



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:20 PM UTC

PDB ID : 6BYW / pdb_00006byw
Title : Structure of GoxA from Pseudoalteromonas luteoviolacea
Authors : Yukl, E.T.; Avalos, D.
Deposited on : 2017-12-21
Resolution : 2.05 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

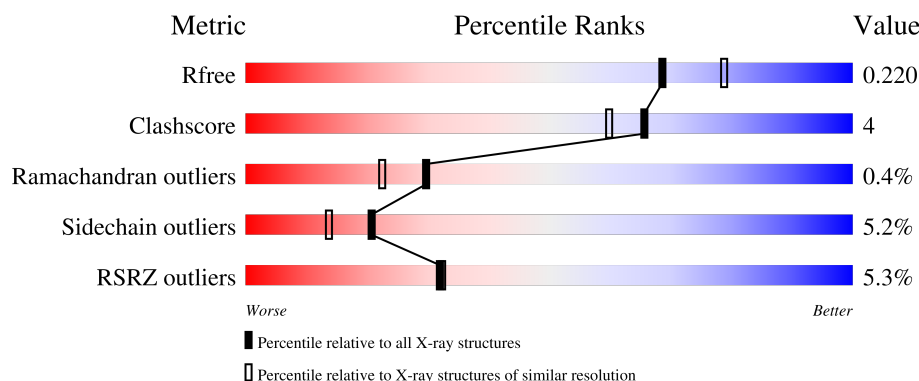
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.05 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	2260 (2.04-2.04)
Clashscore	190562	2333 (2.04-2.04)
Ramachandran outliers	187476	2318 (2.04-2.04)
Sidechain outliers	187428	2318 (2.04-2.04)
RSRZ outliers	180081	2260 (2.04-2.04)

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	816	4% 85% 9% • •
1	B	816	6% 85% 9% • •
1	C	816	5% 84% 10% • 5%
1	D	816	5% 85% 9% • 5%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 49970 atoms, of which 23533 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.

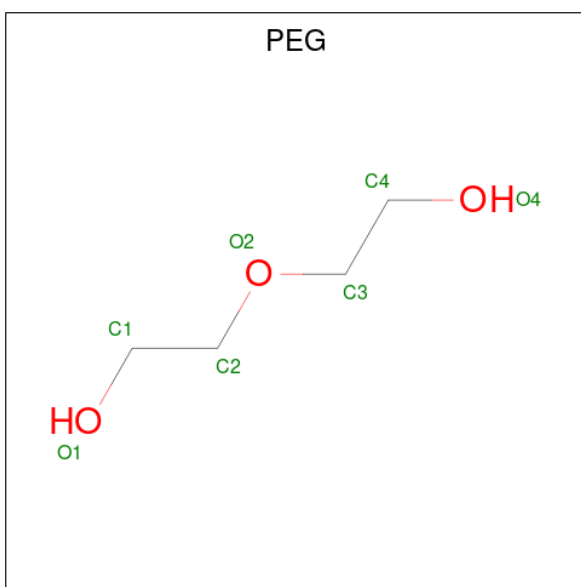
- Molecule 1 is a protein called GoxA.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	B	781	Total	C	H	N	O	S	0	2	0
			12046	3915	5858	1051	1202	20			
1	A	787	Total	C	H	N	O	S	0	3	0
			12157	3946	5913	1063	1215	20			
1	C	778	Total	C	H	N	O	S	0	1	0
			12043	3902	5875	1050	1197	19			
1	D	776	Total	C	H	N	O	S	0	2	0
			11973	3885	5831	1046	1191	20			

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

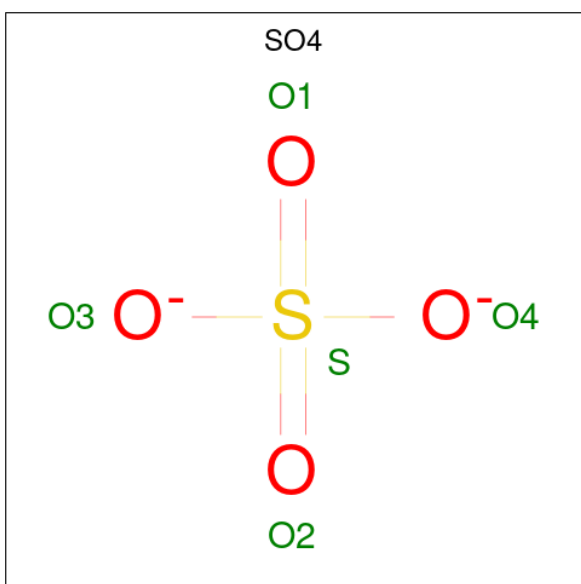
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Mg	0	0
			1	1		
2	A	1	Total	Mg	0	0
			1	1		
2	C	1	Total	Mg	0	0
			1	1		
2	D	1	Total	Mg	0	0
			1	1		

- Molecule 3 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



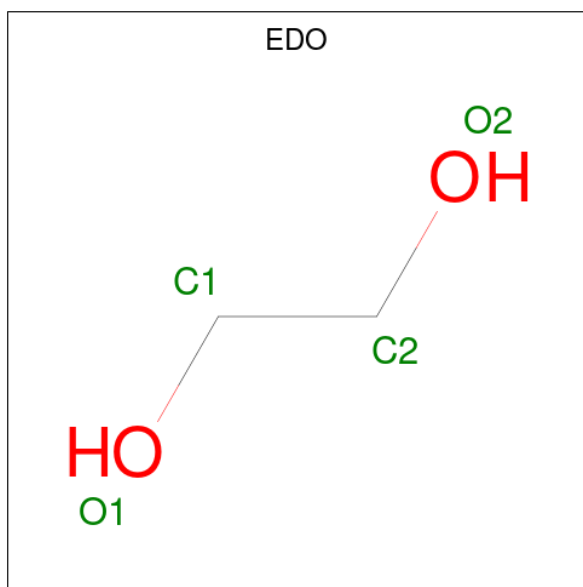
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	H	O	0	0
			17	4	10	3		
3	A	1	Total	C	H	O	0	0
			17	4	10	3		
3	A	1	Total	C	H	O	0	0
			17	4	10	3		
3	C	1	Total	C	H	O	0	0
			17	4	10	3		
3	D	1	Total	C	H	O	0	0
			17	4	10	3		

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	D	1	Total	C	H	O	0	0
			10	2	6	2		

