Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 10:16 am BST

PDB ID	:	1U7N
Title	:	Crystal Structure of the fatty acid/phospholipid synthesis protein PlsX from Enterococcus faecalis V583
Authors	:	Kim, Y.; Li, H.; Collart, F.; Joachimiak, A.; Midwest Center for Structural Genomics (MCSG)
Deposited on	:	2004-08-04
Resolution	:	2.26 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:

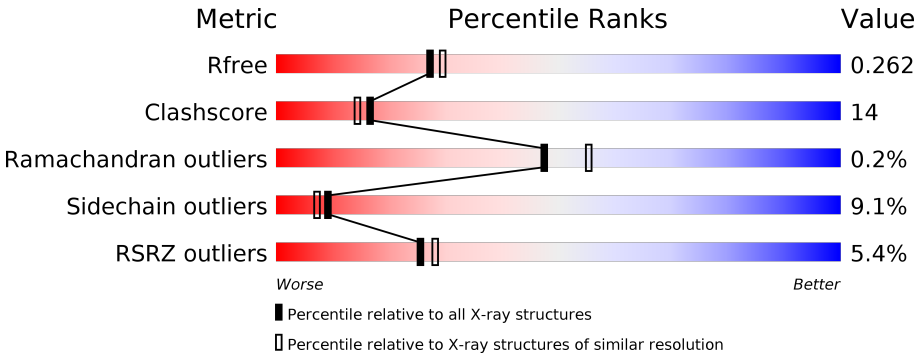
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 2.26 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	1377 (2.26-2.26)
Clashscore	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (2.26-2.26)

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

Mol	Chain	Length	Quality of chain
1	A	336	2% 76% 16% • 5%
1	B	336	8% 66% 24% • 5%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5295 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 Fatty acid/phospholipid synthesis protein plsX.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	318	Total	C	N	O	Se	0	9	0
			2478	1561	420	483	14			
1	B	318	Total	C	N	O	Se	0	10	0
			2494	1575	427	479	13			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	CLONING ARTIFACT	UNP Q82ZE8
A	-1	ASN	-	CLONING ARTIFACT	UNP Q82ZE8
A	0	ALA	-	CLONING ARTIFACT	UNP Q82ZE8
A	1	MSE	MET	MODIFIED RESIDUE	UNP Q82ZE8
A	8	MSE	MET	MODIFIED RESIDUE	UNP Q82ZE8
A	22	MSE	MET	MODIFIED RESIDUE	UNP Q82ZE8
A	79	MSE	MET	MODIFIED RESIDUE	UNP Q82ZE8
A	123	MSE	MET	MODIFIED RESIDUE	UNP Q82ZE8
A	129	MSE	MET	MODIFIED RESIDUE	UNP Q82ZE8
A	138	MSE	MET	MODIFIED RESIDUE	UNP Q82ZE8
A	241	MSE	MET	MODIFIED RESIDUE	UNP Q82ZE8
A	243	MSE	MET	MODIFIED RESIDUE	UNP Q82ZE8
A	244	MSE	MET	MODIFIED RESIDUE	UNP Q82ZE8
A	272	MSE	MET	MODIFIED RESIDUE	UNP Q82ZE8
A	276	MSE	MET	MODIFIED RESIDUE	UNP Q82ZE8
A	315	MSE	MET	MODIFIED RESIDUE	UNP Q82ZE8
B	-2	SER	-	CLONING ARTIFACT	UNP Q82ZE8
B	-1	ASN	-	CLONING ARTIFACT	UNP Q82ZE8
B	0	ALA	-	CLONING ARTIFACT	UNP Q82ZE8
B	1	MSE	MET	MODIFIED RESIDUE	UNP Q82ZE8
B	8	MSE	MET	MODIFIED RESIDUE	UNP Q82ZE8
B	22	MSE	MET	MODIFIED RESIDUE	UNP Q82ZE8
B	79	MSE	MET	MODIFIED RESIDUE	UNP Q82ZE8
B	123	MSE	MET	MODIFIED RESIDUE	UNP Q82ZE8
B	129	MSE	MET	MODIFIED RESIDUE	UNP Q82ZE8

