Full wwPDB X-ray Structure Validation Report (i)

Dec 10, 2023 – 11:46 pm GMT

PDB ID	:	2VL4
Title	:	Structural and biochemical evidence for a boat-like transition state in beta-mannosidases
Authors	:	Tailford, L.E.; Offen, W.A.; Smith, N.L.; Dumon, C.; Moreland, C.; Gratien, J.; Heck, M.P.; Stick, R.V.; Bleriot, Y.; Vasella, A.; Gilbert, H.J.; Davies, G.J.
Deposited on	:	2008-01-08
Resolution	:	1.90 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 (i) 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 (i)) were used in the production of this report:

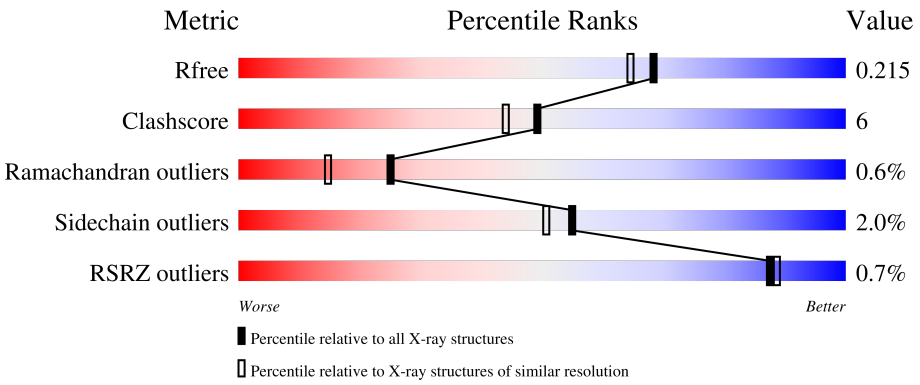
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 1.90 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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 <=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	846	% 86% 11% • •
1	B	846	89% 9% • •

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	EDO	A	1872	-	-	X	-
3	EDO	B	1888	-	-	X	-
4	BR	A	1880	-	-	X	-
5	CL	B	1896	-	-	X	-

2 Entry composition (i)

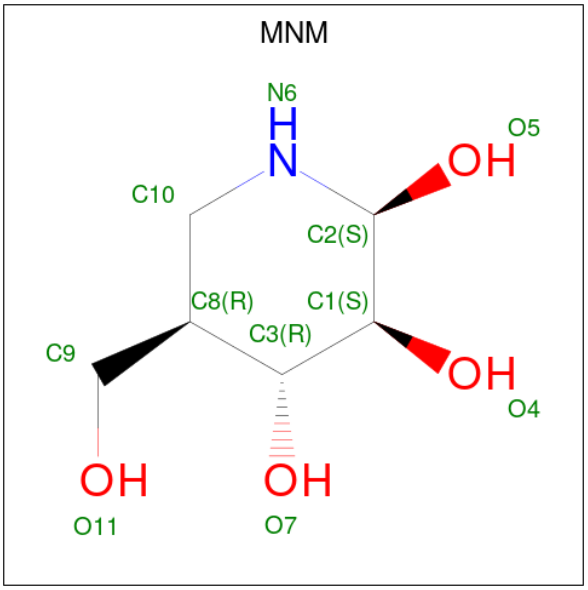
There are 6 unique types of molecules in this entry. The entry contains 15415 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 BETA-MANNOSIDASE.

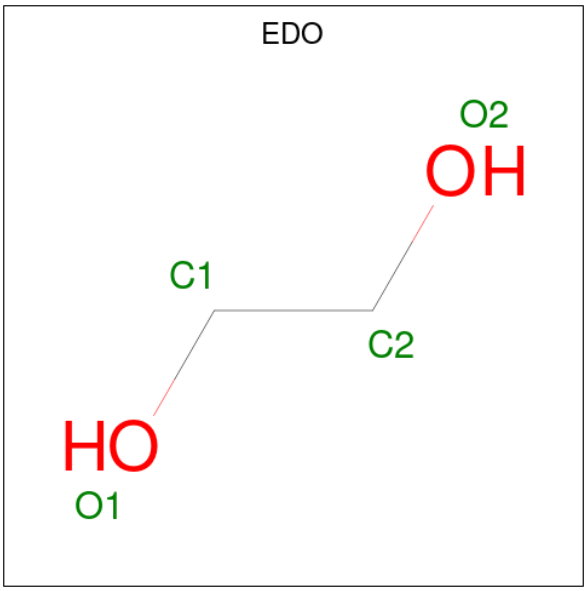
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	836	6894	4422	1158	1281	33	0	19	0
1	B	841	6881	4408	1159	1280	34	0	19	0

- Molecule 2 is (2S,3S,4R,5R)-2,3,4-TRIHYDROXY-5-HYDROXYMETHYL-PIPERIDINE (three-letter code: MNM) (formula: $C_6H_{13}NO_4$).



