Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 02:32 am BST

PDB ID	:	6BYW
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 following versions of software and data (see references ⓘ) were used in the production of this report:

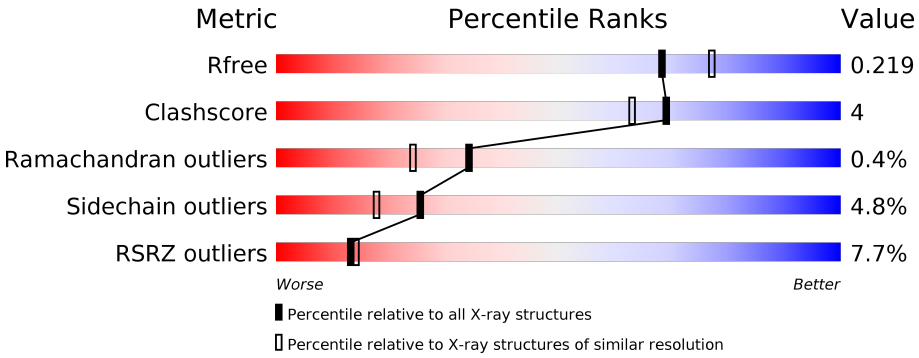
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.05 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}	130704	1692 (2.04-2.04)
Clashscore	141614	1773 (2.04-2.04)
Ramachandran outliers	138981	1752 (2.04-2.04)
Sidechain outliers	138945	1752 (2.04-2.04)
RSRZ outliers	127900	1672 (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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	9% 86% 9% • •
1	B	816	6% 86% 8% • •
1	C	816	7% 84% 10% • 5%
1	D	816	7% 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.

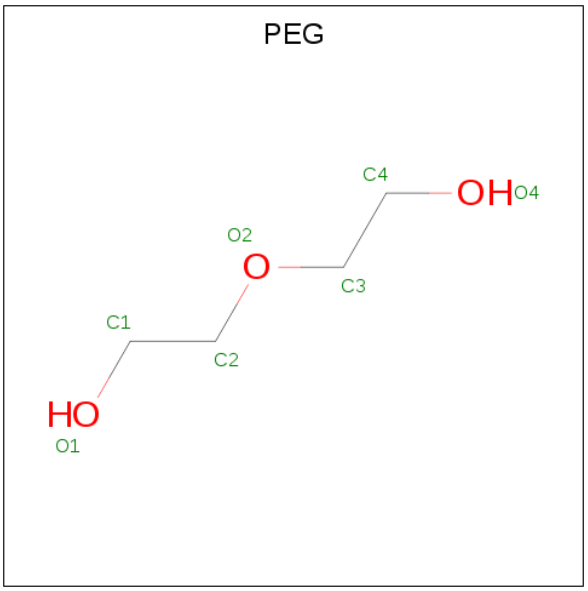
- Molecule 1 is a protein called GoxA.

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 (three-letter code: MG) (formula: Mg).

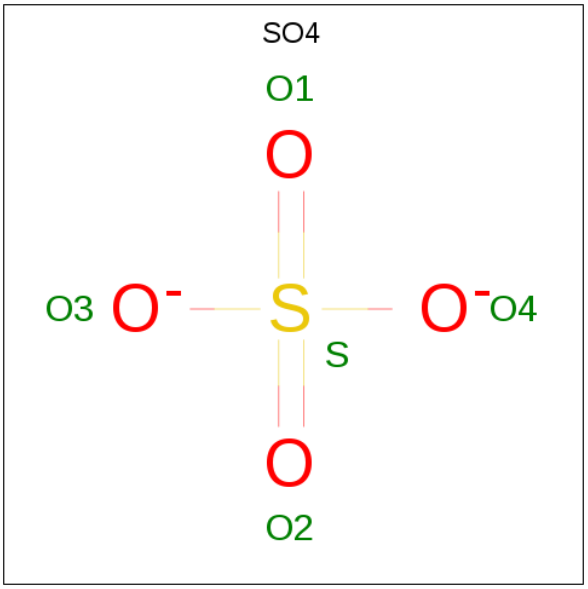
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Mg	0	0
			1	1		
2	A	1	Total	Mg	0	0
			1	1		
2	D	1	Total	Mg	0	0
			1	1		
2	C	1	Total	Mg	0	0
			1	1		

