Full wwPDB X-ray Structure Validation Report (i)

Dec 16, 2023 – 03:50 PM EST

PDB ID	:	4PC4
Title	:	Bombyx mori lipoprotein 6
Authors	:	Pietrzyk, A.J.; Bujacz, A.; Jaskolski, M.; Bujacz, G.
Deposited on	:	2014-04-14
Resolution	:	1.80 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (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 (1)) were used in the production of this report:

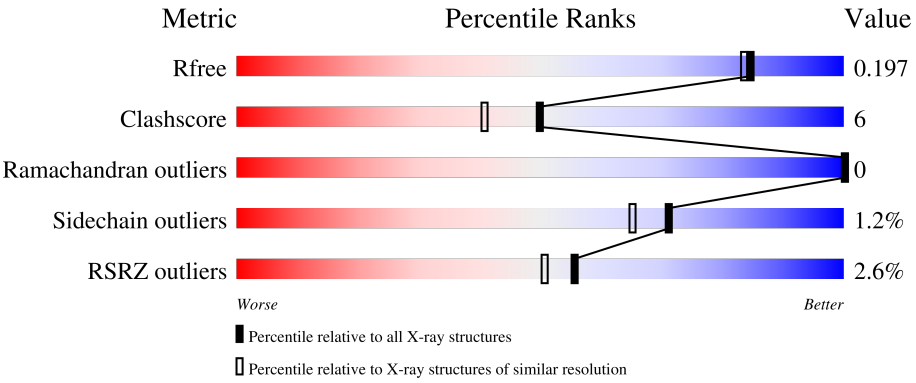
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 1.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	245	89% 8% .
1	B	245	90% 7% .
1	C	245	88% 9% .
1	D	245	87% 10% .
1	E	245	11% 89% 7% . .

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
2	MES	A	302	-	-	X	-
3	EDO	C	302	-	-	X	-
5	IPA	C	306[A]	-	-	X	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 11107 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.

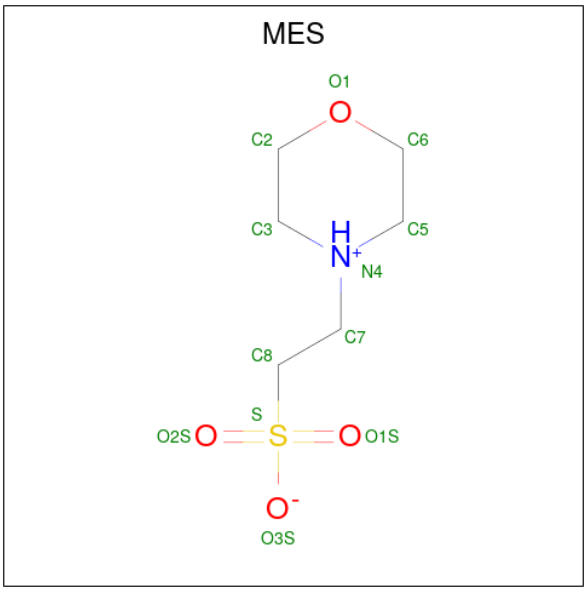
- Molecule 1 is a protein called 30K lipoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	238	Total	C	N	O	S	0	3	0
			1973	1254	341	372	6			
1	B	238	Total	C	N	O	S	0	3	0
			1972	1254	338	374	6			
1	C	240	Total	C	N	O	S	0	7	0
			2007	1279	346	376	6			
1	D	238	Total	C	N	O	S	0	2	0
			1966	1250	338	372	6			
1	E	239	Total	C	N	O	S	0	2	0
			1967	1249	338	374	6			

There are 5 discrepancies between the modelled and reference sequences:

