Full wwPDB X-ray Structure Validation Report (i)

Feb 18, 2024 – 07:26 AM EST

PDB ID	:	4EDL
Title	:	Crystal structure of beta-parvin CH2 domain
Authors	:	Stiegler, A.L.; Draheim, K.M.; Li, X.; Chayen, N.E.; Calderwood, D.A.; Boggon, T.J.
Deposited on	:	2012-03-27
Resolution	:	2.10 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

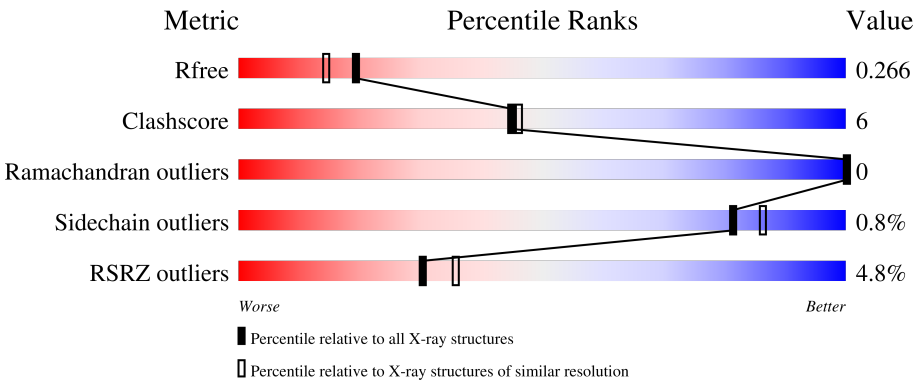
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 2.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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

Mol	Chain	Length	Quality of chain
1	A	133	4%, 90%, 7%, •
1	B	133	3%, 86%, 10%, •
1	C	133	4%, 87%, 8%, 5%
1	D	133	5%, 81%, 14%, 5%
1	E	133	4%, 80%, 15%, • •

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Mol	Chain	Length	Quality of chain
1	F	133	9% 72% 21% 5%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 6593 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Beta-parvin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	129	1065	697	172	194	2	4	0	0
			Total	C	N	O	S			
1	B	128	1054	691	168	193	2	0	0	0
			Total	C	N	O	S			
1	C	127	1043	682	167	192	2	0	0	0
			Total	C	N	O	S			
1	D	127	1043	682	167	192	2	0	0	0
			Total	C	N	O	S			
1	E	128	1054	691	168	193	2	0	0	0
			Total	C	N	O	S			
1	F	126	1032	673	166	191	2	0	0	0

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	232	GLY	-	expression tag	UNP Q9HBI1
A	233	ASN	-	expression tag	UNP Q9HBI1
A	234	SER	-	expression tag	UNP Q9HBI1
B	232	GLY	-	expression tag	UNP Q9HBI1
B	233	ASN	-	expression tag	UNP Q9HBI1
B	234	SER	-	expression tag	UNP Q9HBI1
C	232	GLY	-	expression tag	UNP Q9HBI1
C	233	ASN	-	expression tag	UNP Q9HBI1
C	234	SER	-	expression tag	UNP Q9HBI1
D	232	GLY	-	expression tag	UNP Q9HBI1
D	233	ASN	-	expression tag	UNP Q9HBI1
D	234	SER	-	expression tag	UNP Q9HBI1
E	232	GLY	-	expression tag	UNP Q9HBI1
E	233	ASN	-	expression tag	UNP Q9HBI1
E	234	SER	-	expression tag	UNP Q9HBI1
F	232	GLY	-	expression tag	UNP Q9HBI1
F	233	ASN	-	expression tag	UNP Q9HBI1

