Full wwPDB X-ray Structure Validation Report (i)

Dec 9, 2023 – 04:53 pm GMT

PDB ID	:	2VMF
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	:	2008-01-25
Resolution	:	2.10 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:

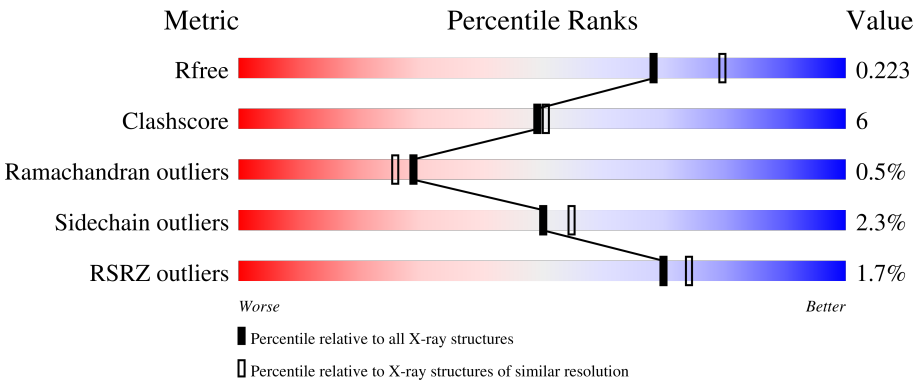
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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	.% 87% 11% ••
1	B	846	2% 86% 12% ••

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	B	1895	-	-	X	-
5	CL	B	1893	-	-	X	-

2 Entry composition (i)

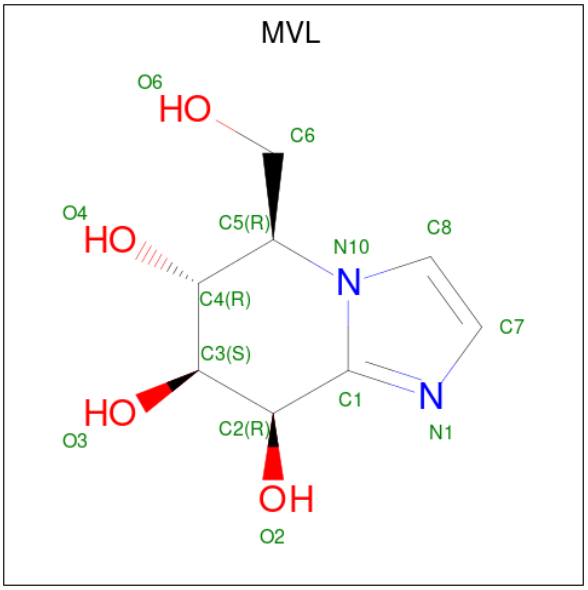
There are 6 unique types of molecules in this entry. The entry contains 14845 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

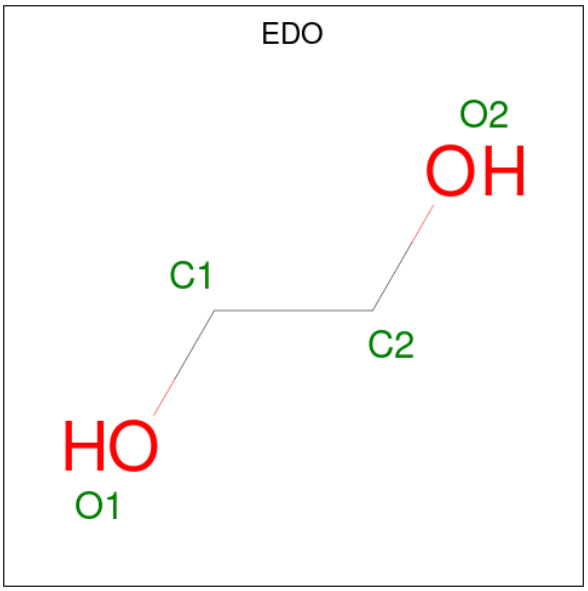
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	835	6803	4371	1136	1263	33	0	19	0
1	B	840	6878	4410	1151	1284	33	0	20	0

- Molecule 2 is (5R,6R,7S,8R)-5-(HYDROXYMETHYL)-5,6,7,8-TETRAHYDROIMIDAZO[1,2-A]PYRIDINE-6,7,8-TRIOL (three-letter code: MVL) (formula: $C_8H_{12}N_2O_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	14	8	2	4	0	0
2	B	1	14	8	2	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	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	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
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	9	Total Br 9 9	0	0
4	B	7	Total Br 7 7	0	0

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

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

- Molecule 6 is water.