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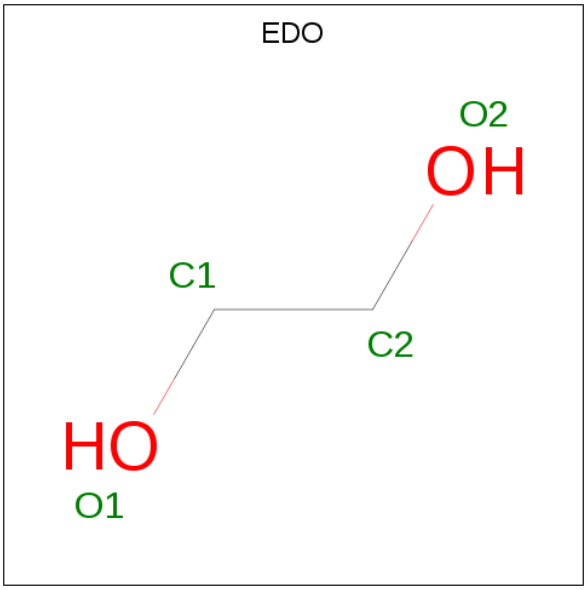
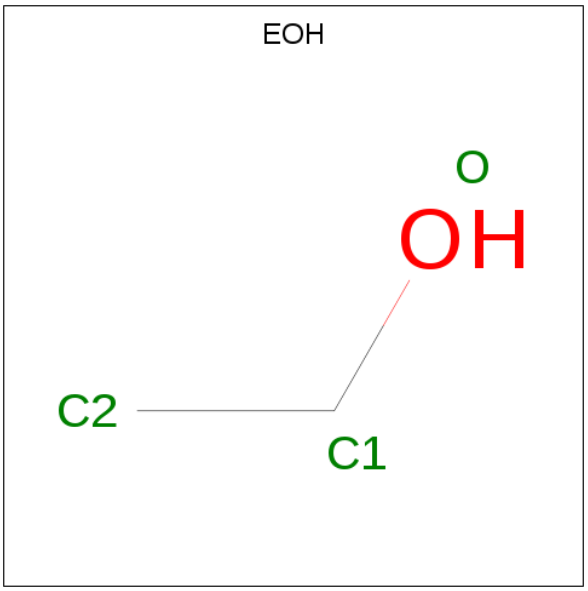
Chain	Residue	Modelled	Actual	Comment	Reference
B	138	MSE	MET	MODIFIED RESIDUE	UNP Q82ZE8
B	241	MSE	MET	MODIFIED RESIDUE	UNP Q82ZE8
B	243	MSE	MET	MODIFIED RESIDUE	UNP Q82ZE8
B	244	MSE	MET	MODIFIED RESIDUE	UNP Q82ZE8
B	272	MSE	MET	MODIFIED RESIDUE	UNP Q82ZE8
B	276	MSE	MET	MODIFIED RESIDUE	UNP Q82ZE8
B	315	MSE	MET	MODIFIED RESIDUE	UNP Q82ZE8

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



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

- Molecule 3 is ETHANOL (three-letter code: EOH) (formula: C_2H_6O).



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

- Molecule 4 is water.

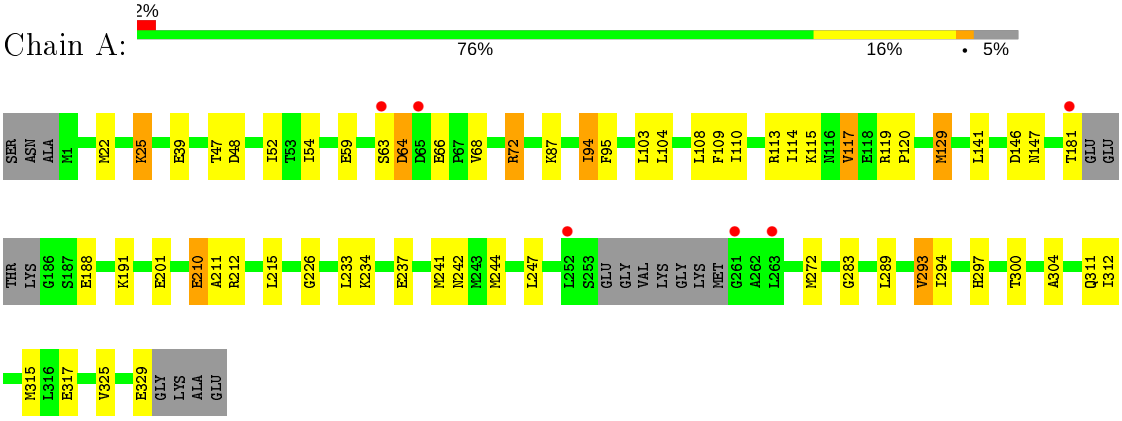
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	183	Total O 183 183	0	0
4	B	124	Total O 124 124	0	0

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.

