Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 04:21 PM GMT

PDB ID	:	4EDN
Title	:	Crystal structure of beta-parvin CH2 domain in complex with paxillin LD1 motif
Authors	:	Stiegler, A.L.; Draheim, K.M.; Li, X.; Chayen, N.E.; Calderwood, D.A.; Boggon, T.J.
Deposited on	:	2012-03-27
Resolution	:	2.90 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

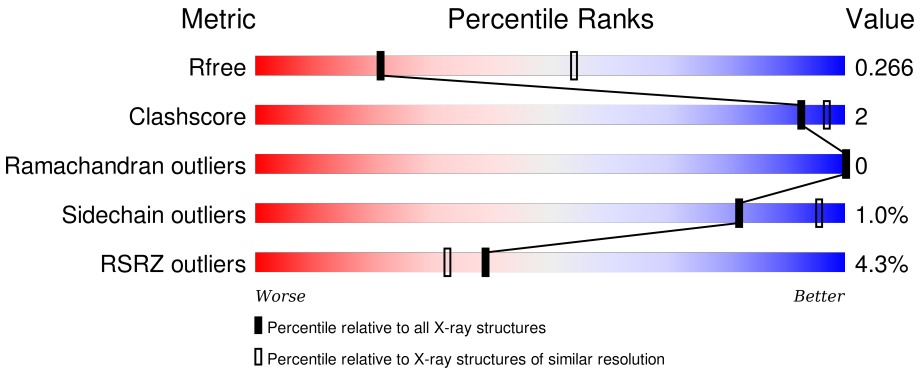
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.90 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}	91344	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)

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. 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	2% 87% 8% 5%
1	B	133	2% 89% 5% 5%
1	C	133	% 89% 7% 5%
1	D	133	2% 90% • 6%
1	E	133	2% 89% 5% • 5%

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Mol	Chain	Length	Quality of chain
1	F	133	2% 86% 8% 6%
1	G	133	5% 86% 8% 6%
1	H	133	2% 91% 6%
1	I	133	9% 87% 6% 7%
1	J	133	11% 88% 6% 6%
2	K	22	5% 45% 9% 45%
2	L	22	5% 77% 14% 9%
2	M	22	36% 9% 55%
2	N	22	14% 50% 5% 45%
2	O	22	55% 45%
2	P	22	5% 50% 50%
2	Q	22	9% 59% 5% 36%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11011 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
1	A	127	Total	C	N	O	S	0	0	0
			1043	682	167	192	2			
1	B	126	Total	C	N	O	S	0	0	0
			1034	677	166	189	2			
1	C	127	Total	C	N	O	S	0	0	0
			1043	682	167	192	2			
1	D	125	Total	C	N	O	S	0	0	0
			1023	671	162	188	2			
1	E	127	Total	C	N	O	S	0	0	0
			1043	682	167	192	2			
1	F	125	Total	C	N	O	S	0	0	0
			1023	671	162	188	2			
1	G	125	Total	C	N	O	S	0	0	0
			1023	671	162	188	2			
1	H	125	Total	C	N	O	S	0	0	0
			1023	671	162	188	2			
1	I	124	Total	C	N	O	S	0	0	0
			1015	667	161	185	2			
1	J	125	Total	C	N	O	S	0	0	0
			1023	671	162	188	2			

There are 30 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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
F	234	SER	-	EXPRESSION TAG	UNP Q9HBI1
G	232	GLY	-	EXPRESSION TAG	UNP Q9HBI1
G	233	ASN	-	EXPRESSION TAG	UNP Q9HBI1
G	234	SER	-	EXPRESSION TAG	UNP Q9HBI1
H	232	GLY	-	EXPRESSION TAG	UNP Q9HBI1
H	233	ASN	-	EXPRESSION TAG	UNP Q9HBI1
H	234	SER	-	EXPRESSION TAG	UNP Q9HBI1
I	232	GLY	-	EXPRESSION TAG	UNP Q9HBI1
I	233	ASN	-	EXPRESSION TAG	UNP Q9HBI1
I	234	SER	-	EXPRESSION TAG	UNP Q9HBI1
J	232	GLY	-	EXPRESSION TAG	UNP Q9HBI1
J	233	ASN	-	EXPRESSION TAG	UNP Q9HBI1
J	234	SER	-	EXPRESSION TAG	UNP Q9HBI1