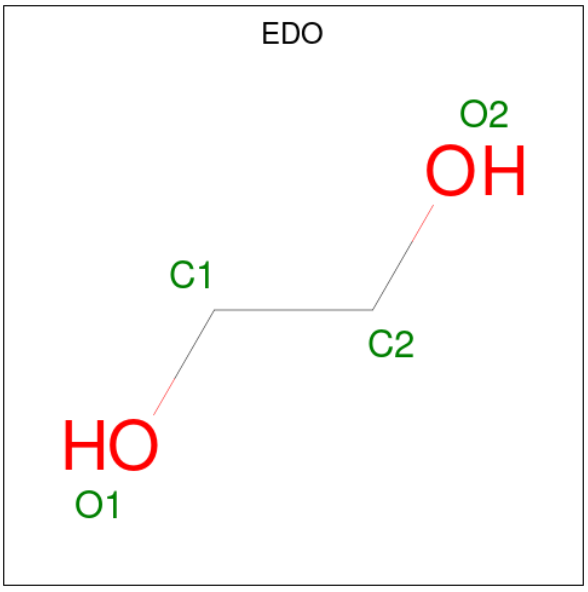
Chain	Residue	Modelled	Actual	Comment	Reference
A	217	ASN	TYR	conflict	UNP A7LIK7
B	217	ASN	TYR	conflict	UNP A7LIK7
C	217	ASN	TYR	conflict	UNP A7LIK7
D	217	ASN	TYR	conflict	UNP A7LIK7
E	217	ASN	TYR	conflict	UNP A7LIK7

- Molecule 2 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).



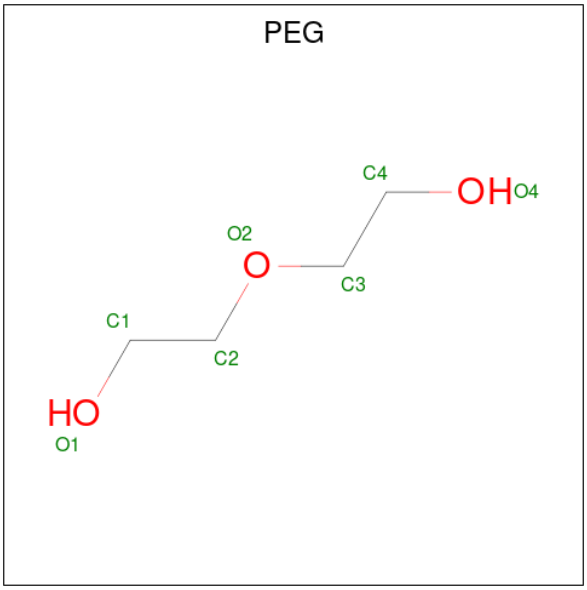
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C N O S 12 6 1 4 1	0	0
2	A	1	Total C N O S 12 6 1 4 1	0	0
2	B	1	Total C N O S 12 6 1 4 1	0	0
2	C	1	Total C N O S 12 6 1 4 1	0	0

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



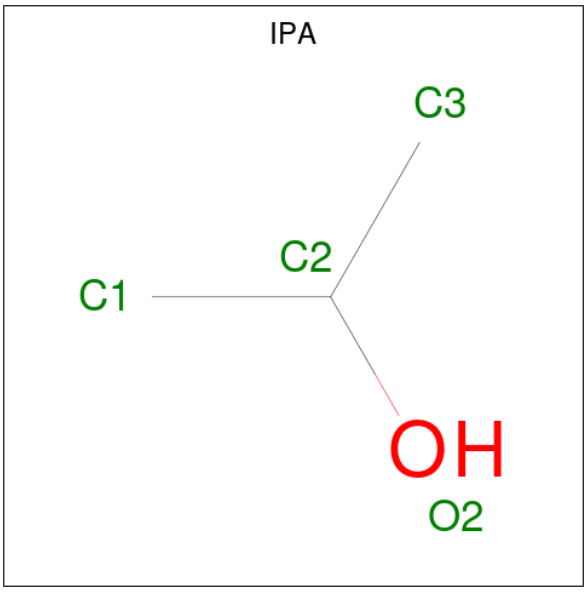
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	C	1	Total C O 4 2 2	0	0
3	C	1	Total C O 4 2 2	0	0

- Molecule 4 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C O 7 4 3	0	0

- Molecule 5 is ISOPROPYL ALCOHOL (three-letter code: IPA) (formula: C_3H_8O).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	1	Total C O 4 3 1	0	0
5	C	1	Total C O 4 3 1	0	0
5	C	1	Total C O 8 6 2	0	1

- Molecule 6 is water.