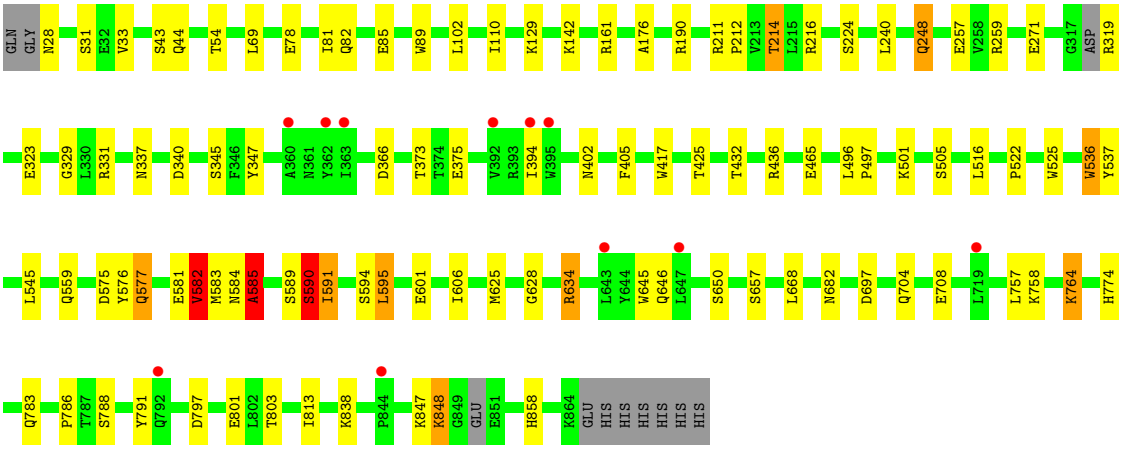
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	468	Total O 468 468	0	0
6	B	481	Total O 481 481	0	0

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.

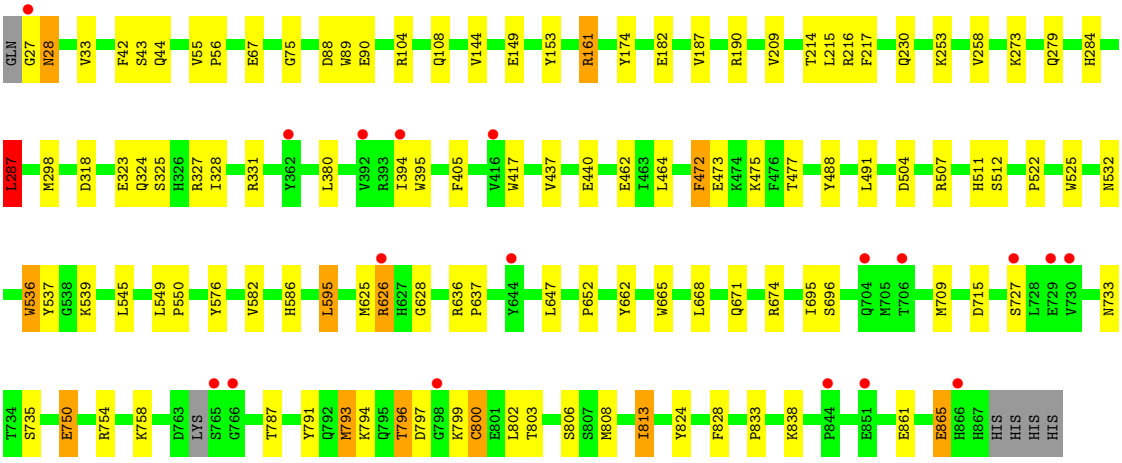
• Molecule 1: BETA-MANNOSIDASE

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	91.05Å 114.66Å 99.09Å 90.00° 113.19° 90.00°	Depositor
Resolution (Å)	37.45 – 2.10 35.60 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.9 (37.45-2.10) 99.9 (35.60-2.10)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.54 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.4.0062	Depositor
R, R_{free}	0.164 , 0.223 0.165 , 0.223	Depositor DCC
R_{free} test set	5385 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å^2)	24.6	Xtriage
Anisotropy	0.023	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 48.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	14845	wwPDB-VP
Average B, all atoms (Å^2)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.63% 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: EDO, CL, MVL, BR

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	0/7019	0.87	10/9538 (0.1%)
1	B	0.88	3/7100 (0.0%)	0.84	6/9649 (0.1%)
All	All	0.88	3/14119 (0.0%)	0.85	16/19187 (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	1	6
1	B	0	1
All	All	1	7

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	865	GLU	CB-CG	-6.13	1.40	1.52
1	B	865	GLU	CG-CD	-5.18	1.44	1.51
1	B	800	CYS	CB-SG	-5.15	1.73	1.81

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	591[A]	ILE	N-CA-C	9.82	137.50	111.00
1	B	473	GLU	N-CA-C	-9.54	85.24	111.00
1	A	583	MET	N-CA-C	-7.99	89.42	111.00
1	A	582	VAL	CB-CA-C	7.76	126.15	111.40
1	A	590	SER	N-CA-C	-6.40	93.72	111.00
1	B	549	LEU	CA-CB-CG	-6.04	101.41	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	190	ARG	NE-CZ-NH1	5.97	123.28	120.30
1	B	287	LEU	CA-CB-CG	5.66	128.31	115.30
1	B	215	LEU	CB-CG-CD1	-5.61	101.47	111.00
1	A	634	ARG	NE-CZ-NH2	-5.48	117.56	120.30
1	B	595	LEU	CA-CB-CG	5.47	127.89	115.30
1	A	340	ASP	CB-CG-OD1	5.46	123.22	118.30
1	A	585	ALA	N-CA-C	5.31	125.33	111.00
1	A	240	LEU	CA-CB-CG	5.23	127.33	115.30
1	A	577	GLN	N-CA-C	5.19	125.00	111.00
1	A	190	ARG	NE-CZ-NH2	-5.03	117.78	120.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	582	VAL	CA

