



Full wwPDB X-ray Structure Validation Report ⓘ

May 18, 2020 – 04:46 am BST

PDB ID : 2ZAD
Title : Crystal Structure of Muconate Cycloisomerase from *Thermotoga maritima* MSB8
Authors : Padmanabhan, B.; Bessho, Y.; Yokoyama, S.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on : 2007-10-03
Resolution : 1.60 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

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

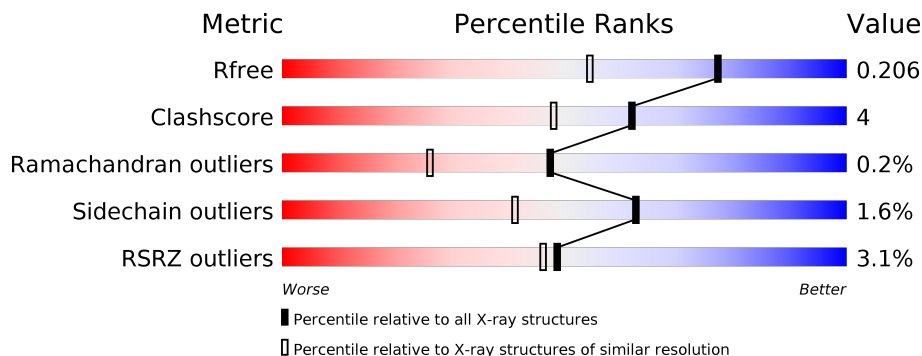
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.60 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	3398 (1.60-1.60)
Clashscore	141614	3665 (1.60-1.60)
Ramachandran outliers	138981	3564 (1.60-1.60)
Sidechain outliers	138945	3563 (1.60-1.60)
RSRZ outliers	127900	3321 (1.60-1.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	345	
1	B	345	
1	C	345	
1	D	345	

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	1PE	D	348	-	-	X	-
4	PEG	A	351	-	-	X	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 12336 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 Muconate cycloisomerase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	344	2734	1734	470	520	2	8	0	6	0
1	B	344	2742	1743	470	519	2	8	0	8	0
1	C	344	2729	1733	467	519	2	8	0	5	0
1	D	344	2720	1726	466	518	2	8	0	4	0

- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

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

- Molecule 3 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: C₁₀H₂₂O₆).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 16 10 6	0	0
3	A	1	Total C O 16 10 6	0	0
3	A	1	Total C O 13 8 5	0	0
3	B	1	Total C O 16 10 6	0	0
3	B	1	Total C O 13 8 5	0	0
3	C	1	Total C O 16 10 6	0	0
3	C	1	Total C O 13 8 5	0	0
3	C	1	Total C O 10 6 4	0	0
3	D	1	Total C O 16 10 6	0	0
3	D	1	Total C O 16 10 6	0	0
3	D	1	Total C O 16 10 6	0	0

- Molecule 4 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



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

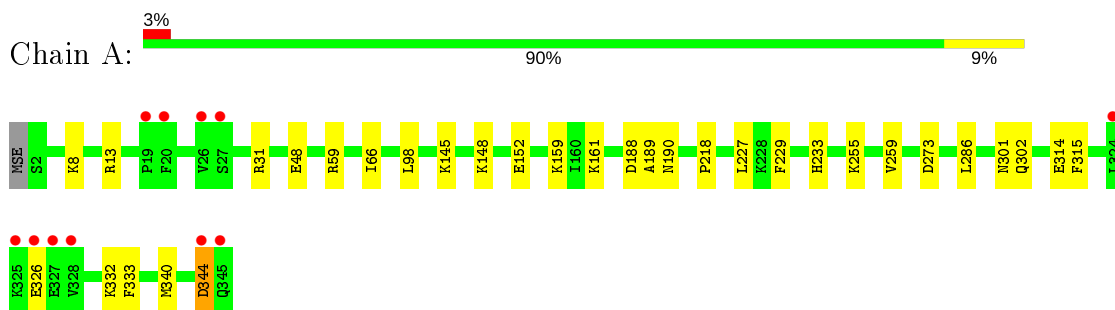
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	292	Total O 292 292	0	0
5	B	313	Total O 313 313	0	0
5	C	321	Total O 321 321	0	0
5	D	292	Total O 292 292	0	0