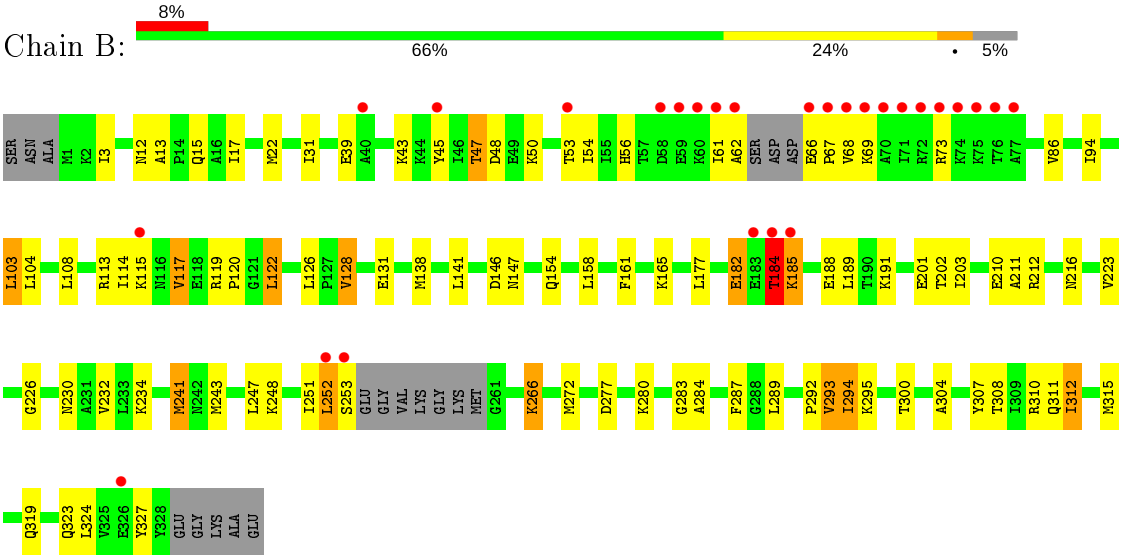
- Molecule 1: Fatty acid/phospholipid synthesis protein plsX

Chain A:



- Molecule 1: Fatty acid/phospholipid synthesis protein plsX

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	62.36Å 82.42Å 147.24Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	73.52 – 2.26 35.96 – 2.26	Depositor EDS
% Data completeness (in resolution range)	99.7 (73.52-2.26) 99.7 (35.96-2.26)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.21 (at 2.27Å)	Xtriage
Refinement program	REFMAC 5.2.0000	Depositor
R, R_{free}	0.206 , 0.262 0.205 , 0.262	Depositor DCC
R_{free} test set	1804 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	30.4	Xtriage
Anisotropy	0.270	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 44.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	5295	wwPDB-VP
Average B, all atoms (Å^2)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.68% 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: EOH, 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	0.61	0/2498	0.71	2/3350 (0.1%)
1	B	0.53	0/2514	0.67	1/3367 (0.0%)
All	All	0.57	0/5012	0.69	3/6717 (0.0%)

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.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	72	ARG	NE-CZ-NH2	-6.54	117.03	120.30
1	B	184	THR	N-CA-C	6.46	128.44	111.00
1	A	72	ARG	NE-CZ-NH1	5.81	123.21	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	184	THR	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	2478	0	2497	71	0
1	B	2494	0	2540	90	0
2	A	4	0	6	0	0
3	A	9	0	18	0	0
3	B	3	0	6	0	0
4	A	183	0	0	13	0
4	B	124	0	0	8	0
All	All	5295	0	5067	143	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 14.