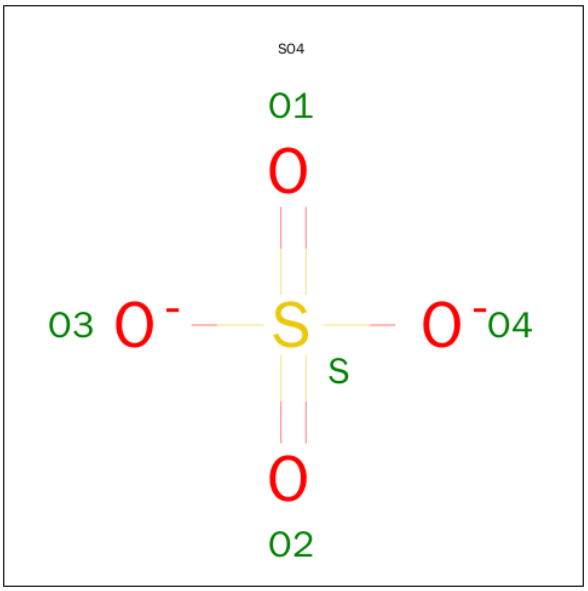
- Molecule 2 is a protein called Paxillin.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
2	K	12	Total C N O 89 54 12 23	0	0	0
2	L	20	Total C N O S 144 87 21 35 1	0	0	0
2	M	10	Total C N O 75 47 10 18	0	0	0
2	N	12	Total C N O 89 54 12 23	0	0	0
2	O	12	Total C N O S 91 56 12 22 1	0	0	0
2	P	11	Total C N O 83 51 11 21	0	0	0
2	Q	14	Total C N O S 104 63 14 26 1	0	0	0

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	0	ACE	-	ACETYLATION	UNP P49023
K	21	NH2	-	AMIDATION	UNP P49023
L	0	ACE	-	ACETYLATION	UNP P49023
L	21	NH2	-	AMIDATION	UNP P49023
M	0	ACE	-	ACETYLATION	UNP P49023
M	21	NH2	-	AMIDATION	UNP P49023
N	0	ACE	-	ACETYLATION	UNP P49023
N	21	NH2	-	AMIDATION	UNP P49023
O	0	ACE	-	ACETYLATION	UNP P49023
O	21	NH2	-	AMIDATION	UNP P49023
P	0	ACE	-	ACETYLATION	UNP P49023
P	21	NH2	-	AMIDATION	UNP P49023
Q	0	ACE	-	ACETYLATION	UNP P49023
Q	21	NH2	-	AMIDATION	UNP P49023

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	1	Total O S 5 4 1	0	0

- Molecule 4 is water.

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

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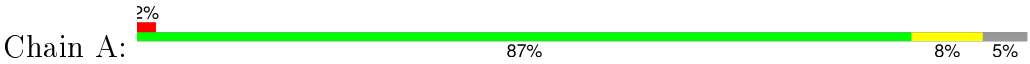
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	4	Total O 4 4	0	0
4	D	1	Total O 1 1	0	0
4	E	6	Total O 6 6	0	0
4	F	2	Total O 2 2	0	0
4	G	2	Total O 2 2	0	0
4	H	5	Total O 5 5	0	0
4	I	5	Total O 5 5	0	0
4	J	6	Total O 6 6	0	0
4	K	1	Total O 1 1	0	0

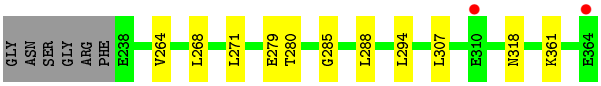
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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

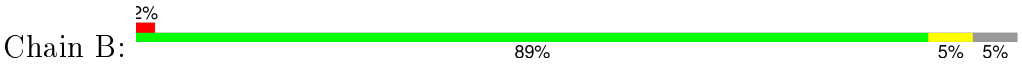
Chain A:





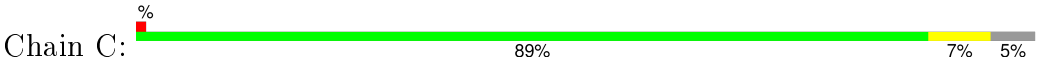
- Molecule 1: Beta-parvin

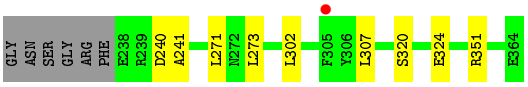
Chain B:



- Molecule 1: Beta-parvin

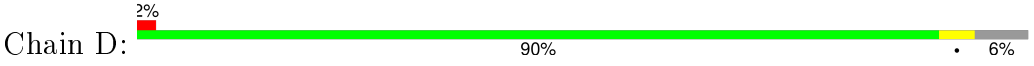
Chain C:

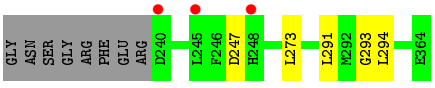




- Molecule 1: Beta-parvin

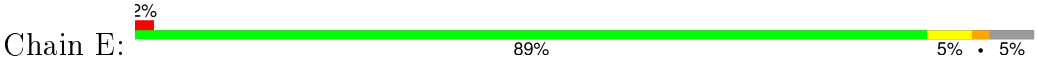
Chain D:

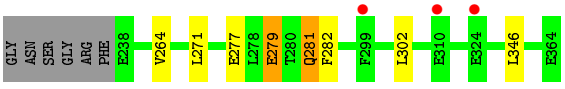




- Molecule 1: Beta-parvin

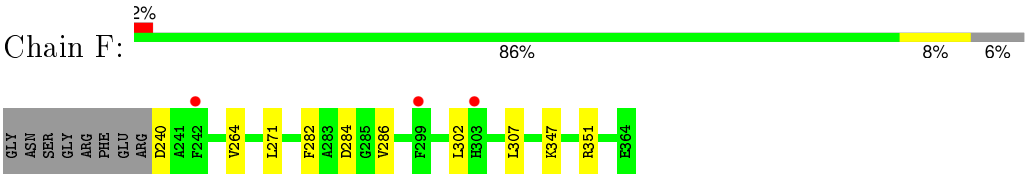
Chain E:





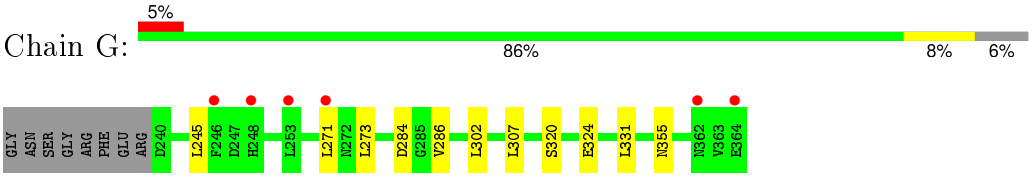
- Molecule 1: Beta-parvin

Chain F:



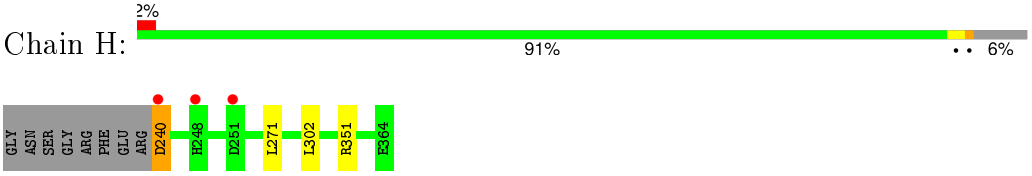
• Molecule 1: Beta-parvin

Chain G:



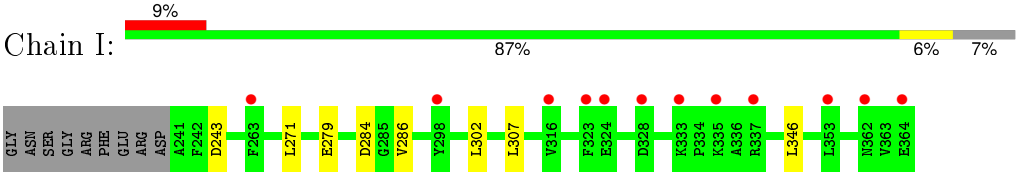
• Molecule 1: Beta-parvin

Chain H:



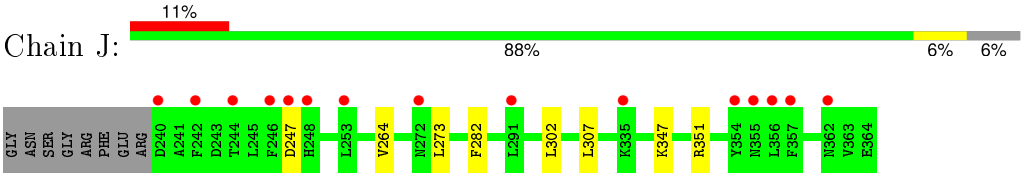
• Molecule 1: Beta-parvin

Chain I:



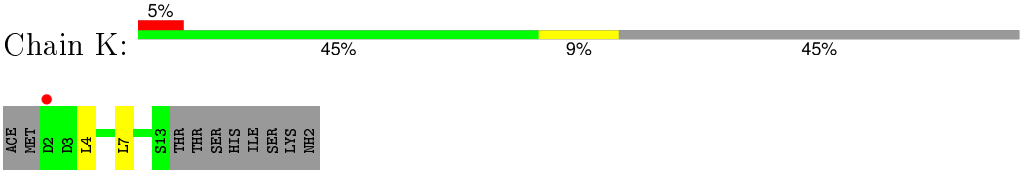
• Molecule 1: Beta-parvin

Chain J:



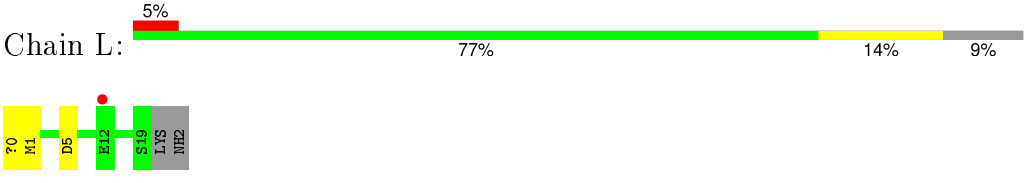
• Molecule 2: Paxillin

Chain K:



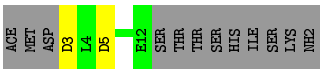
• Molecule 2: Paxillin

Chain L:



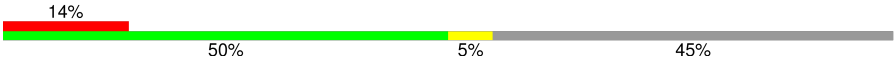
• Molecule 2: Paxillin

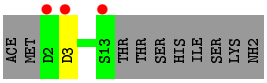
Chain M:



- Molecule 2: Paxillin

Chain N:



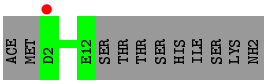


- Molecule 2: Paxillin

Chain O:

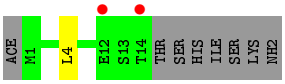
- Molecule 2: Paxillin

Chain P:



- Molecule 2: Paxillin

Chain Q:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	330.74Å 55.84Å 95.55Å 90.00° 97.44° 90.00°	Depositor
Resolution (Å)	50.00 – 2.90 49.73 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.4 (50.00-2.90) 99.3 (49.73-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	2.04 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.228 , 0.265 0.228 , 0.266	Depositor DCC
R_{free} test set	1953 reflections (5.29%)	DCC
Wilson B-factor (Å^2)	77.3	Xtriage
Anisotropy	0.114	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 46.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	1 of 38941 reflections (0.003%)	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	11011	wwPDB-VP
Average B, all atoms (Å^2)	92.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.86% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: SO4, ACE

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	0.36	0/1067	0.45	0/1443
1	B	0.37	0/1058	0.45	0/1431
1	C	0.37	0/1067	0.45	0/1443
1	D	0.37	0/1047	0.45	0/1417
1	E	0.36	0/1067	0.46	0/1443
1	F	0.37	0/1047	0.44	0/1417
1	G	0.37	0/1047	0.45	0/1417
1	H	0.37	0/1047	0.44	0/1417
1	I	0.37	0/1039	0.43	0/1406
1	J	0.37	0/1047	0.46	0/1417
2	K	0.28	0/88	0.47	0/119
2	L	0.42	0/142	0.53	0/193
2	M	0.28	0/74	0.43	0/100
2	N	0.29	0/88	0.49	0/119
2	O	0.29	0/90	0.46	0/121
2	P	0.28	0/82	0.43	0/111
2	Q	0.29	0/103	0.50	0/139
All	All	0.36	0/11200	0.45	0/15153

