



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 11:20 AM UTC

PDB ID : 3SLA / pdb_00003sla
Title : X-ray structure of first four repeats of human beta-catenin
Authors : Gupta, D.; Bienz, M.
Deposited on : 2011-06-24
Resolution : 2.50 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:

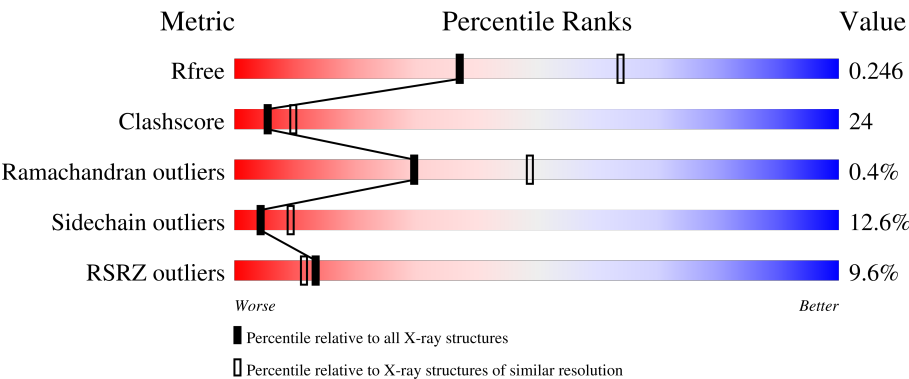
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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 2.50 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}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	168	4% 71% 23% 5% .
1	B	168	2% 66% 24% 7% ..
1	C	168	38% 28% 46% 15% 9% .
1	D	168	% 67% 24% 5% ..
1	E	168	2% 70% 22% . .

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6074 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.

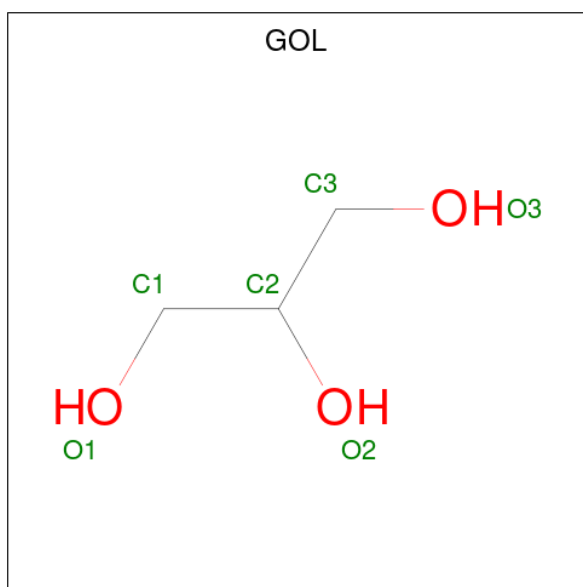
- Molecule 1 is a protein called Catenin beta-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	166	Total	C	N	O	S	0	0	0
			1256	790	226	231	9			
1	B	156	Total	C	N	O	S	0	0	0
			1166	734	213	210	9			
1	C	153	Total	C	N	O	S	0	0	0
			1061	667	193	194	7			
1	D	164	Total	C	N	O	S	0	0	0
			1236	778	221	228	9			
1	E	162	Total	C	N	O	S	0	0	0
			1219	768	222	220	9			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	139	GLY	-	expression tag	UNP P35222
A	140	SER	-	expression tag	UNP P35222
B	139	GLY	-	expression tag	UNP P35222
B	140	SER	-	expression tag	UNP P35222
C	139	GLY	-	expression tag	UNP P35222
C	140	SER	-	expression tag	UNP P35222
D	139	GLY	-	expression tag	UNP P35222
D	140	SER	-	expression tag	UNP P35222
E	139	GLY	-	expression tag	UNP P35222
E	140	SER	-	expression tag	UNP P35222

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

- Molecule 3 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	2	Total	Na	0	0
			2	2		

- Molecule 4 is water.

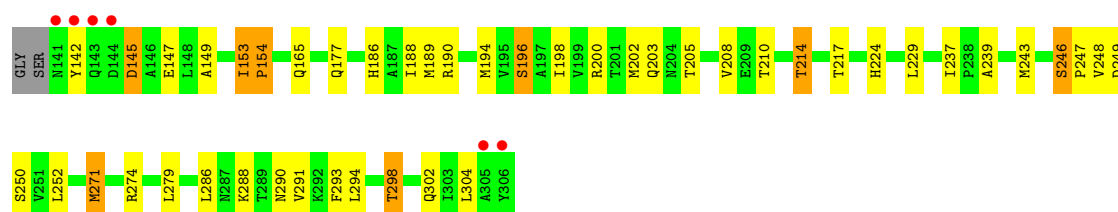
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	18	Total 18	O 18	0	0
4	B	17	Total 17	O 17	0	0
4	C	2	Total 2	O 2	0	0
4	D	21	Total 21	O 21	0	0
4	E	28	Total 28	O 28	0	0

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.

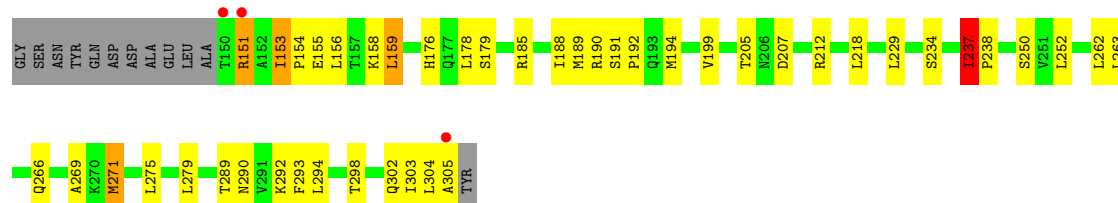
• Molecule 1: Catenin beta-1

Chain A: 