All (143) 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:A:211:ALA:HB3	1:B:234[B]:LYS:HG3	1.42	1.00
1:B:312:ILE:HG22	1:B:315:MSE:CE	1.94	0.98
1:A:108:LEU:HD23	4:A:799:HOH:O	1.65	0.96
1:A:294:ILE:HD11	1:A:315:MSE:HE1	1.50	0.92
1:A:244:MSE:HG2	1:A:272:MSE:HE3	1.52	0.90
1:A:247:LEU:HD12	1:A:272:MSE:HE1	1.55	0.88
1:B:22:MSE:HE2	1:B:47:THR:HG22	1.56	0.86
1:A:234:LYS:HG3	1:B:211:ALA:HB3	1.55	0.85
1:A:311:GLN:HG2	1:A:315:MSE:HE2	1.58	0.85
1:B:22:MSE:HE1	1:B:48:ASP:HB3	1.58	0.85
1:A:25:LYS:HD3	1:A:52:ILE:HD11	1.58	0.83
1:A:241[B]:MSE:HA	1:A:244:MSE:HE2	1.60	0.83
1:A:120:PRO:HG2	4:A:796:HOH:O	1.77	0.82
1:A:247:LEU:HD12	1:A:272:MSE:CE	2.08	0.82
1:A:212:ARG:HD3	4:A:782:HOH:O	1.80	0.82
1:A:241[A]:MSE:HA	1:A:244:MSE:HE2	1.60	0.81
1:A:22:MSE:HE1	1:A:48:ASP:HB3	1.65	0.78
1:A:283:GLY:H	1:A:311:GLN:HE22	1.31	0.78
1:B:294:ILE:HG12	1:B:308:THR:HG23	1.65	0.77
1:A:237:GLU:O	1:A:241[A]:MSE:HG2	1.83	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:39:GLU:HB3	1:B:54:ILE:HG21	1.67	0.76
1:B:184:THR:H	1:B:185:LYS:HB3	1.52	0.74
1:B:128:VAL:CG2	1:B:131:GLU:HB2	2.18	0.74
1:B:188[B]:GLU:HG2	1:B:189:LEU:N	2.04	0.72
1:B:182:GLU:HB2	4:B:657:HOH:O	1.90	0.70
1:A:244:MSE:CG	1:A:272:MSE:HE3	2.22	0.69
1:A:234:LYS:HE3	1:B:211:ALA:HB3	1.76	0.68
1:B:283:GLY:HA3	1:B:294:ILE:CD1	2.26	0.65
1:A:234:LYS:HE3	1:B:211:ALA:CB	2.27	0.65
1:A:312:ILE:HA	1:A:315:MSE:HE3	1.78	0.64
1:A:283:GLY:H	1:A:311:GLN:NE2	1.95	0.64
1:A:234:LYS:HE3	1:B:211:ALA:H	1.61	0.64
1:A:241[A]:MSE:HG3	1:B:212:ARG:NH2	2.13	0.64
1:B:66:GLU:OE1	1:B:68:VAL:HG12	1.97	0.64
1:B:184:THR:N	1:B:185:LYS:HB3	2.13	0.63
1:A:211:ALA:HB3	1:B:234[B]:LYS:CG	2.23	0.62
1:A:129:MSE:HE3	1:A:215:LEU:HB3	1.79	0.62
1:B:312:ILE:HG22	1:B:315:MSE:HE1	1.79	0.62
1:B:312:ILE:HG22	1:B:315:MSE:HE3	1.79	0.62
1:B:251:ILE:O	1:B:252:LEU:HB2	1.97	0.61
1:B:283:GLY:HA3	1:B:294:ILE:HD13	1.84	0.60
1:B:251:ILE:HG21	1:B:266[B]:LYS:HE3	1.84	0.60
1:A:72:ARG:NH2	1:A:109:PHE:CD2	2.69	0.60
1:B:69:LYS:HG2	1:B:73:ARG:NH1	2.17	0.59
1:B:184:THR:H	1:B:185:LYS:CB	2.16	0.59
1:B:128:VAL:HG22	1:B:131:GLU:HB2	1.84	0.59
1:B:182:GLU:O	1:B:185:LYS:HB3	2.02	0.59
1:B:12:ASN:O	1:B:15[B]:GLN:HG2	2.03	0.59