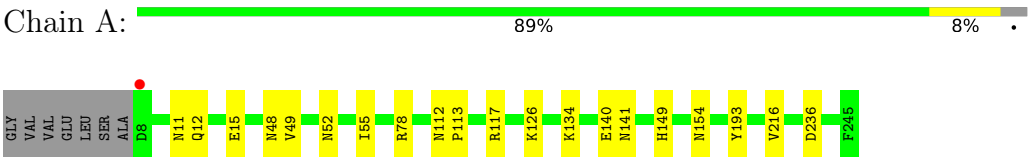
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	268	Total O 268 268	0	0
6	B	274	Total O 274 274	0	0
6	C	302	Total O 302 302	0	0
6	D	171	Total O 171 171	0	0
6	E	116	Total O 116 116	0	0

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.

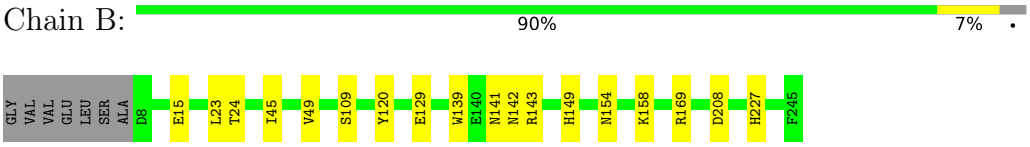
• Molecule 1: 30K lipoprotein

Chain A:



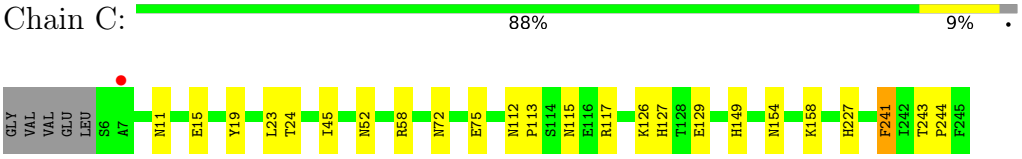
• Molecule 1: 30K lipoprotein

Chain B:



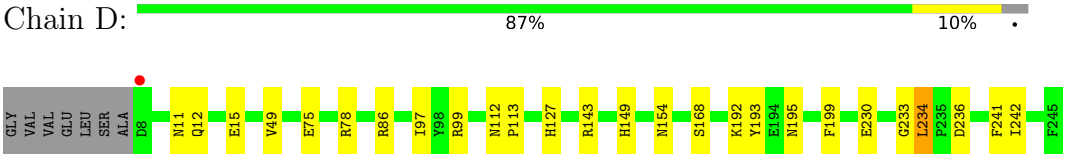
• Molecule 1: 30K lipoprotein

Chain C:



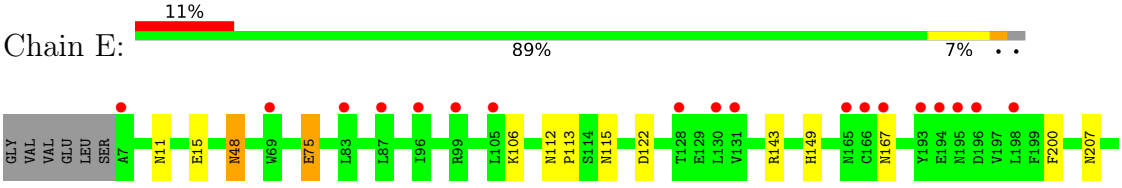
• Molecule 1: 30K lipoprotein

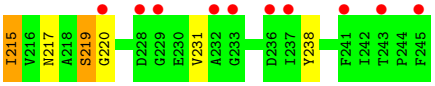
Chain D:



• Molecule 1: 30K lipoprotein

Chain E:




I215
V216
N217
A218
S219
G220
D228
G229
E230
V231
A232
G233
D236
I237
Y238
F241
I242
T243
P244
F245

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	83.21Å 85.75Å 104.47Å 90.00° 104.84° 90.00°	Depositor
Resolution (Å)	47.00 – 1.80 47.05 – 1.80	Depositor EDS
% Data completeness (in resolution range)	94.9 (47.00-1.80) 95.0 (47.05-1.80)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.48 (at 1.79Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.161 , 0.183 0.171 , 0.197	Depositor DCC
R_{free} test set	1265 reflections (1.01%)	wwPDB-VP
Wilson B-factor (Å^2)	26.7	Xtriage
Anisotropy	0.091	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 42.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	11107	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.50% 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: MES, PEG, IPA, 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	0.69	0/2027	0.77	1/2743 (0.0%)
1	B	0.71	0/2026	0.78	1/2742 (0.0%)
1	C	0.70	0/2075	0.80	2/2809 (0.1%)
1	D	0.63	0/2017	0.80	2/2730 (0.1%)
1	E	0.57	0/2018	0.77	2/2734 (0.1%)
All	All	0.66	0/10163	0.78	8/13758 (0.1%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	143	ARG	NE-CZ-NH2	-5.88	117.36	120.30
1	E	143	ARG	NE-CZ-NH1	5.50	123.05	120.30
1	D	143	ARG	NE-CZ-NH2	-5.49	117.56	120.30
1	A	134	LYS	CD-CE-NZ	5.19	123.64	111.70
1	C	241[A]	PHE	CB-CA-C	-5.12	100.15	110.40
1	C	241[B]	PHE	CB-CA-C	-5.12	100.15	110.40
1	D	143	ARG	NE-CZ-NH1	5.10	122.85	120.30
1	B	129	GLU	OE1-CD-OE2	-5.01	117.29	123.30