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

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
3	A	1	4	2	2	0	0
3	A	1	4	2	2	0	0
3	A	1	4	2	2	0	0
3	A	1	4	2	2	0	0
3	A	1	4	2	2	0	0
3	A	1	4	2	2	0	0
3	A	1	4	2	2	0	0
3	A	1	4	2	2	0	0
3	A	1	4	2	2	0	0
3	A	1	4	2	2	0	0
3	A	1	4	2	2	0	0
3	A	1	4	2	2	0	0
3	A	1	4	2	2	0	0
3	A	1	4	2	2	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
3	A	1	4	2	2	0	0
3	B	1	4	2	2	0	0
3	B	1	4	2	2	0	0
3	B	1	4	2	2	0	0
3	B	1	4	2	2	0	0
3	B	1	4	2	2	0	0
3	B	1	4	2	2	0	0
3	B	1	4	2	2	0	0
3	B	1	4	2	2	0	0
3	B	1	4	2	2	0	0
3	B	1	4	2	2	0	0
3	B	1	4	2	2	0	0
3	B	1	4	2	2	0	0
3	B	1	4	2	2	0	0
3	B	1	4	2	2	0	0
3	B	1	4	2	2	0	0
3	B	1	4	2	2	0	0
3	B	1	4	2	2	0	0
3	B	1	4	2	2	0	0
3	B	1	4	2	2	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
3	B	1	4	2	2	0	0

- Molecule 4 is BROMIDE ION (three-letter code: BR) (formula: Br).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Br		
4	A	7	7	7	0	0
4	B	4	4	4	0	0

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
5	A	2	2	2	0	0
5	B	3	3	3	0	0

- Molecule 6 is water.

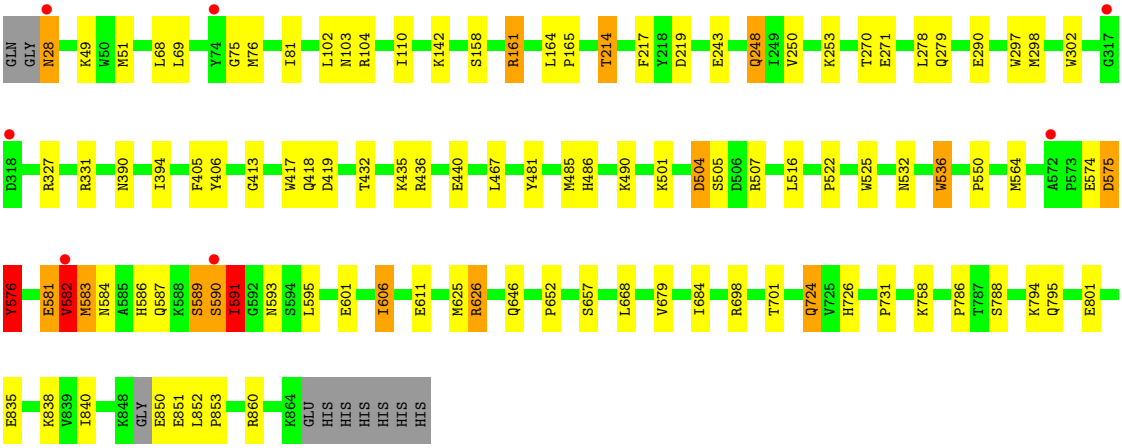
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	700	700	700	0	0
6	B	758	758	758	0	0

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.

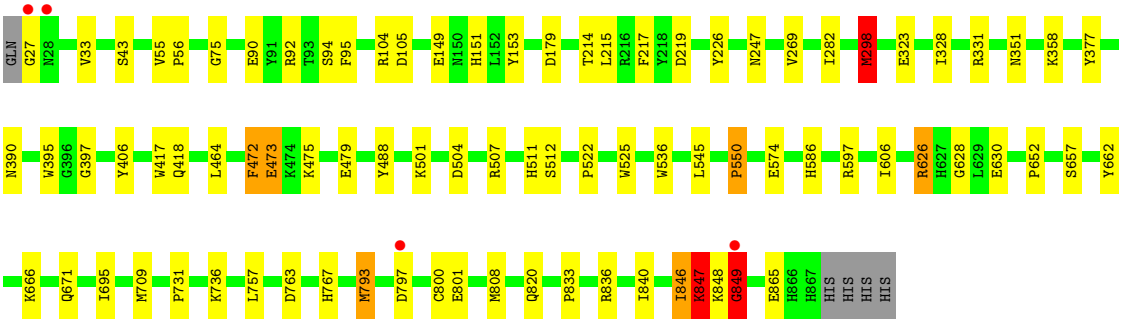
• Molecule 1: BETA-MANNOSIDASE

Chain A:



• Molecule 1: BETA-MANNOSIDASE

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	90.56Å 115.04Å 98.70Å 90.00° 112.59° 90.00°	Depositor
Resolution (Å)	48.91 – 1.90 47.68 – 1.90	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.91-1.90) 100.0 (47.68-1.90)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.66 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.4.0062	Depositor
R, R_{free}	0.162 , 0.215 0.162 , 0.215	Depositor DCC
R_{free} test set	7278 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å^2)	20.0	Xtriage
Anisotropy	0.042	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 52.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	15415	wwPDB-VP
Average B, all atoms (Å^2)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.37% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: CL, MNM, BR, EDO

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	0.87	0/7122	0.85	11/9676 (0.1%)
1	B	0.89	3/7106 (0.0%)	0.80	4/9654 (0.0%)
All	All	0.88	3/14228 (0.0%)	0.83	15/19330 (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	2	6
1	B	0	4
All	All	2	10