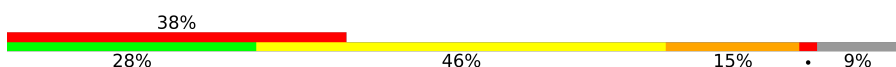


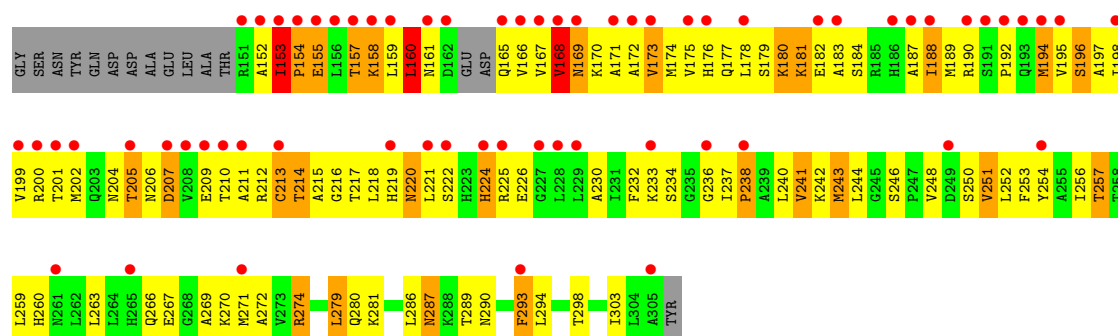
• Molecule 1: Catenin beta-1

Chain B: 



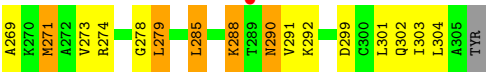
• Molecule 1: Catenin beta-1

Chain C: 

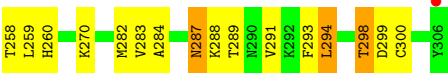


• Molecule 1: Catenin beta-1

Chain D: 



• Molecule 1: Catenin beta-1



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	90.79Å 90.79Å 364.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.71 – 2.50 40.71 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.0 (40.71-2.50) 99.0 (40.71-2.50)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.86 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.218 , 0.277 (Not available) , 0.246	Depositor DCC
R_{free} test set	2719 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	57.4	Xtriage
Anisotropy	0.001	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 46.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6074	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.82% 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

5.1 Standard geometry

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

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	1.23	3/1271 (0.2%)	1.28	5/1720 (0.3%)
1	B	1.14	2/1180 (0.2%)	1.23	3/1600 (0.2%)
1	C	1.34	6/1072 (0.6%)	1.29	6/1456 (0.4%)
1	D	1.18	2/1251 (0.2%)	1.27	7/1695 (0.4%)
1	E	1.23	2/1233 (0.2%)	1.27	6/1668 (0.4%)
All	All	1.22	15/6007 (0.2%)	1.27	27/8139 (0.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	153	ILE	CA-CB	-12.90	1.47	1.54
1	C	154	PRO	N-CD	10.63	1.62	1.47
1	C	207	ASP	CA-CB	9.42	1.68	1.53
1	C	153	ILE	CA-CB	8.16	1.64	1.54
1	C	153	ILE	CA-C	6.11	1.59	1.52
1	E	172	ALA	CA-CB	-5.82	1.44	1.53
1	E	198	ILE	CA-CB	-5.81	1.48	1.54
1	A	153	ILE	CA-CB	5.71	1.56	1.54
1	D	257	THR	CA-CB	5.47	1.62	1.53
1	D	171	ALA	CA-CB	-5.33	1.44	1.53
1	C	241	VAL	CA-CB	-5.21	1.48	1.54
1	C	168	VAL	CA-CB	5.07	1.60	1.54
1	A	229	LEU	N-CA	-5.04	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	199	VAL	CA-CB	-5.04	1.48	1.54
1	A	239	ALA	CA-CB	-5.01	1.45	1.53

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	145	ASP	N-CA-C	8.45	123.20	109.85
1	A	153	ILE	CB-CA-C	-7.16	106.90	113.70
1	D	290	ASN	N-CA-C	6.77	119.61	109.25
1	E	298	THR	N-CA-C	-6.26	104.38	111.07
1	E	186	HIS	N-CA-C	-6.16	104.68	111.82
1	D	246	SER	CA-C-N	6.14	125.76	119.56
1	D	246	SER	C-N-CA	6.14	125.76	119.56
1	D	193	GLN	N-CA-C	-6.13	104.68	111.36
1	B	237	ILE	CB-CA-C	-6.07	107.94	113.70
1	C	160	LEU	N-CA-C	5.99	123.55	110.80
1	A	250	SER	N-CA-C	-5.86	105.80	113.12
1	B	159	LEU	N-CA-C	5.71	117.30	111.14
1	C	286	LEU	CA-C-N	5.65	128.63	120.38
1	C	286	LEU	C-N-CA	5.65	128.63	120.38
1	E	237	ILE	CA-C-N	-5.65	113.85	119.56
1	E	237	ILE	C-N-CA	-5.65	113.85	119.56
1	E	236	GLY	N-CA-C	5.65	120.64	113.24
1	C	161	ASN	N-CA-C	5.59	118.91	111.75
1	B	158	LYS	N-CA-C	-5.54	105.24	111.28
1	A	246	SER	CA-C-N	5.53	125.06	119.19
1	A	246	SER	C-N-CA	5.53	125.06	119.19
1	D	249	ASP	N-CA-C	5.51	118.80	111.75
1	C	153	ILE	N-CA-C	5.33	120.40	108.88
1	D	204	ASN	N-CA-C	5.32	119.32	112.41
1	D	278	GLY	N-CA-C	5.29	119.04	112.64
1	E	182	GLU	N-CA-C	5.17	117.58	111.33
1	C	154	PRO	N-CD-CG	-5.11	95.53	103.20

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	159	LEU	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1256	0	1305	37	0
1	B	1166	0	1214	34	0
1	C	1061	0	1029	161	0
1	D	1236	0	1281	40	0
1	E	1219	0	1282	23	0
2	A	24	0	32	7	0
2	D	12	0	16	2	0
2	E	12	0	16	1	0
3	E	2	0	0	0	0
4	A	18	0	0	1	0
4	B	17	0	0	1	0
4	C	2	0	0	0	0
4	D	21	0	0	3	0
4	E	28	0	0	2	0
All	All	6074	0	6175	289	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 24.

