



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:54 PM UTC

PDB ID : 1L0X / pdb_0000110x
Title : TCR beta chain complexed with streptococcal superantigen SpeA
Authors : Li, H.; Sundberg, E.J.; Mariuzza, R.A.
Deposited on : 2002-02-14
Resolution : 2.80 Å(reported)

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

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

A user guide is available at

<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

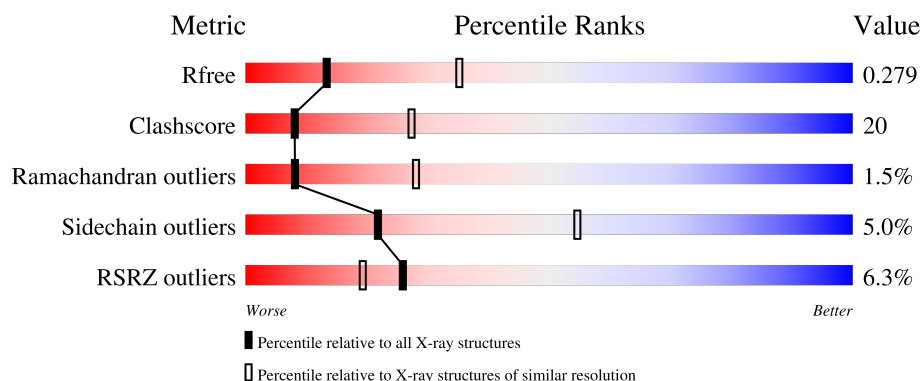
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	238	10% 66% 29% ..
1	C	238	7% 67% 31% ..
2	B	221	5% 59% 37% .
2	D	221	4% 61% 34% 5%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7323 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 14.3.d T cell receptor beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	236	Total	C	N	O	S	0	0	0
			1786	1120	321	339	6			
1	C	236	Total	C	N	O	S	0	0	0
			1782	1117	321	338	6			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	24	GLN	ASN	engineered mutation	UNP P01851
A	74	GLN	ASN	engineered mutation	UNP P01851
A	?	-	GLN	SEE REMARK 999	UNP P01851
A	99	GLY	-	SEE REMARK 999	UNP P01851
A	100	SER	-	SEE REMARK 999	UNP P01851
A	101	TYR	-	SEE REMARK 999	UNP P01851
A	121	GLN	ASN	engineered mutation	UNP P01851
C	24	GLN	ASN	engineered mutation	UNP P01851
C	74	GLN	ASN	engineered mutation	UNP P01851
C	?	-	GLN	SEE REMARK 999	UNP P01851
C	99	GLY	-	SEE REMARK 999	UNP P01851
C	100	SER	-	SEE REMARK 999	UNP P01851
C	101	TYR	-	SEE REMARK 999	UNP P01851
C	121	GLN	ASN	engineered mutation	UNP P01851

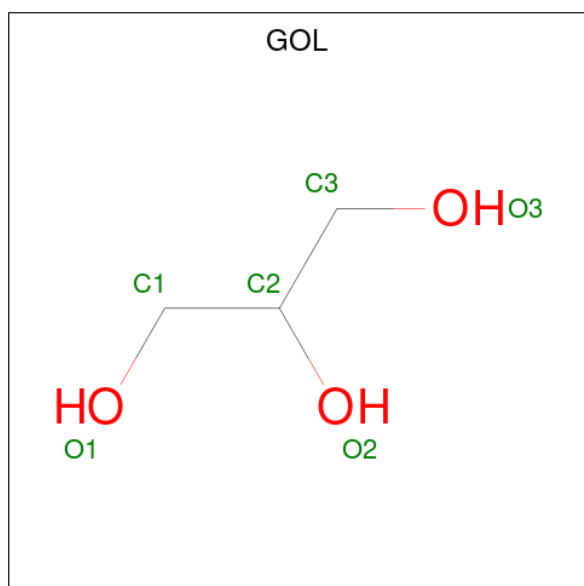
- Molecule 2 is a protein called Exotoxin type A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	221	Total	C	N	O	S	0	0	0
			1765	1126	285	349	5			
2	D	221	Total	C	N	O	S	0	0	0
			1791	1144	289	353	5			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	90	SER	CYS	engineered mutation	UNP P08095
D	90	SER	CYS	engineered mutation	UNP P08095

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

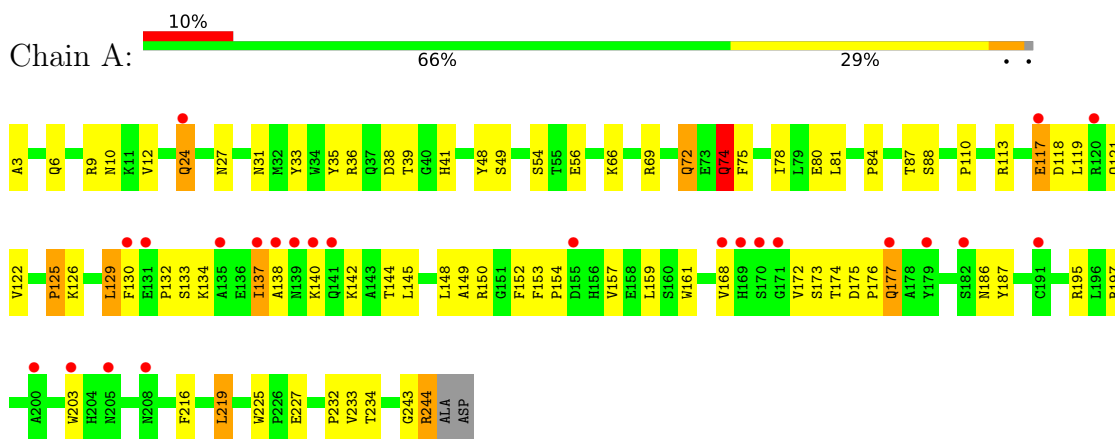
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	53	Total	O	0	0
			53	53		
4	B	32	Total	O	0	0
			32	32		
4	C	42	Total	O	0	0
			42	42		
4	D	54	Total	O	0	0
			54	54		