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	576	TYR	Peptide
1	A	581	GLU	Peptide
1	A	582	VAL	Peptide
1	A	584	ASN	Peptide
1	A	589	SER	Peptide
1	A	590	SER	Peptide
1	B	472	PHE	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	6803	0	6535	67	0
1	B	6878	0	6576	85	0
2	A	14	0	12	1	0
2	B	14	0	12	4	0
3	A	84	0	126	12	0
3	B	76	0	114	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	9	0	0	1	0
4	B	7	0	0	3	0
5	A	4	0	0	1	0
5	B	7	0	0	5	0
6	A	468	0	0	7	0
6	B	481	0	0	13	0
All	All	14845	0	13375	161	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (161) 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)
5:B:1884:CL:CL	6:B:2116:HOH:O	1.90	1.22
4:B:1901:BR:BR	6:B:2473:HOH:O	2.19	1.16
1:A:214[A]:THR:HG22	6:A:2061:HOH:O	1.52	1.09
1:A:432:THR:HG22	1:A:436[B]:ARG:HH12	1.17	1.09
1:A:432:THR:CG2	1:A:436[B]:ARG:HH12	1.69	1.04
1:B:298[A]:MET:SD	5:B:1892:CL:CL	2.55	1.01
1:A:432:THR:HG22	1:A:436[B]:ARG:NH1	1.74	1.00
5:B:1893:CL:CL	6:B:2209:HOH:O	2.21	0.93
1:A:432:THR:CG2	1:A:436[B]:ARG:NH1	2.33	0.90
3:B:1895:EDO:H12	6:B:2167:HOH:O	1.73	0.86
1:B:472:PHE:O	1:B:475:LYS:HB2	1.79	0.83
1:A:375[A]:GLU:OE1	6:A:2227:HOH:O	1.98	0.82
1:B:793:MET:CE	1:B:800:CYS:HB3	2.11	0.80
1:B:27:GLY:HA3	1:B:323:GLU:OE1	1.82	0.79
1:B:665:TRP:CD2	3:B:1900:EDO:H12	2.18	0.78
1:B:33:VAL:HG13	1:B:214:THR:HG23	1.66	0.77
1:B:695:ILE:HG23	3:B:1875:EDO:H22	1.66	0.76
1:B:626[A]:ARG:HG2	1:B:671:GLN:HB3	1.67	0.75
1:B:824:TYR:O	3:B:1900:EDO:H22	1.89	0.73
1:B:230:GLN:HE21	3:B:1899:EDO:H21	1.55	0.72
1:B:149[A]:GLU:OE2	6:B:2094:HOH:O	2.08	0.70
1:B:464:LEU:HD22	1:B:511:HIS:HE1	1.56	0.70
3:B:1877:EDO:C1	6:B:2473:HOH:O	2.40	0.70
1:B:793:MET:HE1	1:B:800:CYS:HB3	1.72	0.69
1:B:88:ASP:CG	1:B:161[B]:ARG:HH21	1.97	0.67
1:B:796:THR:HG22	1:B:799:LYS:HB3	1.76	0.67
1:A:82:GLN:O	1:A:85:GLU:HG2	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:28:ASN:HB2	1:A:323:GLU:OE1	1.96	0.66
4:B:1891:BR:BR	6:B:2234:HOH:O	2.70	0.65
1:B:537:TYR:HE2	2:B:1868:MVL:H8	1.62	0.64
1:B:253:LYS:NZ	1:B:279:GLN:HB3	2.13	0.62
1:B:525:TRP:CE2	3:B:1869:EDO:H22	2.35	0.62
1:B:861[A]:GLU:OE1	6:B:2465:HOH:O	2.16	0.62
1:B:318[B]:ASP:C	1:B:318[B]:ASP:OD2	2.38	0.62
1:A:704:GLN:HB3	1:A:764:LYS:HG2	1.82	0.62
1:A:797:ASP:H	1:A:848:LYS:HD2	1.65	0.61
1:A:536:TRP:CH2	1:A:559:GLN:HB2	2.36	0.61
1:B:665:TRP:CG	3:B:1900:EDO:H12	2.35	0.61
1:B:793:MET:HE2	1:B:800:CYS:HB3	1.83	0.61
1:A:394:ILE:HD11	1:A:405:PHE:CE2	2.36	0.60
1:A:43:SER:HA	3:A:1879:EDO:H12	1.82	0.60
1:A:257:GLU:OE1	1:A:259:ARG:NH1	2.31	0.60
1:A:161:ARG:CB	3:A:1880:EDO:H12	2.32	0.59
1:B:695:ILE:CG2	3:B:1875:EDO:H22	2.34	0.58
1:A:402:ASN:ND2	6:A:2242:HOH:O	2.36	0.58
1:A:110:ILE:HB	1:A:214[A]:THR:HG23	1.85	0.57
1:B:477:THR:HG23	4:B:1882:BR:BR	2.59	0.57
1:A:525:TRP:CE2	3:A:1867:EDO:H22	2.40	0.57
1:A:801[A]:GLU:OE1	1:A:838:LYS:NZ	2.38	0.56
1:B:793:MET:HE3	1:B:802:LEU:CD1	2.36	0.56
1:B:464:LEU:HD22	1:B:511:HIS:CE1	2.38	0.55
1:B:324:GLN:NE2	5:B:1893:CL:CL	2.75	0.55
1:B:750:GLU:O	1:B:754:ARG:HG3	2.07	0.55
1:B:253:LYS:HZ2	1:B:279:GLN:HB3	1.70	0.55
1:B:536:TRP:CE2	1:B:595:LEU:HD23	2.41	0.55
1:B:104:ARG:HG3	1:B:217:PHE:HB3	1.89	0.54
1:A:161:ARG:HB3	3:A:1880:EDO:H12	1.88	0.54
1:A:271[A]:GLU:HG2	6:A:2173:HOH:O	2.08	0.54
1:B:327:ARG:HH11	3:B:1895:EDO:H22	1.73	0.54
1:A:78:GLU:O	1:A:81:ILE:HG12	2.07	0.53
1:A:704:GLN:NE2	1:A:764:LYS:HE3	2.23	0.53
1:A:537[A]:TYR:HE2	2:A:1865:MVL:H8	1.73	0.53
1:A:347:TYR:CE2	3:A:1888:EDO:H12	2.45	0.52
1:B:787:THR:OG1	1:B:806:SER:OG	2.28	0.52
1:A:28:ASN:N	6:A:2001:HOH:O	2.42	0.51
1:A:797:ASP:HB3	1:A:847:LYS:HA	1.91	0.51
1:A:129:LYS:NZ	3:A:1895:EDO:O2	2.36	0.51
1:B:88:ASP:CG	1:B:161[B]:ARG:NH2	2.61	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:697:ASP:HB3	3:A:1899:EDO:H12	1.93	0.51
1:B:793:MET:CE	1:B:802:LEU:HD11	2.42	0.50
1:B:626[A]:ARG:HH22	1:B:674:ARG:HB2	1.77	0.50
1:A:69:LEU:HD22	1:A:81:ILE:HG22	1.93	0.50
