Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 10:05 am BST

PDB ID	:	6S9N
Title	:	Designed Armadillo Repeat protein Lock2 fused to target peptide KRKRKAKLSF
Authors	:	Ernst, P.; Zosel, F.; Reichen, C.; Schuler, B.; Pluckthun, A.
Deposited on	:	2019-07-15
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 ⓘ symbol.

The following versions of software and data (see references ①) were used in the production of this report:

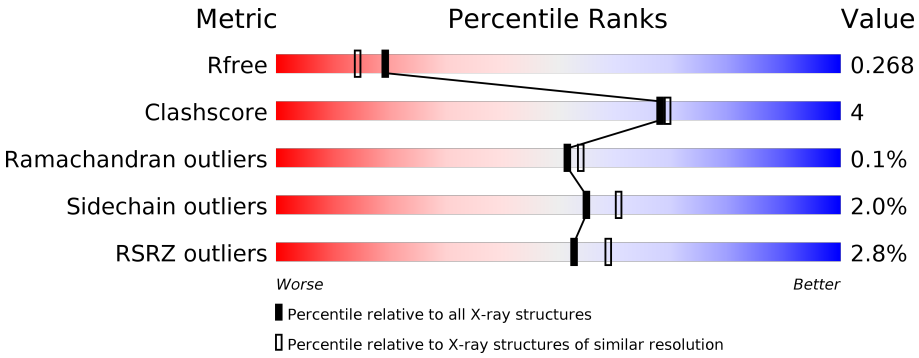
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA,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

1 Overall quality at a glance (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 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	302	2% 89% 9%
1	B	302	% 90% 7%
1	C	302	% 90% 8%
1	D	302	7% 92% 7%
1	E	302	% 92% 6%
1	F	302	6% 89% 9%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 14498 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.

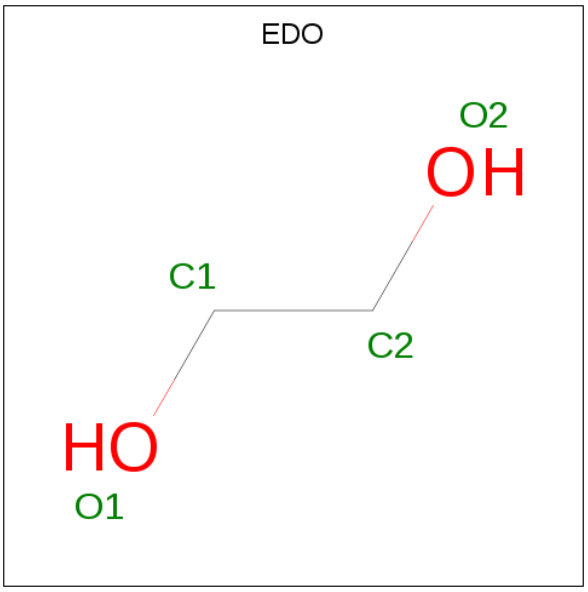
- Molecule 1 is a protein called Lock2_KRKRKAKLSF.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	300	Total	C	N	O	S	0	2	0
			2218	1379	387	450	2			
1	B	299	Total	C	N	O	S	0	3	0
			2225	1383	389	451	2			
1	C	299	Total	C	N	O	S	0	4	0
			2234	1388	392	452	2			
1	D	299	Total	C	N	O	S	0	2	0
			2211	1375	385	449	2			
1	E	301	Total	C	N	O	S	0	1	0
			2218	1380	389	447	2			
1	F	299	Total	C	N	O	S	0	0	0
			2196	1367	383	444	2			

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	5	Total	Ca	0	0
			5	5		
2	A	6	Total	Ca	0	0
			6	6		
2	D	1	Total	Ca	0	0
			1	1		
2	C	6	Total	Ca	0	0
			6	6		

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



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

- Molecule 4 is water.