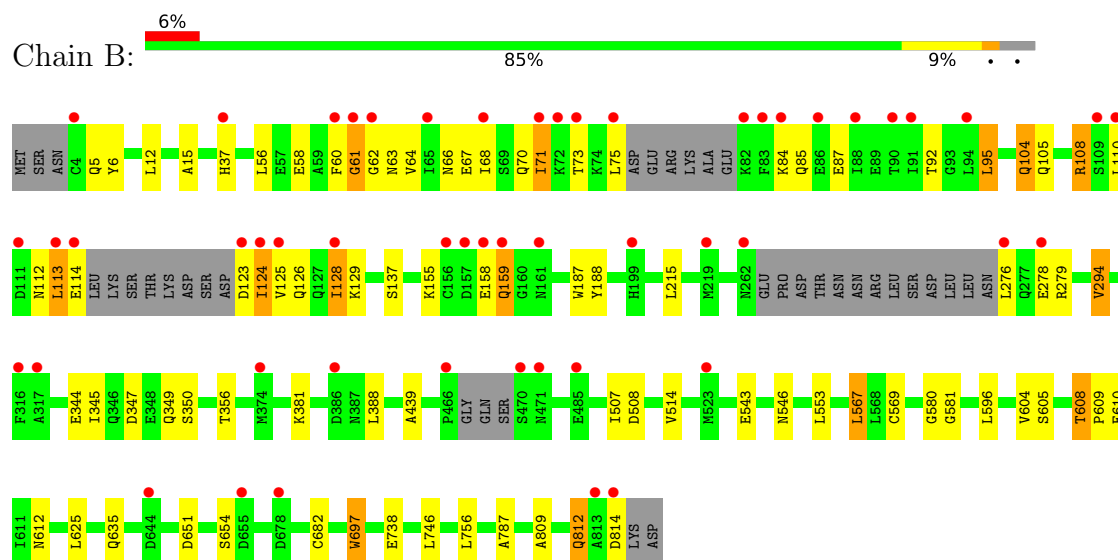
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	453	Total	O	0	0
			453	453		
6	A	355	Total	O	0	0
			355	355		
6	C	440	Total	O	0	0
			440	440		
6	D	393	Total	O	0	1
			394	394		

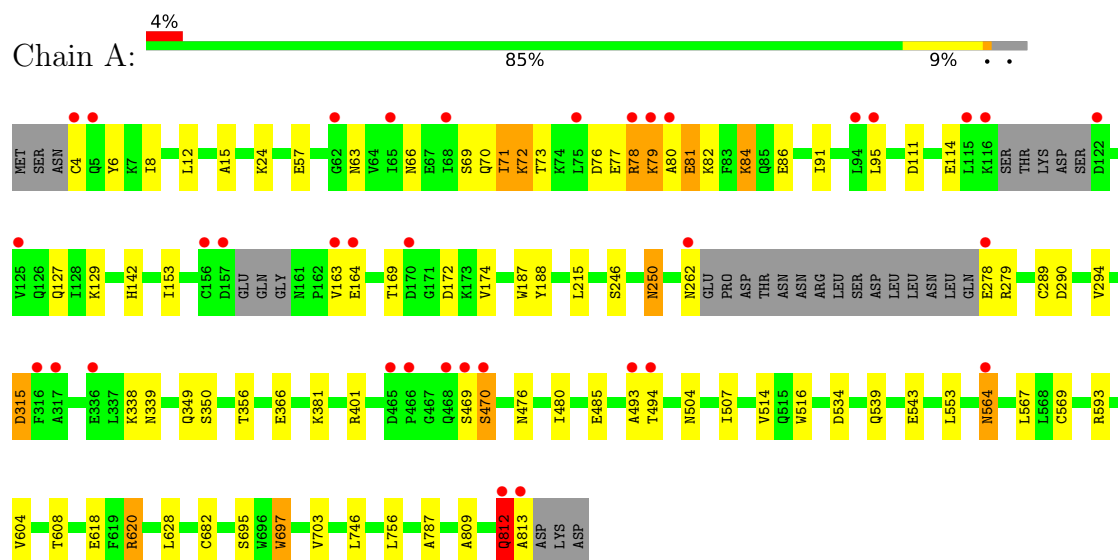
3 Residue-property plots [i](#)

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.