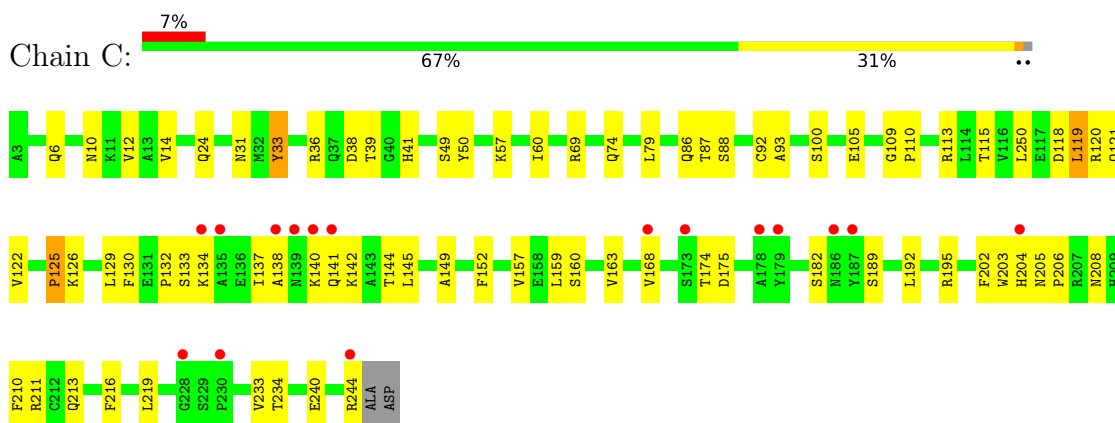
3 Residue-property plots

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.

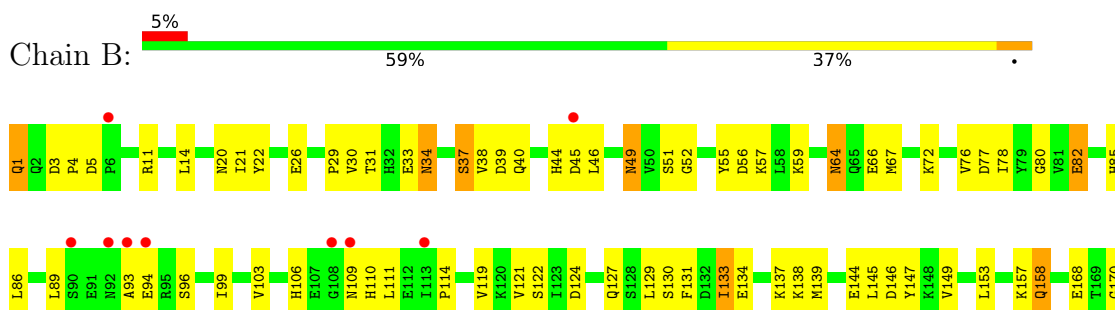
• Molecule 1: 14.3.d T cell receptor beta chain

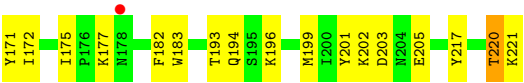


• Molecule 1: 14.3.d T cell receptor beta chain

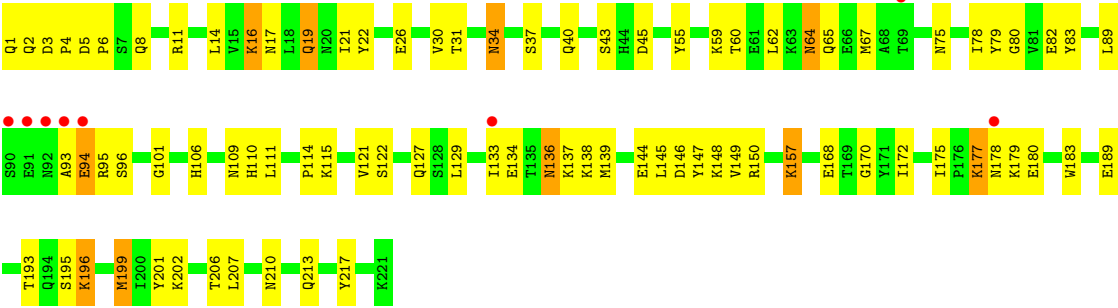


• Molecule 2: Exotoxin type A





● Molecule 2: Exotoxin type A



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	71.40Å 83.25Å 93.58Å 90.00° 91.63° 90.00°	Depositor
Resolution (Å)	40.78 – 2.80 40.78 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.0 (40.78-2.80) 99.0 (40.78-2.80)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.23 (at 2.48Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.232 , 0.278 0.233 , 0.279	Depositor DCC
R_{free} test set	1874 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	44.8	Xtriage
Anisotropy	0.302	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 46.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.020 for h,-k,-l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	7323	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.18% 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: 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	0.46	0/1837	0.89	1/2500 (0.0%)
1	C	0.46	0/1834	0.91	2/2496 (0.1%)
2	B	0.43	0/1806	0.92	2/2446 (0.1%)
2	D	0.46	0/1832	0.91	1/2478 (0.0%)
All	All	0.45	0/7309	0.91	6/9920 (0.1%)