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	1973	0	1913	29	0
1	B	1972	0	1908	22	0
1	C	2007	0	1951	24	0
1	D	1966	0	1902	20	0
1	E	1967	0	1895	14	0
2	A	24	0	26	15	0
2	B	12	0	13	0	0
2	C	12	0	13	0	0
3	A	4	0	6	0	0
3	B	8	0	12	3	0
3	C	8	0	12	6	0
4	B	7	0	10	3	0
5	C	16	0	32	8	0
6	A	268	0	0	5	0
6	B	274	0	0	3	0
6	C	302	0	0	10	0
6	D	171	0	0	7	0
6	E	116	0	0	3	0
All	All	11107	0	9693	113	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 (113) 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)
2:A:302:MES:H22	1:B:142:ASN:HD22	1.09	1.13
1:A:15:GLU:HB2	2:A:302:MES:O2S	1.59	1.03
2:A:302:MES:H22	1:B:142:ASN:ND2	1.87	0.88
1:A:15:GLU:CB	2:A:302:MES:O2S	2.22	0.88
1:A:12:GLN:HG2	2:A:302:MES:H82	1.59	0.85
1:B:149:HIS:HE1	1:B:154:ASN:HD22	1.25	0.84
1:C:149:HIS:HE1	1:C:154:ASN:HD22	1.26	0.83
1:B:24:THR:HG22	6:D:375:HOH:O	1.78	0.83
1:A:149:HIS:HE1	1:A:154:ASN:HD22	1.27	0.81
1:D:149:HIS:HE1	1:D:154:ASN:HD22	1.29	0.79
1:A:15:GLU:HG2	1:A:49[B]:VAL:HG23	1.67	0.77
1:B:149:HIS:CE1	1:B:154:ASN:HD22	2.03	0.77
1:C:149:HIS:CE1	1:C:154:ASN:HD22	2.02	0.76
1:A:149:HIS:CE1	1:A:154:ASN:HD22	2.03	0.76
1:D:168:SER:HB2	6:D:431:HOH:O	1.85	0.76
1:B:15[A]:GLU:HG2	1:B:49:VAL:HG23	1.69	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:149:HIS:CE1	1:D:154:ASN:HD22	2.04	0.74
1:B:109:SER:H	4:B:304:PEG:H32	1.50	0.74
1:D:99:ARG:HD3	1:D:99:ARG:C	2.09	0.72
1:C:117[A]:ARG:NH1	6:C:681:HOH:O	2.23	0.71
1:E:106:LYS:HE2	1:E:122:ASP:OD1	1.89	0.71
1:D:15:GLU:HG2	1:D:49:VAL:HG23	1.74	0.70
1:C:241[A]:PHE:CE2	6:C:583:HOH:O	2.48	0.67
1:A:117[A]:ARG:NH1	6:A:633:HOH:O	2.28	0.66
1:C:149:HIS:HE1	1:C:154:ASN:ND2	1.93	0.65
1:A:149:HIS:HE1	1:A:154:ASN:ND2	1.94	0.64
1:A:78[A]:ARG:NH2	6:A:401:HOH:O	2.29	0.64
1:B:149:HIS:HE1	1:B:154:ASN:ND2	1.95	0.64
1:C:72:ASN:HA	5:C:306[B]:IPA:H2	1.80	0.64
1:D:149:HIS:HE1	1:D:154:ASN:ND2	1.96	0.63
1:A:12:GLN:CG	2:A:302:MES:H82	2.28	0.63
1:C:129:GLU:HB2	6:C:680:HOH:O	1.98	0.63
1:E:75:GLU:CD	1:E:75:GLU:H	2.02	0.63
1:A:15:GLU:HG2	1:A:49[B]:VAL:CG2	2.28	0.62
2:A:302:MES:H71	1:B:143:ARG:HH22	1.63	0.62
1:B:15[A]:GLU:HG2	1:B:49:VAL:CG2	2.29	0.62
1:A:52:ASN:HD21	2:A:302:MES:H52	1.63	0.61
1:E:106:LYS:CE	1:E:122:ASP:OD1	2.49	0.60
1:A:48:ASN:CB	2:A:302:MES:O1S	2.48	0.60
1:C:23[B]:LEU:HD21	1:C:58:ARG:HD2	1.83	0.60
1:A:48:ASN:ND2	2:A:302:MES:O1S	2.35	0.60
5:C:306[A]:IPA:H31	6:C:487:HOH:O	2.01	0.59
1:D:78[B]:ARG:HG2	1:D:86:ARG:HD3	1.84	0.58
1:B:120:TYR:CE2	4:B:304:PEG:H12	2.37	0.58
1:B:227:HIS:HE1	6:B:509:HOH:O	1.86	0.58
1:B:158:LYS:HD2	6:B:654:HOH:O	2.05	0.56
1:D:233:GLY:C	1:D:234:LEU:HD12	2.26	0.56
1:C:15:GLU:HG3	1:C:45:ILE:HG23	1.88	0.56
1:D:15:GLU:HG2	1:D:49:VAL:CG2	2.35	0.56
1:A:149:HIS:HD2	6:A:503:HOH:O	1.89	0.55
1:A:12:GLN:HG2	2:A:302:MES:C8	2.32	0.55
1:B:23:LEU:HD21	6:D:412:HOH:O	2.06	0.55
1:C:227:HIS:HE1	6:C:525:HOH:O	1.90	0.55
1:D:241:PHE:C	1:D:242[B]:ILE:HD12	2.27	0.55
3:C:302:EDO:O2	5:C:306[A]:IPA:H12	2.08	0.54
1:D:127:HIS:CD2	6:D:454:HOH:O	2.61	0.54
3:C:302:EDO:H11	5:C:306[A]:IPA:H13	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:192:LYS:HE2	1:D:195:ASN:HA	1.90	0.53