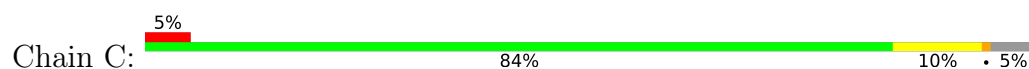
• Molecule 1: GoxA

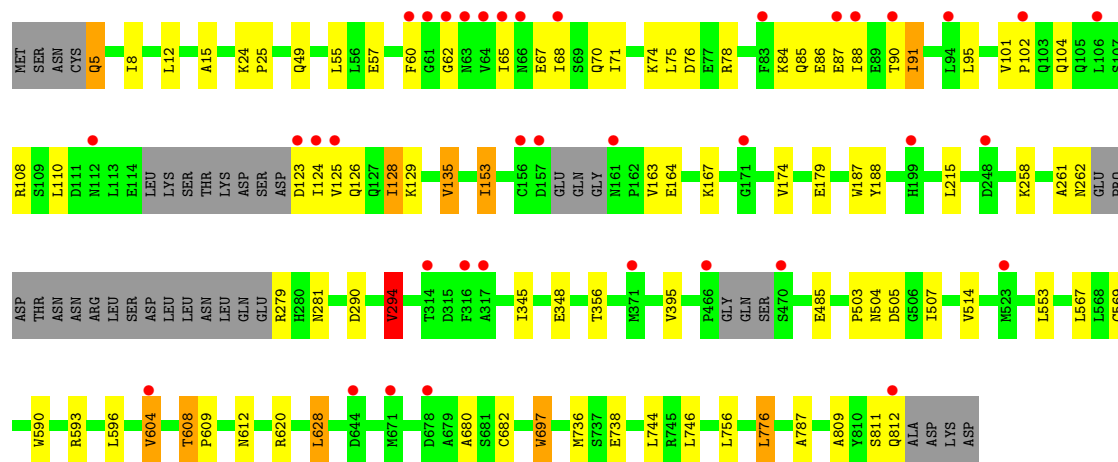


• Molecule 1: GoxA

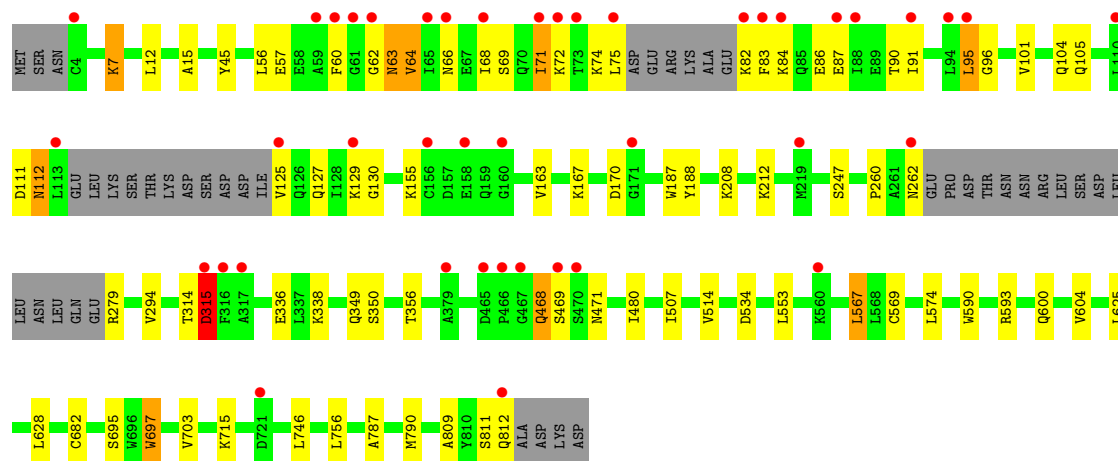
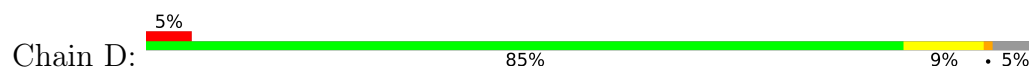


• Molecule 1: GoxA





• Molecule 1: GoxA



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	109.84Å 93.24Å 188.46Å 90.00° 94.88° 90.00°	Depositor
Resolution (Å)	48.28 – 2.05 48.28 – 2.05	Depositor EDS
% Data completeness (in resolution range)	98.8 (48.28-2.05) 98.8 (48.28-2.05)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.89 (at 2.05Å)	Xtriage
Refinement program	PHENIX (1.12_2829: ???)	Depositor
R, R_{free}	0.185 , 0.219 0.187 , 0.220	Depositor DCC
R_{free} test set	11784 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	24.8	Xtriage
Anisotropy	0.459	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 41.8	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	49970	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.30% 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: MG, PEG, SO4, EDO, TRQ

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	0.17	0/6376	0.42	0/8678
1	B	0.18	0/6319	0.45	3/8602 (0.0%)
1	C	0.17	0/6299	0.45	3/8573 (0.0%)
1	D	0.16	0/6274	0.40	0/8542
All	All	0.17	0/25268	0.43	6/34395 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	55	LEU	CA-C-N	9.55	136.92	120.58
1	C	55	LEU	C-N-CA	9.55	136.92	120.58
1	B	110	LEU	CA-C-N	7.97	132.42	120.31
1	B	110	LEU	C-N-CA	7.97	132.42	120.31
1	B	294	VAL	CG1-CB-CG2	5.48	122.86	110.80
1	C	294	VAL	CA-CB-CG2	5.14	119.13	110.40

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	6244	5913	6010	53	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	6188	5858	5955	41	0
1	C	6168	5875	5941	51	2
1	D	6142	5831	5913	42	2
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	14	20	20	1	0
3	B	7	10	10	0	0
3	C	7	10	10	2	0
3	D	7	10	10	0	0
4	B	5	0	0	1	0
4	C	5	0	0	0	0
5	D	4	6	6	0	0
6	A	355	0	0	5	0
6	B	453	0	0	5	0
6	C	440	0	0	5	0
6	D	394	0	0	0	0
All	All	26437	23533	23875	187	2

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 4.