- Molecule 3 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



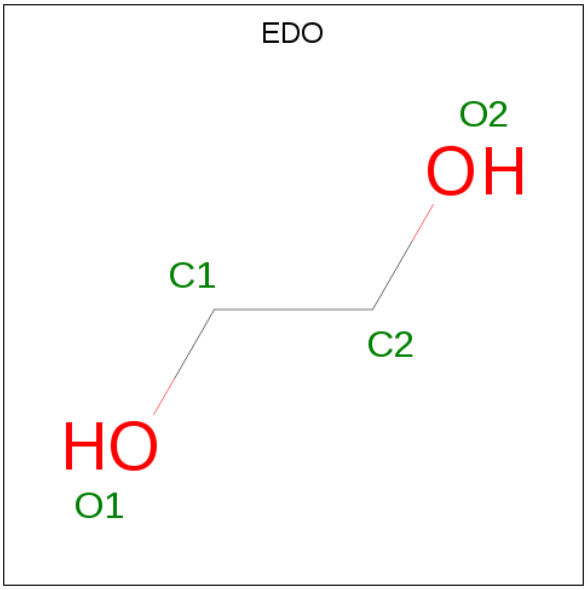
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	H	O	0	0
			17	4	10	3		
3	A	1	Total	C	H	O	0	0
			17	4	10	3		
3	A	1	Total	C	H	O	0	0
			17	4	10	3		
3	C	1	Total	C	H	O	0	0
			17	4	10	3		
3	D	1	Total	C	H	O	0	0
			17	4	10	3		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

- Molecule 6 is water.

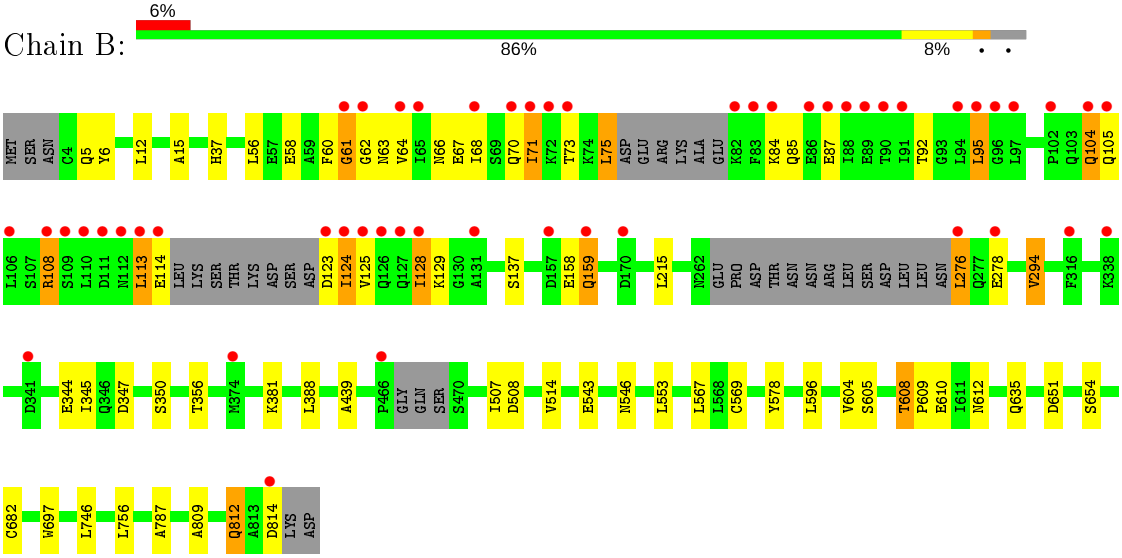
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	453	Total O 453 453	0	0
6	A	355	Total O 355 355	0	0
6	C	440	Total O 440 440	0	0
6	D	393	Total O 394 394	0	1

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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.

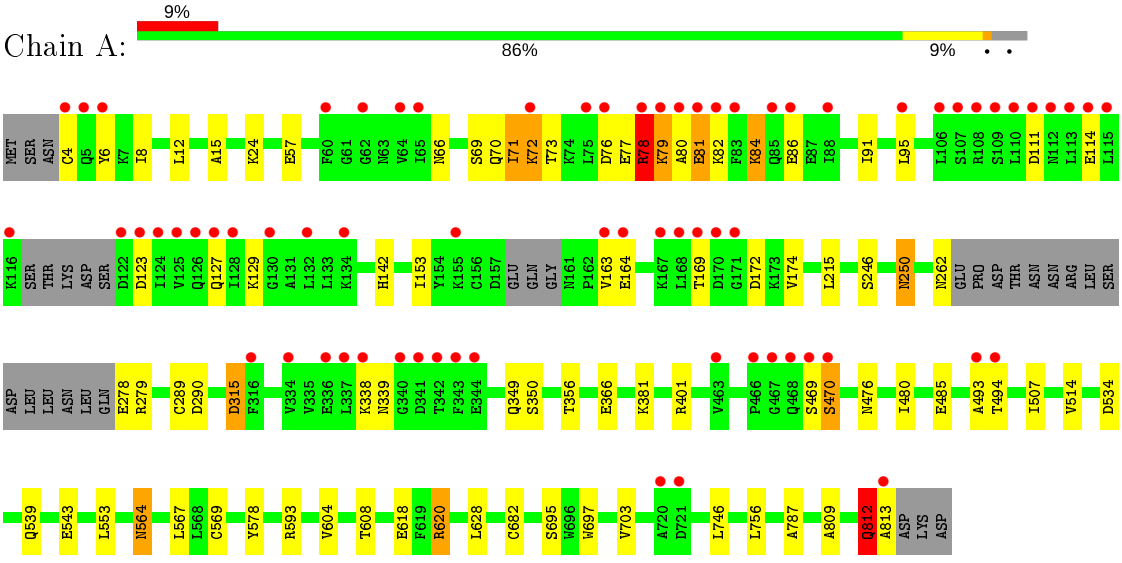
- Molecule 1: GoxA

Chain B:



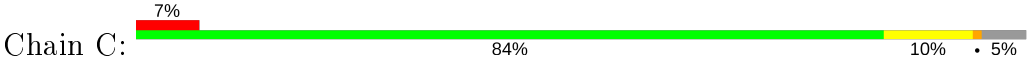
- Molecule 1: GoxA

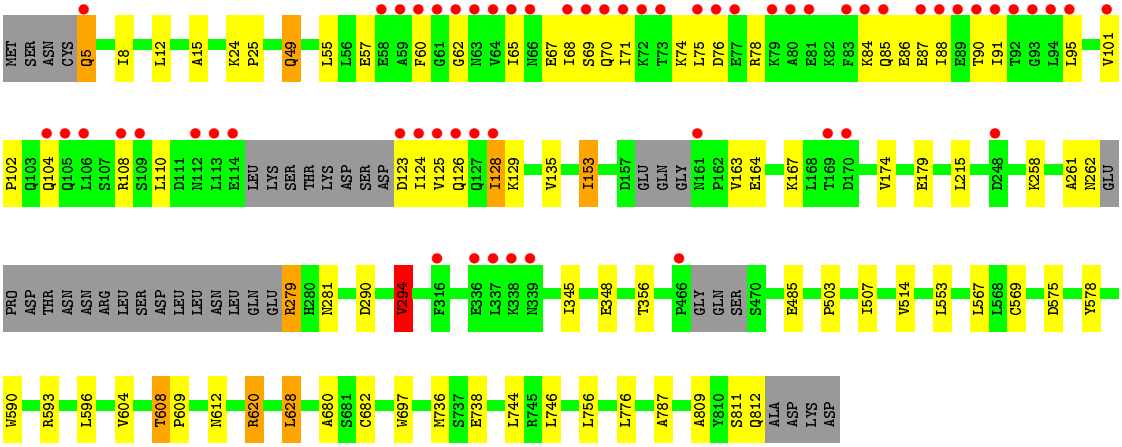
Chain A:



- Molecule 1: GoxA

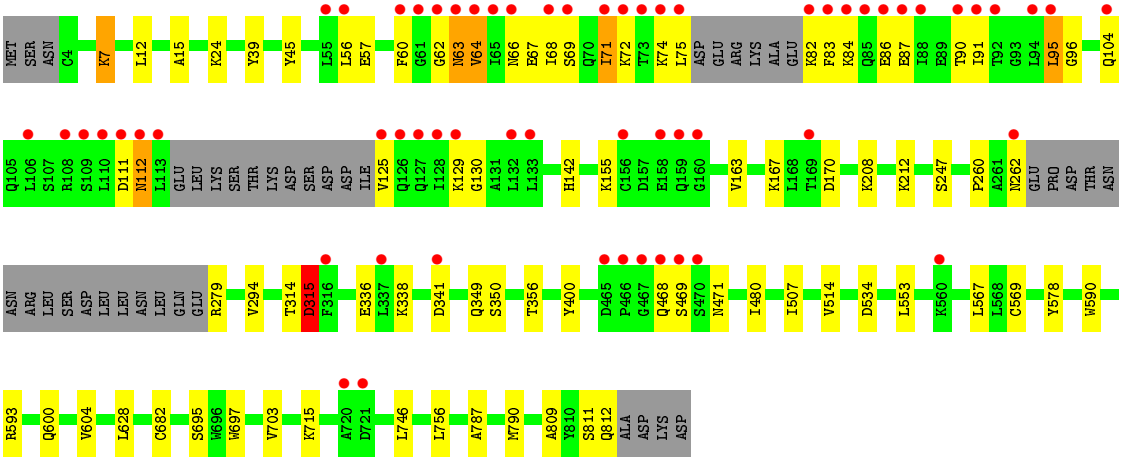
Chain C:





- Molecule 1: GoxA

Chain D:



4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [1]	1.89 (at 2.05Å)	Xtriage
Refinement program	PHENIX (1.12_2829: ???)	Depositor
R, R_{free}	0.185 , 0.219 0.186 , 0.219	Depositor DCC
R_{free} test set	11722 reflections (4.99%)	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 , 45.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: TRQ, MG, PEG, EDO, SO4

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	0.28	0/6376	0.50	0/8678
1	B	0.28	0/6319	0.53	4/8602 (0.0%)
1	C	0.27	0/6299	0.52	3/8573 (0.0%)
1	D	0.27	0/6274	0.50	0/8542
All	All	0.28	0/25268	0.51	7/34395 (0.0%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	294	VAL	CG1-CB-CG2	7.47	122.86	110.90
1	C	294	VAL	CG1-CB-CG2	6.63	121.51	110.90
1	B	276	LEU	CB-CG-CD2	6.61	122.24	111.00
1	B	75	LEU	CB-CG-CD1	6.41	121.89	111.00
1	C	55	LEU	C-N-CA	6.09	136.92	121.70
1	C	294	VAL	CA-CB-CG2	5.49	119.13	110.90
1	B	276	LEU	CB-CG-CD1	5.25	119.93	111.00

There are no chirality outliers.