All (289) 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:C:154:PRO:HB2	1:C:157:THR:OG1	1.41	1.19
1:C:197:ALA:O	1:C:201:THR:HG23	1.44	1.18
1:C:160:LEU:CB	1:C:168:VAL:HA	1.73	1.16
1:C:152:ALA:C	1:C:154:PRO:HD3	1.73	1.14
1:C:219:HIS:O	1:C:222:SER:HB3	1.55	1.05
1:C:212:ARG:CG	1:C:254:TYR:HE2	1.72	1.03
1:C:207:ASP:O	1:C:210:THR:HG22	1.63	0.98
1:C:220:ASN:H	1:C:220:ASN:HD22	0.99	0.98
1:C:212:ARG:HG2	1:C:254:TYR:HE2	1.26	0.97
1:C:158:LYS:HE2	1:C:194:MET:HG2	1.46	0.97
1:C:207:ASP:H	1:C:210:THR:HG21	1.28	0.96
1:C:214:THR:O	1:C:218:LEU:HD12	1.66	0.96
1:C:207:ASP:H	1:C:210:THR:CG2	1.78	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:213:CYS:O	1:C:217:THR:HG23	1.69	0.93
1:A:294:LEU:O	1:A:298:THR:HG23	1.69	0.92
1:C:216:GLY:O	1:C:220:ASN:ND2	2.04	0.91
1:C:195:VAL:HG12	1:C:234:SER:CB	2.02	0.89
1:C:212:ARG:HG2	1:C:254:TYR:CE2	2.07	0.89
1:C:201:THR:O	1:C:205:THR:HG22	1.72	0.87
1:C:263:LEU:HB3	1:C:303:ILE:HG21	1.56	0.86
1:C:154:PRO:HB2	1:C:157:THR:HG1	1.36	0.86
1:C:195:VAL:HG21	1:C:230:ALA:HB1	1.58	0.85
1:C:220:ASN:HD22	1:C:220:ASN:N	1.75	0.84
1:A:302:GLN:HE22	1:C:287:ASN:HB2	1.43	0.83
1:C:220:ASN:H	1:C:220:ASN:ND2	1.75	0.83
1:B:153:ILE:HG23	1:B:194:MET:HE2	1.62	0.81
1:C:289:THR:OG1	1:C:293:PHE:HB2	1.80	0.81
1:A:153:ILE:HB	1:A:154:PRO:HD3	1.62	0.80
1:B:263:LEU:HB3	1:B:303:ILE:HG21	1.61	0.80
1:A:246:SER:HB2	2:A:2:GOL:H32	1.64	0.79
1:C:274:ARG:HG3	1:C:274:ARG:HH11	1.46	0.79
1:C:207:ASP:N	1:C:210:THR:CG2	2.45	0.79
1:A:252:LEU:HD11	1:A:293:PHE:CD2	2.18	0.79
1:D:146:ALA:HB2	1:D:183:ALA:HB1	1.65	0.79
1:A:153:ILE:HG23	1:A:194:MET:HE2	1.65	0.79
1:D:253:PHE:O	1:D:257:THR:HG23	1.84	0.77
1:B:237:ILE:HB	1:B:238:PRO:HD3	1.65	0.77
1:C:252:LEU:O	1:C:256:ILE:HG22	1.84	0.77
1:D:288:LYS:HG3	1:D:288:LYS:O	1.83	0.76
1:D:206:ASN:HD21	2:D:3:GOL:H11	1.50	0.75
1:D:288:LYS:HB3	4:D:9:HOH:O	1.85	0.75
1:C:259:LEU:O	1:C:263:LEU:HD13	1.86	0.74
1:C:237:ILE:HB	1:C:238:PRO:HD3	1.69	0.74
1:C:279:LEU:HD23	1:C:279:LEU:C	2.12	0.74
1:C:188:ILE:HG22	1:C:194:MET:HB3	1.68	0.74
1:C:209:GLU:O	1:C:213:CYS:SG	2.45	0.74
1:B:271:MET:SD	1:B:271:MET:N	2.56	0.73
1:C:160:LEU:O	1:C:167:VAL:HG13	1.89	0.73
1:C:246:SER:CB	1:C:251:VAL:HG21	2.18	0.73
1:A:246:SER:HB2	2:A:2:GOL:C3	2.18	0.73
1:C:207:ASP:N	1:C:210:THR:HG22	2.03	0.72
1:C:176:HIS:HA	1:C:217:THR:HG22	1.70	0.72
1:C:214:THR:O	1:C:218:LEU:CD1	2.37	0.72
1:C:212:ARG:CG	1:C:254:TYR:CE2	2.64	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:196:SER:O	1:C:200:ARG:HG2	1.90	0.72
1:C:216:GLY:O	1:C:219:HIS:HB3	1.91	0.70
1:C:270:LYS:HG3	1:C:271:MET:N	2.05	0.70
1:B:289:THR:OG1	1:B:293:PHE:HB2	1.91	0.70
1:C:240:LEU:O	1:C:243:MET:HB2	1.91	0.70
1:A:145:ASP:OD2	1:A:147:GLU:HB3	1.92	0.70
1:C:207:ASP:C	1:C:210:THR:HG22	2.16	0.69
1:C:194:MET:HE2	1:C:197:ALA:HB3	1.74	0.69
1:C:237:ILE:HD12	1:C:272:ALA:CB	2.22	0.69
1:D:212:ARG:HD3	4:D:17:HOH:O	1.92	0.68
1:C:210:THR:HG23	1:C:211:ALA:N	2.08	0.68
1:C:207:ASP:CA	1:C:210:THR:HG22	2.25	0.67
1:D:145:ASP:C	1:D:145:ASP:OD2	2.38	0.66
1:C:195:VAL:HG12	1:C:234:SER:HB3	1.78	0.65
1:C:207:ASP:N	1:C:210:THR:HG21	2.08	0.65
1:C:246:SER:CB	1:C:251:VAL:CG2	2.73	0.65
1:A:252:LEU:HD11	1:A:293:PHE:CE2	2.32	0.65
1:C:237:ILE:HD12	1:C:272:ALA:HB3	1.78	0.65