All (187) 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:82:LYS:NZ	1:D:111:ASP:O	1.94	0.98
1:A:246:SER:O	6:A:1001:HOH:O	1.90	0.89
1:C:78:ARG:NH2	1:C:87:GLU:OE2	2.06	0.89
1:A:80:ALA:HA	1:A:81:GLU:CB	2.05	0.86
1:C:485:GLU:OE2	6:C:1001:HOH:O	1.99	0.80
1:C:124:ILE:O	1:C:128:ILE:HG23	1.86	0.76
1:B:812:GLN:HG2	6:B:1064:HOH:O	1.85	0.76
1:A:8:ILE:O	1:A:620:ARG:NH2	2.19	0.74
1:B:61:GLY:HA2	1:B:62:GLY:C	2.12	0.73
1:A:80:ALA:HA	1:A:81:GLU:HB2	1.68	0.72
1:A:84:LYS:HD2	1:A:86:GLU:OE1	1.89	0.72
1:B:158:GLU:O	1:B:159:GLN:HB2	1.90	0.71
1:A:250:ASN:N	6:A:1001:HOH:O	2.18	0.70
1:C:8:ILE:O	1:C:620:ARG:NH2	2.25	0.70
1:A:485:GLU:OE1	6:A:1002:HOH:O	2.11	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:349:GLN:OE1	1:D:600:GLN:NE2	2.28	0.67
1:D:469:SER:HA	1:D:471:ASN:ND2	2.09	0.67
1:A:493:ALA:O	1:A:494:THR:OG1	2.13	0.67
1:B:635:GLN:OE1	6:B:1001:HOH:O	2.13	0.66
1:B:61:GLY:HA2	1:B:64:VAL:H	1.60	0.66
1:B:6:TYR:HB2	1:B:345:ILE:HD11	1.78	0.66
1:A:80:ALA:HA	1:A:81:GLU:HB3	1.77	0.66
1:A:4:CYS:SG	6:A:1332:HOH:O	2.54	0.65
1:A:80:ALA:CA	1:A:81:GLU:CB	2.74	0.65
1:C:68:ILE:CG2	1:C:124:ILE:HD11	2.25	0.65
1:B:546:ASN:ND2	6:B:1006:HOH:O	2.29	0.65
1:B:61:GLY:HA2	1:B:63:ASN:N	2.13	0.64
1:C:62:GLY:HA2	1:C:65:ILE:HD13	1.79	0.63
1:A:315[A]:ASP:N	1:A:315[A]:ASP:OD1	2.32	0.62
1:D:468:GLN:O	1:D:469:SER:OG	2.09	0.62
1:D:112:ASN:O	1:D:112:ASN:ND2	2.31	0.62
1:D:315[A]:ASP:N	1:D:315[A]:ASP:OD1	2.33	0.62
1:C:62:GLY:HA2	1:C:65:ILE:CD1	2.30	0.61
1:A:24:LYS:NZ	6:A:1006:HOH:O	2.34	0.60
1:A:142:HIS:CE1	1:A:813:ALA:HA	2.36	0.60
1:A:172:ASP:OD1	1:A:338:LYS:N	2.35	0.59
1:A:91:ILE:O	1:A:95:LEU:HD13	2.03	0.59
1:B:6:TYR:HB2	1:B:345:ILE:CD1	2.33	0.58
1:C:179:GLU:HB2	1:C:628:LEU:HD22	1.85	0.58
1:A:618:GLU:OE2	1:A:620:ARG:NH1	2.37	0.58
1:B:15:ALA:O	1:B:356:THR:HA	2.06	0.56
1:C:68:ILE:HG22	1:C:124:ILE:HD11	1.86	0.56
1:A:80:ALA:CA	1:A:81:GLU:HB3	2.35	0.55
1:C:71:ILE:O	1:C:75:LEU:HD23	2.08	0.54
1:C:124:ILE:HD12	1:C:125:VAL:N	2.23	0.54
1:A:80:ALA:CB	1:A:81:GLU:HB3	2.37	0.54
1:A:84:LYS:CD	1:A:86:GLU:OE1	2.56	0.54
1:C:15:ALA:O	1:C:356:THR:HA	2.08	0.54
1:B:508:ASP:OD2	6:B:1002:HOH:O	2.18	0.53
1:B:682:CYS:SG	1:B:697:TRQ:HB3	2.48	0.53
1:A:469:SER:O	1:A:470:SER:OG	2.21	0.53
1:C:57:GLU:OE2	1:C:129:LYS:NZ	2.41	0.53
1:B:61:GLY:H	1:B:64:VAL:CG2	2.22	0.53
1:C:128:ILE:HG13	1:C:129:LYS:N	2.22	0.53
1:D:91:ILE:O	1:D:95:LEU:HD22	2.08	0.53
1:D:682:CYS:SG	1:D:697:TRQ:HB3	2.48	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:262:ASN:OD1	1:D:279:ARG:NH1	2.42	0.53
1:B:567:LEU:CD2	1:B:604:VAL:HG21	2.39	0.52
1:C:86:GLU:O	1:C:90:THR:HG23	2.10	0.52
1:D:15:ALA:O	1:D:356:THR:HA	2.10	0.52
1:C:279:ARG:NH2	6:C:1006:HOH:O	2.42	0.51
1:D:7:LYS:HG3	1:D:350:SER:HA	1.91	0.51
1:A:682:CYS:SG	1:A:697:TRQ:HB3	2.51	0.51
1:A:15:ALA:O	1:A:356:THR:HA	2.09	0.51
1:C:567:LEU:CD2	1:C:604:VAL:HG21	2.40	0.51
1:B:159:GLN:HA	1:B:159:GLN:OE1	2.10	0.51
1:C:290:ASP:HB3	3:C:902:PEG:H12	1.93	0.51
1:C:49:GLN:NE2	6:C:1014:HOH:O	2.43	0.51
1:A:469:SER:O	1:A:470:SER:CB	2.58	0.50
1:D:62:GLY:O	1:D:63:ASN:C	2.55	0.50
1:A:80:ALA:HB1	1:A:81:GLU:HB3	1.94	0.50
1:A:349:GLN:O	1:A:620:ARG:HD2	2.11	0.50
1:A:564[A]:ASN:N	1:A:564[A]:ASN:OD1	2.45	0.50
1:A:812:GLN:O	1:A:813:ALA:HB2	2.12	0.50
1:D:567:LEU:CD2	1:D:604:VAL:HG21	2.42	0.50
1:D:260:PRO:O	1:D:279:ARG:NH1	2.45	0.49
1:D:314[B]:THR:O	1:D:315[B]:ASP:CB	2.59	0.49
1:A:567:LEU:CD2	1:A:604:VAL:HG21	2.43	0.49
1:C:71:ILE:HG22	1:C:75:LEU:HD23	1.95	0.49
1:B:567:LEU:HD23	1:B:604:VAL:HG21	1.95	0.49
1:A:76:ASP:O	1:A:79:LYS:HE3	2.13	0.49
1:C:68:ILE:HG12	1:C:91:ILE:HD13	1.95	0.48
1:C:682:CYS:SG	1:C:697:TRQ:HB3	2.54	0.48
1:C:612[A]:ASN:ND2	6:C:1019:HOH:O	2.45	0.48
1:D:787:ALA:HB1	1:D:809:ALA:HB1	1.96	0.48
1:C:5:GLN:N	1:C:5:GLN:HE21	2.12	0.47
1:A:71:ILE:HD13	1:A:72:LYS:N	2.29	0.47
1:A:72:LYS:O	1:A:72:LYS:HE2	2.14	0.47
1:C:60:PHE:CD2	1:C:129:LYS:HE3	2.50	0.47
1:A:57:GLU:OE1	1:A:129:LYS:NZ	2.40	0.47
1:C:123:ASP:O	1:C:126:GLN:N	2.46	0.47
1:C:187:TRP:CG	1:C:188:TYR:H	2.33	0.47
1:D:468:GLN:N	1:D:468:GLN:OE1	2.48	0.47
1:A:787:ALA:HB1	1:A:809:ALA:HB1	1.96	0.46
1:C:124:ILE:HD12	1:C:124:ILE:C	2.40	0.46