1:C:19:TYR:CE2	1:C:23[B]:LEU:HD13	2.43	0.53
1:C:149:HIS:HD2	6:C:478:HOH:O	1.91	0.53
1:B:149:HIS:HD2	6:B:485:HOH:O	1.90	0.53
1:C:75:GLU:OE2	3:C:302:EDO:O1	2.26	0.53
1:A:140:GLU:OE1	1:C:23[A]:LEU:HD11	2.09	0.53
1:E:11:ASN:ND2	6:E:303:HOH:O	2.42	0.52
1:D:99:ARG:HD3	1:D:99:ARG:O	2.09	0.52
1:B:15[B]:GLU:HG3	1:B:45:ILE:HG23	1.92	0.52
1:E:149:HIS:HD2	6:E:397:HOH:O	1.93	0.52
1:D:11:ASN:ND2	6:D:302:HOH:O	2.44	0.51
1:D:127:HIS:HD2	6:D:454:HOH:O	1.94	0.50
1:A:78[B]:ARG:HG2	1:A:78[B]:ARG:HH11	1.76	0.50
1:C:158:LYS:HD2	6:C:689:HOH:O	2.12	0.50
1:E:215:ILE:HD12	1:E:220:GLY:HA2	1.94	0.49
6:A:423:HOH:O	1:C:24:THR:HG22	2.12	0.49
1:B:169:ARG:NH1	1:B:208:ASP:OD2	2.33	0.49
1:A:48:ASN:HB3	2:A:302:MES:O1S	2.13	0.48
1:E:200:PHE:CD1	1:E:231:VAL:CG1	2.96	0.48
1:B:139:TRP:HE1	3:B:303:EDO:C2	2.26	0.48
1:A:52:ASN:HD21	2:A:302:MES:C5	2.26	0.48
1:B:142:ASN:HA	3:B:303:EDO:H21	1.95	0.48
1:D:149:HIS:HD2	6:D:427:HOH:O	1.96	0.47
1:A:141:ASN:HD22	1:C:52[B]:ASN:HD22	1.63	0.47
1:E:75:GLU:CD	1:E:75:GLU:N	2.69	0.46
3:C:303:EDO:O1	5:C:304:IPA:H31	2.16	0.46
5:C:306[B]:IPA:H12	6:C:657:HOH:O	2.14	0.46
1:A:11:ASN:ND2	6:A:649:HOH:O	2.48	0.45
1:A:216:VAL:O	1:A:216:VAL:HG12	2.16	0.45
3:C:302:EDO:C2	5:C:306[A]:IPA:C1	2.94	0.45
1:E:231:VAL:HG13	1:E:238:TYR:HB2	1.98	0.45
1:A:55:ILE:HG21	3:B:303:EDO:H11	1.98	0.45
1:C:127[B]:HIS:HD2	6:C:441:HOH:O	2.00	0.44
1:E:200:PHE:CD1	1:E:231:VAL:HG12	2.53	0.44
1:A:52:ASN:HD22	1:B:141:ASN:ND2	2.15	0.44
1:A:78[B]:ARG:HG2	1:A:78[B]:ARG:NH1	2.32	0.44
1:C:19:TYR:CD2	1:C:23[B]:LEU:HD13	2.52	0.44
1:A:12:GLN:HA	2:A:302:MES:H82	2.01	0.43
3:C:302:EDO:O2	5:C:306[A]:IPA:C1	2.67	0.42
1:E:112:ASN:HB2	1:E:113:PRO:CD	2.49	0.42
1:D:75:GLU:OE2	1:D:78[A]:ARG:NH2	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:115:ASN:ND2	6:E:305:HOH:O	2.47	0.42
1:A:193:TYR:CZ	1:A:236:ASP:HB3	2.54	0.41
1:C:11:ASN:ND2	6:C:540:HOH:O	2.52	0.41
1:E:15:GLU:HG3	1:E:48[A]:ASN:OD1	2.20	0.41
1:C:112:ASN:HB2	1:C:113:PRO:CD	2.51	0.41
1:E:217:ASN:ND2	1:E:219:SER:OG	2.54	0.41
1:D:193:TYR:CZ	1:D:236:ASP:HB3	2.56	0.41
1:D:112:ASN:HB2	1:D:113:PRO:CD	2.50	0.41
1:C:19:TYR:HE2	1:C:23[B]:LEU:HD22	1.85	0.41
1:A:112:ASN:HB2	1:A:113:PRO:CD	2.50	0.40
1:B:120:TYR:CZ	4:B:304:PEG:H12	2.56	0.40
1:C:149:HIS:CE1	1:C:154:ASN:ND2	2.77	0.40
2:A:302:MES:C7	1:B:143:ARG:HH22	2.33	0.40
1:C:243:THR:OG1	1:C:244:PRO:HD2	2.21	0.40
1:D:199:PHE:CD1	1:D:242[B]:ILE:HD13	2.57	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	239/245 (98%)	236 (99%)	3 (1%)	0	100	100
1	B	239/245 (98%)	236 (99%)	3 (1%)	0	100	100
1	C	244/245 (100%)	240 (98%)	4 (2%)	0	100	100
1	D	238/245 (97%)	235 (99%)	3 (1%)	0	100	100
1	E	239/245 (98%)	235 (98%)	4 (2%)	0	100	100
All	All	1199/1225 (98%)	1182 (99%)	17 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	215/217 (99%)	214 (100%)	1 (0%)	88 87
1	B	215/217 (99%)	215 (100%)	0	100 100
1	C	220/217 (101%)	218 (99%)	2 (1%)	78 75
1	D	214/217 (99%)	210 (98%)	4 (2%)	57 46
1	E	214/217 (99%)	207 (97%)	7 (3%)	38 23
All	All	1078/1085 (99%)	1064 (99%)	14 (1%)	71 62

