Full wwPDB X-ray Structure Validation Report ⓘ

Oct 26, 2023 – 08:23 PM EDT

PDB ID	:	3RL7
Title	:	Crystal structure of hDLG1-PDZ1 complexed with APC
Authors	:	Zhang, Z.; Li, H.; Wu, G.
Deposited on	:	2011-04-19
Resolution	:	2.30 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

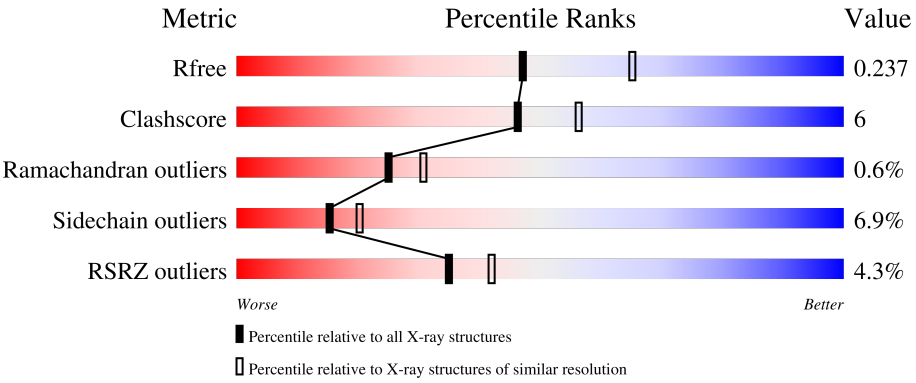
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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	107	67% 15% 16%
1	B	107	68% 15% 17%
1	C	107	2% 72% 9% 19%
1	D	107	3% 71% 11% 14%
1	E	107	7% 70% 6% 23%

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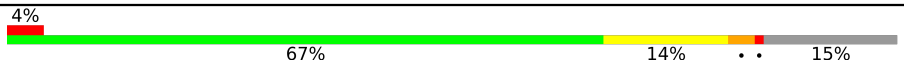
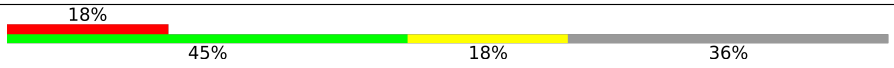
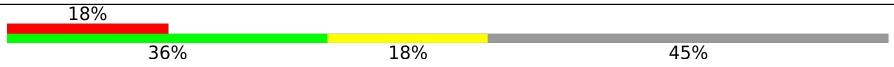
Mol	Chain	Length	Quality of chain
1	F	107	
2	G	11	
2	H	11	
2	I	11	
2	J	11	
2	K	11	
2	L	11	

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 4352 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 Disks large homolog 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	89	Total	C	N	O	S	0	0	0
			682	421	126	134	1			
1	A	90	Total	C	N	O	S	0	0	0
			686	424	124	137	1			
1	C	87	Total	C	N	O	S	0	0	0
			660	406	122	131	1			
1	D	92	Total	C	N	O	S	0	0	0
			705	435	129	139	2			
1	E	82	Total	C	N	O	S	0	0	0
			629	391	116	121	1			
1	F	91	Total	C	N	O	S	0	0	0
			694	429	125	138	2			

There are 54 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	211	MET	-	expression tag	UNP Q12959
B	212	GLY	-	expression tag	UNP Q12959
B	213	HIS	-	expression tag	UNP Q12959
B	214	HIS	-	expression tag	UNP Q12959
B	215	HIS	-	expression tag	UNP Q12959
B	216	HIS	-	expression tag	UNP Q12959
B	217	HIS	-	expression tag	UNP Q12959
B	218	HIS	-	expression tag	UNP Q12959
B	219	MET	-	expression tag	UNP Q12959
A	211	MET	-	expression tag	UNP Q12959
A	212	GLY	-	expression tag	UNP Q12959
A	213	HIS	-	expression tag	UNP Q12959
A	214	HIS	-	expression tag	UNP Q12959
A	215	HIS	-	expression tag	UNP Q12959
A	216	HIS	-	expression tag	UNP Q12959
A	217	HIS	-	expression tag	UNP Q12959
A	218	HIS	-	expression tag	UNP Q12959