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	226	TYR	CD1-CE1	6.12	1.48	1.39
1	B	865	GLU	CG-CD	-5.97	1.43	1.51
1	B	269	VAL	CB-CG2	-5.02	1.42	1.52

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	473	GLU	N-CA-C	-9.88	84.33	111.00
1	A	582	VAL	N-CA-C	9.34	136.23	111.00
1	A	590	SER	C-N-CA	6.24	137.31	121.70
1	B	298[A]	MET	CG-SD-CE	6.16	110.06	100.20
1	B	298[B]	MET	CG-SD-CE	6.16	110.06	100.20
1	A	419	ASP	CB-CG-OD1	5.86	123.58	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	590	SER	N-CA-C	-5.85	95.20	111.00
1	A	591	ILE	N-CA-C	-5.65	95.75	111.00
1	A	219	ASP	CB-CG-OD2	-5.63	113.23	118.30
1	A	591	ILE	N-CA-CB	5.43	123.28	110.80
1	A	28	ASN	CB-CA-C	5.36	121.12	110.40
1	B	179	ASP	CB-CG-OD2	-5.24	113.58	118.30
1	A	504	ASP	CB-CG-OD1	5.23	123.00	118.30
1	A	575	ASP	CB-CA-C	-5.16	100.07	110.40
1	A	504	ASP	CB-CG-OD2	-5.02	113.78	118.30

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	582	VAL	CA
1	A	584[B]	ASN	CA

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	575	ASP	Peptide
1	A	576	TYR	Peptide
1	A	581	GLU	Peptide
1	A	582	VAL	Peptide
1	A	589	SER	Peptide
1	A	590	SER	Peptide
1	B	472	PHE	Peptide
1	B	846	ILE	Peptide
1	B	847	LYS	Peptide
1	B	849	GLY	Peptide

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	6894	0	6670	91	0
1	B	6881	0	6635	66	0
2	A	11	0	13	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	11	0	13	0	0
3	A	60	0	90	11	0
3	B	84	0	126	15	0
4	A	7	0	0	2	0
4	B	4	0	0	0	0
5	A	2	0	0	0	0
5	B	3	0	0	4	0
6	A	700	0	0	17	1
6	B	758	0	0	2	1
All	All	15415	0	13547	163	1

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 6.