1:B:625:MET:HB2	1:B:668:LEU:HD13	1.93	0.50
1:B:636:ARG:HG3	1:B:637:PRO:HA	1.94	0.50
1:B:90:GLU:OE1	1:B:153[A]:TYR:OH	2.17	0.50
1:B:813:ILE:O	1:B:828:PHE:HA	2.11	0.50
1:A:522:PRO:HA	1:A:525:TRP:CD2	2.46	0.49
1:B:328:ILE:HG23	3:B:1876:EDO:H22	1.94	0.49
1:A:601:GLU:HB2	1:A:606:ILE:HD11	1.94	0.49
1:B:522:PRO:HA	1:B:525:TRP:CE2	2.47	0.49
1:B:808[B]:MET:HA	1:B:833:PRO:HB3	1.95	0.48
3:B:1877:EDO:H12	6:B:2473:HOH:O	2.09	0.48
1:A:545:LEU:HD13	1:A:628:GLY:HA3	1.94	0.48
1:B:108:GLN:OE1	1:B:216[A]:ARG:NH1	2.40	0.48
1:A:102:LEU:O	1:A:142:LYS:HE3	2.14	0.48
1:A:536:TRP:CE2	1:A:595:LEU:HD23	2.48	0.48
1:A:373:THR:HG22	1:B:796:THR:OG1	2.13	0.48
1:A:501:LYS:O	1:A:505:SER:HB3	2.14	0.48
1:B:55:VAL:HA	1:B:56:PRO:C	2.33	0.48
1:A:31:SER:OG	1:A:216:ARG:NH1	2.43	0.48
1:A:161:ARG:HB2	3:A:1880:EDO:H12	1.94	0.48
1:A:797:ASP:HB3	1:A:848:LYS:N	2.29	0.47
1:B:394:ILE:HD11	1:B:405:PHE:CE2	2.50	0.47
1:A:337:ASN:HA	1:A:345:SER:O	2.14	0.47
1:A:577:GLN:HB3	4:A:1889:BR:BR	2.69	0.47
1:A:33:VAL:HG13	1:A:214[A]:THR:OG1	2.15	0.47
1:A:537[A]:TYR:HE1	6:A:2318:HOH:O	1.96	0.47
1:A:496:LEU:N	1:A:497:PRO:HD2	2.29	0.47
1:A:522:PRO:HA	1:A:525:TRP:CE2	2.50	0.46
1:B:43:SER:HA	3:B:1878:EDO:H12	1.98	0.46
1:B:464:LEU:CD2	1:B:511:HIS:HE1	2.27	0.46
1:A:54:THR:CG2	1:B:794:LYS:HE3	2.46	0.46
1:A:176:ALA:HB2	1:A:425:THR:HG21	1.98	0.46
1:B:586:HIS:HD2	1:B:652:PRO:O	1.98	0.46
1:A:248:GLN:HE21	1:A:248:GLN:C	2.19	0.46
1:A:582:VAL:O	1:A:585:ALA:HB3	2.16	0.46
1:A:797:ASP:HB3	1:A:848:LYS:H	1.81	0.45
1:B:298[B]:MET:HA	1:B:298[B]:MET:HE3	1.98	0.45
1:B:532:ASN:CG	3:B:1869:EDO:O2	2.54	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:211:ARG:HB3	1:A:212:PRO:CD	2.47	0.45
1:A:646:GLN:O	1:A:657:SER:HA	2.16	0.45
1:B:545:LEU:HD13	1:B:628:GLY:HA3	1.99	0.45
1:B:796:THR:HG23	1:B:797:ASP:N	2.31	0.45
5:B:1886:CL:CL	6:B:2404:HOH:O	2.59	0.44
1:A:758:LYS:HB3	3:A:1892:EDO:H12	2.00	0.44
1:B:504:ASP:OD2	1:B:507:ARG:HD2	2.17	0.44
1:B:793:MET:HE1	1:B:802:LEU:HD11	1.99	0.44
1:B:437:VAL:HG11	1:B:491:LEU:HD11	1.99	0.44
1:A:757:LEU:HB3	1:A:774:HIS:HB3	1.99	0.44
1:B:802:LEU:O	1:B:838:LYS:HA	2.18	0.44
1:A:465:GLU:HA	3:A:1870:EDO:H22	2.00	0.43
1:B:626[B]:ARG:HB3	1:B:671:GLN:HB3	2.00	0.43
1:B:287:LEU:HD12	1:B:287:LEU:N	2.33	0.43
1:A:791:TYR:HA	1:A:803:THR:O	2.18	0.43
1:A:329:GLY:O	3:A:1868:EDO:H11	2.18	0.43
1:A:575:ASP:HB3	1:A:582:VAL:HB	2.01	0.43
1:A:797:ASP:OD2	1:A:848:LYS:HB2	2.19	0.43
1:B:626[A]:ARG:NH2	1:B:671:GLN:OE1	2.52	0.43
1:B:537:TYR:CE2	2:B:1868:MVL:H8	2.48	0.43
1:B:75:GLY:HA2	1:B:582:VAL:HG13	2.00	0.43
1:B:284:HIS:HD2	3:B:1898:EDO:H12	1.83	0.43
1:B:488:TYR:OH	1:B:512:SER:HB2	2.18	0.43
1:B:525:TRP:NE1	3:B:1869:EDO:H22	2.34	0.42
1:B:802:LEU:N	1:B:802:LEU:HD12	2.34	0.42
1:B:55:VAL:HG13	1:B:209:VAL:HB	2.00	0.42
1:A:813:ILE:HG22	1:A:858:HIS:HB3	2.01	0.42
3:B:1895:EDO:H11	6:B:2198:HOH:O	2.20	0.42
1:B:44:GLN:HB2	1:B:89:TRP:CZ3	2.55	0.42
1:B:662:TYR:HA	3:B:1888:EDO:H22	2.02	0.42
1:B:258:VAL:O	1:B:273:LYS:HA	2.20	0.42
1:A:44:GLN:HB2	1:A:89:TRP:CZ3	2.55	0.42
1:A:645:TRP:HA	1:A:646:GLN:HA	1.88	0.42
1:B:42:PHE:HA	1:B:90:GLU:O	2.21	0.41
1:B:709:MET:HA	1:B:758:LYS:O	2.20	0.41
1:B:791:TYR:HA	1:B:803:THR:O	2.19	0.41
1:B:462:GLU:OE2	2:B:1868:MVL:N1	2.54	0.41
1:B:539:LYS:HG2	1:B:595:LEU:HD11	2.03	0.41
1:B:174:TYR:CD2	1:B:187:VAL:HG21	2.55	0.41
1:A:708:GLU:HG2	3:A:1892:EDO:H21	2.03	0.41
1:A:366:ASP:HA	1:A:650:SER:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:727:SER:N	6:B:2418:HOH:O	2.52	0.41
1:A:634:ARG:HD3	1:A:682:ASN:OD1	2.21	0.41
1:B:793:MET:CE	1:B:802:LEU:CD1	2.98	0.41
1:B:797:ASP:CG	6:B:2441:HOH:O	2.59	0.41
1:A:625:MET:HB2	1:A:668:LEU:HD13	2.02	0.41
1:B:327:ARG:HH11	3:B:1895:EDO:C2	2.34	0.41
2:B:1868:MVL:O6	2:B:1868:MVL:C8	2.69	0.41
5:A:1897:CL:CL	6:A:2018:HOH:O	2.60	0.40
1:B:696:SER:O	1:B:733:ASN:HA	2.21	0.40
1:B:380:LEU:HD11	1:B:647:LEU:HD21	2.03	0.40

