
1	A	976	GLN	2.1
1	A	521	ALA	2.1
1	B	190	GLY	2.0
1	D	176	GLY	2.0
1	A	53	THR	2.0
1	B	621	THR	2.0
1	A	170	VAL	2.0
1	D	986	GLY	2.0
1	B	1037	ILE	2.0
1	D	837	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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(\AA^2)	Q<0.9
1	CSO	A	336	7/8	0.92	0.10	40,40,41,41	0
1	CSO	B	336	7/8	0.92	0.11	45,45,47,47	0
1	CSO	D	336	7/8	0.94	0.09	49,49,51,52	0
1	CSO	C	336	7/8	0.95	0.09	36,36,37,38	0

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

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(\AA^2)	Q<0.9
3	GOL	A	2041	6/6	0.72	0.20	47,49,50,50	0
3	GOL	D	2039	6/6	0.78	0.16	54,57,57,58	0
3	GOL	A	2043	6/6	0.81	0.15	58,59,59,59	0
3	GOL	C	2041	6/6	0.82	0.13	47,47,48,48	0
3	GOL	B	2039	6/6	0.83	0.16	42,48,49,49	0
3	GOL	C	2039	6/6	0.84	0.14	36,37,37,38	0
3	GOL	A	2042	6/6	0.85	0.24	42,44,44,45	0
3	GOL	A	2040	6/6	0.87	0.12	46,47,48,48	0
3	GOL	A	2039	6/6	0.92	0.11	37,38,39,39	0
3	GOL	C	2040	6/6	0.92	0.11	41,41,42,44	0
3	GOL	C	2042	6/6	0.93	0.12	38,39,40,40	0
2	NOJ	C	1050	11/11	0.93	0.18	55,57,57,58	0
2	NOJ	D	1050	11/11	0.94	0.15	55,56,58,58	0
2	NOJ	B	1050	11/11	0.94	0.15	56,57,57,58	0
2	NOJ	A	1050	11/11	0.94	0.18	54,56,57,57	0
4	CL	A	2044	1/1	0.98	0.07	34,34,34,34	0
4	CL	B	2040	1/1	0.98	0.04	41,41,41,41	0
4	CL	C	2043	1/1	0.98	0.05	37,37,37,37	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	CL	D	2040	1/1	0.99	0.04	35,35,35,35	0

6.5 Other polymers [i](#)

There are no such residues in this entry.