1:D:811:SER:O	1:D:812:GLN:HB2	2.13	0.46
1:B:113:LEU:HD23	1:B:113:LEU:N	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:347:ASP:OD1	1:B:350:SER:OG	2.26	0.46
1:D:86:GLU:O	1:D:90:THR:OG1	2.33	0.46
1:B:124:ILE:HD12	1:B:125:VAL:H	1.81	0.46
1:D:56:LEU:O	1:D:60:PHE:HD2	1.98	0.45
1:C:348:GLU:O	1:C:620:ARG:HG2	2.16	0.45
1:C:811:SER:O	1:C:812:GLN:HB2	2.16	0.45
1:A:6:TYR:O	1:A:350:SER:OG	2.34	0.45
1:D:60:PHE:HD1	1:D:64:VAL:HG11	1.82	0.45
1:D:95:LEU:HD23	1:D:95:LEU:O	2.16	0.45
1:C:787:ALA:HB1	1:C:809:ALA:HB1	1.98	0.45
1:A:493:ALA:O	1:A:494:THR:CB	2.65	0.45
1:D:60:PHE:HD1	1:D:64:VAL:CG1	2.29	0.45
1:B:187:TRP:CG	1:B:188:TYR:H	2.35	0.44
1:D:71:ILE:HG22	1:D:74:LYS:HD2	2.00	0.44
1:D:187:TRP:CG	1:D:188:TYR:H	2.35	0.44
1:A:187:TRP:CG	1:A:188:TYR:H	2.36	0.44
1:D:514:VAL:HG12	1:D:514:VAL:O	2.18	0.44
1:B:70:GLN:O	1:B:73:THR:HG22	2.18	0.44
1:C:68:ILE:O	1:C:71:ILE:N	2.49	0.44
1:B:612:ASN:ND2	6:B:1029:HOH:O	2.50	0.44
1:B:61:GLY:CA	1:B:64:VAL:H	2.29	0.44
1:C:294:VAL:HG22	3:C:902:PEG:H41	1.99	0.44
1:A:72:LYS:HD3	1:A:72:LYS:C	2.43	0.44
1:D:567:LEU:HD23	1:D:604:VAL:HG21	2.00	0.44
1:B:60:PHE:CD2	1:B:129:LYS:HE2	2.53	0.43
1:B:439:ALA:N	4:B:903:SO4:O1	2.39	0.43
1:A:169:THR:OG1	1:A:338:LYS:HE3	2.18	0.43
1:C:812:GLN:OE1	6:C:1002:HOH:O	2.20	0.43
1:D:125:VAL:CG1	1:D:129:LYS:HE3	2.48	0.43
1:C:153:ILE:HD13	1:C:345:ILE:CD1	2.48	0.43
1:D:262:ASN:OD1	1:D:279:ARG:CZ	2.67	0.43
1:C:101:VAL:HG11	1:C:135:VAL:HG23	1.99	0.43
1:B:787:ALA:HB1	1:B:809:ALA:HB1	2.00	0.43
1:A:514:VAL:HG12	1:A:514:VAL:O	2.18	0.43
1:B:61:GLY:H	1:B:64:VAL:HG23	1.83	0.43
1:B:125:VAL:O	1:B:128:ILE:HG22	2.19	0.43
1:C:88:ILE:HD12	1:C:110:LEU:HB2	2.00	0.43
1:D:155:LYS:O	1:D:163:VAL:HG22	2.18	0.43
1:A:95:LEU:N	1:A:95:LEU:HD12	2.34	0.42
1:A:695:SER:HB2	1:A:703:VAL:HG21	2.01	0.42
1:C:680:ALA:HB3	1:C:776:LEU:HD22	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:608:THR:HG22	1:B:610:GLU:H	1.83	0.42
1:B:68:ILE:HA	1:B:71:ILE:CD1	2.49	0.42
1:A:77:GLU:O	1:A:78:ARG:CB	2.68	0.42
1:B:608:THR:HG23	1:B:609:PRO:HD2	2.01	0.42
1:C:62:GLY:CA	1:C:65:ILE:CD1	2.98	0.42
1:C:514:VAL:HG12	1:C:514:VAL:O	2.20	0.42
1:D:60:PHE:CD1	1:D:64:VAL:HG11	2.53	0.42
1:B:514:VAL:O	1:B:514:VAL:HG12	2.19	0.42
1:C:261:ALA:O	1:C:262:ASN:HB2	2.20	0.42
1:C:504:ASN:CG	1:C:505:ASP:H	2.27	0.42
1:A:71:ILE:HD13	1:A:71:ILE:C	2.45	0.42
1:A:480:ILE:HG21	1:A:507:ILE:HD11	2.02	0.42
1:D:590:TRP:O	1:D:593:ARG:HG2	2.19	0.42
1:B:580:GLY:HA2	1:B:581:GLY:C	2.45	0.41
1:A:504:ASN:HB2	1:A:516:TRP:C	2.45	0.41
1:D:60:PHE:C	1:D:64:VAL:HG21	2.45	0.41
1:C:736:MET:SD	1:C:744:LEU:HD12	2.60	0.41
1:D:45:TYR:CD2	1:D:790:MET:HG2	2.55	0.41
1:A:476:ASN:O	1:A:493:ALA:O	2.39	0.41
1:A:539:GLN:O	1:A:543:GLU:HG3	2.20	0.41
1:A:153:ILE:HD12	1:A:174:VAL:HG21	2.02	0.41
1:A:339:ASN:OD1	1:A:339:ASN:N	2.50	0.41
1:C:24:LYS:HB2	1:C:25:PRO:HD3	2.03	0.41
1:B:92:THR:HA	1:B:95:LEU:HD22	2.03	0.41
1:A:366:GLU:OE1	1:A:401:ARG:NE	2.46	0.41
1:D:69:SER:HA	1:D:72:LYS:HB2	2.03	0.41
1:D:82:LYS:HG3	1:D:83:PHE:N	2.35	0.41
1:C:153:ILE:HD13	1:C:345:ILE:HD12	2.02	0.41
1:C:590:TRP:O	1:C:593:ARG:HG2	2.20	0.41
1:D:112:ASN:ND2	1:D:112:ASN:C	2.77	0.41
1:D:480:ILE:HG21	1:D:507:ILE:HD11	2.02	0.41
1:A:290:ASP:HB3	3:A:902:PEG:H41	2.03	0.41
1:D:208:LYS:HE2	1:D:212:LYS:HD2	2.02	0.41
1:C:503:PRO:HB3	1:C:507:ILE:HD12	2.03	0.41
1:B:105:GLN:HA	1:B:108:ARG:HG3	2.04	0.40
1:C:608:THR:HG23	1:C:609:PRO:HD2	2.02	0.40
1:B:104:GLN:O	1:B:108:ARG:HG2	2.21	0.40
1:B:604:VAL:HG23	1:B:605:SER:N	2.36	0.40
1:B:651:ASP:HB3	1:B:654:SER:HB2	2.01	0.40
1:D:68:ILE:HG21	1:D:125:VAL:HG22	2.04	0.40
1:D:695:SER:HB2	1:D:703:VAL:HG21	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:60:PHE:CE2	1:B:129:LYS:HG3	2.57	0.40
1:A:250:ASN:HA	1:A:289:CYS:O	2.22	0.40
1:C:101:VAL:HG13	1:C:102:PRO:HD2	2.02	0.40
1:B:63:ASN:OD1	1:B:66:ASN:HB2	2.21	0.40
1:B:108:ARG:HG2	1:B:108:ARG:H	1.75	0.40
1:C:258:LYS:HE2	1:C:281:ASN:OD1	2.21	0.40
1:C:62:GLY:CA	1:C:65:ILE:HD12	2.51	0.40
1:D:84:LYS:HB2	1:D:87:GLU:HB2	2.03	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:84:LYS:HZ3	1:D:170:ASP:OD2[1_455]	1.55	0.05
1:C:84:LYS:NZ	1:D:170:ASP:OD2[1_455]	2.17	0.03