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Chain	Residue	Modelled	Actual	Comment	Reference
A	219	MET	-	expression tag	UNP Q12959
C	211	MET	-	expression tag	UNP Q12959
C	212	GLY	-	expression tag	UNP Q12959
C	213	HIS	-	expression tag	UNP Q12959
C	214	HIS	-	expression tag	UNP Q12959
C	215	HIS	-	expression tag	UNP Q12959
C	216	HIS	-	expression tag	UNP Q12959
C	217	HIS	-	expression tag	UNP Q12959
C	218	HIS	-	expression tag	UNP Q12959
C	219	MET	-	expression tag	UNP Q12959
D	211	MET	-	expression tag	UNP Q12959
D	212	GLY	-	expression tag	UNP Q12959
D	213	HIS	-	expression tag	UNP Q12959
D	214	HIS	-	expression tag	UNP Q12959
D	215	HIS	-	expression tag	UNP Q12959
D	216	HIS	-	expression tag	UNP Q12959
D	217	HIS	-	expression tag	UNP Q12959
D	218	HIS	-	expression tag	UNP Q12959
D	219	MET	-	expression tag	UNP Q12959
E	211	MET	-	expression tag	UNP Q12959
E	212	GLY	-	expression tag	UNP Q12959
E	213	HIS	-	expression tag	UNP Q12959
E	214	HIS	-	expression tag	UNP Q12959
E	215	HIS	-	expression tag	UNP Q12959
E	216	HIS	-	expression tag	UNP Q12959
E	217	HIS	-	expression tag	UNP Q12959
E	218	HIS	-	expression tag	UNP Q12959
E	219	MET	-	expression tag	UNP Q12959
F	211	MET	-	expression tag	UNP Q12959
F	212	GLY	-	expression tag	UNP Q12959
F	213	HIS	-	expression tag	UNP Q12959
F	214	HIS	-	expression tag	UNP Q12959
F	215	HIS	-	expression tag	UNP Q12959
F	216	HIS	-	expression tag	UNP Q12959
F	217	HIS	-	expression tag	UNP Q12959
F	218	HIS	-	expression tag	UNP Q12959
F	219	MET	-	expression tag	UNP Q12959

- Molecule 2 is a protein called 11-mer peptide from Adenomatous polyposis coli protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	G	7	Total	C	N	O	0	0	0
			54	35	7	12			

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
2	H	5	Total C N O 33 21 5 7	0	0	0
2	I	5	Total C N O 40 27 5 8	0	0	0
2	J	6	Total C N O 48 32 6 10	0	0	0
2	K	5	Total C N O 36 23 5 8	0	0	0
2	L	4	Total C N O 28 18 4 6	0	0	0

- Molecule 3 is water.

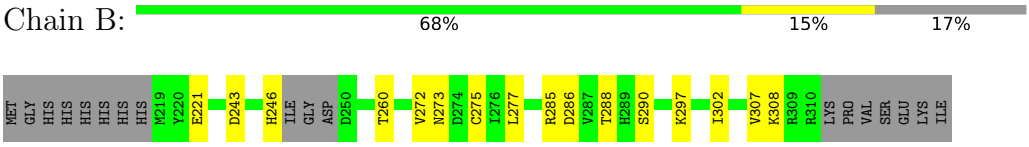
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	54	Total O 54 54	0	0
3	A	1	Total O 1 1	0	0
3	C	1	Total O 1 1	0	0
3	G	1	Total O 1 1	0	0

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.