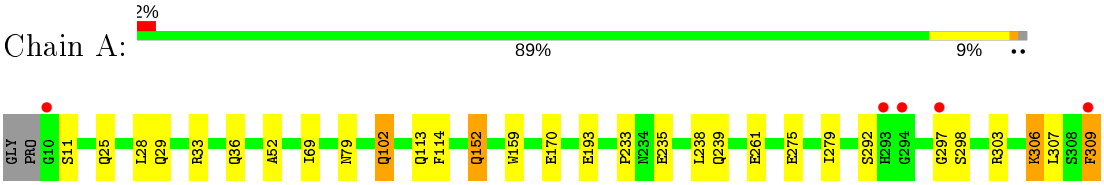
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	216	Total O 216 216	0	0
4	B	233	Total O 233 233	0	0
4	C	230	Total O 230 230	0	0
4	D	144	Total O 144 144	0	0
4	E	173	Total O 173 173	0	0
4	F	178	Total O 178 178	0	0

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.

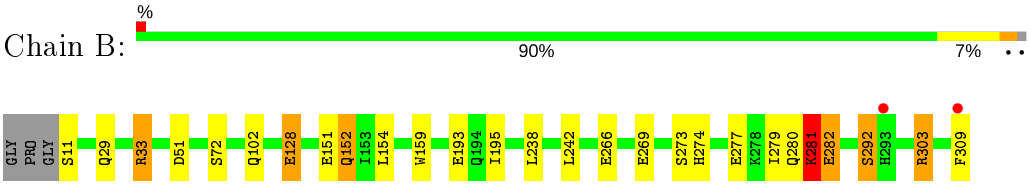
- Molecule 1: Lock2_KRKRKAKLSF

Chain A:



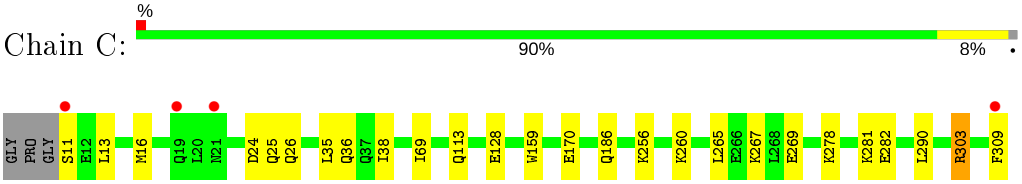
- Molecule 1: Lock2_KRKRKAKLSF

Chain B:



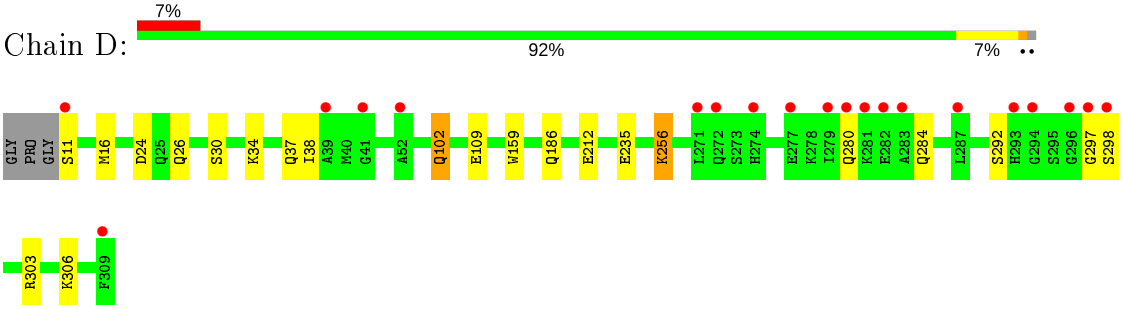
- Molecule 1: Lock2_KRKRKAKLSF

Chain C:



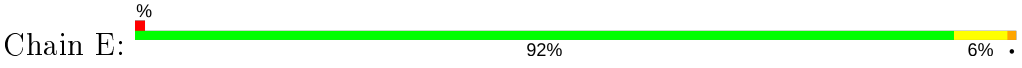
- Molecule 1: Lock2_KRKRKAKLSF

Chain D:



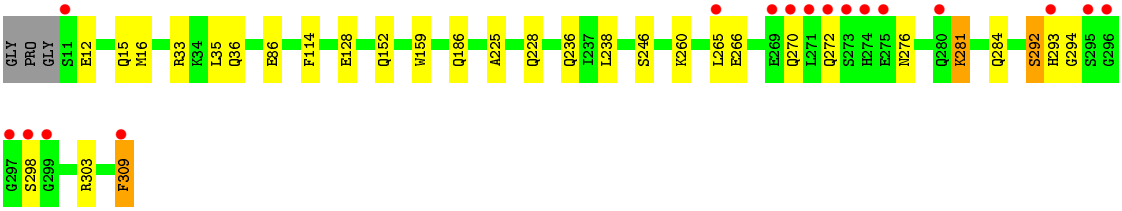
- Molecule 1: Lock2_KRKRKAKLSF

Chain E:



- Molecule 1: Lock2_KRKRKAKLSF

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	55.26Å 85.50Å 194.03Å 90.00° 96.33° 90.00°	Depositor
Resolution (Å)	45.61 – 2.10 45.61 – 2.10	Depositor EDS
% Data completeness (in resolution range)	98.7 (45.61-2.10) 98.7 (45.61-2.10)	Depositor EDS
R_{merge}	0.21	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.87 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.8.0189	Depositor
R, R_{free}	0.223 , 0.262 0.231 , 0.268	Depositor DCC
R_{free} test set	5177 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	25.7	Xtriage
Anisotropy	0.841	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 42.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.009 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	14498	wwPDB-VP
Average B, all atoms (Å^2)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.14% 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: CA, 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	0.98	4/2239 (0.2%)	0.87	2/3036 (0.1%)
1	B	0.94	4/2246 (0.2%)	0.85	6/3045 (0.2%)
1	C	0.90	3/2255 (0.1%)	0.79	0/3057
1	D	0.84	2/2232 (0.1%)	0.81	6/3027 (0.2%)
1	E	0.91	2/2240 (0.1%)	0.87	6/3037 (0.2%)
1	F	0.95	3/2217 (0.1%)	0.88	4/3007 (0.1%)
All	All	0.92	18/13429 (0.1%)	0.85	24/18209 (0.1%)

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	86	GLU	CD-OE1	10.09	1.36	1.25
1	E	128	GLU	CG-CD	7.21	1.62	1.51
1	B	128	GLU	CG-CD	6.79	1.62	1.51
1	F	246	SER	CB-OG	-6.74	1.33	1.42
1	C	128	GLU	CG-CD	6.07	1.61	1.51
1	D	212	GLU	CD-OE2	5.87	1.32	1.25
1	B	152	GLN	CD-OE1	5.82	1.36	1.24
1	D	30	SER	CB-OG	-5.60	1.34	1.42
1	E	128	GLU	CD-OE1	5.54	1.31	1.25
1	A	193	GLU	CD-OE1	5.48	1.31	1.25
1	B	128	GLU	CD-OE1	5.47	1.31	1.25
1	A	170	GLU	CD-OE1	5.44	1.31	1.25
1	C	303[A]	ARG	CZ-NH2	5.42	1.40	1.33
1	C	303[B]	ARG	CZ-NH2	5.42	1.40	1.33
1	A	307	LEU	N-CA	5.40	1.57	1.46
1	B	269	GLU	CD-OE1	5.35	1.31	1.25
1	F	298	SER	CB-OG	-5.10	1.35	1.42
1	A	261	GLU	CD-OE1	5.01	1.31	1.25

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	306	LYS	N-CA-C	7.49	131.23	111.00
1	A	235	GLU	OE1-CD-OE2	-7.34	114.49	123.30
1	E	261	GLU	CA-CB-CG	7.02	128.85	113.40
1	D	306	LYS	CD-CE-NZ	6.60	126.88	111.70
1	D	280	GLN	CA-CB-CG	6.51	127.73	113.40
1	E	309	PHE	CB-CA-C	6.31	123.02	110.40
1	B	193	GLU	OE1-CD-OE2	-6.24	115.81	123.30
1	D	256	LYS	CD-CE-NZ	-6.09	97.69	111.70
1	F	309	PHE	CB-CA-C	-6.05	98.31	110.40
1	B	281	LYS	CA-CB-CG	6.01	126.62	113.40
1	F	281	LYS	CD-CE-NZ	5.87	125.20	111.70
1	F	128	GLU	OE1-CD-OE2	5.80	130.26	123.30
1	B	151	GLU	OE1-CD-OE2	-5.52	116.67	123.30
1	B	303[A]	ARG	NE-CZ-NH1	5.45	123.03	120.30
1	B	303[B]	ARG	NE-CZ-NH1	5.45	123.03	120.30
1	B	152	GLN	CA-CB-CG	5.25	124.94	113.40
1	E	13	LEU	CB-CG-CD1	-5.24	102.09	111.00
1	D	102	GLN	CA-CB-CG	5.24	124.92	113.40
1	F	33	ARG	NE-CZ-NH1	-5.16	117.72	120.30
1	D	109	GLU	OE1-CD-OE2	-5.09	117.20	123.30
1	D	235	GLU	OE1-CD-OE2	-5.06	117.23	123.30
1	E	238	LEU	CA-CB-CG	5.05	126.91	115.30
1	E	186	GLN	CA-CB-CG	5.04	124.49	113.40
1	E	44	GLU	OE1-CD-OE2	-5.03	117.26	123.30

There are no chirality outliers.