There are no symmetry-related clashes.

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	839/846 (99%)	814 (97%)	20 (2%)	5 (1%)	25	21
1	B	851/846 (101%)	823 (97%)	25 (3%)	3 (0%)	34	32
All	All	1690/1692 (100%)	1637 (97%)	45 (3%)	8 (0%)	29	26

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	582	VAL
1	A	585	ALA
1	A	536	TRP
1	A	848	LYS
1	B	536	TRP
1	B	576	TYR
1	A	591[A]	ILE
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	736/754 (98%)	721 (98%)	15 (2%)	55	60
1	B	743/754 (98%)	721 (97%)	22 (3%)	41	44
All	All	1479/1508 (98%)	1442 (98%)	37 (2%)	50	52

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	214[A]	THR
1	A	214[B]	THR
1	A	224	SER
1	A	248	GLN
1	A	319	ARG
1	A	331	ARG
1	A	417	TRP
1	A	516	LEU
1	A	590	SER
1	A	594	SER
1	A	595	LEU
1	A	764	LYS
1	A	783	GLN
1	A	786	PRO
1	A	788	SER
1	B	28[A]	ASN
1	B	28[B]	ASN
1	B	67	GLU
1	B	144	VAL
1	B	161[A]	ARG
1	B	161[B]	ARG
1	B	182[A]	GLU
1	B	287	LEU
1	B	325	SER
1	B	331	ARG
1	B	395	TRP
1	B	417	TRP

