Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 07:29 PM GMT

PDB ID	:	4P1W
Title	:	Crystal structure of Atg13(17BR)-Atg17-Atg29-Atg31 complex
Authors	:	Fujioka, Y.; Noda, N.N.
Deposited on	:	2014-02-27
Resolution	:	3.20 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:

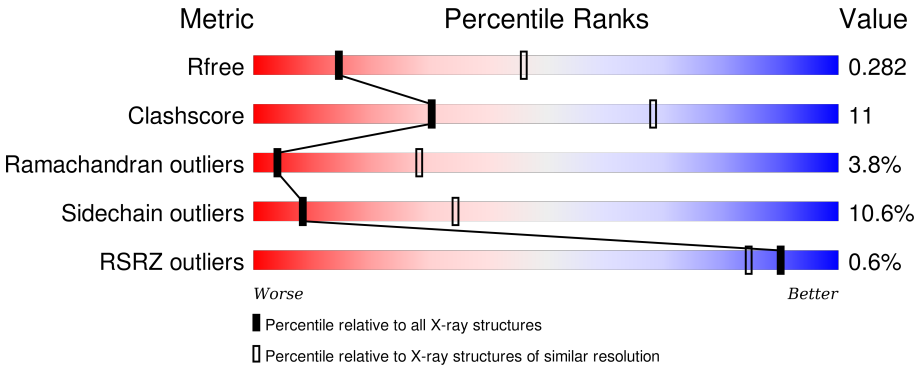
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 3.20 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	1124 (3.24-3.16)
Clashscore	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)
RSRZ outliers	91569	1129 (3.24-3.16)

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	74	% 81% 12% • •
1	D	74	% 80% 7% • 11%
2	B	151	62% 20% 7% • 11%
2	E	151	% 58% 19% 5% • 17%
3	C	413	70% 23% • •

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Mol	Chain	Length	Quality of chain
3	F	413	
4	G	13	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8904 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 Atg29.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	72	Total	C	N	O	S	0	0	0
			448	285	79	83	1			
1	D	66	Total	C	N	O	S	0	0	0
			400	250	71	78	1			

- Molecule 2 is a protein called Atg31.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	135	Total	C	N	O	S	0	0	0
			1009	642	167	198	2			
2	E	126	Total	C	N	O	S	0	0	0
			948	603	159	184	2			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	146	HIS	-	expression tag	UNP C5DEB9
B	147	HIS	-	expression tag	UNP C5DEB9
B	148	HIS	-	expression tag	UNP C5DEB9
B	149	HIS	-	expression tag	UNP C5DEB9
B	150	HIS	-	expression tag	UNP C5DEB9
B	151	HIS	-	expression tag	UNP C5DEB9
E	146	HIS	-	expression tag	UNP C5DEB9
E	147	HIS	-	expression tag	UNP C5DEB9
E	148	HIS	-	expression tag	UNP C5DEB9
E	149	HIS	-	expression tag	UNP C5DEB9
E	150	HIS	-	expression tag	UNP C5DEB9
E	151	HIS	-	expression tag	UNP C5DEB9

- Molecule 3 is a protein called Atg17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	399	Total	C	N	O	S	0	0	0
			3073	1927	527	607	12			
3	F	389	Total	C	N	O	S	0	0	0
			2980	1865	515	589	11			

- Molecule 4 is a protein called Atg13 17BR.

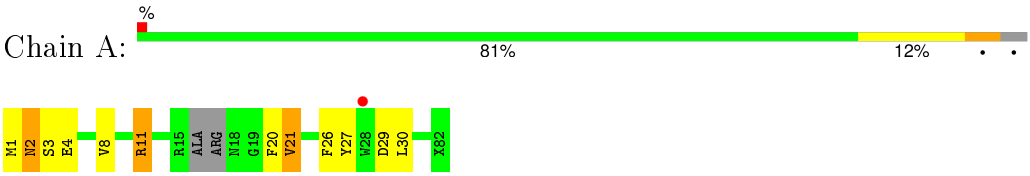
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	G	6	Total	C	N	O	0	0	0
			46	29	9	8			

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.