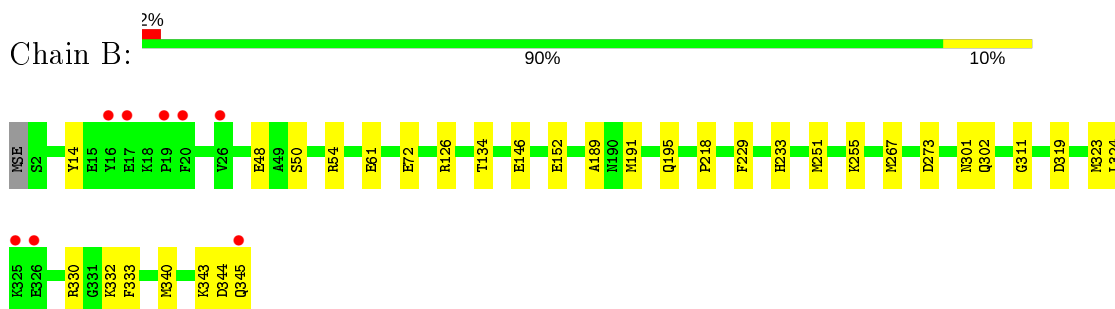
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

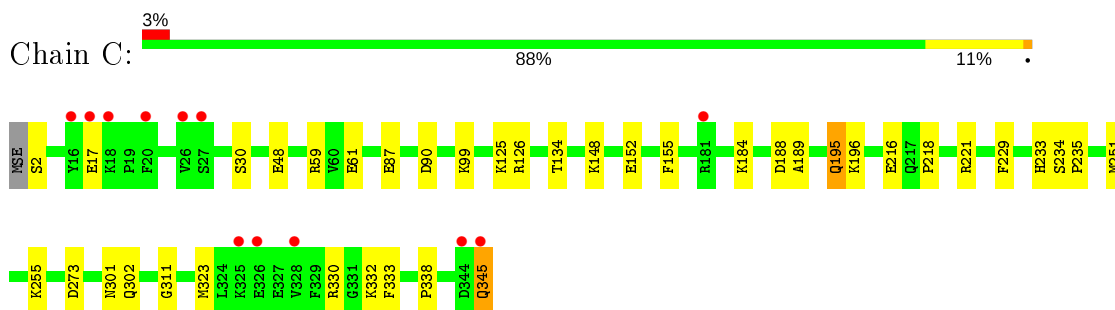
- Molecule 1: Muconate cycloisomerase



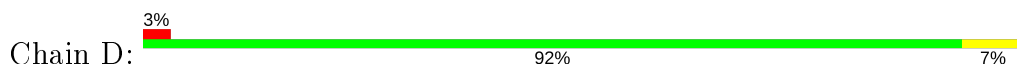
- Molecule 1: Muconate cycloisomerase

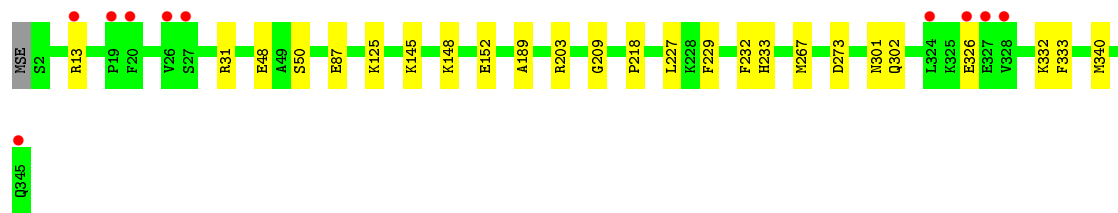


- Molecule 1: Muconate cycloisomerase



- Molecule 1: Muconate cycloisomerase





R345

4 Data and refinement statistics

Property	Value	Source
Space group	P 4	Depositor
Cell constants a, b, c, α , β , γ	112.77Å 112.77Å 122.53Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.60 48.58 – 1.60	Depositor EDS
% Data completeness (in resolution range)	97.7 (20.00-1.60) 97.6 (48.58-1.60)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.59 (at 1.60Å)	Xtrriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.175 , 0.201 0.181 , 0.206	Depositor DCC
R_{free} test set	9901 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	14.0	Xtrriage
Anisotropy	0.344	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 45.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.447 for h,-k,-l	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	12336	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.73% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PEG, MN, 1PE