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	126	LYS
1	C	115	ASN
1	C	126	LYS
1	D	12	GLN
1	D	97	ILE
1	D	230	GLU
1	D	234	LEU
1	E	48[A]	ASN
1	E	48[B]	ASN
1	E	75	GLU
1	E	167	ASN
1	E	207	ASN
1	E	215	ILE
1	E	219	SER

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

Mol	Chain	Res	Type
1	A	11	ASN
1	A	52	ASN
1	A	115	ASN
1	A	141	ASN

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Mol	Chain	Res	Type
1	A	149	HIS
1	A	154	ASN
1	B	11	ASN
1	B	72	ASN
1	B	115	ASN
1	B	127	HIS
1	B	149	HIS
1	B	154	ASN
1	B	227	HIS
1	C	11	ASN
1	C	141	ASN
1	C	149	HIS
1	C	154	ASN
1	C	177	ASN
1	C	227	HIS
1	D	11	ASN
1	D	149	HIS
1	D	154	ASN
1	D	177	ASN
1	D	207	ASN
1	E	11	ASN
1	E	60	ASN
1	E	115	ASN
1	E	141	ASN
1	E	149	HIS
1	E	167	ASN
1	E	177	ASN
1	E	217	ASN
1	E	227	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

14 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	EDO	A	303	-	3,3,3	0.43	0	2,2,2	0.37	0
2	MES	A	301	-	12,12,12	1.99	1 (8%)	14,16,16	1.38	3 (21%)
3	EDO	B	303	-	3,3,3	0.40	0	2,2,2	0.40	0
2	MES	B	301	-	12,12,12	2.09	1 (8%)	14,16,16	1.91	5 (35%)
2	MES	A	302	-	12,12,12	2.21	1 (8%)	14,16,16	4.82	8 (57%)
2	MES	C	301	-	12,12,12	1.90	1 (8%)	14,16,16	1.60	2 (14%)
3	EDO	C	303	-	3,3,3	0.53	0	2,2,2	0.06	0
5	IPA	C	304	-	3,3,3	0.37	0	3,3,3	0.43	0
5	IPA	C	306[B]	-	3,3,3	0.38	0	3,3,3	0.39	0
3	EDO	B	302	-	3,3,3	0.29	0	2,2,2	0.43	0
4	PEG	B	304	-	6,6,6	0.48	0	5,5,5	0.38	0
3	EDO	C	302	-	3,3,3	0.60	0	2,2,2	0.07	0
5	IPA	C	306[A]	-	3,3,3	0.44	0	3,3,3	0.73	0
5	IPA	C	305	-	3,3,3	0.67	0	3,3,3	0.39	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	303	-	-	1/1/1/1	-
2	MES	A	301	-	-	5/6/14/14	0/1/1/1
3	EDO	B	303	-	-	1/1/1/1	-
2	MES	B	301	-	-	3/6/14/14	0/1/1/1
2	MES	A	302	-	-	3/6/14/14	0/1/1/1
2	MES	C	301	-	-	0/6/14/14	0/1/1/1
3	EDO	C	303	-	-	1/1/1/1	-
3	EDO	B	302	-	-	0/1/1/1	-
4	PEG	B	304	-	-	3/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	C	302	-	-	0/1/1/1	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	302	MES	C8-S	-7.26	1.67	1.77
2	A	301	MES	C8-S	-6.29	1.68	1.77
2	B	301	MES	C8-S	-6.09	1.68	1.77
2	C	301	MES	C8-S	-6.01	1.69	1.77

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	302	MES	O3S-S-C8	11.52	124.40	105.77
2	A	302	MES	O1S-S-C8	-7.77	97.55	106.92
2	A	302	MES	O2S-S-C8	-7.35	98.07	106.92
2	C	301	MES	O3S-S-C8	4.72	113.41	105.77
2	A	302	MES	C6-O1-C2	4.27	124.16	109.89
2	A	302	MES	C6-C5-N4	-3.94	104.13	110.10
2	A	302	MES	C2-C3-N4	-3.92	104.16	110.10
2	A	302	MES	O3S-S-O2S	-3.69	102.25	111.27
2	B	301	MES	C2-C3-N4	3.42	115.29	110.10
2	B	301	MES	C6-C5-N4	3.06	114.74	110.10
2	B	301	MES	C5-N4-C3	2.86	115.28	108.83
2	A	301	MES	O1S-S-C8	2.77	110.25	106.92
2	A	302	MES	O2S-S-O1S	2.68	123.22	113.95
2	B	301	MES	O1S-S-C8	2.67	110.13	106.92
2	C	301	MES	O1S-S-C8	2.52	109.95	106.92
2	A	301	MES	O2S-S-O1S	-2.18	106.41	113.95
2	B	301	MES	O2S-S-O1S	-2.14	106.56	113.95
2	A	301	MES	O2S-S-C8	2.06	109.39	106.92