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1043	0	1050	6	0
1	B	1034	0	1044	5	0
1	C	1043	0	1050	7	0
1	D	1023	0	1031	3	0
1	E	1043	0	1050	5	0
1	F	1023	0	1031	7	0
1	G	1023	0	1031	8	0
1	H	1023	0	1031	3	0
1	I	1015	0	1027	6	0
1	J	1023	0	1031	5	0
2	K	89	0	80	1	0
2	L	144	0	135	2	0
2	M	75	0	71	1	0
2	N	89	0	80	0	0
2	O	91	0	87	0	0
2	P	83	0	75	0	0
2	Q	104	0	99	1	0
3	C	5	0	0	0	0
4	A	4	0	0	0	0
4	B	2	0	0	0	0
4	C	4	0	0	0	0
4	D	1	0	0	0	0
4	E	6	0	0	0	0
4	F	2	0	0	0	0
4	G	2	0	0	0	0
4	H	5	0	0	0	0
4	I	5	0	0	0	0
4	J	6	0	0	0	0
4	K	1	0	0	0	0
All	All	11011	0	11003	43	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 2.

All (43) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:0:ACE:H3	2:L:5:ASP:HB2	1.59	0.85
1:A:264:VAL:HG13	1:A:268:LEU:HD12	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:264:VAL:HG11	1:E:282:PHE:HZ	1.66	0.61
1:E:271:LEU:HD22	1:H:302:LEU:HB2	1.86	0.58
1:F:271:LEU:HD22	1:I:302:LEU:HB2	1.86	0.57
1:H:240:ASP:HB3	1:H:351:ARG:HH12	1.69	0.57
1:B:307:LEU:HB3	1:J:273:LEU:HD21	1.88	0.56
1:C:271:LEU:HD22	1:G:302:LEU:HB2	1.89	0.53
1:C:302:LEU:HB2	1:G:271:LEU:HD22	1.91	0.53
1:J:264:VAL:HG11	1:J:282:PHE:HZ	1.74	0.52
1:C:320:SER:O	1:C:324:GLU:HG2	2.11	0.50
1:E:302:LEU:HB2	1:H:271:LEU:HD22	1.93	0.50
1:C:273:LEU:HD21	1:G:307:LEU:HB3	1.94	0.50
1:G:284:ASP:HB3	1:G:286:VAL:HG23	1.94	0.49
1:G:320:SER:O	1:G:324:GLU:HG2	2.14	0.48
1:A:307:LEU:HB3	1:D:273:LEU:HD21	1.96	0.47
1:B:284:ASP:HB3	1:B:286:VAL:HG23	1.96	0.47
1:C:241:ALA:HB2	2:M:3:ASP:HB3	1.97	0.46
1:F:302:LEU:HB2	1:I:271:LEU:HD22	1.97	0.45
1:A:285:GLY:HA3	1:A:318:ASN:HB3	1.97	0.45
1:F:307:LEU:HD11	1:I:307:LEU:HD21	1.99	0.45
1:F:307:LEU:HD21	1:I:307:LEU:HD11	2.00	0.44
1:A:279:GLU:HG2	1:A:280:THR:H	1.83	0.44
1:B:264:VAL:HG11	1:B:282:PHE:HZ	1.83	0.44
2:K:4:LEU:HD12	2:K:7:LEU:HD23	2.00	0.44
1:G:331:LEU:HD21	1:G:355:ASN:HB3	2.00	0.43
1:B:307:LEU:HD11	1:J:307:LEU:HD21	2.01	0.43
1:I:279:GLU:HB3	1:I:346:LEU:HD13	2.01	0.43
1:I:284:ASP:HB3	1:I:286:VAL:HG23	2.01	0.43
1:C:307:LEU:HB3	1:G:273:LEU:HD21	2.00	0.43
1:A:279:GLU:HG2	1:A:280:THR:N	2.34	0.42
1:A:271:LEU:HG	1:A:294:LEU:HD21	2.01	0.42
1:E:277:GLU:O	1:E:281:GLN:HB2	2.19	0.42
1:B:271:LEU:HD22	1:J:302:LEU:HD12	2.01	0.42
1:F:347:LYS:HD3	1:F:351:ARG:HH21	1.85	0.42