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	781/816 (96%)	749 (96%)	28 (4%)	4 (0%)	24	16
1	B	772/816 (95%)	752 (97%)	18 (2%)	2 (0%)	36	30
1	C	768/816 (94%)	743 (97%)	25 (3%)	0	100	100
1	D	769/816 (94%)	737 (96%)	26 (3%)	6 (1%)	16	9
All	All	3090/3264 (95%)	2981 (96%)	97 (3%)	12 (0%)	30	22

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	64	VAL

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Mol	Chain	Res	Type
1	D	315[A]	ASP
1	D	315[B]	ASP
1	B	61	GLY
1	A	78	ARG
1	A	81	GLU
1	D	96	GLY
1	D	63	ASN
1	D	130	GLY
1	A	812	GLN
1	B	159	GLN
1	A	470	SER

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	685/711 (96%)	648 (95%)	37 (5%)	20	12
1	B	679/711 (96%)	634 (93%)	45 (7%)	15	9
1	C	677/711 (95%)	646 (95%)	31 (5%)	24	18
1	D	674/711 (95%)	644 (96%)	30 (4%)	24	18
All	All	2715/2844 (96%)	2572 (95%)	143 (5%)	21	13

All (143) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	5	GLN
1	B	12	LEU
1	B	37	HIS
1	B	56	LEU
1	B	58	GLU
1	B	67	GLU
1	B	71	ILE
1	B	75	LEU
1	B	84	LYS
1	B	85	GLN

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Mol	Chain	Res	Type
1	B	87	GLU
1	B	95	LEU
1	B	104	GLN
1	B	108	ARG
1	B	112	ASN
1	B	113	LEU
1	B	114	GLU
1	B	123	ASP
1	B	124	ILE
1	B	126	GLN
1	B	128	ILE
1	B	137	SER
1	B	155	LYS
1	B	215	LEU
1	B	276	LEU
1	B	278	GLU
1	B	279	ARG
1	B	294	VAL
1	B	344	GLU
1	B	349	GLN
1	B	381	LYS
1	B	388	LEU
1	B	507	ILE
1	B	543	GLU
1	B	553	LEU
1	B	567	LEU
1	B	569	CYS
1	B	596	LEU
1	B	608	THR
1	B	625	LEU
1	B	738	GLU
1	B	746	LEU
1	B	756	LEU
1	B	812	GLN
1	B	814	ASP
1	A	12	LEU
1	A	63	ASN
1	A	66	ASN
1	A	69	SER
1	A	70	GLN
1	A	71	ILE
1	A	72	LYS

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Mol	Chain	Res	Type
1	A	73	THR
1	A	79	LYS
1	A	82	LYS
1	A	84	LYS
1	A	111	ASP
1	A	114	GLU
1	A	127	GLN
1	A	163	VAL
1	A	164	GLU
1	A	215	LEU
1	A	250	ASN
1	A	262	ASN
1	A	278	GLU
1	A	279	ARG
1	A	294	VAL
1	A	315[A]	ASP
1	A	315[B]	ASP
1	A	381	LYS
1	A	534	ASP
1	A	553	LEU
1	A	564[A]	ASN
1	A	564[B]	ASN
1	A	569	CYS
1	A	593	ARG
1	A	608	THR
1	A	620	ARG
1	A	628	LEU
1	A	746	LEU
1	A	756	LEU
1	A	812	GLN
1	C	5	GLN
1	C	12	LEU
1	C	67	GLU
1	C	70	GLN
1	C	74	LYS
1	C	76	ASP
1	C	85	GLN
1	C	91	ILE
1	C	95	LEU
1	C	104	GLN
1	C	108	ARG
1	C	128	ILE

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Mol	Chain	Res	Type
1	C	135	VAL
1	C	153	ILE
1	C	163	VAL
1	C	164	GLU
1	C	167	LYS
1	C	174	VAL
1	C	215	LEU
1	C	294	VAL
1	C	395	VAL
1	C	553	LEU
1	C	569	CYS
1	C	596	LEU
1	C	604	VAL
1	C	608	THR
1	C	628	LEU
1	C	738	GLU
1	C	746	LEU
1	C	756	LEU
1	C	776	LEU
1	D	7	LYS
1	D	12	LEU
1	D	57	GLU
1	D	66	ASN
1	D	71	ILE
1	D	75	LEU
1	D	95	LEU
1	D	101	VAL
1	D	104	GLN
1	D	105	GLN
1	D	112	ASN
1	D	127	GLN
1	D	167	LYS
1	D	247	SER
1	D	294	VAL
1	D	315[A]	ASP
1	D	315[B]	ASP
1	D	336	GLU
1	D	338	LYS
1	D	468	GLN
1	D	534	ASP
1	D	553	LEU
1	D	567	LEU

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Mol	Chain	Res	Type
1	D	569	CYS
1	D	574	LEU
1	D	625	LEU
1	D	628	LEU
1	D	715	LYS
1	D	746	LEU
1	D	756	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	161	ASN
1	B	236	GLN
1	B	284	GLN
1	B	291	ASN
1	B	433	GLN
1	B	632	ASN
1	B	635	GLN
1	A	70	GLN
1	A	103	GLN
1	A	127	GLN
1	A	236	GLN
1	A	280	HIS
1	A	612	ASN
1	A	683	GLN
1	C	284	GLN
1	C	433	GLN
1	C	730	HIS
1	C	734	GLN
1	D	99	HIS
1	D	236	GLN
1	D	600	GLN
1	D	804	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	TRQ	D	697	1	16,17,18	2.58	7 (43%)	16,24,26	3.49	6 (37%)
1	TRQ	B	697	1	16,17,18	2.57	7 (43%)	16,24,26	3.53	6 (37%)
1	TRQ	A	697	1	16,17,18	2.53	6 (37%)	16,24,26	3.53	6 (37%)
1	TRQ	C	697	1	16,17,18	2.54	5 (31%)	16,24,26	3.63	7 (43%)

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	TRQ	D	697	1	-	1/5/19/21	0/2/2/2
1	TRQ	B	697	1	-	1/5/19/21	0/2/2/2
1	TRQ	A	697	1	-	1/5/19/21	0/2/2/2
1	TRQ	C	697	1	-	0/5/19/21	0/2/2/2