1:C:177:GLN:HA	1:C:177:GLN:NE2	2.12	0.64
1:C:158:LYS:CD	1:C:158:LYS:O	2.46	0.64
1:C:178:LEU:O	1:C:184:SER:HB3	1.97	0.64
1:E:291:VAL:HA	1:E:294:LEU:HD22	1.80	0.64
1:C:158:LYS:CE	1:C:194:MET:HG2	2.25	0.64
1:C:294:LEU:O	1:C:298:THR:HG23	1.98	0.64
1:C:174:MET:HA	1:C:177:GLN:HG2	1.78	0.63
1:A:302:GLN:NE2	1:C:287:ASN:HB2	2.11	0.63
1:C:202:MET:HA	1:C:205:THR:CG2	2.28	0.63
1:B:179:SER:O	1:B:185:ARG:NH1	2.32	0.63
1:C:274:ARG:HG3	1:C:274:ARG:NH1	2.14	0.62
1:C:202:MET:HE1	1:C:240:LEU:HD23	1.80	0.62
1:C:220:ASN:ND2	1:C:220:ASN:N	2.36	0.62
1:C:184:SER:O	1:C:187:ALA:HB3	1.99	0.62
1:C:253:PHE:O	1:C:257:THR:OG1	2.18	0.62
1:C:153:ILE:C	1:C:153:ILE:HD13	2.25	0.62
1:C:197:ALA:O	1:C:201:THR:CG2	2.35	0.62
1:B:237:ILE:HD11	1:B:262:LEU:HD13	1.80	0.62
1:C:182:GLU:OE1	1:C:224:HIS:HE1	1.83	0.61
1:D:142:TYR:CD2	1:D:144:ASP:OD2	2.54	0.61
1:D:271:MET:HE1	4:E:83:HOH:O	2.00	0.61
1:B:176:HIS:HE1	4:B:56:HOH:O	1.83	0.61
1:A:149:ALA:O	1:A:153:ILE:HG12	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:153:ILE:N	1:C:154:PRO:HD3	2.16	0.61
1:A:274:ARG:HH12	2:A:7:GOL:H12	1.66	0.60
1:C:169:ASN:HD22	1:C:169:ASN:H	1.48	0.60
1:C:212:ARG:HG3	1:C:254:TYR:HE2	1.65	0.60
1:D:182:GLU:CG	1:D:185:ARG:HH21	2.15	0.60
1:C:207:ASP:O	1:C:210:THR:CG2	2.45	0.59
1:C:176:HIS:CA	1:C:217:THR:HG22	2.31	0.59
1:C:152:ALA:C	1:C:154:PRO:CD	2.64	0.59
1:C:153:ILE:O	1:C:153:ILE:CG1	2.51	0.59
1:D:288:LYS:HD2	1:D:290:ASN:O	2.02	0.58
1:C:153:ILE:O	1:C:153:ILE:HG12	2.02	0.58
1:C:166:VAL:O	1:C:169:ASN:ND2	2.36	0.58
1:C:197:ALA:HA	1:C:200:ARG:HH11	1.68	0.58
1:C:177:GLN:HA	1:C:177:GLN:HE21	1.69	0.58
1:C:232:PHE:HD2	1:C:266:GLN:CD	2.12	0.58
1:C:152:ALA:CB	1:C:154:PRO:HD3	2.34	0.57
1:D:274:ARG:NH1	1:D:304:LEU:O	2.30	0.57
1:C:169:ASN:O	1:C:173:VAL:HG13	2.04	0.57
1:A:210:THR:O	1:A:214:THR:HB	2.03	0.57
1:A:271:MET:HB2	2:A:7:GOL:C3	2.35	0.57
1:B:153:ILE:HB	1:B:154:PRO:HD3	1.85	0.57
1:C:241:VAL:O	1:C:242:LYS:C	2.45	0.57
1:C:195:VAL:HG12	1:C:234:SER:HB2	1.87	0.57
1:D:189:MET:HE3	1:D:226:GLU:HB3	1.87	0.56
1:C:195:VAL:CG1	1:C:234:SER:CB	2.82	0.56
1:D:162:ASP:OD1	2:D:5:GOL:H31	2.06	0.56
1:E:284:ALA:O	1:E:288:LYS:HG3	2.05	0.56
1:C:210:THR:CG2	1:C:211:ALA:N	2.69	0.56
1:E:164:ASP:HB3	1:E:167:VAL:HG13	1.88	0.56
1:C:189:MET:CB	1:C:226:GLU:OE2	2.54	0.55
1:C:180:LYS:HG2	1:C:181:LYS:NZ	2.20	0.55
1:C:248:VAL:O	1:C:251:VAL:HG22	2.07	0.55
1:D:252:LEU:HD11	1:D:285:LEU:HD11	1.89	0.55
1:C:240:LEU:O	1:C:243:MET:N	2.39	0.55
1:C:182:GLU:OE1	1:C:224:HIS:CE1	2.60	0.55
1:C:160:LEU:CB	1:C:168:VAL:CA	2.67	0.55
1:C:180:LYS:H	1:C:180:LYS:HD2	1.72	0.55
1:E:253:PHE:O	1:E:257:THR:OG1	2.25	0.55
1:E:221:LEU:O	1:E:227:GLY:HA3	2.07	0.54
1:B:237:ILE:CD1	1:B:262:LEU:HD13	2.37	0.54
1:C:155:GLU:HA	1:C:155:GLU:OE1	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:294:LEU:O	1:B:298:THR:HG23	2.08	0.53
1:C:178:LEU:O	1:C:184:SER:CB	2.56	0.53
1:B:298:THR:OG1	1:E:287:ASN:ND2	2.42	0.53
1:C:232:PHE:CD2	1:C:266:GLN:CD	2.87	0.53
1:C:224:HIS:ND1	1:C:224:HIS:N	2.56	0.53
1:C:237:ILE:HD12	1:C:272:ALA:HB1	1.91	0.53
1:C:241:VAL:C	1:C:243:MET:N	2.67	0.52
1:A:294:LEU:O	1:A:298:THR:CG2	2.49	0.52
1:C:240:LEU:O	1:C:243:MET:CB	2.56	0.52
1:D:142:TYR:HE1	4:D:68:HOH:O	1.93	0.52
1:A:202:MET:HA	1:A:214:THR:HG21	1.92	0.52