There are no planarity outliers.

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	2218	0	2249	23	0
1	B	2225	0	2256	17	0
1	C	2234	0	2265	24	0
1	D	2211	0	2243	8	0
1	E	2218	0	2257	15	0
1	F	2196	0	2234	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	6	0	0	1	0
2	B	5	0	0	0	0
2	C	6	0	0	2	0
2	D	1	0	0	1	0
3	F	4	0	6	0	0
4	A	216	0	0	2	0
4	B	233	0	0	5	1
4	C	230	0	0	4	1
4	D	144	0	0	1	1
4	E	173	0	0	3	1
4	F	178	0	0	2	2
All	All	14498	0	13510	102	3

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 (102) 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:79:ASN:OD1	1:A:306:LYS:O	1.62	1.17
1:F:36:GLN:HE22	1:F:309:PHE:HD2	1.19	0.89
1:A:28:LEU:HD22	1:A:69:ILE:HD12	1.63	0.81
1:C:265:LEU:CD2	1:C:290:LEU:HD13	2.12	0.80
1:A:25[B]:GLN:OE1	1:A:69:ILE:HD11	1.84	0.78
1:D:16:MET:HE2	1:D:34:LYS:HD2	1.65	0.77
1:A:28:LEU:HD22	1:A:69:ILE:CD1	2.16	0.76
2:C:401:CA:CA	4:C:545:HOH:O	1.61	0.76
1:F:225:ALA:O	1:F:228:GLN:HG3	1.87	0.74
2:A:402:CA:CA	4:E:533:HOH:O	1.66	0.72
1:C:265:LEU:O	1:C:269:GLU:HG3	1.89	0.72
1:C:265:LEU:HD22	1:C:290:LEU:HD13	1.71	0.71
1:F:16:MET:HE2	1:F:35:LEU:CD2	2.22	0.70
1:A:25[A]:GLN:NE2	4:A:501:HOH:O	2.12	0.69
1:C:16:MET:HE2	1:C:35:LEU:CD2	2.21	0.69
2:D:401:CA:CA	4:D:560:HOH:O	1.68	0.69
1:D:256:LYS:NZ	1:D:292:SER:O	2.28	0.67
1:F:292:SER:O	1:F:294:GLY:O	2.13	0.67
2:C:403:CA:CA	4:F:563:HOH:O	1.73	0.65
1:E:16:MET:HE2	1:E:35:LEU:CD2	2.26	0.65
1:C:24:ASP:OD2	1:F:276:ASN:ND2	2.30	0.64
1:C:36:GLN:HE22	1:C:309:PHE:HD1	1.45	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:ARG:HH12	1:A:309:PHE:HB3	1.63	0.63
1:F:266:GLU:O	1:F:270:GLN:HG3	1.99	0.62
1:E:179:GLY:O	4:E:501:HOH:O	2.15	0.62
1:A:29:GLN:OE1	1:A:69:ILE:HD13	2.00	0.62
1:B:242:LEU:HB3	1:B:282:GLU:HG2	1.83	0.61
1:A:33:ARG:NH1	1:A:309:PHE:HB3	2.16	0.61
1:B:277:GLU:O	1:B:281:LYS:HG2	2.03	0.59
1:C:265:LEU:HD21	1:C:290:LEU:HD13	1.85	0.58
1:F:225:ALA:HA	1:F:228:GLN:HG2	1.85	0.58
1:B:29:GLN:OE1	4:B:501:HOH:O	2.17	0.57
1:A:28:LEU:CD2	1:A:69:ILE:HD12	2.33	0.57
1:B:33:ARG:NH2	1:B:309:PHE:CD1	2.74	0.56
1:B:11:SER:N	4:B:510:HOH:O	2.39	0.56
1:B:33:ARG:NH2	1:B:309:PHE:CE1	2.75	0.54
1:A:297:GLY:N	1:D:298:SER:O	2.41	0.54
1:B:292:SER:HB3	4:B:545:HOH:O	2.08	0.54
1:E:239:GLN:HE22	1:E:282:GLU:HG2	1.73	0.53
1:A:298:SER:O	1:D:297:GLY:N	2.39	0.52
1:C:113:GLN:OE1	1:F:152:GLN:NE2	2.40	0.52
1:C:278:LYS:NZ	1:C:282:GLU:OE2	2.43	0.52
1:E:16:MET:HE2	1:E:35:LEU:HG	1.92	0.52
1:C:159:TRP:CD2	1:C:303[B]:ARG:HD2	2.45	0.52