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Mol	Chain	Res	Type
1	B	440	GLU
1	B	626[A]	ARG
1	B	626[B]	ARG
1	B	715	ASP
1	B	735	SER
1	B	750	GLU
1	B	793	MET
1	B	796	THR
1	B	813	ILE
1	B	865	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	108	GLN
1	A	248	GLN
1	A	265[A]	ASN
1	A	704	GLN
1	B	324	GLN
1	B	768	GLN
1	B	867	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 69 ligands modelled in this entry, 27 are monoatomic - leaving 42 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	A	1888	-	3,3,3	0.60	0	2,2,2	0.18	0
3	EDO	A	1869	-	3,3,3	0.73	0	2,2,2	0.34	0
3	EDO	B	1889	-	3,3,3	0.82	0	2,2,2	0.66	0
3	EDO	B	1870	-	3,3,3	0.67	0	2,2,2	0.43	0
3	EDO	B	1895	-	3,3,3	0.59	0	2,2,2	0.24	0
3	EDO	B	1871	-	3,3,3	0.46	0	2,2,2	0.33	0
3	EDO	B	1877	-	3,3,3	0.56	0	2,2,2	0.64	0
3	EDO	B	1899	-	3,3,3	0.35	0	2,2,2	0.89	0
3	EDO	A	1896	-	3,3,3	0.75	0	2,2,2	0.31	0
3	EDO	A	1870	-	3,3,3	0.86	0	2,2,2	0.24	0
3	EDO	A	1875	-	3,3,3	0.67	0	2,2,2	0.38	0
3	EDO	A	1874	-	3,3,3	0.47	0	2,2,2	0.56	0
3	EDO	A	1871	-	3,3,3	0.32	0	2,2,2	1.31	0
3	EDO	B	1872	-	3,3,3	0.81	0	2,2,2	0.10	0
3	EDO	B	1888	-	3,3,3	0.49	0	2,2,2	0.27	0
3	EDO	B	1878	-	3,3,3	0.61	0	2,2,2	0.48	0
3	EDO	B	1898	-	3,3,3	0.44	0	2,2,2	0.55	0
3	EDO	A	1880	-	3,3,3	0.49	0	2,2,2	0.73	0
3	EDO	A	1873	-	3,3,3	0.62	0	2,2,2	0.28	0
2	MVL	A	1865	-	13,15,15	0.65	0	11,22,22	1.39	2 (18%)
3	EDO	A	1878	-	3,3,3	0.91	0	2,2,2	0.30	0
3	EDO	A	1893	-	3,3,3	0.53	0	2,2,2	0.36	0
3	EDO	B	1896	-	3,3,3	0.58	0	2,2,2	0.52	0
3	EDO	B	1894	-	3,3,3	0.52	0	2,2,2	0.43	0
3	EDO	A	1877	-	3,3,3	0.52	0	2,2,2	0.39	0
3	EDO	A	1899	-	3,3,3	0.48	0	2,2,2	0.68	0
3	EDO	B	1876	-	3,3,3	0.74	0	2,2,2	0.19	0
3	EDO	B	1874	-	3,3,3	0.52	0	2,2,2	0.15	0
3	EDO	B	1875	-	3,3,3	0.85	0	2,2,2	0.34	0
3	EDO	A	1879	-	3,3,3	0.60	0	2,2,2	0.67	0
3	EDO	A	1867	-	3,3,3	0.60	0	2,2,2	0.51	0
3	EDO	A	1868	-	3,3,3	0.67	0	2,2,2	0.66	0
3	EDO	A	1876	-	3,3,3	0.58	0	2,2,2	0.09	0
3	EDO	A	1895	-	3,3,3	0.15	0	2,2,2	0.83	0
3	EDO	B	1873	-	3,3,3	0.95	0	2,2,2	0.51	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	EDO	A	1872	-	3,3,3	0.52	0	2,2,2	0.79	0
2	MVL	B	1868	-	13,15,15	0.92	0	11,22,22	1.24	2 (18%)
3	EDO	B	1890	-	3,3,3	0.70	0	2,2,2	0.22	0
3	EDO	A	1866	-	3,3,3	0.62	0	2,2,2	0.33	0
3	EDO	B	1900	-	3,3,3	0.45	0	2,2,2	0.62	0
3	EDO	A	1892	-	3,3,3	0.52	0	2,2,2	0.10	0
3	EDO	B	1869	-	3,3,3	0.53	0	2,2,2	0.46	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	A	1888	-	-	1/1/1/1	-
3	EDO	A	1869	-	-	0/1/1/1	-
3	EDO	B	1889	-	-	0/1/1/1	-
3	EDO	B	1870	-	-	0/1/1/1	-
3	EDO	B	1895	-	-	1/1/1/1	-
3	EDO	B	1871	-	-	0/1/1/1	-
3	EDO	B	1877	-	-	1/1/1/1	-
3	EDO	B	1899	-	-	1/1/1/1	-
3	EDO	A	1896	-	-	1/1/1/1	-
3	EDO	A	1870	-	-	0/1/1/1	-
3	EDO	A	1875	-	-	0/1/1/1	-
3	EDO	A	1874	-	-	0/1/1/1	-
3	EDO	A	1871	-	-	1/1/1/1	-
3	EDO	B	1872	-	-	0/1/1/1	-
3	EDO	B	1888	-	-	0/1/1/1	-
3	EDO	B	1878	-	-	1/1/1/1	-
3	EDO	B	1898	-	-	1/1/1/1	-
3	EDO	A	1880	-	-	1/1/1/1	-
3	EDO	A	1873	-	-	1/1/1/1	-
2	MVL	A	1865	-	-	0/2/22/22	0/1/2/2
3	EDO	A	1878	-	-	0/1/1/1	-
3	EDO	A	1893	-	-	1/1/1/1	-
3	EDO	B	1896	-	-	1/1/1/1	-
3	EDO	B	1894	-	-	0/1/1/1	-
3	EDO	A	1877	-	-	1/1/1/1	-
3	EDO	A	1899	-	-	1/1/1/1	-
3	EDO	B	1876	-	-	0/1/1/1	-
3	EDO	B	1874	-	-	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	A	1879	-	-	1/1/1/1	-
3	EDO	A	1867	-	-	1/1/1/1	-
3	EDO	A	1868	-	-	0/1/1/1	-
3	EDO	A	1876	-	-	0/1/1/1	-
3	EDO	A	1895	-	-	0/1/1/1	-
3	EDO	B	1873	-	-	0/1/1/1	-
3	EDO	A	1872	-	-	1/1/1/1	-
2	MVL	B	1868	-	-	1/2/22/22	0/1/2/2
3	EDO	B	1890	-	-	0/1/1/1	-
3	EDO	A	1866	-	-	1/1/1/1	-
3	EDO	B	1900	-	-	1/1/1/1	-
3	EDO	A	1892	-	-	1/1/1/1	-
3	EDO	B	1869	-	-	0/1/1/1	-