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	A	0	1
2	D	0	1
All	All	0	2

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	21	ILE	N-CA-C	-9.54	103.61	111.81
2	D	21	ILE	N-CA-C	-7.40	105.44	111.81
1	C	119	LEU	N-CA-C	5.72	120.00	113.19
1	A	74	GLN	N-CA-C	5.57	118.56	109.59
2	B	202	LYS	N-CA-C	5.29	117.12	111.36
1	C	109	GLY	N-CA-C	-5.08	106.08	112.23

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	35	TYR	Sidechain
2	D	147	TYR	Sidechain

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	1786	0	1639	62	0
1	C	1782	0	1636	66	0
2	B	1765	0	1675	82	0
2	D	1791	0	1730	64	0
3	B	6	0	8	3	0
3	D	12	0	16	1	0
4	A	53	0	0	4	0
4	B	32	0	0	0	0
4	C	42	0	0	2	0
4	D	54	0	0	3	0
All	All	7323	0	6704	270	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 20.

All (270) 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:A:41:HIS:HB3	4:A:297:HOH:O	1.61	0.99
2:B:109:ASN:HD21	2:B:139:MET:H	1.09	0.97
2:D:17:ASN:HA	2:D:19:GLN:NE2	1.85	0.91
2:D:109:ASN:HD21	2:D:139:MET:H	1.14	0.89
2:D:59:LYS:HB2	2:D:89:LEU:HD13	1.56	0.88
2:B:59:LYS:HB2	2:B:89:LEU:CD1	2.04	0.87
2:B:193:THR:HA	3:B:301:GOL:H2	1.57	0.83
2:D:64:ASN:ND2	2:D:67:MET:H	1.80	0.79
2:B:1:GLN:HB3	2:B:182:PHE:HA	1.66	0.78
1:C:195:ARG:HD2	1:C:195:ARG:N	2.00	0.77
1:A:125:PRO:HB3	1:A:152:PHE:HB3	1.65	0.77
2:B:171:TYR:CE2	2:B:217:TYR:HB2	2.22	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:125:PRO:HB3	1:C:152:PHE:HB3	1.68	0.73
2:B:129:LEU:HD22	2:B:157:LYS:HE2	1.72	0.72
2:D:59:LYS:HB2	2:D:89:LEU:CD1	2.19	0.71
2:B:124:ASP:OD2	2:B:220:THR:HG23	1.91	0.71
2:B:168:GLU:HG2	2:B:221:LYS:HG2	1.73	0.70
2:B:109:ASN:HD21	2:B:139:MET:N	1.88	0.70
2:B:59:LYS:HB2	2:B:89:LEU:HD12	1.71	0.70
1:C:129:LEU:HD23	1:C:130:PHE:N	2.07	0.70
2:D:177:LYS:HD2	2:D:178:ASN:ND2	2.07	0.70
1:C:118:ASP:OD2	1:C:120:ARG:HG3	1.92	0.69
1:A:117:GLU:HG2	1:A:118:ASP:N	2.06	0.69
1:C:163:VAL:HG22	1:C:168:VAL:HG21	1.74	0.68
2:B:122:SER:HA	2:B:127:GLN:HA	1.75	0.67
2:D:4:PRO:HB3	2:D:183:TRP:CZ2	2.30	0.67
2:D:115:LYS:HE2	2:D:210:ASN:HA	1.76	0.67
1:A:6:GLN:HG3	1:A:110:PRO:HD2	1.74	0.67
2:B:34:ASN:HD22	2:B:106:HIS:CD2	2.12	0.67
1:A:66:LYS:NZ	1:A:80:GLU:HG3	2.08	0.67
2:B:89:LEU:HD22	2:B:96:SER:HB3	1.77	0.66
1:C:163:VAL:HG22	1:C:168:VAL:CG2	2.24	0.66
2:B:45:ASP:O	2:B:46:LEU:HD23	1.95	0.66
1:A:233:VAL:HG22	1:A:234:THR:N	2.11	0.65
1:A:134:LYS:CA	1:A:137:ILE:HG12	2.27	0.65
2:B:146:ASP:OD2	2:B:201:TYR:OH	2.15	0.64
1:A:219:LEU:HD22	1:A:232:PRO:HG2	1.79	0.64
2:B:109:ASN:ND2	2:B:138:LYS:HB2	2.13	0.64
2:D:17:ASN:HA	2:D:19:GLN:HE22	1.58	0.64