1:D:159:TRP:CD2	1:D:303:ARG:HD2	2.45	0.52
1:F:16:MET:HE2	1:F:35:LEU:HG	1.91	0.51
1:C:25:GLN:OE1	1:C:69:ILE:HD11	2.09	0.51
1:C:256:LYS:HE2	4:C:653:HOH:O	2.10	0.51
1:C:16:MET:HE2	1:C:35:LEU:HG	1.93	0.51
1:E:33:ARG:NH2	1:E:309:PHE:OXT	2.45	0.50
1:B:238:LEU:HD23	1:B:279:ILE:HD13	1.94	0.50
1:F:186:GLN:NE2	4:F:505:HOH:O	2.43	0.50
1:B:154:LEU:HG	1:B:195:ILE:HD12	1.94	0.50
1:B:51:ASP:OD2	4:B:502:HOH:O	2.20	0.49
1:A:239:GLN:NE2	1:E:26:GLN:OE1	2.45	0.49
1:E:159:TRP:CD2	1:E:303[B]:ARG:HD2	2.48	0.49
1:B:159:TRP:CD2	1:B:303[B]:ARG:HD2	2.48	0.48
1:F:16:MET:CE	1:F:35:LEU:HG	2.43	0.48
1:C:16:MET:HE2	1:C:35:LEU:HD23	1.96	0.48
1:C:11:SER:N	4:C:526:HOH:O	2.47	0.47
1:E:257:GLN:O	1:E:261:GLU:HG2	2.14	0.47
1:A:152:GLN:NE2	1:E:110:GLN:OE1	2.48	0.46
1:F:159:TRP:CD2	1:F:303:ARG:HD2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:16:MET:HE2	1:F:35:LEU:CG	2.46	0.46
1:F:16:MET:HE2	1:F:35:LEU:HD23	1.97	0.46
1:D:37:GLN:HA	1:D:37:GLN:NE2	2.30	0.46
1:F:114:PHE:HE2	1:F:309:PHE:CZ	2.33	0.46
1:A:36:GLN:HE22	1:A:309:PHE:HD1	1.61	0.46
1:A:102:GLN:HA	1:A:102:GLN:OE1	2.15	0.46
1:C:16:MET:CE	1:C:35:LEU:HG	2.46	0.46
1:C:26:GLN:HE21	1:F:236:GLN:HE22	1.65	0.45
1:A:159:TRP:CD2	1:A:303:ARG:HD2	2.52	0.45
1:A:275:GLU:HG3	1:B:273:SER:O	2.16	0.45
1:B:274:HIS:O	1:B:280:GLN:HG3	2.17	0.45
1:A:33:ARG:NH2	1:A:33:ARG:HG2	2.31	0.45
1:E:16:MET:CE	1:E:35:LEU:HG	2.47	0.45
1:A:238:LEU:HD23	1:A:279:ILE:HD13	1.98	0.45
1:B:128:GLU:HB3	4:B:708:HOH:O	2.16	0.45
1:A:113:GLN:OE1	1:A:152:GLN:HG2	2.17	0.44
1:C:260:LYS:HG2	1:C:265:LEU:CD2	2.48	0.44
1:E:16:MET:HE2	1:E:35:LEU:HD23	2.00	0.44
1:C:16:MET:HE2	1:C:35:LEU:CG	2.47	0.44
1:A:233:PRO:HD3	1:B:266[A]:GLU:HB3	2.00	0.43
1:C:13:LEU:HD21	1:C:38:ILE:HD13	2.00	0.43
1:B:159:TRP:CD2	1:B:303[A]:ARG:HD2	2.54	0.43
1:A:114:PHE:HE2	1:A:309:PHE:CZ	2.36	0.42
1:E:159:TRP:CD2	1:E:303[A]:ARG:HD2	2.54	0.42
1:C:159:TRP:CD2	1:C:303[A]:ARG:HD2	2.54	0.42
1:E:10:GLY:HA2	1:E:13:LEU:HD23	2.01	0.42
1:E:280:GLN:NE2	4:E:518:HOH:O	2.49	0.42
1:F:260:LYS:HG2	1:F:265:LEU:HD21	2.02	0.42
1:E:16:MET:HE2	1:E:35:LEU:CG	2.49	0.41
1:F:225:ALA:HA	1:F:228:GLN:CG	2.50	0.41
1:F:272:GLN:OE1	1:F:284:GLN:OE1	2.39	0.41
1:C:170:GLU:HB3	4:C:628:HOH:O	2.19	0.41
1:C:265:LEU:HD22	1:C:290:LEU:CD1	2.46	0.41
1:D:24:ASP:OD1	1:D:26:GLN:HB2	2.21	0.41
1:B:33:ARG:NH2	1:B:72:SER:OG	2.54	0.41
1:C:278:LYS:HD2	1:C:278:LYS:HA	1.92	0.41
1:D:38:ILE:HA	1:D:38:ILE:HD13	1.93	0.41
1:F:260:LYS:HG2	1:F:265:LEU:CD2	2.51	0.41
1:A:52:ALA:HB2	4:A:686:HOH:O	2.21	0.40