1:C:160:LEU:O	1:C:168:VAL:HG22	2.09	0.52
1:B:289:THR:OG1	1:B:293:PHE:CB	2.58	0.52
1:A:203:GLN:HA	1:A:243:MET:HE1	1.92	0.51
1:C:237:ILE:HB	1:C:238:PRO:CD	2.38	0.51
1:D:221:LEU:O	1:D:227:GLY:HA3	2.10	0.51
1:C:266:GLN:HG3	1:C:269:ALA:HB2	1.92	0.51
1:C:181:LYS:H	1:C:181:LYS:HD2	1.75	0.51
1:C:172:ALA:O	1:C:173:VAL:C	2.54	0.50
1:C:152:ALA:CA	1:C:154:PRO:HD3	2.42	0.50
1:C:188:ILE:HG22	1:C:194:MET:CB	2.38	0.50
1:E:260:HIS:HE1	1:E:299:ASP:OD2	1.95	0.50
1:A:286:LEU:HD11	1:A:298:THR:HG22	1.92	0.50
1:A:198:ILE:HD13	1:A:217:THR:HG21	1.93	0.50
1:C:241:VAL:O	1:C:243:MET:N	2.44	0.50
1:C:195:VAL:CG1	1:C:234:SER:HB2	2.42	0.50
1:C:237:ILE:CB	1:C:238:PRO:HD3	2.40	0.50
1:A:186:HIS:HA	1:A:189:MET:HG2	1.92	0.49
1:A:177:GLN:OE1	2:A:4:GOL:H12	2.13	0.49
1:C:190:ARG:O	1:C:192:PRO:HD3	2.12	0.49
1:C:210:THR:O	1:C:214:THR:OG1	2.30	0.49
1:C:152:ALA:HB1	1:C:154:PRO:CD	2.42	0.49
1:C:152:ALA:O	1:C:154:PRO:HD3	2.10	0.48
1:C:152:ALA:HB1	1:C:154:PRO:HD3	1.95	0.48
1:D:143:GLN:O	1:D:143:GLN:HG3	2.11	0.48
1:D:288:LYS:O	1:D:288:LYS:CG	2.58	0.48
1:B:151:ARG:HD2	1:B:151:ARG:N	2.28	0.48
1:A:196:SER:HB2	1:A:200:ARG:NH2	2.28	0.48
1:C:153:ILE:N	1:C:154:PRO:CD	2.76	0.48
1:C:205:THR:C	1:C:206:ASN:OD1	2.56	0.48
1:D:153:ILE:HG23	1:D:194:MET:HE2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:271:MET:HE2	1:A:274:ARG:NH1	2.29	0.47
1:C:174:MET:O	1:C:177:GLN:HB2	2.14	0.47
1:C:181:LYS:HG2	1:C:184:SER:HB2	1.95	0.47
1:D:143:GLN:C	1:D:145:ASP:H	2.21	0.47
1:B:252:LEU:HD23	1:B:293:PHE:CE1	2.49	0.47
1:D:182:GLU:HG3	1:D:185:ARG:HH21	1.79	0.47
1:C:221:LEU:H	1:C:221:LEU:HD12	1.79	0.47
1:C:177:GLN:O	1:C:180:LYS:HD2	2.14	0.47
1:C:181:LYS:O	1:C:184:SER:N	2.47	0.47
1:A:208:VAL:HG13	1:A:248:VAL:HG21	1.97	0.47
1:C:153:ILE:HD13	1:C:153:ILE:O	2.14	0.47
1:D:301:LEU:HA	1:D:301:LEU:HD23	1.55	0.47
1:C:290:ASN:OD1	1:C:290:ASN:C	2.58	0.47
1:D:269:ALA:O	1:D:273:VAL:HG23	2.15	0.47
1:C:218:LEU:HD12	1:C:218:LEU:H	1.80	0.46
1:A:274:ARG:HH12	2:A:7:GOL:C1	2.28	0.46
1:B:237:ILE:CB	1:B:238:PRO:HD3	2.42	0.46
1:C:165:GLN:N	1:C:167:VAL:HG12	2.31	0.46
1:B:302:GLN:HA	1:E:283:VAL:HG11	1.97	0.46
1:C:196:SER:HA	1:C:234:SER:OG	2.16	0.46
1:C:169:ASN:H	1:C:169:ASN:ND2	2.14	0.46
1:C:279:LEU:C	1:C:279:LEU:CD2	2.86	0.46
1:C:195:VAL:HG11	1:C:230:ALA:O	2.16	0.46
1:D:279:LEU:HD12	1:D:304:LEU:HD13	1.98	0.45
1:D:285:LEU:HD23	1:D:285:LEU:HA	1.71	0.45
1:A:290:ASN:OD1	1:A:290:ASN:C	2.60	0.45
1:A:202:MET:HB2	1:A:214:THR:HG23	1.99	0.45
1:B:185:ARG:HD2	1:B:189:MET:CE	2.47	0.45
1:B:190:ARG:O	1:B:192:PRO:HD3	2.16	0.45
1:B:191:SER:O	1:B:194:MET:HB3	2.16	0.45
1:C:294:LEU:HD22	1:E:291:VAL:CG1	2.46	0.45
1:C:152:ALA:CB	1:C:154:PRO:CD	2.95	0.45
1:C:176:HIS:O	1:C:179:SER:OG	2.30	0.45
1:D:149:ALA:O	1:D:153:ILE:HG12	2.17	0.44
1:B:155:GLU:O	1:B:159:LEU:HD12	2.16	0.44
1:C:220:ASN:O	1:C:221:LEU:C	2.60	0.44
1:D:182:GLU:O	1:D:183:ALA:C	2.59	0.44
1:A:202:MET:HG3	1:A:214:THR:CG2	2.48	0.44
1:B:304:LEU:O	1:B:305:ALA:C	2.61	0.44
1:C:216:GLY:O	1:C:217:THR:C	2.61	0.44
1:B:185:ARG:HD2	1:B:189:MET:HE3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:180:LYS:HG2	1:C:181:LYS:HZ2	1.82	0.44
1:B:252:LEU:HD23	1:B:293:PHE:CD1	2.53	0.44
1:D:285:LEU:O	1:D:288:LYS:HG2	2.18	0.44
1:C:169:ASN:O	1:C:173:VAL:CG1	2.65	0.44