There are no planarity outliers.

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	6244	5913	6010	49	0
1	B	6188	5858	5954	39	0
1	C	6168	5875	5941	49	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	2	0
All	All	26437	23533	23874	179	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 (179) 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: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:B:61:GLY:HA2	1:B:62:GLY:C	2.12	0.69
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:469:SER:HA	1:D:471:ASN:ND2	2.09	0.67
1:D:349:GLN:OE1	1:D:600:GLN:NE2	2.28	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:OD1	1:D:315[A]:ASP:N	2.33	0.62
1:A:493:ALA:O	1:A:494:THR:OG1	2.13	0.61
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:124:ILE:HD12	1:C:125:VAL:N	2.23	0.54
1:C:71:ILE:O	1:C:75:LEU:HD23	2.08	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:682:CYS:SG	1:D:697:TRQ:HB3	2.48	0.53
1:D:91:ILE:O	1:D:95:LEU:HD22	2.08	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:OE1	1:B:159:GLN:HA	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:A:80:ALA:HB1	1:A:81:GLU:HB3	1.94	0.50
1:A:564[A]:ASN:N	1:A:564[A]:ASN:OD1	2.45	0.50
1:A:349:GLN:O	1:A:620:ARG:HD2	2.11	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:A:76:ASP:O	1:A:79:LYS:HE3	2.13	0.49
1:B:567:LEU:HD23	1:B:604:VAL:HG21	1.95	0.49
1:D:142:HIS:ND1	6:D:1004:HOH:O	2.35	0.48
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:D:811:SER:O	1:D:812:GLN:HB2	2.13	0.48
1:C:612[A]:ASN:ND2	6:C:1019:HOH:O	2.45	0.48
1:D:24:LYS:NZ	6:D:1012:HOH:O	2.42	0.48
1:D:787:ALA:HB1	1:D:809:ALA:HB1	1.96	0.48
1:C:5:GLN:HE21	1:C:5:GLN:N	2.12	0.47
1:A:71:ILE:HD13	1:A:72:LYS:N	2.29	0.47
1:A:72:LYS:HE2	1:A:72:LYS:O	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:D:468:GLN:OE1	1:D:468:GLN:N	2.48	0.47
1:A:787:ALA:HB1	1:A:809:ALA:HB1	1.96	0.46
1:B:113:LEU:N	1:B:113:LEU:HD23	2.31	0.46
1:D:39:TYR:HH	1:D:400:TYR:HH	1.64	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:62:GLY:O	1:D:63:ASN:C	2.55	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: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:D:71:ILE:HG22	1:D:74:LYS:HD2	2.00	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:347:ASP:OD1	1:B:350:SER:OG	2.26	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:D:567:LEU:HD23	1:D:604:VAL:HG21	2.00	0.44
1:A:169:THR:OG1	1:A:338:LYS:HE3	2.18	0.43
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: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:A:514:VAL:O	1:A:514:VAL:HG12	2.18	0.43
1:B:787:ALA:HB1	1:B:809:ALA:HB1	2.00	0.43
1:D:86:GLU:O	1:D:90:THR:OG1	2.33	0.43
1:B:125:VAL:O	1:B:128:ILE:HG22	2.19	0.43
1:B:61:GLY:H	1:B:64:VAL:HG23	1.83	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:695:SER:HB2	1:A:703:VAL:HG21	2.01	0.42
1:A:95:LEU:HD12	1:A:95:LEU:N	2.34	0.42
1:C:680:ALA:HB3	1:C:776:LEU:HD22	2.01	0.42
1:B:608:THR:HG22	1:B:610:GLU:H	1.83	0.42
1:A:77:GLU:O	1:A:78:ARG:CB	2.68	0.42
1:B:68:ILE:HA	1:B:71:ILE:CD1	2.49	0.42
1:C:124:ILE:C	1:C:124:ILE:HD12	2.40	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:608:THR:HG23	1:B:609:PRO:HD2	2.01	0.42
1:C:514:VAL:O	1:C:514:VAL:HG12	2.20	0.42
1:C:62:GLY:CA	1:C:65:ILE:CD1	2.98	0.42
1:D:60:PHE:CD1	1:D:64:VAL:HG11	2.53	0.42
1:A:6:TYR:O	1:A:350:SER:OG	2.34	0.42
1:B:514:VAL:HG12	1:B:514:VAL:O	2.19	0.42
1:C:261:ALA:O	1:C:262:ASN:HB2	2.20	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: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:A:366:GLU:OE1	1:A:401:ARG:NE	2.46	0.41
1:B:92:THR:HA	1:B:95:LEU:HD22	2.03	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: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
1:A:250:ASN:HA	1:A:289:CYS:O	2.22	0.40
1:B:60:PHE:CE2	1:B:129:LYS:HG3	2.57	0.40
1:C:101:VAL:HG13	1:C:102:PRO:HD2	2.02	0.40
1:B:108:ARG:H	1:B:108:ARG:HG2	1.75	0.40
1:B:63:ASN:OD1	1:B:66:ASN:HB2	2.21	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%)	29	18
1	B	772/816 (95%)	752 (97%)	18 (2%)	2 (0%)	41	31
1	C	768/816 (94%)	743 (97%)	25 (3%)	0	100	100
1	D	769/816 (94%)	737 (96%)	26 (3%)	6 (1%)	19	10
All	All	3090/3264 (95%)	2981 (96%)	97 (3%)	12 (0%)	34	24