2:D:64:ASN:C	2:D:64:ASN:HD22	2.05	0.63
1:A:137:ILE:HG13	1:A:137:ILE:O	1.99	0.63
1:A:142:LYS:HD3	1:A:197:ARG:HD3	1.81	0.63
1:A:233:VAL:HG22	1:A:234:THR:H	1.64	0.62
2:D:5:ASP:HB3	2:D:8:GLN:HG3	1.82	0.62
2:D:122:SER:HA	2:D:127:GLN:HA	1.81	0.62
2:B:34:ASN:HD22	2:B:106:HIS:HD2	1.47	0.62
2:B:11:ARG:HB2	2:B:14:LEU:HD13	1.83	0.61
1:A:122:VAL:HG11	1:A:219:LEU:HD13	1.81	0.61
1:C:79:LEU:HD23	1:C:86:GLN:OE1	2.01	0.61
2:D:17:ASN:CA	2:D:19:GLN:NE2	2.62	0.60
1:A:157:VAL:HG12	1:A:216:PHE:HA	1.81	0.60
1:A:66:LYS:HZ1	1:A:80:GLU:HG3	1.64	0.60
1:A:133:SER:O	1:A:137:ILE:HG23	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:179:LYS:NZ	4:D:345:HOH:O	2.34	0.59
2:D:109:ASN:HD21	2:D:139:MET:N	1.94	0.59
1:C:233:VAL:HG22	1:C:234:THR:H	1.67	0.59
2:D:1:GLN:N	2:D:180:GLU:OE1	2.35	0.59
2:B:145:LEU:O	2:B:149:VAL:HG23	2.02	0.59
2:B:109:ASN:HA	2:B:138:LYS:HD2	1.84	0.58
1:C:122:VAL:HG11	1:C:219:LEU:HD13	1.84	0.58
1:C:182:SER:OG	1:C:189:SER:HB3	2.02	0.58
1:C:233:VAL:HG22	1:C:234:THR:N	2.19	0.58
1:C:31:ASN:HD22	1:C:50:TYR:HA	1.69	0.58
2:B:30:VAL:HG12	2:B:80:GLY:O	2.03	0.58
2:B:168:GLU:HG2	2:B:221:LYS:CG	2.34	0.58
2:B:33:GLU:OE1	2:B:110:HIS:CE1	2.57	0.57
1:C:6:GLN:HG3	1:C:110:PRO:HD2	1.86	0.57
2:B:137:LYS:NZ	2:B:144:GLU:OE1	2.38	0.56
1:C:144:THR:HG22	4:C:287:HOH:O	2.03	0.56
1:C:211:ARG:HB2	1:C:240:GLU:HG2	1.87	0.56
2:D:30:VAL:HG12	2:D:80:GLY:O	2.05	0.56
1:C:205:ASN:HB3	1:C:208:ASN:ND2	2.21	0.56
2:B:51:SER:OG	2:B:56:ASP:HA	2.06	0.56
2:B:114:PRO:HB2	2:B:134:GLU:CG	2.35	0.56
2:B:89:LEU:HD22	2:B:96:SER:CB	2.34	0.56
1:A:36:ARG:NH2	1:A:88:SER:HB2	2.22	0.55
1:A:125:PRO:CB	1:A:152:PHE:HB3	2.36	0.55
1:C:205:ASN:HD22	1:C:208:ASN:ND2	2.05	0.55
2:B:146:ASP:OD1	2:B:172:ILE:HG21	2.07	0.54
2:B:44:HIS:CG	1:C:141:GLN:NE2	2.75	0.54
1:C:250:LEU:HD11	1:C:119:LEU:HD23	1.90	0.54
2:B:4:PRO:HB3	2:B:183:TRP:CZ2	2.42	0.54
1:C:41:HIS:N	1:C:41:HIS:CD2	2.72	0.54
2:B:85:HIS:CE1	2:B:86:LEU:HG	2.43	0.54
1:A:176:PRO:O	1:A:177:GLN:HG3	2.09	0.53
1:C:10:ASN:OD1	1:C:113:ARG:NH1	2.42	0.53
1:C:126:LYS:O	1:C:149:ALA:HA	2.09	0.53
2:D:43:SER:HB2	2:D:65:GLN:HG3	1.91	0.53
2:B:22:TYR:CZ	2:B:26:GLU:HG3	2.44	0.53
1:C:33:TYR:CD1	1:C:33:TYR:N	2.77	0.52
2:B:66:GLU:CD	2:B:66:GLU:H	2.16	0.52
1:C:125:PRO:CB	1:C:152:PHE:HB3	2.36	0.52
2:B:109:ASN:HD22	2:B:138:LYS:HB2	1.74	0.52
2:D:136:ASN:H	2:D:136:ASN:ND2	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:12:VAL:HG21	1:A:219:LEU:CD1	2.39	0.52
2:D:121:VAL:HB	2:D:129:LEU:HB3	1.91	0.52
1:C:92:CYS:SG	1:C:93:ALA:N	2.82	0.52
2:B:64:ASN:ND2	2:B:66:GLU:HB2	2.24	0.52