1:C:270:LYS:HG3	1:C:271:MET:H	1.83	0.44
1:D:145:ASP:OD2	1:D:146:ALA:N	2.50	0.44
1:D:189:MET:HG3	1:D:221:LEU:HD22	1.98	0.44
1:A:246:SER:HA	1:A:247:PRO:HD2	1.79	0.44
1:C:153:ILE:O	1:C:153:ILE:CD1	2.66	0.44
1:C:251:VAL:CG2	1:C:252:LEU:N	2.81	0.43
1:B:156:LEU:HA	1:B:159:LEU:HD12	2.00	0.43
1:B:266:GLN:O	1:B:269:ALA:HB2	2.18	0.43
1:C:279:LEU:HD23	1:C:280:GLN:N	2.31	0.43
1:D:190:ARG:HG2	1:D:226:GLU:OE2	2.19	0.43
1:E:151:ARG:NH1	4:E:24:HOH:O	2.51	0.43
1:A:224:HIS:HB3	4:A:51:HOH:O	2.18	0.43
1:B:188:ILE:HG23	1:B:194:MET:HG2	2.00	0.43
1:B:237:ILE:CD1	1:B:237:ILE:N	2.82	0.43
1:C:215:ALA:HA	1:C:218:LEU:HD13	2.00	0.43
1:D:182:GLU:HG2	1:D:185:ARG:HH21	1.82	0.43
1:D:246:SER:HA	1:D:247:PRO:HD3	1.81	0.43
1:A:189:MET:HE2	1:A:189:MET:HB3	1.93	0.43
1:D:260:HIS:HE1	1:D:299:ASP:OD2	2.01	0.43
1:C:212:ARG:HG3	1:C:254:TYR:CE2	2.48	0.42
1:C:244:LEU:HB2	1:C:281:LYS:HD2	2.00	0.42
1:D:228:LEU:HD22	1:D:262:LEU:HD23	2.00	0.42
1:E:212:ARG:HG2	1:E:212:ARG:HH11	1.85	0.42
1:C:177:GLN:NE2	1:C:177:GLN:CA	2.78	0.42
1:D:186:HIS:O	1:D:190:ARG:HG3	2.19	0.42
1:E:184:SER:O	1:E:188:ILE:HG13	2.20	0.42
1:A:246:SER:HB2	2:A:2:GOL:H31	2.01	0.42
1:D:143:GLN:C	1:D:145:ASP:N	2.77	0.42
1:C:199:VAL:CG1	1:C:236:GLY:HA2	2.50	0.42
1:E:282:MET:SD	1:E:300:CYS:HB3	2.59	0.42
1:A:186:HIS:O	1:A:190:ARG:HG3	2.20	0.42
1:E:287:ASN:HD22	1:E:287:ASN:HA	1.66	0.42
1:C:218:LEU:HA	1:C:221:LEU:HD13	2.02	0.42
1:E:233:LYS:HE3	2:E:8:GOL:O3	2.20	0.42
1:D:142:TYR:CG	1:D:144:ASP:OD2	2.73	0.41
1:C:158:LYS:O	1:C:158:LYS:HD2	2.18	0.41
1:E:200:ARG:HE	1:E:200:ARG:HB2	1.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:188:ILE:HG23	1:A:194:MET:HG2	2.01	0.41
1:E:252:LEU:HD21	1:E:289:THR:HG21	2.01	0.41
1:C:293:PHE:N	1:C:293:PHE:CD1	2.89	0.41
1:E:252:LEU:HD23	1:E:293:PHE:CD2	2.55	0.41
1:E:259:LEU:HA	1:E:259:LEU:HD23	1.75	0.41
1:C:158:LYS:O	1:C:158:LYS:HD3	2.21	0.41
1:C:171:ALA:O	1:C:175:VAL:N	2.46	0.41
1:C:257:THR:O	1:C:260:HIS:HB3	2.21	0.41
1:E:169:ASN:O	1:E:173:VAL:HG23	2.21	0.41
1:C:220:ASN:C	1:C:222:SER:N	2.77	0.41
1:B:205:THR:HG1	1:B:207:ASP:H	1.69	0.41
1:B:237:ILE:HD13	1:B:237:ILE:H	1.84	0.41
1:C:205:THR:OG1	1:C:210:THR:HG21	2.21	0.41
1:D:303:ILE:O	1:D:303:ILE:HG22	2.21	0.41
1:E:294:LEU:HD12	1:E:294:LEU:HA	1.92	0.41
1:A:203:GLN:HA	1:A:243:MET:CE	2.51	0.41
1:C:198:ILE:HA	1:C:201:THR:OG1	2.21	0.41
1:B:290:ASN:OD1	1:B:290:ASN:C	2.64	0.40
1:C:180:LYS:HE2	1:C:180:LYS:HB3	1.95	0.40
1:A:304:LEU:HA	1:A:304:LEU:HD23	1.72	0.40
1:C:237:ILE:CD1	1:C:272:ALA:HB3	2.50	0.40
1:C:246:SER:CB	1:C:251:VAL:HG23	2.51	0.40
1:B:237:ILE:N	1:B:237:ILE:HD13	2.36	0.40
1:C:181:LYS:O	1:C:183:ALA:N	2.54	0.40
1:C:199:VAL:HG13	1:C:236:GLY:HA2	2.04	0.40
1:E:219:HIS:HA	1:E:258:THR:OG1	2.21	0.40
1:A:291:VAL:CG2	1:E:294:LEU:HB3	2.51	0.40
1:B:178:LEU:HD23	1:B:178:LEU:HA	1.82	0.40
1:B:212:ARG:HG3	1:B:250:SER:OG	2.21	0.40
1:C:270:LYS:CG	1:C:271:MET:N	2.81	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	150/168 (89%)	147 (98%)	3 (2%)	0	100	100
1	B	154/168 (92%)	150 (97%)	4 (3%)	0	100	100
1	C	149/168 (89%)	126 (85%)	20 (13%)	3 (2%)	6	10
1	D	162/168 (96%)	161 (99%)	1 (1%)	0	100	100
1	E	160/168 (95%)	158 (99%)	2 (1%)	0	100	100
All	All	775/840 (92%)	742 (96%)	30 (4%)	3 (0%)	30	49