All (163) 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:B:626[A]:ARG:HH11	1:B:626[A]:ARG:CG	1.58	1.15
1:B:797[A]:ASP:OD2	5:B:1896:CL:CL	2.02	1.15
1:A:161:ARG:HB3	6:A:2135:HOH:O	1.52	1.05
1:A:214[A]:THR:HG22	6:A:2091:HOH:O	1.57	1.03
1:B:390:ASN:ND2	3:B:1883:EDO:H21	1.74	1.03
1:B:626[A]:ARG:HG3	1:B:626[A]:ARG:NH1	1.45	1.02
1:B:390:ASN:HD22	3:B:1883:EDO:H21	1.24	1.00
1:A:298:MET:CE	1:A:302:TRP:HB3	1.92	0.98
1:B:695:ILE:HG23	3:B:1874:EDO:H22	1.52	0.91
1:A:467:LEU:HD22	1:A:485:MET:HE1	1.54	0.86
1:B:797[A]:ASP:CG	5:B:1896:CL:CL	2.51	0.86
1:A:248[A]:GLN:C	1:A:248[A]:GLN:HE21	1.78	0.86
1:B:793:MET:SD	1:B:800[B]:CYS:SG	2.73	0.85
1:A:481:TYR:CZ	1:A:485:MET:HE2	2.11	0.85
1:A:298:MET:HE3	1:A:302:TRP:HB3	1.57	0.84
1:A:626:ARG:HG3	6:A:2571:HOH:O	1.78	0.84
1:B:298[A]:MET:HE3	1:B:351:ASN:HB2	1.62	0.81
4:A:1880:BR:BR	6:A:2579:HOH:O	2.53	0.79
1:A:69:LEU:HD22	1:A:81:ILE:HG22	1.64	0.79
1:A:584[B]:ASN:HB3	6:A:2504:HOH:O	1.84	0.77
1:B:33:VAL:HG13	1:B:214:THR:HG23	1.66	0.76
1:A:583:MET:O	1:A:584[B]:ASN:ND2	2.19	0.76
3:A:1888:EDO:H21	6:A:2634:HOH:O	1.85	0.76
1:A:601:GLU:HA	1:A:606:ILE:HD11	1.69	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:486:HIS:HB2	6:A:2436:HOH:O	1.87	0.73
1:A:298:MET:HE3	1:A:302:TRP:CB	2.20	0.72
1:B:298[A]:MET:CE	1:B:351:ASN:HB2	2.19	0.71
1:A:786:PRO:HA	1:A:860[B]:ARG:NE	2.06	0.70
5:B:1889:CL:CL	6:B:2609:HOH:O	2.47	0.70
1:A:564:MET:HG3	1:A:611[A]:GLU:HG2	1.74	0.70
1:A:467:LEU:HB3	1:A:485:MET:CE	2.22	0.69
1:B:298[A]:MET:CE	1:B:351:ASN:HD22	2.07	0.68
5:B:1894:CL:CL	6:B:2239:HOH:O	2.48	0.68
1:A:214[A]:THR:HG21	6:A:2197:HOH:O	1.95	0.67
1:B:472:PHE:O	1:B:475:LYS:HB2	1.95	0.66
1:A:110:ILE:HB	1:A:214[A]:THR:HG23	1.78	0.66
1:A:852:LEU:HD12	1:A:853:PRO:HD2	1.79	0.65
1:B:153:TYR:CE2	3:B:1888:EDO:H21	2.32	0.64
1:A:584[B]:ASN:OD1	1:A:593:ASN:ND2	2.26	0.64
1:B:626[A]:ARG:HH11	1:B:626[A]:ARG:HG3	0.65	0.64
1:B:695:ILE:CG2	3:B:1874:EDO:H22	2.26	0.63
1:A:576:TYR:HD1	1:A:576:TYR:H	1.44	0.63
1:A:390:ASN:HD22	3:A:1876:EDO:H11	1.63	0.63
1:B:848:LYS:O	1:B:849:GLY:C	2.38	0.62
1:A:601:GLU:CA	1:A:606:ILE:HD11	2.29	0.61
1:A:576:TYR:CD1	1:A:576:TYR:N	2.69	0.61
1:A:248[A]:GLN:NE2	1:A:250:VAL:H	2.00	0.60
1:A:467:LEU:HB3	1:A:485:MET:HE3	1.84	0.58
1:A:51:MET:CE	6:A:2024:HOH:O	2.52	0.58
1:A:758:LYS:HG3	6:A:2629:HOH:O	2.05	0.57
1:B:298[B]:MET:HA	1:B:298[B]:MET:HE3	1.84	0.57
1:A:576:TYR:HD1	1:A:576:TYR:N	2.02	0.57
1:A:801:GLU:HG2	1:A:840:ILE:HG12	1.86	0.57
1:A:394:ILE:HD11	1:A:405:PHE:CE2	2.39	0.57
1:A:525:TRP:CD1	3:A:1872:EDO:H21	2.40	0.57
1:A:248[B]:GLN:OE1	1:A:278:LEU:HB2	2.05	0.56
1:B:92:ARG:NH1	3:B:1888:EDO:O2	2.38	0.56
1:A:550:PRO:HB3	3:A:1872:EDO:H12	1.89	0.54
1:B:153:TYR:HE2	3:B:1888:EDO:H21	1.71	0.54
1:B:247:ASN:HD22	1:B:282:ILE:HD13	1.72	0.54
1:B:731:PRO:HG2	1:B:736:LYS:HE2	1.88	0.54
1:A:795:GLN:NE2	1:A:850:GLU:HB2	2.23	0.54
1:B:298[A]:MET:HE2	1:B:351:ASN:HD22	1.71	0.54
1:B:33:VAL:HG13	1:B:214:THR:CG2	2.37	0.54
1:A:270:THR:HG21	1:A:290:GLU:O	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:846:ILE:HG22	1:B:847:LYS:CA	2.38	0.53
1:A:467:LEU:HB3	1:A:485:MET:HE1	1.90	0.53
1:B:626[A]:ARG:CG	1:B:626[A]:ARG:NH1	2.30	0.53
1:B:33:VAL:CG1	1:B:214:THR:HG23	2.38	0.53
1:A:248[A]:GLN:HG3	1:A:279:GLN:O	2.07	0.53
1:A:522:PRO:HA	1:A:525:TRP:CD2	2.44	0.52
1:A:298:MET:HE2	1:A:302:TRP:HB3	1.87	0.52
1:B:377:TYR:CE2	3:B:1893:EDO:H21	2.45	0.52
1:A:243:GLU:OE1	6:A:2229:HOH:O	2.19	0.52
1:B:153:TYR:HD2	3:B:1888:EDO:O1	1.93	0.52
1:A:838:LYS:HE3	1:A:840:ILE:HD11	1.91	0.51
1:B:464:LEU:HD22	1:B:511:HIS:HE1	1.75	0.51
1:A:75:GLY:HA2	1:A:582:VAL:HG13	1.91	0.51
1:A:271:GLU:HG2	6:A:2262:HOH:O	2.10	0.51
1:A:51:MET:HE3	6:A:2024:HOH:O	2.11	0.51