1:B:39:GLU:HB2	1:B:43:LYS:HE2	1.84	0.58
1:A:115:LYS:HE3	1:A:329:GLU:HG3	1.85	0.57
1:B:247:LEU:HG	1:B:272:MSE:HE1	1.85	0.57
1:A:234:LYS:CG	1:B:211:ALA:HB3	2.29	0.57
1:B:283:GLY:H	1:B:311:GLN:HE22	1.53	0.56
1:A:241[A]:MSE:HE3	1:B:212:ARG:HH21	1.70	0.56
1:A:72:ARG:NE	4:A:646:HOH:O	2.24	0.56
1:A:22:MSE:HE3	4:A:581:HOH:O	2.06	0.55
1:A:146:ASP:OD1	1:B:188[B]:GLU:OE1	2.25	0.55
1:A:247:LEU:HD12	1:A:272:MSE:HE2	1.88	0.55
1:A:297:HIS:HD2	4:A:692:HOH:O	1.90	0.55
1:A:300:THR:OG1	1:A:304:ALA:HB3	2.07	0.55
1:B:188[B]:GLU:CG	1:B:189:LEU:N	2.70	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:210:GLU:HG3	4:B:783:HOH:O	2.06	0.55
1:A:63:SER:HA	1:A:64:ASP:OD2	2.07	0.54
1:B:158:LEU:HD23	1:B:324:LEU:HD22	1.90	0.54
1:A:211:ALA:CB	1:B:234[B]:LYS:HE3	2.37	0.54
1:B:241:MSE:HE1	4:B:710:HOH:O	2.08	0.54
1:A:22:MSE:HE3	1:A:22:MSE:HA	1.90	0.54
1:B:138:MSE:HE3	1:B:141:LEU:CD2	2.39	0.53
1:A:22:MSE:CE	4:A:581:HOH:O	2.55	0.53
1:B:61:ILE:O	1:B:62:ALA:O	2.26	0.53
1:A:283:GLY:N	1:A:311:GLN:HE22	2.05	0.53
1:A:39:GLU:HB3	1:A:54:ILE:HG21	1.90	0.53
1:A:289:LEU:CD2	4:A:799:HOH:O	2.58	0.52
1:A:94:ILE:HG23	1:A:293:VAL:HB	1.92	0.52
1:B:39:GLU:HG2	1:B:56:HIS:ND1	2.23	0.52
1:A:247:LEU:CD1	1:A:272:MSE:HE1	2.35	0.51
1:A:211:ALA:HB3	1:B:234[B]:LYS:HE3	1.91	0.51
1:B:292:PRO:HB3	1:B:315:MSE:HE3	1.92	0.51
1:A:25:LYS:HD3	1:A:52:ILE:CD1	2.35	0.51
1:A:87:LYS:HD3	1:A:110:ILE:O	2.10	0.50
1:B:289:LEU:HD12	1:B:293:VAL:CG1	2.42	0.50
1:B:312:ILE:CG2	1:B:315:MSE:CE	2.79	0.50
1:B:182:GLU:OE1	1:B:184:THR:HB	2.11	0.49
1:A:25:LYS:HE3	4:A:617:HOH:O	2.11	0.49
1:B:122:LEU:HD22	1:B:284:ALA:HB1	1.94	0.49
1:B:312:ILE:HA	1:B:315:MSE:HE2	1.94	0.49
1:A:147:ASN:ND2	1:A:226:GLY:H	2.10	0.49
1:B:248:LYS:HE2	4:B:777:HOH:O	2.12	0.49
1:B:126:LEU:CD1	1:B:138:MSE:HE2	2.43	0.48
1:A:289:LEU:HD21	4:A:799:HOH:O	2.13	0.48
1:A:108:LEU:HA	4:A:741:HOH:O	2.12	0.48
1:A:325:VAL:O	1:A:329:GLU:HB3	2.14	0.48
1:B:310[B]:ARG:HG3	4:B:583:HOH:O	2.14	0.48
1:A:94:ILE:HG12	1:A:95:PHE:N	2.29	0.48
1:A:242:ASN:HD21	1:B:216:ASN:HD21	1.61	0.47
1:B:15[A]:GLN:HG2	1:B:45:TYR:CZ	2.49	0.47
1:A:141:LEU:HD13	1:A:233:LEU:HD22	1.97	0.47
1:A:234:LYS:HD2	4:B:507:HOH:O	2.15	0.47