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	153	ILE
1	C	160	LEU
1	C	225	ARG

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	136/140 (97%)	124 (91%)	12 (9%)	9	20
1	B	126/140 (90%)	117 (93%)	9 (7%)	13	29
1	C	99/140 (71%)	69 (70%)	30 (30%)	0	0
1	D	134/140 (96%)	120 (90%)	14 (10%)	7	14
1	E	132/140 (94%)	118 (89%)	14 (11%)	6	14
All	All	627/700 (90%)	548 (87%)	79 (13%)	4	9

All (79) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	142	TYR
1	A	154	PRO

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Mol	Chain	Res	Type
1	A	165	GLN
1	A	196	SER
1	A	205	THR
1	A	214	THR
1	A	237	ILE
1	A	249	ASP
1	A	271	MET
1	A	279	LEU
1	A	288	LYS
1	A	298	THR
1	B	151	ARG
1	B	218	LEU
1	B	229	LEU
1	B	234	SER
1	B	237	ILE
1	B	271	MET
1	B	275	LEU
1	B	279	LEU
1	B	292	LYS
1	C	153	ILE
1	C	155	GLU
1	C	157	THR
1	C	158	LYS
1	C	168	VAL
1	C	169	ASN
1	C	170	LYS
1	C	173	VAL
1	C	180	LYS
1	C	181	LYS
1	C	188	ILE
1	C	194	MET
1	C	196	SER
1	C	204	ASN
1	C	205	THR
1	C	213	CYS
1	C	214	THR
1	C	220	ASN
1	C	224	HIS
1	C	233	LYS
1	C	238	PRO
1	C	243	MET
1	C	250	SER

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Mol	Chain	Res	Type
1	C	251	VAL
1	C	257	THR
1	C	267	GLU
1	C	274	ARG
1	C	279	LEU
1	C	287	ASN
1	C	293	PHE
1	D	143	GLN
1	D	144	ASP
1	D	145	ASP
1	D	148	LEU
1	D	179	SER
1	D	237	ILE
1	D	246	SER
1	D	271	MET
1	D	279	LEU
1	D	285	LEU
1	D	288	LYS
1	D	291	VAL
1	D	292	LYS
1	D	302	GLN
1	E	148	LEU
1	E	156	LEU
1	E	166	VAL
1	E	167	VAL
1	E	177	GLN
1	E	196	SER
1	E	200	ARG
1	E	237	ILE
1	E	249	ASP
1	E	257	THR
1	E	270	LYS
1	E	287	ASN
1	E	294	LEU
1	E	298	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	169	ASN
1	A	186	HIS
1	A	287	ASN

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Mol	Chain	Res	Type
1	A	302	GLN
1	B	161	ASN
1	B	165	GLN
1	B	224	HIS
1	B	265	HIS
1	C	177	GLN
1	C	220	ASN
1	C	223	HIS
1	C	224	HIS
1	C	265	HIS
1	C	287	ASN
1	C	302	GLN
1	D	206	ASN
1	D	265	HIS
1	D	287	ASN
1	E	204	ASN
1	E	260	HIS
1	E	265	HIS
1	E	280	GLN
1	E	287	ASN
1	E	290	ASN
1	E	302	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 2 are monoatomic - leaving 8 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	$\# Z > 2$
2	GOL	E	6	-	5,5,5	0.37	0	5,5,5	0.47	0
2	GOL	A	2	-	5,5,5	0.52	0	5,5,5	0.86	0
2	GOL	D	5	-	5,5,5	0.33	0	5,5,5	0.65	0
2	GOL	A	7	-	5,5,5	0.50	0	5,5,5	1.20	1 (20%)
2	GOL	D	3	-	5,5,5	0.38	0	5,5,5	0.40	0
2	GOL	A	4	-	5,5,5	0.55	0	5,5,5	0.72	0
2	GOL	A	1	-	5,5,5	0.56	0	5,5,5	0.55	0
2	GOL	E	8	-	5,5,5	0.70	0	5,5,5	0.80	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	E	6	-	-	2/4/4/4	-
2	GOL	A	2	-	-	1/4/4/4	-
2	GOL	D	5	-	-	3/4/4/4	-
2	GOL	A	7	-	-	2/4/4/4	-
2	GOL	D	3	-	-	3/4/4/4	-
2	GOL	A	4	-	-	3/4/4/4	-
2	GOL	A	1	-	-	2/4/4/4	-
2	GOL	E	8	-	-	2/4/4/4	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	7	GOL	O3-C3-C2	2.18	120.20	110.38