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	0.45	0/2779	0.60	0/3717
1	B	0.48	0/2797	0.62	0/3742
1	C	0.47	0/2775	0.63	0/3713
1	D	0.47	0/2763	0.60	0/3698
All	All	0.47	0/11114	0.61	0/14870

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	B	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	344	ASP	Peptide

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	2734	0	2779	23	0
1	B	2742	0	2803	22	1
1	C	2729	0	2775	32	0
1	D	2720	0	2761	19	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	45	0	61	4	0
3	B	29	0	39	2	0
3	C	39	0	52	7	0
3	D	48	0	66	10	0
4	A	14	0	20	4	0
4	B	7	0	10	0	0
4	D	7	0	10	0	0
5	A	292	0	0	3	1
5	B	313	0	0	5	0
5	C	321	0	0	7	1
5	D	292	0	0	5	0
All	All	12336	0	11376	99	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (99) 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:C:255:LYS:HG3	5:C:510:HOH:O	1.59	1.03
1:C:134:THR:HB	1:C:323:MSE:HE1	1.42	1.00
1:D:232:PHE:HB3	3:D:348:1PE:H131	1.50	0.94
1:B:134:THR:HB	1:B:323:MSE:HE1	1.57	0.87
1:B:134:THR:HB	1:B:323:MSE:CE	2.09	0.83
1:C:184:LYS:NZ	3:C:349:1PE:H142	1.96	0.80
1:C:134:THR:HB	1:C:323:MSE:CE	2.16	0.76
1:C:184:LYS:HZ1	3:C:349:1PE:H142	1.50	0.75
1:C:152[B]:GLU:HA	1:C:152[B]:GLU:OE1	1.88	0.74
1:B:195:GLN:HG3	5:B:639:HOH:O	1.87	0.73
3:D:348:1PE:H122	5:D:854:HOH:O	1.90	0.71
1:C:195:GLN:HE21	1:C:196:LYS:H	1.38	0.70
1:A:59:ARG:HH12	4:A:351:PEG:H42	1.56	0.70
1:A:255:LYS:O	1:B:255:LYS:NZ	2.18	0.70
3:D:348:1PE:H152	5:D:767:HOH:O	1.92	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:148:LYS:HG3	1:A:152:GLU:OE2	1.95	0.67
1:D:232:PHE:HB3	3:D:348:1PE:C13	2.23	0.66
1:C:189:ALA:HB3	1:C:218:PRO:HA	1.78	0.64
1:B:152:GLU:HG3	5:B:695:HOH:O	1.98	0.63
1:C:330:ARG:HA	3:C:348:1PE:H142	1.81	0.62
1:B:189:ALA:HB3	1:B:218:PRO:HA	1.82	0.62
3:D:348:1PE:C15	5:D:767:HOH:O	2.46	0.61
3:A:349:1PE:H121	5:A:482:HOH:O	2.00	0.61
1:B:343:LYS:HE2	1:B:345:GLN:O	2.00	0.61
1:A:13:ARG:HG2	1:A:31[A]:ARG:HG2	1.83	0.60
1:D:145:LYS:HE2	5:D:797:HOH:O	1.99	0.60
1:A:59:ARG:NH1	4:A:351:PEG:H42	2.16	0.60
1:A:189:ALA:HB3	1:A:218:PRO:HA	1.84	0.59
1:D:189:ALA:HB3	1:D:218:PRO:HA	1.83	0.59
1:A:8:LYS:HE3	5:A:557:HOH:O	2.02	0.59
1:D:203:ARG:NH2	5:D:854:HOH:O	2.36	0.59
1:D:148:LYS:HG3	1:D:152:GLU:OE2	2.04	0.58
1:C:345:GLN:HG2	5:C:445:HOH:O	2.03	0.57
1:D:13:ARG:HG2	1:D:31:ARG:HG2	1.86	0.57
1:C:152[B]:GLU:CA	1:C:152[B]:GLU:OE1	2.53	0.56
3:C:348:1PE:H141	5:C:606:HOH:O	2.06	0.55
1:B:301:ASN:ND2	1:B:332:LYS:H	2.04	0.55
1:A:13:ARG:HG2	1:A:31[B]:ARG:HG2	1.88	0.55
1:C:301:ASN:ND2	1:C:332:LYS:H	2.05	0.55
1:C:195:GLN:HE21	1:C:196:LYS:N	2.04	0.54
1:D:301:ASN:ND2	1:D:332:LYS:H	2.05	0.54
1:B:330:ARG:HA	3:B:348:1PE:H242	1.89	0.54