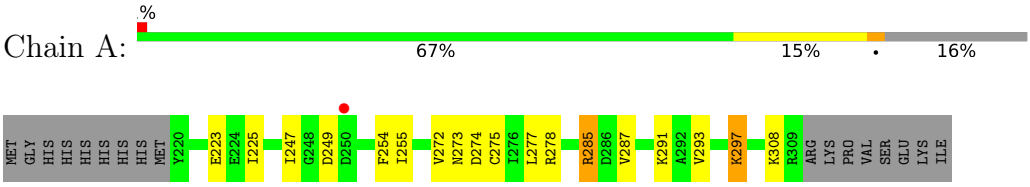
• Molecule 1: Disks large homolog 1

Chain B:



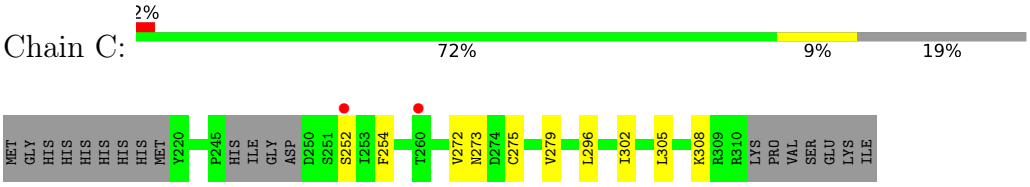
• Molecule 1: Disks large homolog 1

Chain A:



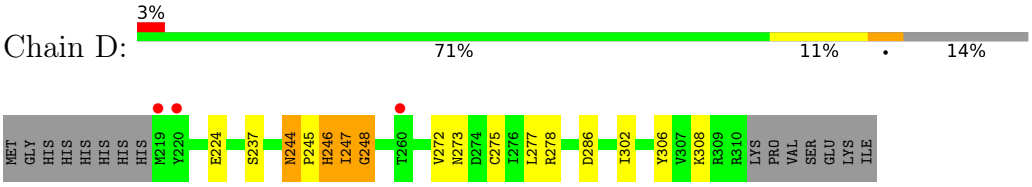
• Molecule 1: Disks large homolog 1

Chain C:



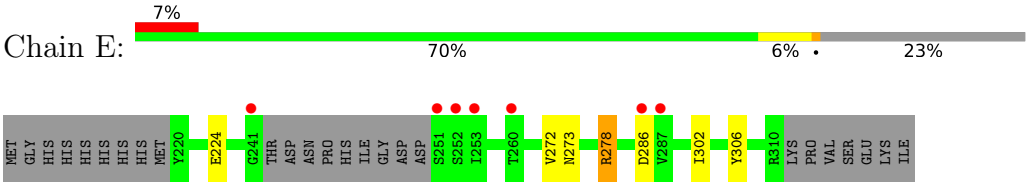
• Molecule 1: Disks large homolog 1

Chain D:



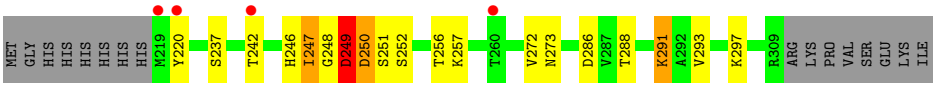
• Molecule 1: Disks large homolog 1

Chain E:



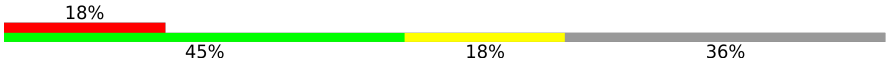
• Molecule 1: Disks large homolog 1

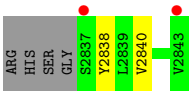
Chain F:



• Molecule 2: 11-mer peptide from Adenomatous polyposis coli protein

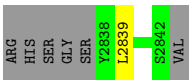
Chain G:





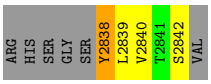
• Molecule 2: 11-mer peptide from Adenomatous polyposis coli protein

Chain H:



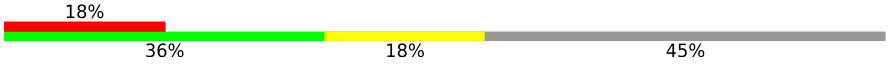
• Molecule 2: 11-mer peptide from Adenomatous polyposis coli protein

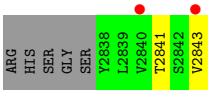
Chain I:



• Molecule 2: 11-mer peptide from Adenomatous polyposis coli protein

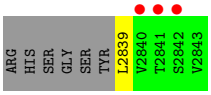
Chain J:





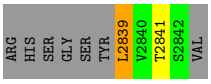
• Molecule 2: 11-mer peptide from Adenomatous polyposis coli protein

Chain K:



• Molecule 2: 11-mer peptide from Adenomatous polyposis coli protein

Chain L:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 3	Depositor
Cell constants a, b, c, α, β, γ	105.63Å 105.63Å 50.83Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.30 45.74 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.8 (50.00-2.30) 99.9 (45.74-2.30)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.98 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.193 , 0.231 0.205 , 0.237	Depositor DCC
R_{free} test set	1392 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å^2)	29.5	Xtriage
Anisotropy	0.295	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 28.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.52$, $< L^2 > = 0.36$	Xtriage
Estimated twinning fraction	0.166 for -h,-k,l 0.226 for h,-h-k,-l 0.135 for -k,-h,-l	Xtriage
Reported twinning fraction	0.262 for H, K, L 0.239 for h+k,-k,-l 0.261 for -h,-k,l 0.238 for K, H, -L	Depositor
Outliers	0 of 28157 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	4352	wwPDB-VP
Average B, all atoms (Å^2)	38.0	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 29.43 % 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 1.5529e-03. 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

5.1 Standard geometry

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	0.34	0/693	0.54	0/934
1	B	0.33	0/688	0.54	0/925
1	C	0.35	0/664	0.52	0/892
1	D	0.42	0/712	0.56	0/958
1	E	0.30	0/633	0.50	0/848
1	F	0.34	0/701	0.59	0/944
2	G	0.40	0/54	0.43	0/72
2	H	0.45	0/32	0.81	0/43
2	I	0.40	0/40	0.52	0/54
2	J	0.39	0/48	0.59	0/64
2	K	0.46	0/35	0.90	0/46
2	L	0.40	0/27	0.54	0/36
All	All	0.35	0/4327	0.55	0/5816