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	4	GOL	O1-C1-C2-C3
2	A	7	GOL	C1-C2-C3-O3
2	D	5	GOL	O1-C1-C2-C3
2	E	6	GOL	C1-C2-C3-O3
2	E	6	GOL	O2-C2-C3-O3
2	E	8	GOL	O2-C2-C3-O3
2	A	4	GOL	C1-C2-C3-O3
2	D	3	GOL	O1-C1-C2-C3
2	D	3	GOL	C1-C2-C3-O3
2	E	8	GOL	C1-C2-C3-O3
2	A	4	GOL	O1-C1-C2-O2
2	A	7	GOL	O2-C2-C3-O3
2	D	5	GOL	O1-C1-C2-O2
2	A	1	GOL	O2-C2-C3-O3
2	A	2	GOL	O1-C1-C2-O2
2	A	1	GOL	C1-C2-C3-O3
2	D	5	GOL	O2-C2-C3-O3
2	D	3	GOL	O1-C1-C2-O2

There are no ring outliers.

6 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2	GOL	3	0
2	D	5	GOL	1	0
2	A	7	GOL	3	0
2	D	3	GOL	1	0
2	A	4	GOL	1	0
2	E	8	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	166/168 (98%)	-0.22	6 (3%) 46 41	33, 48, 77, 122	0
1	B	156/168 (92%)	-0.10	3 (1%) 66 62	39, 57, 83, 95	0
1	C	153/168 (91%)	1.86	63 (41%) 0 0	40, 95, 127, 137	0
1	D	164/168 (97%)	-0.28	2 (1%) 76 73	34, 50, 85, 121	0
1	E	162/168 (96%)	-0.42	3 (1%) 66 62	32, 44, 74, 107	0
All	All	801/840 (95%)	0.15	77 (9%) 13 11	32, 54, 111, 137	0

All (77) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	152	ALA	6.6
1	C	153	ILE	6.2
1	E	145	ASP	6.1
1	A	141	ASN	5.9
1	C	166	VAL	5.8
1	A	143	GLN	5.8
1	C	162	ASP	5.6
1	A	306	TYR	5.5
1	C	165	GLN	5.2
1	C	168	VAL	5.2
1	C	157	THR	5.1
1	A	142	TYR	5.0
1	C	151	ARG	5.0
1	C	167	VAL	4.8
1	C	161	ASN	4.7
1	C	249	ASP	4.5
1	C	156	LEU	4.1
1	C	208	VAL	3.9
1	C	305	ALA	3.8
1	C	173	VAL	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	305	ALA	3.6
1	C	207	ASP	3.6
1	D	289	THR	3.5
1	C	186	HIS	3.5
1	C	228	LEU	3.4
1	C	183	ALA	3.4
1	C	236	GLY	3.2
1	C	171	ALA	3.2
1	C	154	PRO	3.1
1	C	159	LEU	3.1
1	C	193	GLN	3.1
1	A	305	ALA	3.1
1	C	211	ALA	3.1
1	B	151	ARG	3.1
1	C	175	VAL	3.1
1	C	225	ARG	3.0
1	C	155	GLU	2.9
1	C	224	HIS	2.9
1	E	306	TYR	2.9
1	C	192	PRO	2.9
1	C	238	PRO	2.9
1	C	254	TYR	2.9
1	D	142	TYR	2.9
1	C	221	LEU	2.8
1	C	222	SER	2.8
1	C	209	GLU	2.8
1	C	198	ILE	2.8
1	C	169	ASN	2.8
1	C	200	ARG	2.6
1	C	182	GLU	2.6
1	C	293	PHE	2.5
1	C	195	VAL	2.5
1	C	158	LYS	2.5
1	C	219	HIS	2.5
1	C	202	MET	2.5
1	C	213	CYS	2.5
1	C	229	LEU	2.5
1	E	146	ALA	2.5
1	C	205	THR	2.4
1	C	190	ARG	2.4
1	C	265	HIS	2.4
1	C	187	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	172	ALA	2.4
1	C	201	THR	2.3
1	C	176	HIS	2.3
1	C	188	ILE	2.3
1	C	271	MET	2.3
1	C	233	LYS	2.3
1	C	194	MET	2.2
1	A	144	ASP	2.2
1	C	178	LEU	2.1
1	C	210	THR	2.1
1	C	191	SER	2.1
1	C	227	GLY	2.1
1	C	261	ASN	2.0
1	B	150	THR	2.0
1	C	199	VAL	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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(Å ²)	Q<0.9
2	GOL	D	3	6/6	0.82	0.17	93,103,107,108	0
2	GOL	A	1	6/6	0.83	0.20	72,74,76,81	0
2	GOL	A	7	6/6	0.84	0.23	69,77,80,98	0
2	GOL	A	2	6/6	0.86	0.20	74,87,90,90	0
2	GOL	D	5	6/6	0.88	0.19	77,83,88,89	0
2	GOL	E	6	6/6	0.90	0.16	85,92,98,103	0
2	GOL	E	8	6/6	0.91	0.18	62,69,72,73	0
3	NA	E	2	1/1	0.91	0.18	68,68,68,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	GOL	A	4	6/6	0.92	0.15	67,72,77,79	0
3	NA	E	1	1/1	0.95	0.15	54,54,54,54	0

6.5 Other polymers [i](#)

There are no such residues in this entry.