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	64	VAL
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 (i)

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%)	647 (94%)	38 (6%)	21	13
1	B	679/711 (96%)	641 (94%)	38 (6%)	21	12
1	C	677/711 (95%)	645 (95%)	32 (5%)	26	18
1	D	674/711 (95%)	648 (96%)	26 (4%)	32	25
All	All	2715/2844 (96%)	2581 (95%)	134 (5%)	25	17

All (134) 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
1	B	87	GLU
1	B	95	LEU
1	B	104	GLN
1	B	108	ARG
1	B	113	LEU
1	B	114	GLU
1	B	123	ASP
1	B	124	ILE
1	B	128	ILE
1	B	137	SER
1	B	215	LEU
1	B	276	LEU
1	B	278	GLU
1	B	294	VAL

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Mol	Chain	Res	Type
1	B	344	GLU
1	B	381	LYS
1	B	388	LEU
1	B	507	ILE
1	B	543	GLU
1	B	553	LEU
1	B	569	CYS
1	B	578	TYR
1	B	596	LEU
1	B	608	THR
1	B	746	LEU
1	B	756	LEU
1	B	812	GLN
1	B	814	ASP
1	A	12	LEU
1	A	66	ASN
1	A	69	SER
1	A	70	GLN
1	A	71	ILE
1	A	72	LYS
1	A	73	THR
1	A	78	ARG
1	A	79	LYS
1	A	82	LYS
1	A	84	LYS
1	A	111	ASP
1	A	114	GLU
1	A	123	ASP
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	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

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Mol	Chain	Res	Type
1	A	564[B]	ASN
1	A	569	CYS
1	A	578	TYR
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	49	GLN
1	C	67	GLU
1	C	69	SER
1	C	70	GLN
1	C	74	LYS
1	C	76	ASP
1	C	85	GLN
1	C	95	LEU
1	C	104	GLN
1	C	108	ARG
1	C	128	ILE
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	279	ARG
1	C	294	VAL
1	C	553	LEU
1	C	569	CYS
1	C	575	ASP
1	C	578	TYR
1	C	596	LEU
1	C	608	THR
1	C	620	ARG
1	C	628	LEU
1	C	738	GLU
1	C	746	LEU
1	C	756	LEU

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Mol	Chain	Res	Type
1	D	7	LYS
1	D	12	LEU
1	D	57	GLU
1	D	66	ASN
1	D	67	GLU
1	D	71	ILE
1	D	75	LEU
1	D	95	LEU
1	D	104	GLN
1	D	112	ASN
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	341	ASP
1	D	534	ASP
1	D	553	LEU
1	D	569	CYS
1	D	578	TYR
1	D	628	LEU
1	D	715	LYS
1	D	746	LEU
1	D	756	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	127	GLN
1	D	471	ASN
1	D	600	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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	13,17,18	4.84	7 (53%)	14,24,26	3.60	4 (28%)
1	TRQ	A	697	1	13,17,18	4.85	6 (46%)	14,24,26	3.55	3 (21%)
1	TRQ	C	697	1	13,17,18	4.72	5 (38%)	14,24,26	3.74	5 (35%)
1	TRQ	B	697	1	13,17,18	4.78	7 (53%)	14,24,26	3.56	4 (28%)

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	-	0/4/19/21	0/2/2/2
1	TRQ	A	697	1	-	0/4/19/21	0/2/2/2
1	TRQ	C	697	1	-	0/4/19/21	0/2/2/2
1	TRQ	B	697	1	-	0/4/19/21	0/2/2/2