1:A:679:VAL:HG23	1:A:698:ARG:HD2	1.93	0.51
1:A:606:ILE:HD12	1:A:606:ILE:N	2.26	0.51
1:B:104:ARG:HG3	1:B:217:PHE:HB3	1.93	0.51
1:A:522:PRO:HA	1:A:525:TRP:CE2	2.45	0.51
1:A:525:TRP:CG	3:A:1872:EDO:H21	2.46	0.51
1:A:601:GLU:HA	1:A:606:ILE:CD1	2.38	0.50
1:A:646:GLN:O	1:A:657:SER:HA	2.11	0.50
1:B:808[A]:MET:HA	1:B:833:PRO:HB3	1.94	0.50
1:A:586:HIS:HD2	1:A:652:PRO:O	1.95	0.50
1:A:102:LEU:O	1:A:142:LYS:HE3	2.11	0.50
3:A:1867:EDO:H22	6:A:2693:HOH:O	2.12	0.50
1:A:486:HIS:CE1	1:A:490:LYS:HE3	2.47	0.49
1:B:586:HIS:HD2	1:B:652:PRO:O	1.96	0.49
1:A:625:MET:HB2	1:A:668:LEU:HD13	1.94	0.49
1:A:584[B]:ASN:ND2	1:A:587:GLN:CB	2.75	0.49
1:B:328:ILE:HG23	3:B:1871:EDO:H22	1.95	0.48
1:A:679:VAL:CG2	1:A:698:ARG:HD2	2.44	0.48
1:B:43:SER:HA	3:B:1873:EDO:H12	1.96	0.48
1:B:406:TYR:OH	1:B:418:GLN:NE2	2.45	0.48
1:A:104:ARG:HG3	1:A:217:PHE:HB3	1.94	0.47
1:A:248[B]:GLN:OE1	1:A:278:LEU:CB	2.61	0.47
1:A:606:ILE:N	1:A:606:ILE:CD1	2.77	0.47
1:B:479:GLU:H	1:B:479:GLU:CD	2.17	0.47
1:A:584[B]:ASN:ND2	1:A:587:GLN:HB2	2.29	0.47
1:B:358:LYS:HE2	3:B:1883:EDO:H22	1.96	0.47
1:A:406:TYR:OH	1:A:418:GLN:NE2	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:76:MET:HE3	6:A:2502:HOH:O	2.14	0.47
1:B:27:GLY:HA3	1:B:323:GLU:OE1	2.15	0.47
1:A:501:LYS:O	1:A:505:SER:HB3	2.15	0.46
1:B:105:ASP:HB2	1:B:219:ASP:HA	1.98	0.46
1:B:801:GLU:HG2	1:B:840:ILE:HG12	1.97	0.46
1:B:545:LEU:HD13	1:B:628:GLY:HA3	1.98	0.46
1:B:55:VAL:HA	1:B:56:PRO:C	2.36	0.46
1:B:657:SER:O	1:B:666:LYS:HD2	2.16	0.45
1:A:158:SER:HB3	1:A:161:ARG:HG2	1.99	0.45
1:B:501:LYS:HA	1:B:501:LYS:HD2	1.79	0.45
1:A:51:MET:HG2	6:A:2024:HOH:O	2.15	0.45
1:A:758:LYS:NZ	1:A:835:GLU:OE2	2.46	0.45
1:B:488:TYR:OH	1:B:512:SER:HB2	2.16	0.45
1:B:522:PRO:HA	1:B:525:TRP:CE2	2.50	0.45
1:A:583:MET:C	1:A:584[B]:ASN:ND2	2.70	0.45
1:A:724:GLN:HB3	1:A:726:HIS:CE1	2.52	0.45
1:B:597:ARG:HG2	1:B:606:ILE:HD13	1.99	0.45
1:B:626[B]:ARG:HB3	1:B:671:GLN:HB3	1.99	0.45
1:B:820:GLN:HA	1:B:820:GLN:OE1	2.17	0.44
1:A:467:LEU:CD2	1:A:485:MET:HE1	2.36	0.44
1:B:75:GLY:O	1:B:586:HIS:HE1	2.01	0.44
1:B:395:TRP:CH2	1:B:397:GLY:HA3	2.53	0.44
1:B:95:PHE:CE1	1:B:215:LEU:HD11	2.53	0.43
1:A:584[B]:ASN:ND2	1:A:587:GLN:HB3	2.34	0.43
1:A:164:LEU:N	1:A:165:PRO:HD2	2.32	0.43
1:A:504:ASP:OD2	1:A:507:ARG:HD2	2.18	0.43
1:A:532:ASN:CG	3:A:1872:EDO:O2	2.56	0.43
1:B:464:LEU:HD22	1:B:511:HIS:CE1	2.54	0.43
1:B:662:TYR:HA	3:B:1872:EDO:H22	2.01	0.43
1:B:709:MET:HB3	1:B:757:LEU:HD11	2.00	0.43
1:B:90:GLU:OE1	1:B:153:TYR:OH	2.32	0.43
1:A:390:ASN:HD22	3:A:1876:EDO:C1	2.31	0.43
1:A:481:TYR:CZ	1:A:485:MET:CE	2.94	0.42
1:B:298[A]:MET:HE3	1:B:351:ASN:CB	2.41	0.42
1:A:525:TRP:CD2	3:A:1872:EDO:H21	2.55	0.42
1:B:507:ARG:NH1	3:B:1871:EDO:O1	2.49	0.42
1:A:248[A]:GLN:HE22	1:A:250:VAL:H	1.64	0.42
1:A:435:LYS:HA	1:A:435:LYS:HD2	1.89	0.42
1:A:684:ILE:HD12	4:A:1880:BR:BR	2.75	0.41
1:B:153:TYR:CD2	3:B:1888:EDO:H21	2.55	0.41
1:A:248[A]:GLN:NE2	1:A:250:VAL:N	2.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:327:ARG:O	3:A:1877:EDO:H12	2.21	0.41
1:B:574:GLU:H	1:B:574:GLU:CD	2.24	0.41
1:A:248[A]:GLN:HE22	1:A:250:VAL:N	2.19	0.41
1:B:507:ARG:HH21	1:B:507:ARG:HD2	1.76	0.41
1:A:51:MET:SD	1:A:68:LEU:HD11	2.61	0.41
1:A:701:THR:HG23	1:A:731:PRO:HA	2.03	0.41
3:A:1876:EDO:H12	6:A:2345:HOH:O	2.21	0.41
1:B:763:ASP:OD2	1:B:767:HIS:HB3	2.20	0.41
1:A:110:ILE:HB	1:A:214[A]:THR:CG2	2.51	0.40
1:A:536:TRP:O	1:A:595[B]:LEU:HD21	2.20	0.40
1:B:94[A]:SER:HG	1:B:151:HIS:HD1	1.65	0.40
1:A:297:TRP:CZ2	1:A:413:GLY:HA2	2.57	0.40
1:A:432[B]:THR:O	1:A:436[B]:ARG:HG3	2.22	0.40
1:A:574:GLU:H	1:A:574:GLU:CD	2.25	0.40
1:B:504:ASP:OD2	1:B:507:ARG:HD2	2.22	0.40
1:B:626[A]:ARG:HD3	1:B:630:GLU:CD	2.42	0.40