1:A:39:GLU:CB	1:A:54:ILE:HG21	2.45	0.46
1:B:119:ARG:NH1	1:B:146:ASP:O	2.45	0.46
1:B:280:LYS:HA	1:B:307:TYR:CD2	2.51	0.46
1:A:22:MSE:HE1	1:A:25:LYS:HZ1	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:147:ASN:ND2	1:B:226:GLY:H	2.12	0.46
1:B:230:ASN:ND2	1:B:234[B]:LYS:HE2	2.31	0.46
1:B:289:LEU:HD12	1:B:293:VAL:HG11	1.98	0.46
1:B:230:ASN:O	1:B:234[B]:LYS:HG2	2.16	0.46
1:B:13:ALA:HB2	1:B:17:ILE:HD13	1.98	0.45
1:B:294:ILE:CG1	1:B:308:THR:HG23	2.40	0.45
1:B:277:ASP:OD2	1:B:280:LYS:HE2	2.16	0.45
1:B:319[B]:GLN:O	1:B:323:GLN:HG3	2.17	0.45
1:A:272:MSE:HG3	1:B:243:MSE:SE	2.67	0.45
1:A:115:LYS:CE	1:A:329:GLU:HG3	2.46	0.45
1:B:283:GLY:CA	1:B:294:ILE:HD13	2.46	0.45
1:B:283:GLY:N	1:B:311:GLN:HE22	2.14	0.44
1:B:3:ILE:HD12	1:B:31:ILE:HG21	1.99	0.44
1:B:66:GLU:OE2	1:B:69:LYS:HB2	2.17	0.44
1:B:177:LEU:HD21	1:B:232:VAL:HG21	1.99	0.44
1:A:234:LYS:CE	1:B:211:ALA:H	2.31	0.44
1:A:210:GLU:HA	1:B:234[B]:LYS:HZ2	1.83	0.44
1:B:22:MSE:HE3	4:B:749:HOH:O	2.17	0.43
1:B:248:LYS:O	1:B:251:ILE:O	2.36	0.43
1:A:103:LEU:HD22	4:A:729:HOH:O	2.17	0.43
1:B:300:THR:OG1	1:B:304:ALA:HB3	2.18	0.43
1:B:312:ILE:HA	1:B:315:MSE:CE	2.48	0.43
1:A:119:ARG:HA	1:A:120:PRO:HD2	1.86	0.43
1:B:103:LEU:HD12	1:B:295:LYS:HB2	2.00	0.43
1:A:289:LEU:HD12	1:A:293:VAL:HG13	2.01	0.43
1:B:210:GLU:HB3	4:B:507:HOH:O	2.20	0.42
1:A:114:ILE:HB	1:A:117:VAL:HG13	2.01	0.42
1:B:202:THR:HG21	1:B:327:TYR:CE1	2.54	0.42
1:B:119:ARG:HA	1:B:120:PRO:HD2	1.93	0.42
1:B:154[B]:GLN:O	1:B:158:LEU:HG	2.20	0.42
1:A:119:ARG:NH2	4:A:714:HOH:O	2.53	0.41
1:B:185:LYS:HA	1:B:185:LYS:HD3	1.75	0.41
1:A:211:ALA:H	1:B:234[B]:LYS:HE3	1.85	0.41
1:A:72:ARG:NH2	1:A:109:PHE:CG	2.88	0.41
1:A:312:ILE:HA	1:A:315:MSE:CE	2.49	0.40
1:B:114:ILE:HB	1:B:117:VAL:CG1	2.51	0.40
1:B:114:ILE:HB	1:B:117:VAL:HG13	2.02	0.40
1:B:138:MSE:HE3	1:B:141:LEU:HD21	2.03	0.40
1:B:161:PHE:O	1:B:165:LYS:HG2	2.21	0.40
1:A:211:ALA:H	1:B:234[B]:LYS:CE	2.34	0.40
1:B:22:MSE:CE	1:B:48:ASP:HB3	2.41	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	321/336 (96%)	319 (99%)	2 (1%)	0	100 100
1	B	322/336 (96%)	312 (97%)	9 (3%)	1 (0%)	41 46
All	All	643/672 (96%)	631 (98%)	11 (2%)	1 (0%)	47 55