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	697	TRQ	CH2-CZ2	-12.05	1.40	1.54
1	D	697	TRQ	CH2-CZ2	-11.81	1.40	1.54
1	B	697	TRQ	CH2-CZ2	-11.74	1.40	1.54
1	C	697	TRQ	CH2-CZ2	-11.25	1.41	1.54
1	C	697	TRQ	CE2-CZ2	-7.99	1.39	1.50
1	D	697	TRQ	CE2-CZ2	-7.94	1.39	1.50
1	D	697	TRQ	CD1-NE1	-7.92	1.24	1.36
1	A	697	TRQ	CE2-CZ2	-7.91	1.39	1.50
1	C	697	TRQ	CD1-NE1	-7.82	1.24	1.36
1	B	697	TRQ	CE2-CZ2	-7.77	1.39	1.50
1	B	697	TRQ	CD1-NE1	-7.73	1.24	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	697	TRQ	CD1-NE1	-7.71	1.24	1.36
1	C	697	TRQ	CD2-CE3	-3.58	1.37	1.44
1	D	697	TRQ	CD2-CE3	-3.55	1.37	1.44
1	B	697	TRQ	CD2-CE3	-3.51	1.37	1.44
1	A	697	TRQ	CD2-CE3	-3.43	1.37	1.44
1	A	697	TRQ	CZ3-CE3	2.62	1.39	1.34
1	B	697	TRQ	CZ3-CE3	2.60	1.39	1.34
1	C	697	TRQ	CZ3-CE3	2.58	1.39	1.34
1	D	697	TRQ	CZ3-CE3	2.56	1.39	1.34
1	A	697	TRQ	O6-CH2	-2.09	1.19	1.24
1	D	697	TRQ	O6-CH2	-2.08	1.19	1.24
1	B	697	TRQ	O6-CH2	-2.06	1.19	1.24
1	B	697	TRQ	CB-CG	2.05	1.54	1.51
1	D	697	TRQ	CB-CG	2.00	1.54	1.51

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	697	TRQ	CZ2-CE2-NE1	11.74	138.69	119.94
1	D	697	TRQ	CZ2-CE2-NE1	11.48	138.27	119.94
1	B	697	TRQ	CZ2-CE2-NE1	11.46	138.24	119.94
1	C	697	TRQ	CZ2-CE2-NE1	11.39	138.13	119.94
1	B	697	TRQ	CD2-CE2-NE1	-4.64	102.14	109.64
1	C	697	TRQ	CD2-CE2-NE1	-4.53	102.31	109.64
1	A	697	TRQ	CD2-CE2-NE1	-4.51	102.34	109.64
1	D	697	TRQ	CD2-CE2-NE1	-4.48	102.40	109.64
1	C	697	TRQ	O6-CH2-CZ2	4.07	121.28	118.51
1	D	697	TRQ	CB-CG-CD1	-3.79	123.28	127.97
1	B	697	TRQ	CB-CG-CD1	-3.61	123.50	127.97
1	C	697	TRQ	CB-CG-CD1	-3.59	123.54	127.97
1	A	697	TRQ	CB-CG-CD1	-3.07	124.18	127.97
1	D	697	TRQ	O6-CH2-CZ2	3.06	120.59	118.51
1	B	697	TRQ	O6-CH2-CZ2	2.55	120.24	118.51
1	C	697	TRQ	O7-CZ2-CE2	-2.37	119.33	121.84

There are no chirality outliers.

There are no torsion outliers.

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	A	697	TRQ	1	0
1	C	697	TRQ	1	0
1	B	697	TRQ	1	0

5.5 Carbohydrates (i)

There are no carbohydrates 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	D	902	-	6,6,6	0.46	0	5,5,5	0.43	0
3	PEG	A	903	-	6,6,6	0.46	0	5,5,5	0.27	0
5	EDO	D	903	-	3,3,3	0.49	0	2,2,2	0.27	0
3	PEG	A	902	-	6,6,6	0.49	0	5,5,5	1.11	0
4	SO4	C	903	-	4,4,4	0.16	0	6,6,6	0.18	0
3	PEG	C	902	-	6,6,6	0.56	0	5,5,5	0.43	0
3	PEG	B	902	-	6,6,6	0.48	0	5,5,5	0.23	0
4	SO4	B	903	-	4,4,4	0.11	0	6,6,6	0.20	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	D	902	-	-	2/4/4/4	-
3	PEG	A	903	-	-	1/4/4/4	-
5	EDO	D	903	-	-	0/1/1/1	-
3	PEG	A	902	-	-	3/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PEG	C	902	-	-	2/4/4/4	-
3	PEG	B	902	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (8) 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	D	902	PEG	O1-C1-C2-O2
3	A	903	PEG	O2-C3-C4-O4
3	D	902	PEG	O2-C3-C4-O4
3	A	902	PEG	C1-C2-O2-C3
3	C	902	PEG	O2-C3-C4-O4

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	902	PEG	1	0
3	C	902	PEG	2	0
4	B	903	SO4	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, 95^{th} 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%)	0.31	70 (8%)	9 10	19, 37, 83, 116	0
1	B	780/816 (95%)	0.21	51 (6%)	18 20	15, 28, 79, 122	0
1	C	777/816 (95%)	0.23	59 (7%)	13 14	16, 29, 74, 109	0
1	D	775/816 (94%)	0.28	61 (7%)	12 13	17, 33, 86, 139	0
All	All	3118/3264 (95%)	0.26	241 (7%)	13 14	15, 32, 81, 139	0