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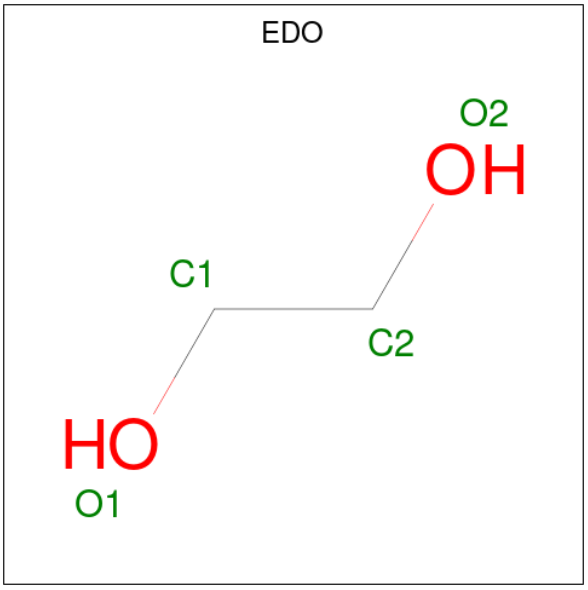
Chain	Residue	Modelled	Actual	Comment	Reference
F	234	SER	-	expression tag	UNP Q9HBI1

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



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

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

- Molecule 3 is water.

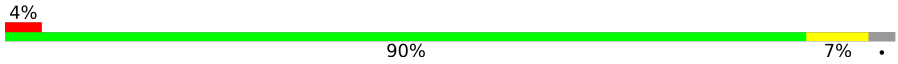
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	41	41	41	0	0
			Total	O		
3	B	55	55	55	0	0
			Total	O		
3	C	37	37	37	0	0
			Total	O		
3	D	38	38	38	0	0
			Total	O		
3	E	36	36	36	0	0
			Total	O		
3	F	27	27	27	0	0

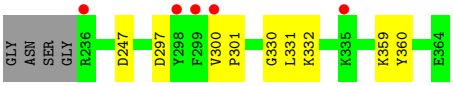
3 Residue-property plots (i)

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

• Molecule 1: Beta-parvin

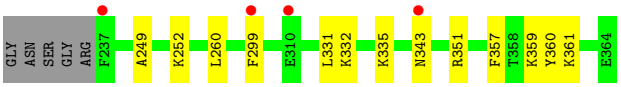
Chain A:





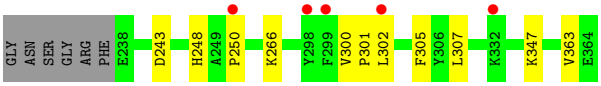
• Molecule 1: Beta-parvin

Chain B:



• Molecule 1: Beta-parvin

Chain C:

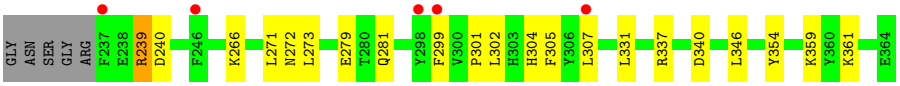


• Molecule 1: Beta-parvin

Chain D:

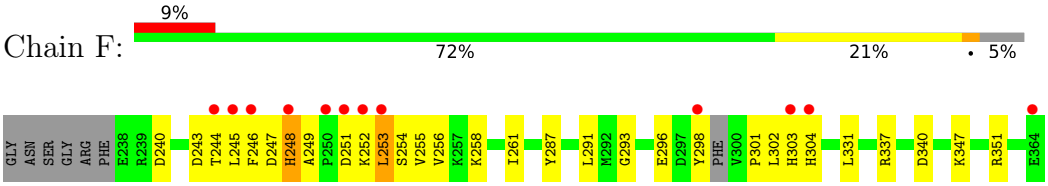
• Molecule 1: Beta-parvin

Chain E:



• Molecule 1: Beta-parvin

Chain F:


9%
72%
21%
5%
GLY
ASN
SER
GLY
ARG
PHE
E238
R239
D240
D243
T244
L245
F246
D247
H248
A249
P250
D251
K252
L253
S254
V255
V256
K257
K258
I261
Y287
L291
M292
G293
E296
D297
Y298
PHE
V300
P301
L302
H303
H304
L331
R337
D340
K347
R351
E364