1:C:345:GLN:HA	5:C:498:HOH:O	2.09	0.52
1:C:251:MSE:HE3	5:C:510:HOH:O	2.09	0.52
1:A:145:LYS:HE2	5:A:624:HOH:O	2.09	0.51
1:D:232:PHE:CD1	3:D:348:1PE:H241	2.45	0.51
1:B:345:GLN:O	1:B:345:GLN:HG2	2.10	0.51
1:B:229:PHE:O	1:B:233:HIS:HD2	1.94	0.50
1:C:195:GLN:NE2	1:C:196:LYS:H	2.08	0.50
1:C:125:LYS:HE3	1:D:87:GLU:OE1	2.12	0.50
1:A:161:LYS:NZ	1:A:190:ASN:HD21	2.09	0.50
1:B:48:GLU:H	1:B:302:GLN:NE2	2.09	0.50
1:D:229:PHE:HA	3:D:348:1PE:H251	1.92	0.50
1:C:148:LYS:HE3	5:C:588:HOH:O	2.11	0.50
1:C:229:PHE:O	1:C:233:HIS:HD2	1.94	0.50
1:C:48:GLU:H	1:C:302:GLN:NE2	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:319:ASP:OD2	1:B:323:MSE:HE2	2.13	0.48
1:A:59:ARG:HH12	4:A:351:PEG:C4	2.24	0.48
1:A:259:VAL:HG23	1:A:286:LEU:HD21	1.96	0.47
1:A:48:GLU:H	1:A:302:GLN:NE2	2.12	0.47
1:B:146:GLU:HG3	5:B:555:HOH:O	2.14	0.47
1:A:301:ASN:ND2	1:A:332:LYS:H	2.12	0.47
1:C:184:LYS:HZ3	3:C:349:1PE:C14	2.28	0.47
1:D:229:PHE:O	1:D:233:HIS:HD2	1.98	0.47
1:B:54:ARG:NH1	1:B:191:MSE:HE2	2.29	0.47
1:A:315:PHE:CE1	3:A:349:1PE:H232	2.50	0.45
1:C:87:GLU:OE1	1:D:125:LYS:HE3	2.17	0.45
1:D:301:ASN:HD22	1:D:333:PHE:HD2	1.65	0.45
1:C:184:LYS:HZ3	3:C:349:1PE:H142	1.74	0.45
1:A:301:ASN:HD22	1:A:333:PHE:HD2	1.64	0.44
1:B:14:TYR:HB3	1:B:324:LEU:HD22	2.00	0.44
1:A:314:GLU:HG3	3:A:349:1PE:H231	2.00	0.44
1:B:251:MSE:HE3	5:B:743:HOH:O	2.16	0.44
1:C:155:PHE:CD1	1:C:338:PRO:HB3	2.53	0.44
1:D:232:PHE:HB2	3:D:348:1PE:C25	2.48	0.44
1:A:229:PHE:O	1:A:233:HIS:HD2	2.01	0.44
1:B:126:ARG:HD2	1:B:311:GLY:HA2	1.99	0.44
1:C:126:ARG:HD2	1:C:311:GLY:HA2	2.00	0.43
1:C:301:ASN:HD22	1:C:333:PHE:HD2	1.65	0.43
1:D:48:GLU:H	1:D:302:GLN:NE2	2.17	0.43
1:A:315:PHE:CZ	3:A:349:1PE:H232	2.54	0.43
1:B:50:SER:H	1:B:267:MSE:SE	2.52	0.42
1:D:209:GLY:HA2	3:D:349:1PE:H131	2.01	0.42
1:C:184:LYS:NZ	3:C:349:1PE:C14	2.73	0.42
1:A:59:ARG:HH22	4:A:351:PEG:H21	1.85	0.41
1:A:66:ILE:HD11	1:A:98:LEU:HD23	2.00	0.41
1:C:48:GLU:H	1:C:302:GLN:HE22	1.68	0.41
1:B:345:GLN:O	1:B:345:GLN:CG	2.68	0.41
1:A:48:GLU:H	1:A:302:GLN:HE22	1.67	0.41
1:A:159[A]:LYS:HE3	1:A:188:ASP:HB2	2.02	0.41
1:B:301:ASN:HD22	1:B:333:PHE:HD2	1.69	0.41
1:C:221:ARG:HD3	5:C:632:HOH:O	2.20	0.41
1:C:90:ASP:OD1	1:C:99:LYS:HE3	2.20	0.41
1:C:188:ASP:HA	1:C:216:GLU:HB2	2.03	0.41
1:C:234:SER:HB2	1:C:235:PRO:HD2	2.02	0.41
1:D:50:SER:H	1:D:267:MSE:SE	2.53	0.41
1:B:146:GLU:HG3	5:B:696:HOH:O	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:232:PHE:HB2	3:D:348:1PE:H252	2.03	0.40
3:B:348:1PE:H252	3:B:348:1PE:H241	1.85	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:255:LYS:NZ	5:A:526:HOH:O[4_565]	1.96	0.24
5:C:460:HOH:O	5:C:647:HOH:O[3_555]	2.14	0.06