1:E:279:GLU:HB3	1:E:346:LEU:HD13	2.02	0.41
1:F:284:ASP:HB3	1:F:286:VAL:HG23	2.02	0.41
1:C:240:ASP:OD1	1:C:351:ARG:NH1	2.52	0.41
1:F:264:VAL:HG11	1:F:282:PHE:HZ	1.86	0.41
1:G:245:LEU:HD13	2:Q:4:LEU:HD11	2.03	0.41
1:J:347:LYS:HD3	1:J:351:ARG:HH21	1.86	0.41
1:D:291:LEU:HA	1:D:294:LEU:HD12	2.03	0.40
1:D:293:GLY:HA3	2:L:1:MET:CE	2.50	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	125/133 (94%)	120 (96%)	5 (4%)	0	100	100
1	B	124/133 (93%)	121 (98%)	3 (2%)	0	100	100
1	C	125/133 (94%)	123 (98%)	2 (2%)	0	100	100
1	D	123/133 (92%)	118 (96%)	5 (4%)	0	100	100
1	E	125/133 (94%)	121 (97%)	4 (3%)	0	100	100
1	F	123/133 (92%)	120 (98%)	3 (2%)	0	100	100
1	G	123/133 (92%)	115 (94%)	8 (6%)	0	100	100
1	H	123/133 (92%)	121 (98%)	2 (2%)	0	100	100
1	I	122/133 (92%)	118 (97%)	4 (3%)	0	100	100
1	J	123/133 (92%)	121 (98%)	2 (2%)	0	100	100
2	K	10/22 (46%)	10 (100%)	0	0	100	100
2	L	18/22 (82%)	16 (89%)	2 (11%)	0	100	100
2	M	8/22 (36%)	8 (100%)	0	0	100	100
2	N	10/22 (46%)	10 (100%)	0	0	100	100
2	O	10/22 (46%)	10 (100%)	0	0	100	100
2	P	9/22 (41%)	9 (100%)	0	0	100	100
2	Q	12/22 (54%)	11 (92%)	1 (8%)	0	100	100
All	All	1313/1484 (88%)	1272 (97%)	41 (3%)	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	118/122 (97%)	116 (98%)	2 (2%)	68 91
1	B	117/122 (96%)	116 (99%)	1 (1%)	84 96
1	C	118/122 (97%)	118 (100%)	0	100 100
1	D	116/122 (95%)	115 (99%)	1 (1%)	84 96
1	E	118/122 (97%)	116 (98%)	2 (2%)	68 91
1	F	116/122 (95%)	115 (99%)	1 (1%)	84 96
1	G	116/122 (95%)	116 (100%)	0	100 100
1	H	116/122 (95%)	115 (99%)	1 (1%)	84 96
1	I	115/122 (94%)	114 (99%)	1 (1%)	84 96
1	J	116/122 (95%)	115 (99%)	1 (1%)	84 96
2	K	10/18 (56%)	10 (100%)	0	100 100
2	L	17/18 (94%)	17 (100%)	0	100 100
2	M	8/18 (44%)	7 (88%)	1 (12%)	6 17
2	N	10/18 (56%)	9 (90%)	1 (10%)	9 28
2	O	10/18 (56%)	10 (100%)	0	100 100
2	P	9/18 (50%)	9 (100%)	0	100 100
2	Q	12/18 (67%)	12 (100%)	0	100 100
All	All	1242/1346 (92%)	1230 (99%)	12 (1%)	82 95

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	288	LEU
1	A	361	LYS
1	B	279	GLU
1	D	247	ASP
1	E	279	GLU
1	E	281	GLN
1	F	240	ASP

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Mol	Chain	Res	Type
1	H	240	ASP
1	I	243	ASP
1	J	247	ASP
2	M	5	ASP
2	N	3	ASP