All (3) 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)
4:B:677:HOH:O	4:D:630:HOH:O[1_445]	2.02	0.18
4:E:637:HOH:O	4:F:628:HOH:O[2_454]	2.13	0.07
4:C:728:HOH:O	4:F:637:HOH:O[1_455]	2.17	0.03

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	300/302 (99%)	299 (100%)	1 (0%)	0	100	100
1	B	300/302 (99%)	300 (100%)	0	0	100	100
1	C	301/302 (100%)	300 (100%)	1 (0%)	0	100	100
1	D	299/302 (99%)	298 (100%)	1 (0%)	0	100	100
1	E	300/302 (99%)	300 (100%)	0	0	100	100
1	F	297/302 (98%)	296 (100%)	0	1 (0%)	41	41
All	All	1797/1812 (99%)	1793 (100%)	3 (0%)	1 (0%)	51	54

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	293	HIS

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	232/231 (100%)	227 (98%)	5 (2%)	52 57
1	B	233/231 (101%)	227 (97%)	6 (3%)	46 50
1	C	234/231 (101%)	231 (99%)	3 (1%)	69 75
1	D	232/231 (100%)	228 (98%)	4 (2%)	60 67
1	E	232/231 (100%)	228 (98%)	4 (2%)	60 67
1	F	230/231 (100%)	225 (98%)	5 (2%)	52 57
All	All	1393/1386 (100%)	1366 (98%)	27 (2%)	55 63

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	SER
1	A	102	GLN
1	A	152	GLN
1	A	292	SER
1	A	309	PHE
1	B	33	ARG
1	B	102	GLN
1	B	152	GLN
1	B	281	LYS
1	B	282	GLU
1	B	292	SER
1	C	186	GLN
1	C	267	LYS
1	C	281	LYS
1	D	11	SER
1	D	102	GLN
1	D	186	GLN
1	D	284	GLN
1	E	128	GLU
1	E	261	GLU
1	E	267	LYS
1	E	269	GLU
1	F	12	GLU
1	F	15	GLN
1	F	238	LEU
1	F	281	LYS
1	F	292	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	37	GLN
1	A	79	ASN
1	A	152	GLN
1	A	169	ASN
1	A	239	GLN
1	A	272	GLN
1	A	280	GLN
1	B	29	GLN
1	B	253	ASN
1	C	280	GLN
1	D	26	GLN
1	D	37	GLN
1	D	169	ASN
1	D	270	GLN
1	D	280	GLN
1	E	26	GLN
1	E	110	GLN
1	E	144	GLN
1	E	239	GLN
1	E	272	GLN
1	E	284	GLN
1	E	291	GLN
1	F	169	ASN
1	F	236	GLN
1	F	239	GLN
1	F	284	GLN
1	F	291	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 (i)