2:B:119:VAL:HG21	2:B:133:ILE:HD13	1.92	0.52
1:C:129:LEU:HD21	1:C:145:LEU:HD22	1.92	0.52
1:C:250:LEU:HD13	1:C:118:ASP:O	2.10	0.52
1:C:202:PHE:O	1:C:208:ASN:ND2	2.43	0.51
1:C:125:PRO:HB3	1:C:152:PHE:CD2	2.45	0.51
2:B:30:VAL:HG23	2:B:55:TYR:OH	2.10	0.51
1:A:129:LEU:HD23	1:A:130:PHE:H	1.76	0.51
2:B:196:LYS:HA	2:B:199:MET:HE2	1.93	0.51
2:D:175:ILE:HB	2:D:213:GLN:HB2	1.92	0.51
2:D:64:ASN:HD22	2:D:67:MET:H	1.58	0.51
2:D:111:LEU:HD12	2:D:136:ASN:HA	1.92	0.51
2:B:170:GLY:HA2	2:B:217:TYR:O	2.12	0.50
2:D:22:TYR:CZ	2:D:26:GLU:HG3	2.46	0.50
1:C:57:LYS:HE2	2:D:16:LYS:O	2.11	0.50
1:A:69:ARG:HD2	1:A:74:GLN:O	2.11	0.50
2:D:64:ASN:HD21	2:D:67:MET:H	1.56	0.50
2:D:30:VAL:HG23	2:D:55:TYR:OH	2.11	0.50
2:D:196:LYS:O	2:D:199:MET:HG3	2.12	0.50
1:A:153:PHE:CD1	1:A:154:PRO:HA	2.46	0.50
1:A:161:TRP:CD1	1:A:172:VAL:HG13	2.47	0.50
1:A:78:ILE:N	1:A:78:ILE:HD12	2.27	0.50
1:C:60:ILE:O	1:C:60:ILE:HG13	2.12	0.50
2:B:33:GLU:OE1	2:B:106:HIS:CE1	2.65	0.49
2:D:4:PRO:HB3	2:D:183:TRP:CH2	2.47	0.49
2:B:52:GLY:HA3	2:B:55:TYR:CE2	2.47	0.49
2:D:11:ARG:HB3	2:D:168:GLU:OE1	2.12	0.49
2:B:11:ARG:CB	2:B:14:LEU:HD13	2.43	0.49
2:D:144:GLU:O	2:D:148:LYS:HG3	2.12	0.49
1:A:41:HIS:N	1:A:41:HIS:CD2	2.79	0.49
2:D:136:ASN:HD22	2:D:136:ASN:C	2.19	0.49
2:B:82:GLU:HA	2:B:99:ILE:HG22	1.95	0.49
2:D:60:THR:HG23	2:D:60:THR:O	2.13	0.49
2:D:202:LYS:HD3	4:D:331:HOH:O	2.11	0.49
1:A:12:VAL:HG23	1:A:12:VAL:O	2.13	0.49
2:D:170:GLY:HA2	2:D:217:TYR:O	2.13	0.49
2:B:37:SER:HB3	2:B:72:LYS:O	2.13	0.48
2:D:193:THR:HB	3:D:302:GOL:H2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:85:HIS:O	2:B:86:LEU:HB2	2.13	0.48
2:D:5:ASP:CG	2:D:6:PRO:HD2	2.38	0.48
1:A:10:ASN:OD1	1:A:113:ARG:NH1	2.46	0.48
2:B:76:VAL:HB	2:B:103:VAL:HG13	1.94	0.48
1:C:204:HIS:O	1:C:206:PRO:HD3	2.13	0.48
1:C:175:ASP:OD1	1:C:195:ARG:NH1	2.44	0.48
2:D:109:ASN:ND2	2:D:139:MET:H	1.96	0.48
1:A:144:THR:HG23	1:A:144:THR:O	2.12	0.48
1:A:140:LYS:C	1:A:142:LYS:H	2.21	0.48
1:C:159:LEU:C	1:C:159:LEU:HD23	2.38	0.48
2:B:129:LEU:HD12	2:B:130:SER:H	1.78	0.48
1:A:126:LYS:O	1:A:149:ALA:HA	2.14	0.48
1:A:3:ALA:N	1:A:27:ASN:OD1	2.47	0.47
2:B:1:GLN:HB2	2:B:182:PHE:HB3	1.96	0.47
2:B:34:ASN:HB2	2:B:106:HIS:CD2	2.50	0.47
1:C:12:VAL:HG11	1:C:219:LEU:HD12	1.96	0.47
2:B:194:GLN:HG3	3:B:301:GOL:H12	1.96	0.47
2:D:34:ASN:OD1	2:D:75:ASN:HB3	2.15	0.47
2:D:106:HIS:CE1	2:D:110:HIS:HE2	2.32	0.47
1:A:216:PHE:O	1:A:234:THR:HG23	2.13	0.47
2:D:114:PRO:HB2	2:D:134:GLU:HG2	1.96	0.47
1:A:145:LEU:HD21	1:A:203:TRP:CZ3	2.49	0.47
2:B:1:GLN:HG3	2:B:182:PHE:HB2	1.97	0.47