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	697	TRQ	CD1-NE1	-5.78	1.24	1.36
1	C	697	TRQ	CD1-NE1	-5.71	1.24	1.36
1	B	697	TRQ	CD1-NE1	-5.65	1.24	1.36
1	A	697	TRQ	CD1-NE1	-5.63	1.24	1.36
1	B	697	TRQ	CE2-NE1	-4.58	1.31	1.38
1	C	697	TRQ	CE2-NE1	-4.45	1.31	1.38
1	D	697	TRQ	CE2-NE1	-4.39	1.31	1.38
1	A	697	TRQ	CE2-NE1	-4.30	1.31	1.38
1	C	697	TRQ	CD1-CG	-3.41	1.33	1.38
1	B	697	TRQ	CD1-CG	-3.33	1.33	1.38
1	D	697	TRQ	CD1-CG	-3.29	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	697	TRQ	CD1-CG	-3.23	1.33	1.38
1	C	697	TRQ	CE2-CZ2	-3.02	1.39	1.50
1	D	697	TRQ	CE2-CZ2	-3.00	1.39	1.50
1	A	697	TRQ	CE2-CZ2	-2.99	1.39	1.50
1	B	697	TRQ	CE2-CZ2	-2.94	1.39	1.50
1	A	697	TRQ	CH2-CZ2	-2.81	1.40	1.53
1	D	697	TRQ	CH2-CZ2	-2.75	1.40	1.53
1	B	697	TRQ	CH2-CZ2	-2.73	1.40	1.53
1	C	697	TRQ	CH2-CZ2	-2.62	1.41	1.53
1	A	697	TRQ	O6-CH2	-2.07	1.19	1.24
1	D	697	TRQ	O6-CH2	-2.07	1.19	1.24
1	B	697	TRQ	CB-CG	2.06	1.54	1.50
1	B	697	TRQ	O6-CH2	-2.05	1.19	1.24
1	D	697	TRQ	CB-CG	2.02	1.54	1.50

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	697	TRQ	CD1-NE1-CE2	9.55	121.27	109.49
1	C	697	TRQ	CD1-NE1-CE2	9.47	121.17	109.49
1	A	697	TRQ	CD1-NE1-CE2	9.32	120.99	109.49
1	D	697	TRQ	CD1-NE1-CE2	9.31	120.98	109.49
1	C	697	TRQ	CD1-CG-CD2	6.23	111.58	105.95
1	A	697	TRQ	CD1-CG-CD2	6.09	111.45	105.95
1	D	697	TRQ	CD1-CG-CD2	5.85	111.23	105.95
1	B	697	TRQ	CD1-CG-CD2	5.80	111.19	105.95
1	A	697	TRQ	CZ2-CE2-NE1	4.70	138.69	127.25
1	D	697	TRQ	CZ2-CE2-NE1	4.53	138.27	127.25
1	B	697	TRQ	CZ2-CE2-NE1	4.51	138.24	127.25
1	C	697	TRQ	CZ2-CE2-NE1	4.47	138.13	127.25
1	C	697	TRQ	CG-CD1-NE1	-4.38	103.58	109.22
1	C	697	TRQ	CE2-CD2-CG	-4.38	101.36	107.16
1	D	697	TRQ	CE2-CD2-CG	-4.30	101.46	107.16
1	A	697	TRQ	CG-CD1-NE1	-4.28	103.71	109.22
1	A	697	TRQ	CE2-CD2-CG	-4.27	101.50	107.16
1	B	697	TRQ	CE2-CD2-CG	-4.22	101.56	107.16
1	B	697	TRQ	CG-CD1-NE1	-4.18	103.84	109.22
1	D	697	TRQ	CG-CD1-NE1	-4.11	103.93	109.22
1	B	697	TRQ	CD2-CE2-NE1	-2.79	102.14	107.20
1	C	697	TRQ	CD2-CE2-NE1	-2.69	102.31	107.20
1	A	697	TRQ	CD2-CE2-NE1	-2.67	102.34	107.20
1	D	697	TRQ	CD2-CE2-NE1	-2.64	102.40	107.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	697	TRQ	O7-CZ2-CH2	2.03	120.98	118.39

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	D	697	TRQ	CA-CB-CG-CD2
1	B	697	TRQ	CA-CB-CG-CD2
1	A	697	TRQ	CA-CB-CG-CD1

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	D	697	TRQ	1	0
1	B	697	TRQ	1	0
1	A	697	TRQ	1	0
1	C	697	TRQ	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 4 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	$\# Z > 2$
3	PEG	A	903	-	6,6,6	0.48	0	5,5,5	0.27	0
3	PEG	D	902	-	6,6,6	0.47	0	5,5,5	0.42	0
4	SO4	C	903	-	4,4,4	0.26	0	6,6,6	0.12	0
4	SO4	B	903	-	4,4,4	0.21	0	6,6,6	0.20	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PEG	C	902	-	6,6,6	0.57	0	5,5,5	0.43	0
3	PEG	B	902	-	6,6,6	0.49	0	5,5,5	0.22	0
3	PEG	A	902	-	6,6,6	0.50	0	5,5,5	1.10	0
5	EDO	D	903	-	3,3,3	0.46	0	2,2,2	0.31	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	PEG	A	903	-	-	1/4/4/4	-
3	PEG	D	902	-	-	2/4/4/4	-
3	PEG	C	902	-	-	3/4/4/4	-
3	PEG	B	902	-	-	0/4/4/4	-
3	PEG	A	902	-	-	3/4/4/4	-
5	EDO	D	903	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	902	PEG	C4-C3-O2-C2
3	C	902	PEG	O1-C1-C2-O2
3	A	902	PEG	O2-C3-C4-O4
3	A	903	PEG	O2-C3-C4-O4
3	D	902	PEG	O1-C1-C2-O2
3	D	902	PEG	O2-C3-C4-O4
3	A	902	PEG	C1-C2-O2-C3
3	C	902	PEG	O2-C3-C4-O4
3	C	902	PEG	C4-C3-O2-C2

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	903	SO4	1	0
3	C	902	PEG	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	902	PEG	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	786/816 (96%)	0.19	35 (4%)	38	38	21, 41, 90, 124	3 (0%)
1	B	780/816 (95%)	0.02	52 (6%)	24	23	15, 31, 86, 129	2 (0%)
1	C	777/816 (95%)	0.05	37 (4%)	35	36	17, 33, 81, 116	1 (0%)
1	D	775/816 (94%)	0.14	42 (5%)	31	31	19, 37, 91, 156	2 (0%)
All	All	3118/3264 (95%)	0.10	166 (5%)	32	32	15, 35, 89, 156	8 (0%)