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1865	MVL	C4-C3-C2	2.68	114.31	110.24
2	B	1868	MVL	C3-C4-C5	2.32	115.28	111.37
2	A	1865	MVL	O2-C2-C3	2.29	113.36	108.55
2	B	1868	MVL	O2-C2-C3	2.17	113.11	108.55

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1879	EDO	O1-C1-C2-O2
3	A	1871	EDO	O1-C1-C2-O2
3	A	1888	EDO	O1-C1-C2-O2
3	A	1899	EDO	O1-C1-C2-O2
3	B	1896	EDO	O1-C1-C2-O2
3	B	1898	EDO	O1-C1-C2-O2
3	B	1899	EDO	O1-C1-C2-O2
3	A	1896	EDO	O1-C1-C2-O2
3	B	1878	EDO	O1-C1-C2-O2
3	A	1867	EDO	O1-C1-C2-O2
3	A	1872	EDO	O1-C1-C2-O2
3	A	1892	EDO	O1-C1-C2-O2
3	B	1877	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
3	B	1895	EDO	O1-C1-C2-O2
3	B	1900	EDO	O1-C1-C2-O2
3	A	1866	EDO	O1-C1-C2-O2
3	A	1873	EDO	O1-C1-C2-O2
3	A	1877	EDO	O1-C1-C2-O2
2	B	1868	MVL	N10-C5-C6-O6
3	A	1880	EDO	O1-C1-C2-O2
3	A	1893	EDO	O1-C1-C2-O2

There are no ring outliers.

21 monomers are involved in 36 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1888	EDO	1	0
3	B	1895	EDO	4	0
3	B	1877	EDO	2	0
3	B	1899	EDO	1	0
3	A	1870	EDO	1	0
3	B	1888	EDO	1	0
3	B	1878	EDO	1	0
3	B	1898	EDO	1	0
3	A	1880	EDO	3	0
2	A	1865	MVL	1	0
3	A	1899	EDO	1	0
3	B	1876	EDO	1	0
3	B	1875	EDO	2	0
3	A	1879	EDO	1	0
3	A	1867	EDO	1	0
3	A	1868	EDO	1	0
3	A	1895	EDO	1	0
2	B	1868	MVL	4	0
3	B	1900	EDO	3	0
3	A	1892	EDO	2	0
3	B	1869	EDO	3	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (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	835/846 (98%)	-0.23	11 (1%)	77	80	14, 23, 39, 57	9 (1%)
1	B	840/846 (99%)	-0.23	18 (2%)	63	68	13, 23, 40, 52	5 (0%)
All	All	1675/1692 (98%)	-0.23	29 (1%)	70	74	13, 23, 39, 57	14 (0%)

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	394	ILE	3.0
1	A	363	ILE	2.8
1	B	394	ILE	2.8
1	B	798	GLY	2.8
1	B	727	SER	2.7
1	A	360	ALA	2.6
1	B	866	HIS	2.6
1	A	643	LEU	2.6
1	B	729	GLU	2.5
1	B	27	GLY	2.5
1	B	766	GLY	2.5
1	B	730	VAL	2.4
1	A	792	GLN	2.3
1	B	644	TYR	2.3
1	B	416	VAL	2.3
1	B	765	SER	2.2
1	A	647	LEU	2.2
1	B	851	GLU	2.2
1	A	844	PRO	2.2
1	B	706	THR	2.2
1	B	844	PRO	2.2
1	A	395	TRP	2.1
1	A	719	LEU	2.1
1	B	392	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	362	TYR	2.1
1	A	362	TYR	2.1
1	B	704	GLN	2.0
1	A	392	VAL	2.0
1	B	626[A]	ARG	2.0