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	348/345 (101%)	333 (96%)	13 (4%)	2 (1%)	25	8
1	B	350/345 (101%)	332 (95%)	18 (5%)	0	100	100
1	C	347/345 (101%)	333 (96%)	14 (4%)	0	100	100
1	D	346/345 (100%)	331 (96%)	14 (4%)	1 (0%)	41	21
All	All	1391/1380 (101%)	1329 (96%)	59 (4%)	3 (0%)	47	26

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	326	GLU
1	A	326	GLU
1	A	344	ASP

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	295/283 (104%)	291 (99%)	4 (1%)	67	47
1	B	297/283 (105%)	293 (99%)	4 (1%)	69	50
1	C	294/283 (104%)	286 (97%)	8 (3%)	44	20
1	D	293/283 (104%)	290 (99%)	3 (1%)	76	61
All	All	1179/1132 (104%)	1160 (98%)	19 (2%)	62	41

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	227	LEU
1	A	273	ASP
1	A	340	MSE
1	A	344	ASP
1	B	61	GLU
1	B	72	GLU
1	B	273	ASP
1	B	340	MSE
1	C	2	SER
1	C	17	GLU
1	C	30	SER
1	C	59	ARG
1	C	61	GLU
1	C	195	GLN
1	C	273	ASP
1	C	345	GLN
1	D	227	LEU
1	D	273	ASP
1	D	340	MSE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	81	ASN
1	A	190	ASN
1	A	233	HIS
1	A	301	ASN
1	A	302	GLN
1	B	81	ASN
1	B	233	HIS
1	B	301	ASN
1	B	302	GLN
1	C	81	ASN
1	C	195	GLN
1	C	233	HIS
1	C	301	ASN
1	C	302	GLN
1	D	81	ASN
1	D	301	ASN
1	D	302	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 19 ligands modelled in this entry, 4 are monoatomic - leaving 15 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	1PE	D	349	-	15,15,15	0.44	0	14,14,14	0.34	0
4	PEG	A	351	-	6,6,6	0.47	0	5,5,5	0.37	0
3	1PE	A	348	-	15,15,15	0.34	0	14,14,14	0.72	0
3	1PE	B	348	-	12,12,15	0.43	0	11,11,14	0.29	0
3	1PE	C	348	-	12,12,15	0.42	0	11,11,14	0.34	0
3	1PE	D	348	-	15,15,15	0.44	0	14,14,14	0.42	0
4	PEG	A	350	-	6,6,6	0.48	0	5,5,5	0.22	0
3	1PE	A	349	-	12,12,15	0.48	0	11,11,14	0.17	0
3	1PE	C	349	-	9,9,15	0.42	0	8,8,14	0.46	0
4	PEG	D	350	-	6,6,6	0.44	0	5,5,5	0.26	0
4	PEG	B	349	-	6,6,6	0.42	0	5,5,5	0.34	0
3	1PE	D	347	-	15,15,15	0.47	0	14,14,14	0.33	0
3	1PE	C	347	-	15,15,15	0.42	0	14,14,14	0.34	0
3	1PE	B	347	-	15,15,15	0.38	0	14,14,14	0.50	0
3	1PE	A	347	-	15,15,15	0.45	0	14,14,14	0.31	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	1PE	D	349	-	-	5/13/13/13	-
4	PEG	A	351	-	-	3/4/4/4	-
3	1PE	A	348	-	-	0/13/13/13	-
3	1PE	B	348	-	-	7/10/10/13	-
3	1PE	C	348	-	-	6/10/10/13	-
3	1PE	D	348	-	-	8/13/13/13	-
4	PEG	A	350	-	-	3/4/4/4	-