All (1) 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)
6:A:2108:HOH:O	6:B:2124:HOH:O[1_655]	2.03	0.17

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	851/846 (101%)	829 (97%)	16 (2%)	6 (1%)	22 12
1	B	853/846 (101%)	829 (97%)	20 (2%)	4 (0%)	29 18
All	All	1704/1692 (101%)	1658 (97%)	36 (2%)	10 (1%)	25 15

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	576	TYR
1	A	582	VAL
1	A	583	MET
1	A	591	ILE
1	A	851	GLU
1	B	847	LYS
1	B	849	GLY
1	A	536	TRP
1	B	536	TRP
1	B	550	PRO

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	751/754 (100%)	729 (97%)	22 (3%)	42	35
1	B	751/754 (100%)	740 (98%)	11 (2%)	65	62
All	All	1502/1508 (100%)	1469 (98%)	33 (2%)	55	47

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	ASN
1	A	49	LYS
1	A	103	ASN
1	A	161	ARG
1	A	214[A]	THR
1	A	214[B]	THR
1	A	248[A]	GLN
1	A	248[B]	GLN
1	A	253	LYS
1	A	331	ARG
1	A	417	TRP
1	A	440	GLU
1	A	516	LEU

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Mol	Chain	Res	Type
1	A	576	TYR
1	A	581	GLU
1	A	589	SER
1	A	591	ILE
1	A	606	ILE
1	A	626	ARG
1	A	724	GLN
1	A	788	SER
1	A	794	LYS
1	B	149[A]	GLU
1	B	298[A]	MET
1	B	298[B]	MET
1	B	331	ARG
1	B	417	TRP
1	B	473	GLU
1	B	550	PRO
1	B	626[A]	ARG
1	B	626[B]	ARG
1	B	793	MET
1	B	836	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	242	ASN
1	A	274	GLN
1	A	418	GLN
1	A	486	HIS
1	A	726	HIS
1	B	247	ASN
1	B	274	GLN
1	B	279	GLN
1	B	337	ASN
1	B	351	ASN
1	B	388	ASN
1	B	418	GLN
1	B	586	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 54 ligands modelled in this entry, 16 are monoatomic - leaving 38 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	EDO	B	1871	-	3,3,3	0.98	0	2,2,2	0.33	0
3	EDO	B	1893	-	3,3,3	0.41	0	2,2,2	0.33	0
3	EDO	A	1872	-	3,3,3	0.49	0	2,2,2	0.22	0
3	EDO	A	1877	-	3,3,3	1.14	0	2,2,2	0.89	0
3	EDO	A	1876	-	3,3,3	0.60	0	2,2,2	0.81	0
3	EDO	A	1873	-	3,3,3	0.80	0	2,2,2	0.31	0
3	EDO	A	1869	-	3,3,3	0.59	0	2,2,2	0.24	0
3	EDO	B	1883	-	3,3,3	0.54	0	2,2,2	0.69	0
3	EDO	B	1878	-	3,3,3	0.42	0	2,2,2	1.25	0
3	EDO	B	1881	-	3,3,3	0.64	0	2,2,2	0.16	0
3	EDO	A	1866	-	3,3,3	0.57	0	2,2,2	0.36	0
3	EDO	B	1874	-	3,3,3	1.07	0	2,2,2	0.51	0
3	EDO	A	1870	-	3,3,3	0.36	0	2,2,2	0.17	0
3	EDO	B	1880	-	3,3,3	0.47	0	2,2,2	0.27	0
3	EDO	B	1890	-	3,3,3	0.40	0	2,2,2	0.77	0
3	EDO	B	1892	-	3,3,3	0.57	0	2,2,2	0.07	0
3	EDO	A	1874	-	3,3,3	0.67	0	2,2,2	0.32	0
3	EDO	B	1879	-	3,3,3	0.50	0	2,2,2	0.53	0
3	EDO	B	1891	-	3,3,3	0.51	0	2,2,2	0.20	0
3	EDO	B	1875	-	3,3,3	0.54	0	2,2,2	0.71	0
3	EDO	B	1895	-	3,3,3	0.44	0	2,2,2	0.52	0
3	EDO	A	1868	-	3,3,3	0.75	0	2,2,2	0.24	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	EDO	B	1869	-	3,3,3	0.82	0	2,2,2	0.16	0
3	EDO	B	1870	-	3,3,3	0.59	0	2,2,2	0.34	0