All (241) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	115	LEU	8.4
1	B	110	LEU	7.7
1	B	83	PHE	7.7
1	D	75	LEU	7.6
1	C	62	GLY	7.3
1	D	61	GLY	7.0
1	C	68	ILE	6.8
1	D	469	SER	6.7
1	D	73	THR	6.6
1	D	83	PHE	6.4
1	B	73	THR	6.4
1	D	84	LYS	6.4
1	B	68	ILE	6.3
1	C	65	ILE	6.3
1	D	68	ILE	6.3
1	D	86	GLU	6.2
1	D	129	LYS	6.1
1	B	61	GLY	6.1
1	C	88	ILE	6.0
1	D	71	ILE	5.7
1	B	124	ILE	5.7

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Mol	Chain	Res	Type	RSRZ
1	D	94	LEU	5.7
1	C	61	GLY	5.6
1	C	83	PHE	5.5
1	D	467	GLY	5.5
1	A	116	LYS	5.5
1	C	75	LEU	5.4
1	B	125	VAL	5.2
1	C	123	ASP	5.0
1	C	124	ILE	5.0
1	A	466	PRO	4.9
1	D	721	ASP	4.8
1	A	467	GLY	4.7
1	B	276	LEU	4.6
1	B	71	ILE	4.6
1	C	80	ALA	4.6
1	D	112	ASN	4.5
1	B	91	ILE	4.5
1	B	128	ILE	4.5
1	D	65	ILE	4.4
1	A	340	GLY	4.4
1	B	113	LEU	4.4
1	C	94	LEU	4.3
1	D	72	LYS	4.3
1	B	159	GLN	4.3
1	B	88	ILE	4.3
1	B	86	GLU	4.2
1	A	813	ALA	4.2
1	D	87	GLU	4.2
1	C	125	VAL	4.2
1	A	170	ASP	4.1
1	D	111	ASP	4.1
1	C	76	ASP	4.1
1	C	81	GLU	4.1
1	A	78	ARG	4.1
1	C	79	LYS	4.1
1	C	70	GLN	4.0
1	D	110	LEU	4.0
1	D	316	PHE	3.9
1	C	114	GLU	3.8
1	A	337	LEU	3.8
1	D	468	GLN	3.8
1	C	170	ASP	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	83	PHE	3.8
1	C	66	ASN	3.7
1	A	112	ASN	3.7
1	B	316	PHE	3.7
1	A	113	LEU	3.7
1	C	60	PHE	3.7
1	B	94	LEU	3.7
1	C	63	ASN	3.7
1	B	109	SER	3.6
1	A	122	ASP	3.6
1	C	69	SER	3.6
1	D	69	SER	3.6
1	B	82	LYS	3.6
1	D	64	VAL	3.5
1	C	85	GLN	3.5
1	D	126	GLN	3.5
1	D	66	ASN	3.4
1	D	466	PRO	3.4
1	A	110	LEU	3.4
1	C	95	LEU	3.4
1	D	74	LYS	3.4
1	C	112	ASN	3.4
1	A	316	PHE	3.4
1	C	316	PHE	3.4
1	D	60	PHE	3.4
1	A	132	LEU	3.4
1	C	106	LEU	3.4
1	C	77	GLU	3.4
1	A	62	GLY	3.4
1	A	167	LYS	3.3
1	D	82	LYS	3.3
1	A	81	GLU	3.3
1	C	64	VAL	3.3
1	B	90	THR	3.3
1	A	124	ILE	3.3
1	D	88	ILE	3.3
1	B	84	LYS	3.3
1	C	466	PRO	3.3
1	B	105	GLN	3.3
1	C	93	GLY	3.2
1	A	88	ILE	3.2
1	A	5	GLN	3.2