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	80.89Å 52.58Å 82.33Å 90.00° 101.49° 90.00°	Depositor
Resolution (Å)	50.00 – 2.10 44.05 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.2 (50.00-2.10) 99.2 (44.05-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	2.12 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.215 , 0.266 0.214 , 0.266	Depositor DCC
R_{free} test set	1990 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	34.5	Xtriage
Anisotropy	0.229	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 49.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.000 for l,-k,h	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	6593	wwPDB-VP
Average B, all atoms (Å^2)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 75.65 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.2129e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: EDO

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	0/1090	0.66	0/1473
1	B	0.58	0/1079	0.64	0/1459
1	C	0.58	0/1067	0.65	0/1443
1	D	0.58	0/1067	0.69	0/1443
1	E	0.55	0/1079	0.64	0/1459
1	F	0.53	0/1054	0.65	1/1424 (0.1%)
All	All	0.57	0/6436	0.66	1/8701 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	331	LEU	CA-CB-CG	5.08	126.98	115.30

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	1065	0	1072	7	0
1	B	1054	0	1059	10	0
1	C	1043	0	1050	7	0
1	D	1043	0	1050	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	1054	0	1059	16	0
1	F	1032	0	1040	35	0
2	A	16	0	24	0	0
2	B	4	0	6	0	0
2	C	8	0	12	0	0
2	D	24	0	36	2	0
2	E	4	0	6	1	0
2	F	12	0	18	0	0
3	A	41	0	0	0	0
3	B	55	0	0	0	0
3	C	37	0	0	1	0
3	D	38	0	0	2	0
3	E	36	0	0	4	0
3	F	27	0	0	1	0
All	All	6593	0	6432	83	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 (83) 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:F:243:ASP:OD1	1:F:347:LYS:HE3	1.61	1.00
1:F:243:ASP:OD1	1:F:347:LYS:CE	2.19	0.90
1:E:273:LEU:HD21	1:F:244:THR:OG1	1.75	0.85
1:D:247:ASP:OD1	1:D:248:HIS:N	2.12	0.82
1:F:303:HIS:NE2	1:F:304:HIS:CD2	2.51	0.79
1:B:359:LYS:HD3	1:B:360:TYR:CE2	2.21	0.75
1:F:293:GLY:HA2	1:F:298:TYR:HB2	1.69	0.74
1:F:303:HIS:CD2	1:F:304:HIS:CD2	2.77	0.72
1:B:359:LYS:HD3	1:B:360:TYR:CZ	2.24	0.72
1:E:302:LEU:HD21	1:F:252:LYS:HE2	1.76	0.68
1:C:363:VAL:O	3:C:515:HOH:O	2.12	0.68
1:F:247:ASP:OD1	1:F:248:HIS:N	2.27	0.68
1:F:246:PHE:CE2	1:F:347:LYS:HB2	2.31	0.66
1:D:251:ASP:OD1	1:D:252:LYS:N	2.28	0.65
1:F:337:ARG:HB2	1:F:340:ASP:OD2	1.97	0.65
1:E:361:LYS:NZ	3:E:521:HOH:O	2.30	0.64
1:D:363:VAL:HG12	1:D:364:GLU:HG3	1.80	0.63
1:E:279:GLU:HG3	1:E:346:LEU:HD13	1.81	0.62
1:F:303:HIS:NE2	1:F:304:HIS:NE2	2.49	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:363:VAL:CG1	1:D:364:GLU:HG3	2.31	0.61
1:E:239:ARG:HG3	1:E:240:ASP:N	2.16	0.61
1:F:252:LYS:O	1:F:255:VAL:HB	2.01	0.61
1:E:340:ASP:OD2	3:E:533:HOH:O	2.15	0.60
1:D:257:LYS:HD3	2:D:403:EDO:H12	1.84	0.59
1:E:281:GLN:HG2	2:E:401:EDO:H22	1.85	0.58
1:A:330:GLY:O	1:C:266:LYS:HE2	2.03	0.58
1:C:302:LEU:HD23	1:C:305:PHE:CE1	2.39	0.58
1:D:275:VAL:HG13	1:D:281:GLN:OE1	2.05	0.57
1:B:357:PHE:O	1:B:361:LYS:HB3	2.05	0.56