3	EDO	A	1888	-	3,3,3	0.32	0	2,2,2	0.88	0
3	EDO	A	1887	-	3,3,3	0.37	0	2,2,2	0.80	0
3	EDO	B	1872	-	3,3,3	0.50	0	2,2,2	0.24	0
3	EDO	B	1876	-	3,3,3	1.24	0	2,2,2	1.21	0
3	EDO	B	1877	-	3,3,3	0.60	0	2,2,2	0.50	0
3	EDO	A	1871	-	3,3,3	0.61	0	2,2,2	0.25	0
3	EDO	B	1882	-	3,3,3	0.50	0	2,2,2	0.27	0
2	MNM	B	1868	-	9,11,11	1.21	1 (11%)	10,15,15	2.02	2 (20%)
2	MNM	A	1865	-	9,11,11	1.07	1 (11%)	10,15,15	1.82	1 (10%)
3	EDO	B	1888	-	3,3,3	0.31	0	2,2,2	0.69	0
3	EDO	A	1867	-	3,3,3	0.76	0	2,2,2	0.20	0
3	EDO	A	1875	-	3,3,3	0.60	0	2,2,2	0.13	0
3	EDO	B	1873	-	3,3,3	0.65	0	2,2,2	0.63	0
3	EDO	A	1884	-	3,3,3	0.51	0	2,2,2	0.07	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	EDO	B	1871	-	-	1/1/1/1	-
3	EDO	B	1893	-	-	1/1/1/1	-
3	EDO	A	1872	-	-	1/1/1/1	-
3	EDO	A	1877	-	-	0/1/1/1	-
3	EDO	A	1876	-	-	1/1/1/1	-
3	EDO	A	1873	-	-	0/1/1/1	-
3	EDO	A	1869	-	-	1/1/1/1	-
3	EDO	B	1883	-	-	1/1/1/1	-
3	EDO	B	1878	-	-	0/1/1/1	-
3	EDO	B	1881	-	-	0/1/1/1	-
3	EDO	A	1866	-	-	0/1/1/1	-
3	EDO	B	1874	-	-	0/1/1/1	-
3	EDO	A	1870	-	-	0/1/1/1	-
3	EDO	B	1880	-	-	1/1/1/1	-
3	EDO	B	1890	-	-	1/1/1/1	-
3	EDO	B	1892	-	-	1/1/1/1	-
3	EDO	A	1874	-	-	0/1/1/1	-
3	EDO	B	1879	-	-	0/1/1/1	-
3	EDO	B	1891	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	B	1875	-	-	0/1/1/1	-
3	EDO	B	1895	-	-	1/1/1/1	-
3	EDO	A	1868	-	-	1/1/1/1	-
3	EDO	B	1869	-	-	0/1/1/1	-
3	EDO	B	1870	-	-	0/1/1/1	-
3	EDO	A	1888	-	-	1/1/1/1	-
3	EDO	A	1887	-	-	1/1/1/1	-
3	EDO	B	1872	-	-	0/1/1/1	-
3	EDO	B	1876	-	-	0/1/1/1	-
3	EDO	B	1877	-	-	1/1/1/1	-
3	EDO	A	1871	-	-	0/1/1/1	-
3	EDO	B	1882	-	-	0/1/1/1	-
2	MNM	B	1868	-	-	0/2/19/19	0/1/1/1
2	MNM	A	1865	-	-	0/2/19/19	0/1/1/1
3	EDO	B	1888	-	-	1/1/1/1	-
3	EDO	A	1867	-	-	0/1/1/1	-
3	EDO	A	1875	-	-	1/1/1/1	-
3	EDO	B	1873	-	-	1/1/1/1	-
3	EDO	A	1884	-	-	1/1/1/1	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1868	MNM	C8-C3	2.46	1.56	1.53
2	A	1865	MNM	C8-C3	2.13	1.55	1.53

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1865	MNM	C10-N6-C2	5.39	119.38	108.98
2	B	1868	MNM	C10-N6-C2	5.16	118.92	108.98
2	B	1868	MNM	O4-C1-C2	2.62	114.08	109.39

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1875	EDO	O1-C1-C2-O2
3	B	1880	EDO	O1-C1-C2-O2
3	A	1876	EDO	O1-C1-C2-O2
3	B	1883	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
3	B	1890	EDO	O1-C1-C2-O2
3	B	1892	EDO	O1-C1-C2-O2
3	B	1893	EDO	O1-C1-C2-O2
3	B	1895	EDO	O1-C1-C2-O2
3	B	1888	EDO	O1-C1-C2-O2
3	A	1872	EDO	O1-C1-C2-O2
3	B	1873	EDO	O1-C1-C2-O2
3	A	1888	EDO	O1-C1-C2-O2
3	A	1868	EDO	O1-C1-C2-O2
3	B	1871	EDO	O1-C1-C2-O2
3	A	1884	EDO	O1-C1-C2-O2
3	A	1887	EDO	O1-C1-C2-O2
3	A	1869	EDO	O1-C1-C2-O2
3	B	1877	EDO	O1-C1-C2-O2

There are no ring outliers.