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	67	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	262/253 (104%)	244 (93%)	18 (7%)	15 14
1	B	263/253 (104%)	234 (89%)	29 (11%)	6 4
All	All	525/506 (104%)	478 (91%)	47 (9%)	9 7

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	LYS
1	A	47	THR

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Mol	Chain	Res	Type
1	A	59	GLU
1	A	64	ASP
1	A	66	GLU
1	A	68	VAL
1	A	94	ILE
1	A	104	LEU
1	A	113	ARG
1	A	117	VAL
1	A	129	MSE
1	A	181	THR
1	A	188	GLU
1	A	191	LYS
1	A	201	GLU
1	A	210	GLU
1	A	293	VAL
1	A	317	GLU
1	B	47	THR
1	B	50	LYS
1	B	53	THR
1	B	86	VAL
1	B	94	ILE
1	B	103	LEU
1	B	104	LEU
1	B	108	LEU
1	B	113	ARG
1	B	115	LYS
1	B	117	VAL
1	B	122	LEU
1	B	128	VAL
1	B	182	GLU
1	B	184	THR
1	B	185	LYS
1	B	191	LYS
1	B	201	GLU
1	B	203	ILE
1	B	223	VAL
1	B	241	MSE
1	B	252	LEU
1	B	253	SER
1	B	266[A]	LYS
1	B	266[B]	LYS
1	B	287	PHE

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Mol	Chain	Res	Type
1	B	293	VAL
1	B	294	ILE
1	B	312	ILE

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

Mol	Chain	Res	Type
1	A	26	GLN
1	A	88	ASN
1	A	147	ASN
1	A	204	ASN
1	A	216	ASN
1	A	230	ASN
1	A	297	HIS
1	A	311	GLN
1	B	88	ASN
1	B	147	ASN
1	B	216	ASN
1	B	281	HIS
1	B	311	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry

5 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	EOH	B	404	-	2,2,2	0.49	0	1,1,1	0.08	0
3	EOH	A	403	-	2,2,2	0.48	0	1,1,1	0.00	0
3	EOH	A	401	-	2,2,2	0.49	0	1,1,1	0.15	0
3	EOH	A	402	-	2,2,2	0.51	0	1,1,1	0.05	0
2	EDO	A	405	-	3,3,3	0.49	0	2,2,2	0.35	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
2	EDO	A	405	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	405	EDO	O1-C1-C2-O2

There are no ring outliers.

No monomer is involved in short contacts.

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	305/336 (90%)	-0.03	6 (1%) 65 68	14, 23, 39, 48	2 (0%)
1	B	305/336 (90%)	0.47	27 (8%) 9 10	16, 33, 57, 61	12 (3%)
All	All	610/672 (90%)	0.22	33 (5%) 25 28	14, 28, 48, 61	14 (2%)

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	61	ILE	11.2
1	B	62	ALA	8.0
1	A	65	ASP	7.2
1	B	60	LYS	7.0
1	B	71	ILE	5.9
1	B	252	LEU	5.3
1	B	68	VAL	5.0
1	A	63	SER	4.7
1	B	59	GLU	4.3
1	B	66	GLU	4.3
1	B	69	LYS	3.8
1	B	70	ALA	3.8
1	B	77	ALA	3.6
1	B	76	THR	3.4
1	B	40	ALA	3.3
1	B	326[A]	GLU	3.3
1	B	75	LYS	3.2
1	B	67	PRO	3.1
1	B	58	ASP	3.0
1	B	73	ARG	2.9
1	B	184	THR	2.9
1	B	74	LYS	2.9
1	B	253	SER	2.8
1	B	72	ARG	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	45	TYR	2.8
1	A	252	LEU	2.6
1	A	181	THR	2.4
1	B	185	LYS	2.3
1	B	53	THR	2.3
1	B	115	LYS	2.2
1	A	263	LEU	2.2
1	A	261	GLY	2.1
1	B	183	GLU	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 carbohydrates in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	EOH	B	404	3/3	0.39	0.32	68,68,68,68	0
2	EDO	A	405	4/4	0.75	0.15	43,47,49,51	0
3	EOH	A	403	3/3	0.76	0.29	37,37,37,37	0
3	EOH	A	402	3/3	0.83	0.25	35,35,35,37	0
3	EOH	A	401	3/3	0.85	0.51	49,49,49,49	0

6.5 Other polymers (i)

There are no such residues in this entry.