1:E:331:LEU:HD13	1:E:359:LYS:HD2	1.87	0.56
1:F:249:ALA:HB1	1:F:252:LYS:HB3	1.87	0.55
1:A:331:LEU:CD2	1:A:359:LYS:HD2	2.38	0.54
1:A:331:LEU:HD21	1:A:359:LYS:HD2	1.90	0.54
1:F:302:LEU:N	1:F:302:LEU:HD23	2.23	0.53
1:B:343:ASN:CG	1:F:254:SER:HB2	2.28	0.53
1:D:243:ASP:OD1	1:D:347:LYS:HE3	2.10	0.51
1:E:301:PRO:HB2	1:E:304:HIS:HD2	1.76	0.51
1:F:253:LEU:O	1:F:256:VAL:N	2.43	0.51
1:F:296:GLU:HG2	1:F:298:TYR:CZ	2.45	0.51
1:D:269:ASN:ND2	3:D:502:HOH:O	2.45	0.49
1:F:296:GLU:HB3	1:F:298:TYR:CE2	2.48	0.49
1:F:240:ASP:OD2	1:F:351:ARG:NH1	2.46	0.48
1:D:251:ASP:HA	2:D:406:EDO:O2	2.14	0.48
1:F:240:ASP:HB2	3:F:518:HOH:O	2.13	0.48
1:C:302:LEU:HD13	1:C:307:LEU:HD11	1.95	0.48
1:F:246:PHE:CD2	1:F:347:LYS:HD2	2.48	0.48
1:D:267:HIS:HA	1:D:270:LYS:HE2	1.96	0.47
1:B:249:ALA:CB	1:B:252:LYS:HE2	2.45	0.47
1:F:301:PRO:HG2	1:F:304:HIS:ND1	2.29	0.46
1:E:307:LEU:HD21	1:F:245:LEU:HD12	1.97	0.46
1:F:243:ASP:OD1	1:F:347:LYS:NZ	2.49	0.45
1:F:301:PRO:HB2	1:F:303:HIS:CE1	2.50	0.45
1:B:335:LYS:HB3	1:B:351:ARG:HD3	1.98	0.45
1:D:238:GLU:HG3	1:D:239:ARG:H	1.81	0.45
1:F:258:LYS:O	1:F:261:ILE:HG22	2.17	0.45
1:F:301:PRO:HG2	1:F:304:HIS:HD1	1.81	0.45
1:E:271:LEU:O	1:F:244:THR:HG23	2.17	0.45
1:F:249:ALA:HB1	1:F:252:LYS:CB	2.47	0.44
1:F:303:HIS:CD2	1:F:304:HIS:HD2	2.34	0.44
1:D:252:LYS:HD3	1:D:252:LYS:HA	1.64	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:248:HIS:C	1:C:250:PRO:HD3	2.39	0.43
1:A:332:LYS:HB3	1:A:332:LYS:HE3	1.89	0.43
1:E:272:ASN:ND2	3:E:528:HOH:O	2.51	0.43
1:C:243:ASP:OD1	1:C:347:LYS:HD3	2.19	0.42
1:F:251:ASP:O	1:F:254:SER:OG	2.28	0.42
1:E:301:PRO:HB2	1:E:304:HIS:CD2	2.54	0.42
1:F:293:GLY:O	1:F:298:TYR:N	2.53	0.42
1:F:296:GLU:HB3	1:F:298:TYR:CD2	2.55	0.42
1:A:297:ASP:HB2	1:E:337:ARG:HD3	2.02	0.42
1:D:261:ILE:HD11	1:D:275:VAL:O	2.20	0.41
1:E:354:TYR:OH	3:E:506:HOH:O	2.22	0.41
1:A:300:VAL:HA	1:A:301:PRO:HD3	1.94	0.41
1:F:287:TYR:O	1:F:291:LEU:HB2	2.21	0.41
1:B:260:LEU:HA	1:B:260:LEU:HD23	1.85	0.41
1:B:331:LEU:HD12	1:B:332:LYS:H	1.84	0.41
1:B:299:PHE:O	1:B:299:PHE:CD1	2.74	0.41
1:F:293:GLY:CA	1:F:298:TYR:HB2	2.45	0.40
1:B:249:ALA:HB1	1:B:252:LYS:HE2	2.02	0.40
1:A:359:LYS:HD3	1:A:360:TYR:CZ	2.56	0.40
1:C:300:VAL:HA	1:C:301:PRO:HD3	1.95	0.40
1:D:258:LYS:O	1:D:261:ILE:HG22	2.20	0.40
1:D:337:ARG:NH2	3:D:503:HOH:O	2.54	0.40
1:E:302:LEU:HD23	1:E:305:PHE:CE1	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	127/133 (96%)	124 (98%)	3 (2%)	0	100	100
1	B	126/133 (95%)	125 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	125/133 (94%)	122 (98%)	3 (2%)	0	100	100
1	D	125/133 (94%)	121 (97%)	4 (3%)	0	100	100
1	E	126/133 (95%)	125 (99%)	1 (1%)	0	100	100
1	F	122/133 (92%)	120 (98%)	2 (2%)	0	100	100
All	All	751/798 (94%)	737 (98%)	14 (2%)	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	120/122 (98%)	119 (99%)	1 (1%)	81	86
1	B	119/122 (98%)	119 (100%)	0	100	100
1	C	118/122 (97%)	118 (100%)	0	100	100
1	D	118/122 (97%)	118 (100%)	0	100	100
1	E	119/122 (98%)	116 (98%)	3 (2%)	47	52
1	F	117/122 (96%)	115 (98%)	2 (2%)	60	67
All	All	711/732 (97%)	705 (99%)	6 (1%)	81	86