2:B:31:THR:HA	2:B:78:ILE:O	2.15	0.47
2:B:33:GLU:OE1	2:B:106:HIS:ND1	2.47	0.47
1:A:122:VAL:HG11	1:A:219:LEU:CD1	2.45	0.47
2:B:59:LYS:HB2	2:B:89:LEU:HD11	1.93	0.47
1:C:244:ARG:HG3	1:C:244:ARG:HH11	1.80	0.47
1:A:119:LEU:O	1:A:225:TRP:HZ3	1.98	0.47
2:B:121:VAL:HG21	2:B:131:PHE:HE2	1.80	0.46
1:C:140:LYS:C	1:C:142:LYS:H	2.24	0.46
2:B:182:PHE:CZ	2:B:205:GLU:HG2	2.50	0.46
1:C:122:VAL:HG21	1:C:219:LEU:HD11	1.97	0.46
1:C:244:ARG:HG3	1:C:244:ARG:NH1	2.30	0.46
1:C:14:VAL:HG12	1:C:118:ASP:HA	1.97	0.46
1:C:38:ASP:O	1:C:41:HIS:N	2.49	0.46
2:D:145:LEU:HD12	2:D:207:LEU:HD12	1.96	0.46
1:A:12:VAL:HG21	1:A:219:LEU:HD12	1.98	0.46
2:D:146:ASP:OD2	2:D:201:TYR:OH	2.23	0.46
1:A:41:HIS:ND1	4:A:298:HOH:O	2.36	0.46
1:C:69:ARG:HD2	1:C:74:GLN:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1:GLN:O	2:D:2:GLN:C	2.58	0.46
1:C:163:VAL:CG2	1:C:168:VAL:HG21	2.43	0.46
2:B:106:HIS:ND1	2:B:110:HIS:NE2	2.64	0.46
1:C:36:ARG:NH2	1:C:88:SER:HB2	2.31	0.46
1:A:74:GLN:HG3	1:A:75:PHE:N	2.31	0.45
1:A:31:ASN:HA	1:A:49:SER:O	2.17	0.45
1:A:33:TYR:CD1	1:A:33:TYR:N	2.84	0.45
2:B:29:PRO:HD3	2:B:147:TYR:CZ	2.52	0.45
1:A:72:GLN:HA	1:A:72:GLN:HE21	1.82	0.45
2:B:39:ASP:CG	2:B:40:GLN:H	2.25	0.45
1:C:31:ASN:HA	1:C:49:SER:O	2.17	0.45
2:D:17:ASN:HA	2:D:19:GLN:HE21	1.77	0.45
2:D:189:GLU:HG3	4:D:338:HOH:O	2.17	0.45
1:A:233:VAL:CG2	1:A:234:THR:N	2.78	0.45
1:C:122:VAL:HG11	1:C:219:LEU:CD1	2.46	0.45
1:A:233:VAL:CG2	1:A:234:THR:H	2.29	0.45
2:D:136:ASN:H	2:D:136:ASN:HD22	1.63	0.44
2:D:83:TYR:CE1	2:D:195:SER:HB3	2.53	0.44
2:B:172:ILE:O	2:B:183:TRP:HA	2.18	0.44
1:A:148:LEU:HG	4:A:295:HOH:O	2.17	0.44
2:B:33:GLU:OE1	2:B:110:HIS:HE1	2.00	0.44
2:B:175:ILE:N	2:B:175:ILE:HD12	2.32	0.44
1:C:125:PRO:HB3	1:C:152:PHE:CB	2.43	0.44
2:B:77:ASP:OD2	2:B:106:HIS:ND1	2.50	0.44
1:A:129:LEU:CD2	1:A:130:PHE:N	2.81	0.44
2:D:17:ASN:CA	2:D:19:GLN:HE22	2.25	0.44
1:A:38:ASP:O	1:A:39:THR:C	2.60	0.44
2:B:158:GLN:OE1	2:B:158:GLN:N	2.50	0.43
2:B:66:GLU:CD	2:B:66:GLU:N	2.76	0.43
1:C:87:THR:HG23	1:C:115:THR:HA	1.99	0.43
1:C:174:THR:HG22	1:C:175:ASP:N	2.32	0.43
1:C:125:PRO:CA	1:C:152:PHE:HB3	2.48	0.43
1:C:100:SER:OG	1:C:105:GLU:HG3	2.18	0.43
1:A:159:LEU:C	1:A:159:LEU:HD23	2.43	0.43
1:A:243:GLY:O	1:A:244:ARG:C	2.61	0.43
2:D:5:ASP:N	2:D:8:GLN:OE1	2.49	0.43
2:B:1:GLN:CB	2:B:182:PHE:HA	2.45	0.43
1:C:24:GLN:HG3	4:C:281:HOH:O	2.18	0.43
2:B:64:ASN:ND2	2:B:67:MET:H	2.18	0.42
1:A:125:PRO:HB3	1:A:152:PHE:CB	2.44	0.42
2:D:145:LEU:O	2:D:149:VAL:HG23	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:44:HIS:CG	1:C:141:GLN:HE21	2.37	0.42