3	1PE	A	349	-	-	5/10/10/13	-
3	1PE	C	349	-	-	4/7/7/13	-
4	PEG	D	350	-	-	2/4/4/4	-
4	PEG	B	349	-	-	4/4/4/4	-
3	1PE	D	347	-	-	4/13/13/13	-
3	1PE	C	347	-	-	3/13/13/13	-
3	1PE	B	347	-	-	7/13/13/13	-
3	1PE	A	347	-	-	6/13/13/13	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (67) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	348	1PE	OH4-C13-C23-OH3
3	B	347	1PE	OH4-C13-C23-OH3
3	D	348	1PE	OH4-C13-C23-OH3
4	A	350	PEG	O2-C3-C4-O4
3	C	349	1PE	OH2-C12-C22-OH3
4	A	351	PEG	O2-C3-C4-O4
3	C	348	1PE	OH6-C15-C25-OH5
3	D	348	1PE	OH2-C12-C22-OH3
4	A	350	PEG	O1-C1-C2-O2
4	B	349	PEG	O2-C3-C4-O4
3	A	347	1PE	OH7-C16-C26-OH6
3	D	349	1PE	OH4-C13-C23-OH3
4	D	350	PEG	O1-C1-C2-O2
3	B	347	1PE	OH2-C12-C22-OH3
3	D	347	1PE	OH4-C13-C23-OH3
3	C	349	1PE	OH5-C14-C24-OH4
3	A	349	1PE	OH4-C13-C23-OH3
3	D	348	1PE	OH5-C14-C24-OH4
4	A	351	PEG	O1-C1-C2-O2
3	C	348	1PE	OH2-C12-C22-OH3
3	D	349	1PE	OH2-C12-C22-OH3
3	C	347	1PE	OH6-C15-C25-OH5
3	B	348	1PE	OH4-C13-C23-OH3
3	A	347	1PE	OH6-C15-C25-OH5
3	D	348	1PE	C14-C24-OH4-C13
4	B	349	PEG	C4-C3-O2-C2
3	A	349	1PE	OH6-C15-C25-OH5
3	C	349	1PE	C12-C22-OH3-C23
3	D	348	1PE	C24-C14-OH5-C25
3	D	349	1PE	C14-C24-OH4-C13
3	A	347	1PE	C14-C24-OH4-C13
3	A	349	1PE	C12-C22-OH3-C23
3	B	348	1PE	C12-C22-OH3-C23
3	A	347	1PE	C25-C15-OH6-C26
4	B	349	PEG	O1-C1-C2-O2
3	B	347	1PE	C24-C14-OH5-C25
3	D	347	1PE	OH5-C14-C24-OH4
3	D	347	1PE	OH2-C12-C22-OH3
3	B	347	1PE	C23-C13-OH4-C24

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Mol	Chain	Res	Type	Atoms
3	D	348	1PE	C13-C23-OH3-C22
3	B	348	1PE	C14-C24-OH4-C13
3	C	349	1PE	C23-C13-OH4-C24
3	C	348	1PE	C13-C23-OH3-C22
3	C	347	1PE	C14-C24-OH4-C13
3	A	349	1PE	OH5-C14-C24-OH4
3	D	348	1PE	C25-C15-OH6-C26
3	A	347	1PE	C24-C14-OH5-C25
3	B	348	1PE	OH5-C14-C24-OH4
3	B	347	1PE	C13-C23-OH3-C22
3	B	347	1PE	C14-C24-OH4-C13
3	D	349	1PE	C24-C14-OH5-C25
3	D	348	1PE	C23-C13-OH4-C24
3	B	348	1PE	C13-C23-OH3-C22
3	A	349	1PE	C14-C24-OH4-C13
3	D	349	1PE	OH6-C15-C25-OH5
3	A	347	1PE	C16-C26-OH6-C15
3	C	348	1PE	OH5-C14-C24-OH4
4	B	349	PEG	C1-C2-O2-C3
3	B	348	1PE	C24-C14-OH5-C25
4	A	350	PEG	C4-C3-O2-C2
3	B	348	1PE	OH2-C12-C22-OH3
3	B	347	1PE	OH5-C14-C24-OH4
3	C	348	1PE	C14-C24-OH4-C13
3	D	347	1PE	OH7-C16-C26-OH6
4	D	350	PEG	O2-C3-C4-O4
4	A	351	PEG	C4-C3-O2-C2
3	C	347	1PE	C23-C13-OH4-C24

There are no ring outliers.