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	686	0	682	12	0
1	B	682	0	678	7	0
1	C	660	0	662	8	0
1	D	705	0	704	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	629	0	641	2	0
1	F	694	0	691	18	0
2	G	54	0	54	2	0
2	H	33	0	33	1	0
2	I	40	0	40	4	0
2	J	48	0	49	3	0
2	K	36	0	40	0	0
2	L	28	0	31	1	0
3	A	1	0	0	0	0
3	B	54	0	0	0	0
3	C	1	0	0	0	0
3	G	1	0	0	0	0
All	All	4352	0	4305	54	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 (54) 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:249:ASP:HB2	1:F:250:ASP:HA	1.58	0.83
1:B:243:ASP:OD2	1:B:288:THR:HG23	1.81	0.79
1:D:245:PRO:HD2	2:I:2838:TYR:HB2	1.63	0.78
1:F:247:ILE:HG22	1:F:248:GLY:H	1.50	0.76
1:F:248:GLY:O	1:F:249:ASP:HB3	1.83	0.75
1:F:247:ILE:HG22	1:F:248:GLY:N	2.02	0.75
1:F:249:ASP:CB	1:F:250:ASP:HA	2.20	0.68
1:C:272:VAL:O	1:C:273:ASN:HB2	1.94	0.67
1:F:246:HIS:O	1:F:246:HIS:ND1	2.29	0.66
1:F:247:ILE:CG2	1:F:248:GLY:H	2.05	0.62
2:H:2839:LEU:HD21	2:I:2840:VAL:HG21	1.83	0.60
1:E:272:VAL:O	1:E:273:ASN:HB2	2.04	0.57
1:A:255:ILE:HG12	1:A:274:ASP:HB2	1.86	0.56
1:F:248:GLY:O	1:F:249:ASP:CB	2.53	0.54
1:B:286:ASP:OD1	1:A:285:ARG:NH1	2.40	0.54
1:C:296:LEU:HD21	1:C:305:LEU:HD21	1.90	0.54
1:A:275:CYS:HB2	1:A:308:LYS:HG2	1.89	0.53
1:B:288:THR:HG22	1:B:290:SER:H	1.74	0.52
1:D:277:LEU:HD21	1:D:308:LYS:HD3	1.91	0.52
1:A:254:PHE:HA	1:A:274:ASP:O	2.10	0.52
1:F:272:VAL:O	1:F:273:ASN:HB2	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:288:THR:OG1	1:F:291:LYS:HG2	2.12	0.50
1:F:293:VAL:O	1:F:297:LYS:HG2	2.12	0.50
1:A:272:VAL:O	1:A:273:ASN:HB2	2.11	0.50
1:A:287:VAL:HB	1:A:291:LYS:HB2	1.92	0.50
1:F:256:THR:HB	2:G:2838:TYR:HB2	1.96	0.48
1:F:246:HIS:O	1:F:247:ILE:HB	2.14	0.48
1:D:272:VAL:O	1:D:273:ASN:HB2	2.15	0.47
1:F:246:HIS:O	1:F:246:HIS:CG	2.63	0.47
1:D:278:ARG:HB2	1:D:306:TYR:HB2	1.97	0.46
1:C:252:SER:HB2	1:C:275:CYS:SG	2.55	0.46
1:A:293:VAL:CG1	1:A:297:LYS:HE2	2.46	0.46
1:D:237:SER:HA	2:I:2842:SER:HA	1.97	0.45
1:B:275:CYS:O	1:B:307:VAL:HA	2.16	0.45
1:F:246:HIS:O	1:F:247:ILE:CB	2.63	0.45
1:A:277:LEU:HD21	1:A:308:LYS:HD3	1.99	0.44
1:D:246:HIS:C	1:D:248:GLY:N	2.68	0.44
1:B:277:LEU:HD21	1:B:308:LYS:HE3	2.00	0.44
1:A:247:ILE:CD1	1:F:252:SER:OG	2.65	0.44
1:A:255:ILE:CG1	1:A:274:ASP:HB2	2.48	0.43
1:B:285:ARG:HB3	1:A:285:ARG:NH1	2.33	0.43
2:I:2838:TYR:HB3	2:I:2839:LEU:H	1.64	0.43
1:C:296:LEU:HD13	2:J:2843:VAL:HG11	2.00	0.43
1:F:237:SER:HB2	1:F:257:LYS:HB3	2.01	0.42
1:C:296:LEU:HB3	2:J:2843:VAL:HG11	2.00	0.42
1:E:278:ARG:HB3	1:E:306:TYR:HB2	2.01	0.42
1:F:242:THR:HA	1:F:251:SER:HB2	2.01	0.42
1:B:272:VAL:O	1:B:273:ASN:HB2	2.20	0.42
1:D:244:ASN:O	1:D:247:ILE:HG12	2.20	0.42
1:C:279:VAL:HG21	1:C:296:LEU:HG	2.03	0.41
1:A:223:GLU:OE1	1:A:225:ILE:HD11	2.21	0.41
1:C:275:CYS:HB3	1:C:308:LYS:HG2	2.02	0.41
1:C:296:LEU:HB3	2:J:2843:VAL:CG1	2.50	0.41
2:G:2840:VAL:HG21	2:L:2839:LEU:HD23	2.03	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	88/107 (82%)	84 (96%)	4 (4%)	0	100 100
1	B	85/107 (79%)	81 (95%)	4 (5%)	0	100 100
1	C	83/107 (78%)	78 (94%)	5 (6%)	0	100 100
1	D	90/107 (84%)	84 (93%)	5 (6%)	1 (1%)	14 15
1	E	78/107 (73%)	72 (92%)	6 (8%)	0	100 100
1	F	89/107 (83%)	79 (89%)	8 (9%)	2 (2%)	6 5
2	G	5/11 (46%)	5 (100%)	0	0	100 100
2	H	3/11 (27%)	3 (100%)	0	0	100 100
2	I	3/11 (27%)	3 (100%)	0	0	100 100
2	J	4/11 (36%)	4 (100%)	0	0	100 100
2	K	3/11 (27%)	3 (100%)	0	0	100 100
2	L	2/11 (18%)	2 (100%)	0	0	100 100
All	All	533/708 (75%)	498 (93%)	32 (6%)	3 (1%)	25 31

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	249	ASP
1	F	247	ILE
1	D	248	GLY