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301	MES	C8-C7-N4-C3
2	A	301	MES	C8-C7-N4-C5
2	A	301	MES	C7-C8-S-O1S
2	A	301	MES	C7-C8-S-O2S
2	A	301	MES	C7-C8-S-O3S

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Mol	Chain	Res	Type	Atoms
2	A	302	MES	N4-C7-C8-S
2	B	301	MES	C8-C7-N4-C3
4	B	304	PEG	O2-C3-C4-O4
2	B	301	MES	C7-C8-S-O3S
2	A	302	MES	C8-C7-N4-C3
2	A	302	MES	C8-C7-N4-C5
3	A	303	EDO	O1-C1-C2-O2
3	B	303	EDO	O1-C1-C2-O2
4	B	304	PEG	C1-C2-O2-C3
2	B	301	MES	C7-C8-S-O2S
4	B	304	PEG	C4-C3-O2-C2
3	C	303	EDO	O1-C1-C2-O2

There are no ring outliers.

8 monomers are involved in 30 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	303	EDO	3	0
2	A	302	MES	15	0
3	C	303	EDO	1	0
5	C	304	IPA	1	0
5	C	306[B]	IPA	2	0
4	B	304	PEG	3	0
3	C	302	EDO	5	0
5	C	306[A]	IPA	5	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	238/245 (97%)	-0.74	1 (0%) 92 90	18, 28, 49, 89	0
1	B	238/245 (97%)	-0.63	0 100 100	17, 26, 43, 69	0
1	C	240/245 (97%)	-0.57	1 (0%) 92 90	19, 27, 44, 81	0
1	D	238/245 (97%)	-0.35	1 (0%) 92 90	23, 40, 61, 91	0
1	E	239/245 (97%)	0.50	28 (11%) 4 3	22, 51, 88, 106	0
All	All	1193/1225 (97%)	-0.36	31 (2%) 56 51	17, 32, 66, 106	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	7	ALA	7.0
1	E	7	ALA	6.3
1	E	193	TYR	4.3
1	E	83	LEU	3.9
1	E	105	LEU	3.8
1	E	166	CYS	3.6
1	E	198	LEU	3.4
1	E	194	GLU	3.3
1	E	233	GLY	3.3
1	E	131	VAL	3.1
1	E	245	PHE	3.1
1	A	8	ASP	3.0
1	E	220	GLY	3.0
1	E	167	ASN	3.0
1	E	130	LEU	2.9
1	D	8	ASP	2.8
1	E	87	LEU	2.7
1	E	237	ILE	2.7
1	E	165	ASN	2.6
1	E	232	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	E	96	ILE	2.5
1	E	128	THR	2.5
1	E	196	ASP	2.4
1	E	236	ASP	2.4
1	E	195	ASN	2.3
1	E	99	ARG	2.2
1	E	243	THR	2.2
1	E	229	GLY	2.2
1	E	69	TRP	2.2
1	E	241	PHE	2.1
1	E	228	ASP	2.1

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, 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
2	MES	A	302	12/12	0.67	0.23	44,50,65,67	12
3	EDO	C	302	4/4	0.73	0.17	64,72,74,75	0
3	EDO	C	303	4/4	0.79	0.20	67,70,70,71	0
4	PEG	B	304	7/7	0.82	0.33	48,50,54,59	0
2	MES	C	301	12/12	0.84	0.17	51,58,62,69	12
5	IPA	C	305	4/4	0.84	0.14	38,42,48,50	0
2	MES	B	301	12/12	0.91	0.14	35,43,45,48	12
5	IPA	C	304	4/4	0.92	0.17	52,53,55,57	0
3	EDO	B	303	4/4	0.93	0.26	37,43,45,47	0
2	MES	A	301	12/12	0.93	0.13	49,55,68,71	0
3	EDO	A	303	4/4	0.95	0.12	37,52,57,64	0
3	EDO	B	302	4/4	0.96	0.17	34,35,41,43	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	IPA	C	306[A]	4/4	0.96	0.19	19,20,20,23	4
5	IPA	C	306[B]	4/4	0.96	0.19	29,31,31,32	4

6.5 Other polymers (i)

There are no such residues in this entry.