12 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1871	EDO	2	0
3	B	1893	EDO	1	0
3	A	1872	EDO	5	0
3	A	1877	EDO	1	0
3	A	1876	EDO	3	0
3	B	1883	EDO	3	0
3	B	1874	EDO	2	0
3	A	1888	EDO	1	0
3	B	1872	EDO	1	0
3	B	1888	EDO	5	0
3	A	1867	EDO	1	0
3	B	1873	EDO	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 (i)

6.1 Protein, DNA and RNA chains (i)

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	836/846 (98%)	-0.34	7 (0%)	86	87	10, 19, 37, 53	0
1	B	841/846 (99%)	-0.50	4 (0%)	91	92	10, 19, 35, 48	5 (0%)
All	All	1677/1692 (99%)	-0.42	11 (0%)	87	88	10, 19, 37, 53	5 (0%)

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	27	GLY	3.5
1	A	582	VAL	3.3
1	A	317	GLY	3.3
1	A	572	ALA	2.7
1	A	318	ASP	2.6
1	B	849	GLY	2.5
1	A	28	ASN	2.4
1	B	28[A]	ASN	2.4
1	A	74	TYR	2.4
1	B	797[A]	ASP	2.3
1	A	590	SER	2.2

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	EDO	B	1874	4/4	0.76	0.17	24,25,26,30	0
3	EDO	B	1895	4/4	0.80	0.17	52,53,53,56	0
3	EDO	B	1890	4/4	0.82	0.15	50,52,52,52	0
3	EDO	A	1875	4/4	0.82	0.12	46,46,47,48	0
3	EDO	B	1876	4/4	0.84	0.13	21,24,26,26	0
3	EDO	A	1877	4/4	0.86	0.17	20,26,27,28	0
3	EDO	B	1891	4/4	0.86	0.12	41,42,43,45	0
3	EDO	B	1883	4/4	0.86	0.15	31,32,33,33	0
3	EDO	A	1872	4/4	0.87	0.15	28,29,32,33	0
5	CL	B	1894	1/1	0.87	0.13	43,43,43,43	1
3	EDO	A	1876	4/4	0.89	0.13	27,28,28,32	0
3	EDO	B	1888	4/4	0.89	0.24	41,42,42,43	0
3	EDO	A	1869	4/4	0.89	0.12	37,38,39,41	0
3	EDO	A	1888	4/4	0.91	0.14	30,30,32,34	0
3	EDO	B	1892	4/4	0.91	0.18	45,46,46,47	0
3	EDO	A	1867	4/4	0.91	0.14	15,25,28,32	0
3	EDO	A	1887	4/4	0.91	0.17	37,40,41,43	0
3	EDO	B	1873	4/4	0.92	0.15	29,29,30,32	0
3	EDO	B	1878	4/4	0.92	0.11	23,25,26,34	0
3	EDO	B	1869	4/4	0.92	0.12	19,19,23,24	0
3	EDO	B	1872	4/4	0.93	0.12	38,38,39,41	0
3	EDO	A	1870	4/4	0.94	0.10	29,31,31,33	0
3	EDO	B	1893	4/4	0.94	0.15	46,48,49,52	0
3	EDO	B	1870	4/4	0.94	0.12	26,29,30,31	0
5	CL	A	1889	1/1	0.94	0.09	60,60,60,60	0
3	EDO	B	1871	4/4	0.94	0.12	13,27,29,32	0
3	EDO	B	1877	4/4	0.95	0.10	24,25,29,29	0
5	CL	A	1885	1/1	0.95	0.25	27,27,27,27	1
3	EDO	B	1879	4/4	0.96	0.14	22,23,26,26	0
3	EDO	B	1880	4/4	0.96	0.10	31,31,34,34	0
3	EDO	A	1866	4/4	0.96	0.07	21,25,26,27	0
3	EDO	A	1873	4/4	0.96	0.09	18,22,22,29	0
3	EDO	A	1868	4/4	0.96	0.10	17,19,24,25	0
3	EDO	A	1871	4/4	0.96	0.07	17,21,24,24	0
3	EDO	B	1881	4/4	0.97	0.08	21,21,22,24	0
3	EDO	B	1882	4/4	0.97	0.06	27,28,29,30	0
3	EDO	A	1884	4/4	0.97	0.08	24,28,29,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	EDO	A	1874	4/4	0.97	0.12	22,23,23,24	0
2	MNM	B	1868	11/11	0.98	0.11	13,15,16,18	0
3	EDO	B	1875	4/4	0.98	0.12	18,21,23,24	0
4	BR	A	1879	1/1	0.98	0.10	17,17,17,17	1
5	CL	B	1896	1/1	0.98	0.18	29,29,29,29	1
4	BR	A	1883	1/1	0.99	0.10	21,21,21,21	1
4	BR	A	1886	1/1	0.99	0.07	27,27,27,27	1
4	BR	B	1884	1/1	0.99	0.07	23,23,23,23	1
4	BR	B	1885	1/1	0.99	0.13	20,20,20,20	1
4	BR	B	1886	1/1	0.99	0.12	17,17,17,17	1
4	BR	B	1887	1/1	0.99	0.10	30,30,30,30	1
4	BR	A	1878	1/1	0.99	0.08	21,21,21,21	1
2	MNM	A	1865	11/11	0.99	0.09	12,15,16,17	0
5	CL	B	1889	1/1	0.99	0.07	23,23,23,23	0
4	BR	A	1881	1/1	0.99	0.04	20,20,20,20	1
4	BR	A	1882	1/1	0.99	0.15	18,18,18,18	1
4	BR	A	1880	1/1	1.00	0.07	24,24,24,24	1

6.5 Other polymers (i)

There are no such residues in this entry.