Of 19 ligands modelled in this entry, 18 are monoatomic - leaving 1 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	F	401	-	3,3,3	0.37	0	2,2,2	0.43	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	F	401	-	-	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
3	F	401	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	300/302 (99%)	0.09	5 (1%)	70	74	20, 27, 52, 83	0
1	B	299/302 (99%)	-0.02	2 (0%)	87	89	22, 28, 45, 63	0
1	C	299/302 (99%)	0.14	4 (1%)	77	80	22, 28, 57, 79	0
1	D	299/302 (99%)	0.42	20 (6%)	17	22	25, 37, 79, 91	0
1	E	301/302 (99%)	0.21	3 (0%)	82	85	21, 32, 54, 93	0
1	F	299/302 (99%)	0.31	17 (5%)	23	29	22, 30, 70, 91	0
All	All	1797/1812 (99%)	0.19	51 (2%)	53	59	20, 30, 60, 93	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	293	HIS	7.0
1	F	295	SER	6.2
1	D	309	PHE	5.8
1	D	279	ILE	5.8
1	D	293	HIS	5.6
1	E	9	PRO	5.6
1	D	274	HIS	5.3
1	C	11	SER	5.3
1	A	293	HIS	5.1
1	F	298	SER	4.9
1	E	309	PHE	4.6
1	A	10	GLY	4.3
1	D	11	SER	4.3
1	F	309	PHE	4.3
1	F	11	SER	3.7
1	F	297	GLY	3.7
1	A	294	GLY	3.5
1	D	277	GLU	3.2
1	C	309	PHE	3.1

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Mol	Chain	Res	Type	RSRZ
1	F	296	GLY	3.1
1	A	309	PHE	3.1
1	D	294	GLY	3.1
1	D	52	ALA	2.9
1	B	293	HIS	2.9
1	F	270	GLN	2.9
1	B	309	PHE	2.8
1	F	273	SER	2.7
1	D	283	ALA	2.7
1	C	21	ASN	2.7
1	D	296	GLY	2.7
1	E	10	GLY	2.6
1	C	19	GLN	2.6
1	F	272	GLN	2.6
1	F	274	HIS	2.6
1	F	275	GLU	2.5
1	F	271	LEU	2.5
1	F	265	LEU	2.5
1	F	299	GLY	2.5
1	D	39	ALA	2.5
1	D	41	GLY	2.4
1	D	280	GLN	2.4
1	D	282	GLU	2.3
1	D	272	GLN	2.3
1	A	297	GLY	2.3
1	D	287	LEU	2.1
1	D	297	GLY	2.1
1	F	280	GLN	2.1
1	D	298	SER	2.1
1	D	271	LEU	2.0
1	D	281	LYS	2.0
1	F	269	GLU	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

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	EDO	F	401	4/4	0.84	0.24	49,49,51,57	0
2	CA	A	403	1/1	0.89	0.06	36,36,36,36	0
2	CA	C	403	1/1	0.90	0.07	33,33,33,33	0
2	CA	C	406	1/1	0.93	0.12	61,61,61,61	0
2	CA	C	404	1/1	0.94	0.05	37,37,37,37	0
2	CA	B	405	1/1	0.96	0.05	45,45,45,45	0
2	CA	A	405	1/1	0.96	0.04	27,27,27,27	0
2	CA	B	401	1/1	0.96	0.10	27,27,27,27	0
2	CA	D	401	1/1	0.97	0.05	35,35,35,35	0
2	CA	A	401	1/1	0.97	0.06	31,31,31,31	0
2	CA	A	402	1/1	0.97	0.04	34,34,34,34	0
2	CA	C	405	1/1	0.97	0.05	33,33,33,33	0
2	CA	B	403	1/1	0.98	0.05	36,36,36,36	0
2	CA	B	402	1/1	0.98	0.06	29,29,29,29	0
2	CA	B	404	1/1	0.98	0.05	40,40,40,40	0
2	CA	C	402	1/1	0.98	0.06	26,26,26,26	0
2	CA	A	406	1/1	0.98	0.08	37,37,37,37	0
2	CA	C	401	1/1	0.98	0.08	30,30,30,30	0
2	CA	A	404	1/1	0.99	0.09	26,26,26,26	0

6.5 Other polymers

There are no such residues in this entry.