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Mol	Chain	Res	Type	RSRZ
1	D	127	GLN	3.2
1	B	106	LEU	3.2
1	D	133	LEU	3.2
1	A	82	LYS	3.2
1	C	108	ARG	3.1
1	A	114	GLU	3.1
1	A	343	PHE	3.1
1	D	132	LEU	3.1
1	D	91	ILE	3.1
1	A	721	ASP	3.1
1	C	71	ILE	3.1
1	C	84	LYS	3.1
1	B	64	VAL	3.1
1	A	168	LEU	3.1
1	C	89	GLU	3.0
1	A	341	ASP	3.0
1	C	87	GLU	3.0
1	C	113	LEU	3.0
1	C	90	THR	3.0
1	B	72	LYS	3.0
1	B	62	GLY	3.0
1	D	85	GLN	3.0
1	B	123	ASP	3.0
1	A	80	ALA	3.0
1	D	341	ASP	3.0
1	D	158	GLU	3.0
1	D	55	LEU	3.0
1	A	128	ILE	2.9
1	C	91	ILE	2.9
1	A	336	GLU	2.9
1	D	90	THR	2.9
1	D	159	GLN	2.9
1	B	127	GLN	2.9
1	D	106	LEU	2.9
1	A	127	GLN	2.9
1	B	97	LEU	2.9
1	A	75	LEU	2.9
1	D	104	GLN	2.8
1	B	466	PRO	2.8
1	D	128	ILE	2.8
1	D	262	ASN	2.8
1	C	248	ASP	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	87	GLU	2.8
1	B	112	ASN	2.8
1	C	338	LYS	2.8
1	C	73	THR	2.8
1	A	85	GLN	2.8
1	A	468	GLN	2.8
1	A	493	ALA	2.7
1	A	111	ASP	2.7
1	A	169	THR	2.7
1	D	95	LEU	2.7
1	D	108	ARG	2.7
1	C	92	THR	2.7
1	A	95	LEU	2.7
1	A	64	VAL	2.7
1	D	113	LEU	2.7
1	D	337	LEU	2.7
1	B	96	GLY	2.6
1	B	65	ILE	2.6
1	B	89	GLU	2.6
1	A	155	LYS	2.6
1	D	156	CYS	2.6
1	A	338	LYS	2.6
1	A	125	VAL	2.6
1	B	814	ASP	2.6
1	B	170	ASP	2.6
1	A	720	ALA	2.5
1	B	104	GLN	2.5
1	C	72	LYS	2.5
1	A	109	SER	2.5
1	B	114	GLU	2.5
1	C	109	SER	2.5
1	C	104	GLN	2.5
1	A	106	LEU	2.5
1	D	560	LYS	2.5
1	D	92	THR	2.4
1	C	127	GLN	2.4
1	C	101	VAL	2.4
1	B	126	GLN	2.4
1	A	164	GLU	2.4
1	A	79	LYS	2.4
1	D	63	ASN	2.4
1	B	95	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	56	LEU	2.4
1	C	105	GLN	2.4
1	B	102	PRO	2.4
1	C	59	ALA	2.4
1	A	494	THR	2.4
1	D	62	GLY	2.4
1	A	60	PHE	2.4
1	C	161	ASN	2.4
1	C	339	ASN	2.4
1	B	278	GLU	2.3
1	D	720	ALA	2.3
1	B	374	MET	2.3
1	A	342	THR	2.3
1	C	169	THR	2.3
1	A	470	SER	2.3
1	A	469	SER	2.3
1	D	109	SER	2.3
1	C	336	GLU	2.3
1	B	111	ASP	2.3
1	D	465	ASP	2.3
1	A	130	GLY	2.3
1	A	171	GLY	2.3
1	D	160	GLY	2.2
1	A	163	VAL	2.2
1	A	123	ASP	2.2
1	A	4	CYS	2.2
1	C	128	ILE	2.2
1	B	341	ASP	2.2
1	C	58	GLU	2.2
1	C	126	GLN	2.2
1	A	72	LYS	2.2
1	A	6	TYR	2.2
1	A	344	GLU	2.2
1	A	107	SER	2.1
1	A	463	VAL	2.1
1	A	108	ARG	2.1
1	B	338	LYS	2.1
1	B	70	GLN	2.1
1	A	334	VAL	2.1
1	B	131	ALA	2.1
1	A	76	ASP	2.1
1	D	470	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	169	THR	2.1
1	B	108	ARG	2.0
1	C	5	GLN	2.0
1	A	134	LYS	2.0
1	A	126	GLN	2.0
1	A	65	ILE	2.0
1	C	337	LEU	2.0
1	B	157	ASP	2.0
1	A	86	GLU	2.0
1	D	125	VAL	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, 95^{th} 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	0.18	19,20,30,47	0
1	TRQ	D	697	16/17	0.96	0.17	19,20,29,32	0
1	TRQ	C	697	16/17	0.97	0.16	16,17,34,44	0
1	TRQ	B	697	16/17	0.97	0.17	15,16,31,32	0

6.3 Carbohydrates (i)

There are no carbohydrates 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, 95^{th} 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	0.53	0.31	50,63,76,76	0
3	PEG	A	903	7/7	0.71	0.26	46,61,93,93	0
3	PEG	C	902	7/7	0.85	0.21	34,55,72,80	0
3	PEG	A	902	7/7	0.88	0.19	52,63,77,77	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	PEG	B	902	7/7	0.91	0.11	33,46,57,64	0
5	EDO	D	903	4/4	0.92	0.11	49,59,65,78	0
4	SO4	C	903	5/5	0.92	0.28	56,66,76,88	0
4	SO4	B	903	5/5	0.95	0.25	72,76,104,107	0
2	MG	C	901	1/1	0.98	0.06	20,20,20,20	0
2	MG	A	901	1/1	0.98	0.13	24,24,24,24	0
2	MG	D	901	1/1	0.98	0.16	23,23,23,23	0
2	MG	B	901	1/1	0.98	0.10	18,18,18,18	0

6.5 Other polymers (i)

There are no such residues in this entry.