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	247	ASP
1	E	239	ARG
1	E	266	LYS
1	E	299	PHE
1	F	248	HIS
1	F	253	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

17 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	$\#\|Z\| > 2$
2	EDO	F	402	-	3,3,3	0.36	0	2,2,2	0.57	0
2	EDO	A	404	-	3,3,3	0.42	0	2,2,2	0.55	0
2	EDO	C	401	-	3,3,3	0.52	0	2,2,2	0.32	0
2	EDO	D	405	-	3,3,3	0.49	0	2,2,2	0.44	0
2	EDO	C	402	-	3,3,3	0.53	0	2,2,2	0.37	0
2	EDO	D	401	-	3,3,3	0.42	0	2,2,2	0.54	0
2	EDO	B	401	-	3,3,3	0.39	0	2,2,2	0.47	0
2	EDO	D	403	-	3,3,3	0.51	0	2,2,2	0.49	0
2	EDO	A	402	-	3,3,3	0.56	0	2,2,2	0.23	0
2	EDO	F	401	-	3,3,3	0.49	0	2,2,2	0.44	0
2	EDO	F	403	-	3,3,3	0.60	0	2,2,2	0.27	0
2	EDO	A	401	-	3,3,3	0.55	0	2,2,2	0.30	0
2	EDO	D	406	-	3,3,3	0.50	0	2,2,2	0.25	0
2	EDO	A	403	-	3,3,3	0.45	0	2,2,2	0.16	0
2	EDO	D	404	-	3,3,3	0.38	0	2,2,2	0.50	0
2	EDO	D	402	-	3,3,3	0.51	0	2,2,2	0.47	0
2	EDO	E	401	-	3,3,3	0.55	0	2,2,2	0.23	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	F	402	-	-	1/1/1/1	-
2	EDO	A	404	-	-	0/1/1/1	-
2	EDO	C	401	-	-	1/1/1/1	-
2	EDO	D	405	-	-	1/1/1/1	-
2	EDO	C	402	-	-	0/1/1/1	-
2	EDO	D	401	-	-	0/1/1/1	-
2	EDO	B	401	-	-	1/1/1/1	-
2	EDO	D	403	-	-	1/1/1/1	-
2	EDO	A	402	-	-	0/1/1/1	-
2	EDO	F	401	-	-	1/1/1/1	-
2	EDO	F	403	-	-	1/1/1/1	-
2	EDO	A	401	-	-	0/1/1/1	-
2	EDO	D	406	-	-	0/1/1/1	-
2	EDO	A	403	-	-	0/1/1/1	-
2	EDO	D	404	-	-	1/1/1/1	-
2	EDO	D	402	-	-	0/1/1/1	-
2	EDO	E	401	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	401	EDO	O1-C1-C2-O2
2	D	403	EDO	O1-C1-C2-O2
2	F	402	EDO	O1-C1-C2-O2
2	B	401	EDO	O1-C1-C2-O2
2	D	404	EDO	O1-C1-C2-O2
2	F	401	EDO	O1-C1-C2-O2
2	F	403	EDO	O1-C1-C2-O2
2	D	405	EDO	O1-C1-C2-O2