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	73/89 (82%)	69 (94%)	4 (6%)	21 30
1	B	72/89 (81%)	67 (93%)	5 (7%)	15 20
1	C	70/89 (79%)	68 (97%)	2 (3%)	42 58
1	D	75/89 (84%)	68 (91%)	7 (9%)	9 10
1	E	66/89 (74%)	62 (94%)	4 (6%)	18 25
1	F	74/89 (83%)	69 (93%)	5 (7%)	16 21
2	G	7/10 (70%)	7 (100%)	0	100 100
2	H	4/10 (40%)	4 (100%)	0	100 100
2	I	5/10 (50%)	4 (80%)	1 (20%)	1 1
2	J	6/10 (60%)	5 (83%)	1 (17%)	2 2
2	K	5/10 (50%)	4 (80%)	1 (20%)	1 1
2	L	4/10 (40%)	2 (50%)	2 (50%)	0 0
All	All	461/594 (78%)	429 (93%)	32 (7%)	15 20

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	221	GLU
1	B	246	HIS
1	B	260	THR
1	B	297	LYS
1	B	302	ILE
1	A	249	ASP
1	A	278	ARG
1	A	285	ARG
1	A	297	LYS
1	C	254	PHE
1	C	302	ILE
1	D	224	GLU
1	D	244	ASN
1	D	246	HIS
1	D	247	ILE
1	D	275	CYS
1	D	286	ASP
1	D	302	ILE
1	E	224	GLU
1	E	278	ARG
1	E	286	ASP
1	E	302	ILE

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Mol	Chain	Res	Type
1	F	220	TYR
1	F	249	ASP
1	F	250	ASP
1	F	286	ASP
1	F	291	LYS
2	I	2838	TYR
2	J	2841	THR
2	K	2839	LEU
2	L	2839	LEU
2	L	2841	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	231	ASN
1	D	244	ASN
1	E	266	GLN
1	F	244	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

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	90/107 (84%)	0.39	1 (1%) 80 85	27, 32, 42, 45	0
1	B	89/107 (83%)	0.36	0 100 100	27, 32, 42, 47	0
1	C	87/107 (81%)	0.49	2 (2%) 60 67	31, 38, 47, 53	0
1	D	92/107 (85%)	0.48	3 (3%) 46 53	27, 34, 43, 47	0
1	E	82/107 (76%)	0.65	7 (8%) 10 14	38, 44, 49, 50	0
1	F	91/107 (85%)	0.38	4 (4%) 34 41	34, 38, 44, 48	0
2	G	7/11 (63%)	1.16	2 (28%) 0 0	57, 58, 59, 59	0
2	H	5/11 (45%)	0.45	0 100 100	37, 38, 43, 50	0
2	I	5/11 (45%)	0.71	0 100 100	53, 54, 55, 57	0
2	J	6/11 (54%)	1.14	2 (33%) 0 0	45, 47, 50, 53	0
2	K	5/11 (45%)	2.37	3 (60%) 0 0	65, 65, 73, 75	0
2	L	4/11 (36%)	0.97	0 100 100	76, 82, 84, 93	0
All	All	563/708 (79%)	0.49	24 (4%) 35 42	27, 37, 49, 93	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	252	SER	5.2
1	D	220	TYR	4.9
1	E	241	GLY	4.1
1	F	220	TYR	3.4
1	C	252	SER	3.3
1	E	286	ASP	3.3
2	K	2842	SER	3.1
1	A	250	ASP	3.0
1	E	253	ILE	2.9
2	K	2841	THR	2.9
1	D	219	MET	2.8

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Mol	Chain	Res	Type	RSRZ
1	F	219	MET	2.8
2	J	2843	VAL	2.6
1	D	260	THR	2.5
2	K	2840	VAL	2.5
2	G	2843	VAL	2.5
1	E	260	THR	2.4
1	E	251	SER	2.3
2	G	2837	SER	2.3
1	F	242	THR	2.2
2	J	2840	VAL	2.2
1	F	260	THR	2.2
1	E	287	VAL	2.2
1	C	260	THR	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 monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.