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

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

1 ligand is 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	SO4	C	401	-	4,4,4	0.33	0	6,6,6	0.08	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	SO4	C	401	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	127/133 (95%)	0.38	2 (1%) 74 72	49, 67, 106, 125	0
1	B	126/133 (94%)	0.23	2 (1%) 74 72	51, 68, 92, 112	0
1	C	127/133 (95%)	0.38	1 (0%) 87 86	69, 85, 109, 127	0
1	D	125/133 (93%)	0.42	3 (2%) 62 57	58, 83, 143, 172	0
1	E	127/133 (95%)	0.49	3 (2%) 62 57	70, 90, 114, 121	0
1	F	125/133 (93%)	0.36	3 (2%) 62 57	67, 91, 122, 138	0
1	G	125/133 (93%)	0.34	6 (4%) 34 28	72, 97, 132, 151	0
1	H	125/133 (93%)	0.41	3 (2%) 62 57	71, 94, 136, 151	0
1	I	124/133 (93%)	0.82	12 (9%) 10 6	79, 99, 139, 151	0
1	J	125/133 (93%)	0.91	15 (12%) 6 3	70, 102, 159, 183	0
2	K	12/22 (54%)	0.29	1 (8%) 14 9	66, 84, 113, 146	0
2	L	19/22 (86%)	0.74	1 (5%) 30 23	69, 86, 107, 112	0
2	M	10/22 (45%)	0.09	0 100 100	106, 112, 123, 134	0
2	N	12/22 (54%)	0.74	3 (25%) 1 0	121, 129, 157, 172	0
2	O	12/22 (54%)	0.79	0 100 100	103, 111, 125, 128	0
2	P	11/22 (50%)	1.09	1 (9%) 11 7	121, 130, 156, 167	0
2	Q	14/22 (63%)	0.78	2 (14%) 4 2	114, 118, 132, 142	0
All	All	1346/1484 (90%)	0.49	58 (4%) 39 32	49, 90, 136, 183	0

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	335	LYS	5.9
1	I	362	ASN	5.4
2	K	2	ASP	4.8
1	D	245	LEU	4.7

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Mol	Chain	Res	Type	RSRZ
1	J	247	ASP	4.6
1	I	364	GLU	4.5
1	J	356	LEU	4.3
2	L	12	GLU	4.3
1	J	240	ASP	4.2
1	J	248	HIS	3.8
2	Q	14	THR	3.8
1	E	310	GLU	3.6
1	J	357	PHE	3.4
1	G	364	GLU	3.2
1	J	244	THR	3.1
1	G	246	PHE	3.1
1	D	248	HIS	3.0
1	D	240	ASP	2.9
1	G	248	HIS	2.9
1	J	354	TYR	2.8
1	B	364	GLU	2.7
1	B	239	ARG	2.7
1	C	305	PHE	2.7
2	Q	12	GLU	2.7
1	F	299	PHE	2.6
1	I	337	ARG	2.6
1	I	335	LYS	2.6
1	A	310	GLU	2.5
1	E	299	PHE	2.5
1	H	240	ASP	2.5
1	I	323	PHE	2.5
1	J	253	LEU	2.4
1	H	251	ASP	2.4
1	I	324	GLU	2.4
1	I	328	ASP	2.4
1	G	362	ASN	2.4
1	I	333	LYS	2.4
2	N	2	ASP	2.3
1	J	355	ASN	2.3
1	F	242	PHE	2.2
1	G	253	LEU	2.2
1	G	271	LEU	2.2
2	N	13	SER	2.2
2	N	3	ASP	2.2
1	A	364	GLU	2.2
1	I	316	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	I	263	PHE	2.1
1	J	291	LEU	2.1
1	J	242	PHE	2.1
1	J	362	ASN	2.1
1	H	248	HIS	2.1
1	I	353	LEU	2.1
1	F	303	HIS	2.0
2	P	2	ASP	2.0
1	E	324	GLU	2.0
1	I	298	TYR	2.0
1	J	272	ASN	2.0
1	J	246	PHE	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å^2)	Q<0.9
3	SO4	C	401	5/5	0.92	0.24	0.05	98,99,102,102	0

6.5 Other polymers (i)

There are no such residues in this entry.