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	403	EDO	1	0
2	D	406	EDO	1	0
2	E	401	EDO	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	129/133 (96%)	0.04	5 (3%)	39	45	27, 41, 70, 83	1 (0%)
1	B	128/133 (96%)	0.10	4 (3%)	49	55	26, 44, 70, 103	0
1	C	127/133 (95%)	0.09	5 (3%)	39	45	26, 44, 72, 87	0
1	D	127/133 (95%)	0.12	6 (4%)	31	37	28, 43, 85, 113	0
1	E	128/133 (96%)	0.29	5 (3%)	39	45	28, 48, 74, 89	0
1	F	126/133 (94%)	0.56	12 (9%)	8	10	31, 56, 112, 147	0
All	All	765/798 (95%)	0.20	37 (4%)	30	36	26, 45, 83, 147	1 (0%)

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	299	PHE	10.2
1	F	250	PRO	6.3
1	F	248	HIS	4.8
1	F	298	TYR	4.7
1	F	244	THR	4.5
1	F	245	LEU	4.4
1	D	298	TYR	4.4
1	B	299	PHE	4.4
1	C	299	PHE	3.8
1	B	237	PHE	3.8
1	E	299	PHE	3.5
1	F	304	HIS	3.3
1	F	364	GLU	3.2
1	C	298	TYR	3.2
1	D	253	LEU	3.1
1	E	237	PHE	3.0
1	A	299	PHE	2.9
1	A	236	ARG	2.8
1	F	246	PHE	2.8

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Mol	Chain	Res	Type	RSRZ
1	E	307	LEU	2.8
1	C	302	LEU	2.7
1	F	303	HIS	2.7
1	D	249	ALA	2.6
1	E	246	PHE	2.6
1	F	252	LYS	2.5
1	D	248	HIS	2.5
1	B	310	GLU	2.5
1	C	250	PRO	2.5
1	F	251	ASP	2.4
1	C	332	LYS	2.3
1	D	250	PRO	2.2
1	A	335	LYS	2.2
1	E	298	TYR	2.1
1	A	298	TYR	2.1
1	A	300	VAL	2.0
1	B	343	ASN	2.0
1	F	253	LEU	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	EDO	F	403	4/4	0.66	0.23	58,61,63,64	0
2	EDO	A	403	4/4	0.70	0.21	65,67,67,69	0
2	EDO	C	402	4/4	0.78	0.17	57,59,60,61	0
2	EDO	A	402	4/4	0.80	0.15	45,49,52,52	0
2	EDO	E	401	4/4	0.81	0.17	51,53,54,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	EDO	D	403	4/4	0.86	0.17	50,51,54,59	0
2	EDO	D	405	4/4	0.86	0.14	52,59,63,66	0
2	EDO	F	401	4/4	0.87	0.16	54,58,61,66	0
2	EDO	A	401	4/4	0.87	0.16	48,49,51,53	0
2	EDO	A	404	4/4	0.89	0.24	53,57,59,59	0
2	EDO	C	401	4/4	0.90	0.11	55,55,57,58	0
2	EDO	D	402	4/4	0.91	0.19	47,50,52,53	0
2	EDO	F	402	4/4	0.91	0.10	56,57,57,60	0
2	EDO	D	404	4/4	0.91	0.19	55,57,59,66	0
2	EDO	D	401	4/4	0.92	0.11	48,51,52,54	0
2	EDO	D	406	4/4	0.93	0.18	50,53,54,58	0
2	EDO	B	401	4/4	0.95	0.11	39,49,51,55	0

6.5 Other polymers (i)

There are no such residues in this entry.