7 monomers are involved in 27 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	349	1PE	1	0
4	A	351	PEG	4	0
3	B	348	1PE	2	0
3	C	348	1PE	2	0
3	D	348	1PE	9	0
3	A	349	1PE	4	0
3	C	349	1PE	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, 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	336/345 (97%)	-0.30	11 (3%) 46 43	12, 19, 32, 46	0
1	B	336/345 (97%)	-0.30	8 (2%) 59 56	13, 18, 33, 43	0
1	C	336/345 (97%)	-0.30	12 (3%) 42 40	13, 18, 34, 43	0
1	D	336/345 (97%)	-0.31	10 (2%) 50 48	12, 19, 33, 44	0
All	All	1344/1380 (97%)	-0.30	41 (3%) 49 46	12, 18, 33, 46	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	326	GLU	7.4
1	C	326	GLU	5.3
1	C	20	PHE	5.1
1	A	326	GLU	5.0
1	B	20	PHE	4.9
1	D	27	SER	4.6
1	B	19	PRO	4.3
1	A	324	LEU	4.3
1	D	324	LEU	4.0
1	A	328	VAL	3.9
1	D	326	GLU	3.8
1	C	16	TYR	3.8
1	B	345	GLN	3.7
1	D	328	VAL	3.7
1	A	19	PRO	3.5
1	D	345	GLN	3.5
1	B	325	LYS	3.4
1	C	345	GLN	3.2
1	A	344	ASP	3.2
1	C	325	LYS	3.1
1	D	26	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	16	TYR	2.9
1	A	26	VAL	2.9
1	A	325	LYS	2.9
1	C	18	LYS	2.9
1	D	327	GLU	2.7
1	B	17	GLU	2.6
1	D	20	PHE	2.5
1	C	27	SER	2.5
1	A	20	PHE	2.3
1	A	327	GLU	2.3
1	C	328	VAL	2.3
1	A	27[A]	SER	2.2
1	C	344	ASP	2.2
1	B	26	VAL	2.2
1	D	13	ARG	2.1
1	C	26	VAL	2.1
1	C	17	GLU	2.1
1	C	181	ARG	2.0
1	A	345	GLN	2.0
1	D	19	PRO	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 carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	1PE	D	348	16/16	0.69	0.25	42,45,47,47	0
3	1PE	A	349	13/16	0.69	0.21	44,45,48,49	0
4	PEG	B	349	7/7	0.73	0.16	48,49,50,50	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	1PE	D	347	16/16	0.79	0.19	38,43,51,52	0
4	PEG	A	350	7/7	0.81	0.11	41,41,44,45	0
3	1PE	B	348	13/16	0.83	0.14	41,42,45,46	0
4	PEG	A	351	7/7	0.83	0.14	39,39,41,42	0
3	1PE	C	349	10/16	0.85	0.13	39,44,45,45	0
3	1PE	D	349	16/16	0.86	0.15	39,40,47,49	0
3	1PE	C	348	13/16	0.86	0.15	40,41,47,49	0
4	PEG	D	350	7/7	0.88	0.11	46,46,47,47	0
3	1PE	A	347	16/16	0.88	0.11	40,43,46,47	0
3	1PE	C	347	16/16	0.91	0.12	29,33,40,41	0
3	1PE	B	347	16/16	0.92	0.10	32,37,39,40	0
3	1PE	A	348	16/16	0.96	0.09	19,21,28,32	0
2	MN	C	346	1/1	0.98	0.32	16,16,16,16	0
2	MN	D	346	1/1	0.99	0.32	15,15,15,15	0
2	MN	B	346	1/1	0.99	0.31	17,17,17,17	0
2	MN	A	346	1/1	0.99	0.28	15,15,15,15	0

6.5 Other polymers [i](#)

There are no such residues in this entry.