All (166) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	316	PHE	7.2
1	A	813	ALA	6.7
1	B	316	PHE	6.4
1	D	316	PHE	6.1
1	C	316	PHE	5.3
1	D	75	LEU	4.7
1	D	83	PHE	4.5
1	B	83	PHE	4.3
1	A	80	ALA	4.2
1	A	262	ASN	4.2
1	B	61	GLY	4.1
1	D	68	ILE	4.1
1	B	75	LEU	4.0
1	D	160	GLY	3.9
1	C	64	VAL	3.9
1	A	317	ALA	3.9
1	C	61	GLY	3.8
1	B	814	ASP	3.8
1	C	161	ASN	3.8
1	D	73	THR	3.7
1	B	124	ILE	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	73	THR	3.6
1	D	59	ALA	3.6
1	D	317	ALA	3.6
1	D	469	SER	3.6
1	B	276	LEU	3.5
1	D	129	LYS	3.5
1	C	94	LEU	3.5
1	B	94	LEU	3.4
1	B	4	CYS	3.4
1	A	493	ALA	3.4
1	D	65	ILE	3.4
1	A	466	PRO	3.4
1	B	466	PRO	3.3
1	C	65	ILE	3.3
1	C	68	ILE	3.3
1	A	122	ASP	3.3
1	B	68	ILE	3.3
1	C	157	ASP	3.3
1	D	470	SER	3.3
1	C	88	ILE	3.3
1	A	163	VAL	3.2
1	B	88	ILE	3.2
1	A	157	ASP	3.2
1	C	317	ALA	3.2
1	B	110	LEU	3.2
1	D	465	ASP	3.2
1	D	262	ASN	3.2
1	B	813	ALA	3.1
1	B	91	ILE	3.1
1	B	90	THR	3.1
1	C	123	ASP	3.0
1	A	4	CYS	3.0
1	D	812	GLN	2.9
1	B	159	GLN	2.9
1	A	115	LEU	2.9
1	D	87	GLU	2.9
1	D	467	GLY	2.9
1	B	678	ASP	2.9
1	D	71	ILE	2.9
1	A	336	GLU	2.9
1	C	812	GLN	2.8
1	B	128	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	219	MET	2.8
1	B	655	ASP	2.8
1	B	62	GLY	2.8
1	B	156	CYS	2.8
1	C	112	ASN	2.7
1	A	75	LEU	2.7
1	D	94	LEU	2.7
1	B	278	GLU	2.7
1	A	278	GLU	2.7
1	C	124	ILE	2.7
1	B	158	GLU	2.7
1	D	158	GLU	2.7
1	C	156	CYS	2.7
1	D	315[A]	ASP	2.6
1	D	4	CYS	2.6
1	B	471	ASN	2.6
1	C	125	VAL	2.6
1	D	61	GLY	2.6
1	B	374	MET	2.6
1	B	60	PHE	2.6
1	D	91	ILE	2.6
1	C	678	ASP	2.6
1	C	106	LEU	2.6
1	D	113	LEU	2.6
1	C	60	PHE	2.5
1	B	485	GLU	2.5
1	C	66	ASN	2.5
1	A	494	THR	2.5
1	B	470	SER	2.5
1	B	37	HIS	2.5
1	B	523	MET	2.5
1	B	644	ASP	2.4
1	B	84	LYS	2.4
1	B	113	LEU	2.4
1	C	199	HIS	2.4
1	D	88	ILE	2.4
1	A	95	LEU	2.4
1	C	83	PHE	2.4
1	C	87	GLU	2.4
1	C	644	ASP	2.4
1	A	65	ILE	2.4
1	C	470	SER	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	466	PRO	2.4
1	B	199	HIS	2.4
1	D	95	LEU	2.4
1	A	78	ARG	2.4
1	A	469	SER	2.4
1	C	466	PRO	2.4
1	B	86	GLU	2.3
1	A	156	CYS	2.3
1	B	71	ILE	2.3
1	D	66	ASN	2.3
1	B	72	LYS	2.3
1	A	812	GLN	2.3
1	A	564[A]	ASN	2.3
1	A	62	GLY	2.3
1	A	79	LYS	2.3
1	C	671	MET	2.3
1	C	314	THR	2.2
1	D	156	CYS	2.2
1	D	171	GLY	2.2
1	D	219	MET	2.2
1	D	110	LEU	2.2
1	B	262	ASN	2.2
1	B	109	SER	2.2
1	B	123	ASP	2.2
1	C	62	GLY	2.2
1	D	72	LYS	2.2
1	C	171	GLY	2.1
1	B	317	ALA	2.1
1	C	63	ASN	2.1
1	C	371	MET	2.1
1	B	111	ASP	2.1
1	B	386	ASP	2.1
1	C	90	THR	2.1
1	C	102	PRO	2.1
1	A	468	GLN	2.1
1	C	604	VAL	2.1
1	D	379	ALA	2.1
1	A	116	LYS	2.1
1	D	84	LYS	2.1
1	A	470	SER	2.1
1	D	82	LYS	2.1
1	A	94	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	170	ASP	2.1
1	A	465	ASP	2.1
1	D	721	ASP	2.1
1	B	65	ILE	2.1
1	B	82	LYS	2.1
1	A	68	ILE	2.1
1	B	125	VAL	2.1
1	D	60	PHE	2.1
1	D	125	VAL	2.1
1	B	114	GLU	2.0
1	C	523	MET	2.0
1	B	161	ASN	2.0
1	B	157	ASP	2.0
1	A	5	GLN	2.0
1	C	248	ASP	2.0
1	D	560	LYS	2.0
1	A	125	VAL	2.0
1	A	164	GLU	2.0
1	D	62	GLY	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(Å ²)	Q<0.9
1	TRQ	A	697	16/17	0.95	0.09	19,20,30,47	0
1	TRQ	D	697	16/17	0.95	0.07	19,20,29,32	0
1	TRQ	C	697	16/17	0.97	0.06	16,17,34,44	0
1	TRQ	B	697	16/17	0.97	0.05	15,16,31,32	0

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
3	PEG	D	902	7/7	0.77	0.18	50,63,76,76	0
3	PEG	A	903	7/7	0.80	0.20	46,61,93,93	0
4	SO4	C	903	5/5	0.81	0.10	56,66,76,88	0
5	EDO	D	903	4/4	0.84	0.16	49,59,65,78	0
3	PEG	C	902	7/7	0.86	0.16	34,55,72,80	0
4	SO4	B	903	5/5	0.87	0.10	72,76,104,107	0
3	PEG	A	902	7/7	0.89	0.14	52,63,77,77	0
3	PEG	B	902	7/7	0.91	0.10	33,46,57,64	0
2	MG	D	901	1/1	0.97	0.03	23,23,23,23	0
2	MG	C	901	1/1	0.98	0.06	20,20,20,20	0
2	MG	B	901	1/1	0.98	0.04	18,18,18,18	0
2	MG	A	901	1/1	0.99	0.04	24,24,24,24	0

6.5 Other polymers [i](#)

There are no such residues in this entry.