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

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

6.3 Carbohydrates (i)

There are no 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	A	1892	4/4	0.82	0.26	49,50,52,53	0
3	EDO	A	1888	4/4	0.83	0.13	38,39,39,41	0
3	EDO	A	1896	4/4	0.83	0.31	42,44,45,48	0
3	EDO	A	1871	4/4	0.85	0.15	32,32,32,40	0
3	EDO	A	1877	4/4	0.86	0.18	44,45,45,45	0
3	EDO	A	1874	4/4	0.86	0.12	52,52,52,53	0
3	EDO	A	1878	4/4	0.88	0.16	23,28,30,30	0
3	EDO	B	1875	4/4	0.88	0.14	26,29,33,34	0
3	EDO	A	1879	4/4	0.89	0.15	34,36,37,39	0
3	EDO	A	1899	4/4	0.91	0.16	30,32,34,37	0
3	EDO	A	1873	4/4	0.91	0.17	33,37,40,40	0
3	EDO	B	1888	4/4	0.91	0.12	34,35,37,38	0
3	EDO	B	1889	4/4	0.91	0.14	24,24,25,26	0
3	EDO	B	1900	4/4	0.91	0.22	31,35,38,39	0
3	EDO	A	1893	4/4	0.92	0.17	48,48,49,50	0
3	EDO	B	1873	4/4	0.92	0.15	19,19,21,25	0
3	EDO	B	1895	4/4	0.92	0.33	41,42,42,44	0
3	EDO	B	1896	4/4	0.92	0.25	45,46,46,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	EDO	B	1899	4/4	0.92	0.11	34,38,40,43	0
3	EDO	A	1868	4/4	0.92	0.12	17,25,28,37	0
4	BR	B	1901	1/1	0.92	0.22	46,46,46,46	1
3	EDO	B	1898	4/4	0.93	0.13	28,37,40,45	0
3	EDO	B	1894	4/4	0.93	0.11	46,46,47,48	0
3	EDO	A	1880	4/4	0.93	0.13	31,34,35,40	0
3	EDO	B	1878	4/4	0.93	0.13	29,30,30,32	0
5	CL	B	1884	1/1	0.93	0.12	26,26,26,26	1
3	EDO	B	1869	4/4	0.94	0.11	27,28,30,33	0
4	BR	A	1889	1/1	0.94	0.13	58,58,58,58	1
3	EDO	B	1870	4/4	0.94	0.12	22,23,27,28	0
5	CL	B	1883	1/1	0.94	0.15	31,31,31,31	1
3	EDO	A	1872	4/4	0.94	0.17	31,31,32,33	0
3	EDO	B	1877	4/4	0.95	0.16	35,35,38,40	0
3	EDO	A	1867	4/4	0.95	0.08	24,25,25,26	0
4	BR	B	1891	1/1	0.95	0.18	57,57,57,57	1
3	EDO	A	1895	4/4	0.95	0.18	33,33,38,39	0
5	CL	A	1898	1/1	0.95	0.04	44,44,44,44	0
3	EDO	B	1876	4/4	0.95	0.09	18,23,29,30	0
3	EDO	B	1890	4/4	0.95	0.13	26,29,30,30	0
5	CL	B	1893	1/1	0.95	0.10	28,28,28,28	1
3	EDO	A	1870	4/4	0.96	0.13	17,23,25,29	0
5	CL	A	1897	1/1	0.96	0.08	37,37,37,37	1
3	EDO	B	1872	4/4	0.96	0.09	18,20,20,22	0
4	BR	A	1890	1/1	0.96	0.18	46,46,46,46	1
4	BR	B	1882	1/1	0.96	0.05	34,34,34,34	1
3	EDO	A	1869	4/4	0.96	0.09	26,28,28,31	0
5	CL	A	1891	1/1	0.97	0.32	36,36,36,36	1
3	EDO	A	1866	4/4	0.97	0.16	22,23,25,27	0
4	BR	A	1894	1/1	0.97	0.25	45,45,45,45	1
2	MVL	A	1865	14/14	0.97	0.11	11,16,17,18	0
2	MVL	B	1868	14/14	0.97	0.12	13,16,18,21	0
3	EDO	A	1875	4/4	0.97	0.10	26,27,28,33	0
5	CL	B	1897	1/1	0.97	0.10	22,22,22,22	1
4	BR	B	1887	1/1	0.98	0.12	25,25,25,25	1
3	EDO	B	1871	4/4	0.98	0.12	28,29,29,32	0
3	EDO	B	1874	4/4	0.98	0.08	21,24,25,26	0
5	CL	B	1892	1/1	0.98	0.10	29,29,29,29	1
3	EDO	A	1876	4/4	0.98	0.11	15,18,21,22	0
4	BR	A	1882	1/1	0.98	0.10	20,20,20,20	1
4	BR	A	1885	1/1	0.99	0.12	22,22,22,22	1
4	BR	A	1886	1/1	0.99	0.08	26,26,26,26	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	BR	A	1881	1/1	0.99	0.07	24,24,24,24	1
5	CL	B	1885	1/1	0.99	0.09	26,26,26,26	0
4	BR	A	1883	1/1	0.99	0.11	16,16,16,16	1
4	BR	A	1884	1/1	0.99	0.14	19,19,19,19	1
4	BR	B	1881	1/1	0.99	0.13	16,16,16,16	1
5	CL	B	1886	1/1	1.00	0.13	16,16,16,16	0
4	BR	B	1880	1/1	1.00	0.17	20,20,20,20	1
4	BR	B	1879	1/1	1.00	0.08	24,24,24,24	1
5	CL	A	1887	1/1	1.00	0.13	16,16,16,16	0

6.5 Other polymers (i)

There are no such residues in this entry.