2:D:146:ASP:O	2:D:150:ARG:HG3	2.19	0.42
2:B:26:GLU:CD	2:B:26:GLU:C	2.88	0.42
2:B:57:LYS:HB3	2:B:89:LEU:HD21	2.01	0.42
1:C:160:SER:OG	1:C:213:GLN:HB3	2.20	0.42
2:B:121:VAL:HB	2:B:129:LEU:HB3	2.02	0.42
1:C:129:LEU:HD23	1:C:130:PHE:H	1.80	0.42
2:B:149:VAL:HG12	2:B:153:LEU:HD12	2.01	0.42
1:A:24:GLN:HE21	1:A:24:GLN:HB2	1.67	0.42
1:A:174:THR:HG22	1:A:175:ASP:N	2.34	0.42
1:C:175:ASP:HB2	1:C:192:LEU:HD12	2.02	0.42
2:D:31:THR:HG22	2:D:79:TYR:CD1	2.55	0.42
1:C:38:ASP:O	1:C:39:THR:C	2.63	0.42
2:D:40:GLN:NE2	2:D:45:ASP:O	2.53	0.42
1:A:54:SER:HA	2:B:20:ASN:OD1	2.20	0.41
1:C:31:ASN:ND2	1:C:50:TYR:HA	2.35	0.41
1:A:132:PRO:HB2	1:A:137:ILE:HG22	2.02	0.41
1:A:186:ASN:ND2	1:A:187:TYR:CE1	2.89	0.41
2:D:30:VAL:HG13	2:D:30:VAL:O	2.20	0.41
1:A:81:LEU:HB2	4:A:286:HOH:O	2.21	0.41
1:C:133:SER:O	1:C:134:LYS:C	2.63	0.41
2:B:111:LEU:HD21	2:B:138:LYS:HG2	2.03	0.41
2:B:203:ASP:OD1	2:B:203:ASP:C	2.64	0.41
1:A:9:ARG:HD3	1:A:110:PRO:HG2	2.02	0.41
1:A:129:LEU:CD2	1:A:130:PHE:H	2.34	0.41
2:D:157:LYS:HA	2:D:157:LYS:HE2	2.03	0.41
1:C:132:PRO:HD2	1:C:203:TRP:CZ2	2.56	0.41
2:D:94:GLU:O	2:D:95:ARG:HB2	2.20	0.41
1:A:173:SER:O	1:A:195:ARG:NH1	2.50	0.41
2:B:33:GLU:CD	2:B:110:HIS:HE1	2.28	0.41
2:D:31:THR:HA	2:D:78:ILE:O	2.21	0.41
2:B:82:GLU:CA	2:B:99:ILE:HG22	2.51	0.41
2:B:194:GLN:HG3	3:B:301:GOL:H31	2.02	0.41
1:C:195:ARG:HD2	1:C:195:ARG:H	1.84	0.41
2:D:89:LEU:HD22	2:D:96:SER:HB2	2.03	0.41
1:A:48:TYR:CE1	1:A:56:GLU:HB2	2.56	0.41
1:C:145:LEU:HD11	1:C:210:PHE:CG	2.56	0.41
1:C:157:VAL:HG12	1:C:216:PHE:HA	2.04	0.40
2:D:111:LEU:CD2	2:D:138:LYS:HG2	2.51	0.40
1:A:133:SER:O	1:A:134:LYS:C	2.63	0.40
1:A:157:VAL:HG12	1:A:216:PHE:CA	2.50	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:30:VAL:O	2:B:30:VAL:HG13	2.21	0.40
2:B:129:LEU:HD12	2:B:130:SER:N	2.37	0.40
1:C:163:VAL:O	1:C:163:VAL:HG23	2.21	0.40
2:B:109:ASN:ND2	2:B:139:MET:H	1.94	0.40
1:C:87:THR:O	1:C:88:SER:HB2	2.21	0.40
2:B:38:VAL:HG21	2:B:49:ASN:HB2	2.03	0.40
1:C:203:TRP:HE3	1:C:210:PHE:CE2	2.39	0.40
1:A:38:ASP:O	1:A:41:HIS:N	2.50	0.40
2:D:62:LEU:HD23	2:D:101:GLY:HA2	2.04	0.40
2:D:109:ASN:O	2:D:137:LYS:HA	2.22	0.40
2:D:172:ILE:O	2:D:183:TRP:HA	2.22	0.40
2:D:206:THR:HG22	2:D:207:LEU:N	2.36	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	234/238 (98%)	215 (92%)	18 (8%)	1 (0%)	30	60
1	C	234/238 (98%)	215 (92%)	17 (7%)	2 (1%)	14	41
2	B	219/221 (99%)	202 (92%)	11 (5%)	6 (3%)	4	15
2	D	219/221 (99%)	201 (92%)	13 (6%)	5 (2%)	5	18
All	All	906/918 (99%)	833 (92%)	59 (6%)	14 (2%)	8	28

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	34	ASN
2	B	93	ALA
2	B	177	LYS

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Mol	Chain	Res	Type
1	C	138	ALA
2	D	93	ALA
2	D	177	LYS
1	A	138	ALA
2	B	37	SER
2	B	94	GLU
2	D	34	ASN
2	B	3	ASP
2	D	37	SER
2	D	94	GLU
1	C	137	ILE

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	184/202 (91%)	168 (91%)	16 (9%)	9	30
1	C	184/202 (91%)	181 (98%)	3 (2%)	55	83
2	B	195/208 (94%)	187 (96%)	8 (4%)	27	62
2	D	202/208 (97%)	191 (95%)	11 (5%)	20	51
All	All	765/820 (93%)	727 (95%)	38 (5%)	22	54

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	GLN
1	A	72	GLN
1	A	74	GLN
1	A	84	PRO
1	A	87	THR
1	A	117	GLU
1	A	121	GLN
1	A	125	PRO
1	A	129	LEU
1	A	137	ILE

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Mol	Chain	Res	Type
1	A	150	ARG
1	A	168	VAL
1	A	177	GLN
1	A	219	LEU
1	A	227	GLU
1	A	244	ARG
2	B	1	GLN
2	B	5	ASP
2	B	49	ASN
2	B	64	ASN
2	B	82	GLU
2	B	133	ILE
2	B	158	GLN
2	B	220	THR
1	C	33	TYR
1	C	121	GLN
1	C	125	PRO
2	D	3	ASP
2	D	14	LEU
2	D	16	LYS
2	D	19	GLN
2	D	64	ASN
2	D	82	GLU
2	D	133	ILE
2	D	136	ASN
2	D	157	LYS
2	D	196	LYS
2	D	199	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	GLN
1	A	27	ASN
1	A	30	ASN
1	A	31	ASN
1	A	37	GLN
1	A	41	HIS
1	A	72	GLN
1	A	121	GLN
1	A	177	GLN
1	A	186	ASN

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Mol	Chain	Res	Type
1	A	215	GLN
1	A	236	ASN
2	B	34	ASN
2	B	64	ASN
2	B	65	GLN
2	B	109	ASN
2	B	127	GLN
2	B	143	GLN
1	C	27	ASN
1	C	31	ASN
1	C	121	GLN
1	C	208	ASN
1	C	235	GLN
2	D	1	GLN
2	D	19	GLN
2	D	49	ASN
2	D	64	ASN
2	D	75	ASN
2	D	109	ASN
2	D	136	ASN
2	D	156	ASN
2	D	178	ASN
2	D	210	ASN

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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

3 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GOL	D	302	-	5,5,5	1.24	1 (20%)	5,5,5	0.92	0
3	GOL	D	303	-	5,5,5	1.20	1 (20%)	5,5,5	0.95	0
3	GOL	B	301	-	5,5,5	0.98	0	5,5,5	1.13	1 (20%)

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	D	302	-	-	4/4/4/4	-
3	GOL	D	303	-	-	4/4/4/4	-
3	GOL	B	301	-	-	2/4/4/4	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	302	GOL	O2-C2	2.31	1.50	1.43
3	D	303	GOL	O2-C2	2.04	1.49	1.43

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	301	GOL	O3-C3-C2	-2.26	100.19	110.38

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	301	GOL	C1-C2-C3-O3
3	B	301	GOL	O2-C2-C3-O3
3	D	302	GOL	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
3	D	303	GOL	O1-C1-C2-O2
3	D	303	GOL	O1-C1-C2-C3
3	D	303	GOL	C1-C2-C3-O3
3	D	303	GOL	O2-C2-C3-O3
3	D	302	GOL	O2-C2-C3-O3
3	D	302	GOL	O1-C1-C2-C3
3	D	302	GOL	O1-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	302	GOL	1	0
3	B	301	GOL	3	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	236/238 (99%)	0.56	24 (10%) 12 9	14, 39, 71, 86	0
1	C	236/238 (99%)	0.48	16 (6%) 23 17	16, 38, 74, 87	0
2	B	221/221 (100%)	0.57	10 (4%) 38 30	21, 43, 60, 78	0
2	D	221/221 (100%)	0.34	8 (3%) 46 37	17, 39, 55, 77	0
All	All	914/918 (99%)	0.49	58 (6%) 26 19	14, 40, 69, 87	0

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	140	LYS	5.1
1	C	139	ASN	4.9
1	A	141	GLN	3.6
1	C	135	ALA	3.5
2	B	108	GLY	3.5
2	D	93	ALA	3.5
2	D	92	ASN	3.4
1	C	138	ALA	3.4
2	B	92	ASN	3.4
1	C	178	ALA	3.3
1	A	179	TYR	3.3
1	C	140	LYS	3.3
1	A	135	ALA	3.3
1	A	200	ALA	3.2
2	D	91	GLU	3.1
2	D	90	SER	3.0
1	A	138	ALA	3.0
1	C	141	GLN	3.0
2	B	93	ALA	2.9
1	A	182	SER	2.8
2	D	94	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	169	HIS	2.8
1	A	203	TRP	2.7
2	B	90	SER	2.7
1	A	120	ARG	2.7
1	A	139	ASN	2.7
2	B	94	GLU	2.7
1	C	228	GLY	2.6
1	C	134	LYS	2.6
2	B	178	ASN	2.5
2	D	133	ILE	2.5
1	A	177	GLN	2.5
1	C	186	ASN	2.5
2	B	45	ASP	2.4
1	C	179	TYR	2.4
1	A	117	GLU	2.4
1	A	131	GLU	2.4
2	B	109	ASN	2.4
1	A	171	GLY	2.4
1	A	170	SER	2.3
1	C	244	ARG	2.3
1	A	208	ASN	2.3
1	C	173	SER	2.3
1	C	187	TYR	2.3
2	D	69	THR	2.2
2	D	178	ASN	2.2
1	A	191	CYS	2.2
1	C	168	VAL	2.2
2	B	113	ILE	2.2
1	A	205	ASN	2.2
1	C	230	PRO	2.2
1	A	137	ILE	2.1
1	C	204	HIS	2.1
2	B	6	PRO	2.1
1	A	24	GLN	2.1
1	A	130	PHE	2.1
1	A	168	VAL	2.0
1	A	155	ASP	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](#)

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($\text{\AA}^2$)	Q<0.9
3	GOL	D	303	6/6	0.83	0.14	39,45,47,50	0
3	GOL	D	302	6/6	0.86	0.14	32,36,39,40	0
3	GOL	B	301	6/6	0.86	0.16	36,40,42,42	0

6.5 Other polymers [i](#)

There are no such residues in this entry.