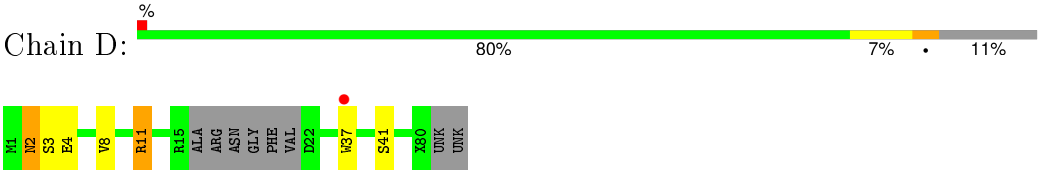
- Molecule 1: Atg29

Chain A:



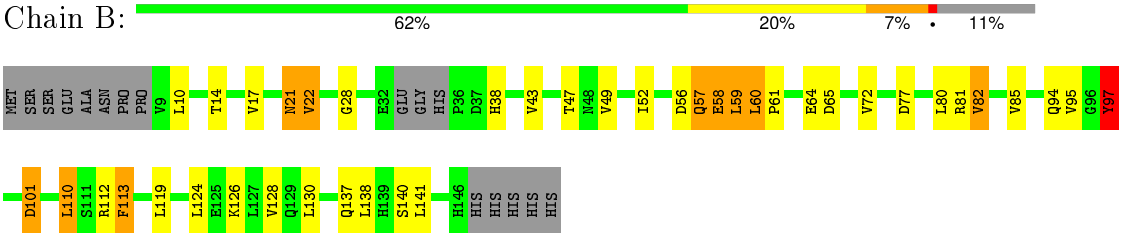
- Molecule 1: Atg29

Chain D:



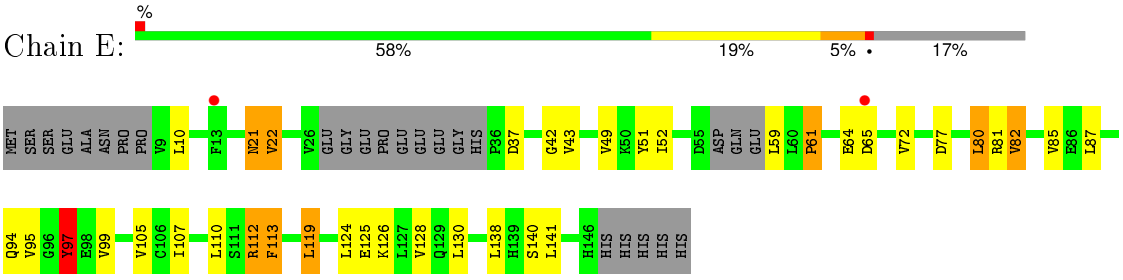
- Molecule 2: Atg31

Chain B:



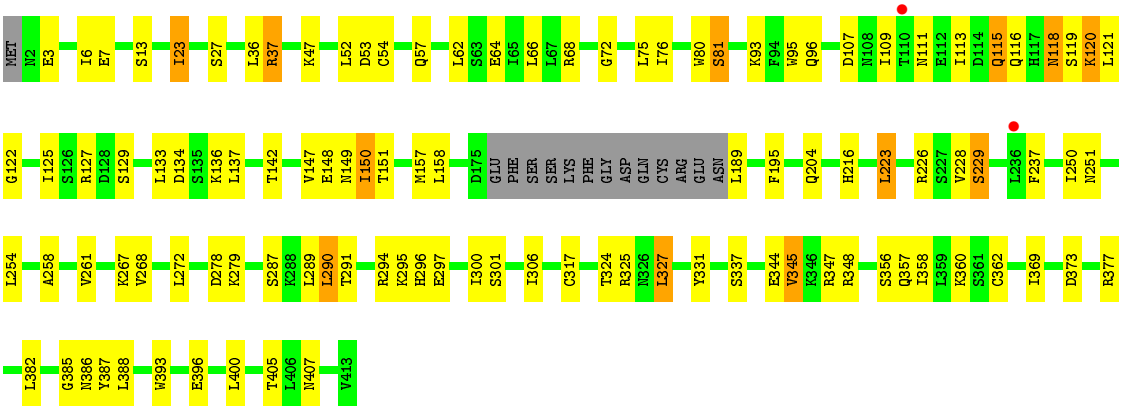
- Molecule 2: Atg31

Chain E:



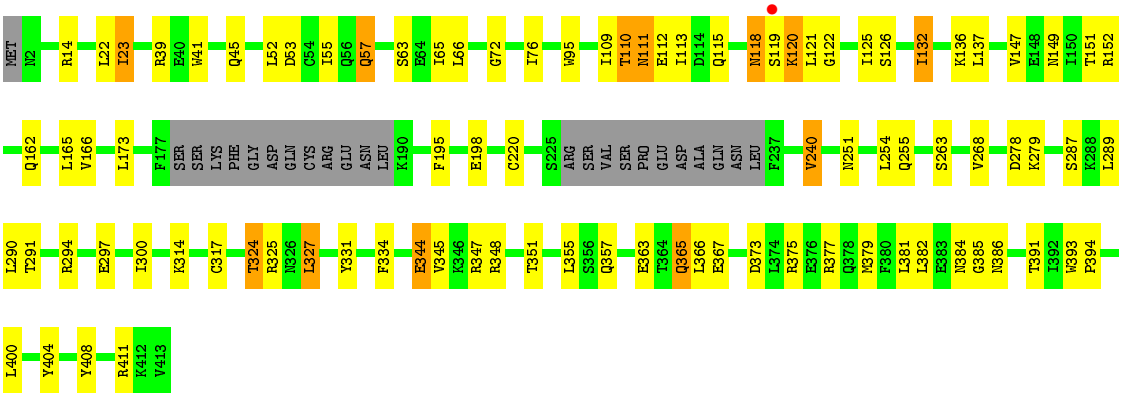
- Molecule 3: Atg17

Chain C:



- Molecule 3: Atg17

Chain F:



- Molecule 4: Atg13 17BR

Chain G:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	148.35Å 63.99Å 184.60Å 90.00° 109.25° 90.00°	Depositor
Resolution (Å)	44.26 – 3.20 44.26 – 3.20	Depositor EDS
% Data completeness (in resolution range)	89.7 (44.26-3.20) 89.7 (44.26-3.20)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.09 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.257 , 0.293 0.248 , 0.282	Depositor DCC
R_{free} test set	5548 reflections (12.58%)	DCC
Wilson B-factor (Å^2)	78.5	Xtriage
Anisotropy	0.406	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 77.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 54566 reflections	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	8904	wwPDB-VP
Average B, all atoms (Å^2)	117.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.85% 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

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	0.52	0/300	0.64	0/410
1	D	0.51	0/261	0.56	0/358
2	B	0.53	0/1026	0.75	0/1400
2	E	0.44	0/963	0.69	0/1314
3	C	0.50	0/3115	0.70	1/4224 (0.0%)
3	F	0.42	0/3018	0.62	0/4092
4	G	0.52	0/46	0.57	0/59
All	All	0.47	0/8729	0.67	1/11857 (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})
3	C	115	GLN	N-CA-C	5.26	125.22	111.00

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	448	0	271	12	0
1	D	400	0	210	6	0
2	B	1009	0	925	34	0
2	E	948	0	874	32	0
3	C	3073	0	2869	80	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	2980	0	2754	59	0
4	G	46	0	45	2	0
All	All	8904	0	7948	185	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 11.

All (185) 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)
3:C:111:ASN:HA	3:C:120:LYS:HA	1.40	1.03
3:C:109:ILE:HG21	3:C:121:LEU:HD13	1.48	0.93
3:F:111:ASN:HA	3:F:120:LYS:HA	1.48	0.92
1:D:8:VAL:HG12	2:E:72:VAL:HB	1.65	0.77
3:C:96:GLN:HE21	3:C:133:LEU:HB2	1.50	0.77
2:B:21:ASN:HD22	2:B:22:VAL:N	1.84	0.75
2:B:112:ARG:O	2:B:113:PHE:HB2	1.85	0.75
2:B:56:ASP:O	2:B:58:GLU:N	2.20	0.75
1:A:8:VAL:HG12	2:B:72:VAL:HB	1.68	0.75
3:C:76:ILE:O	3:C:81:SER:HB2	1.87	0.75
3:C:385:GLY:O	3:C:387:TYR:N	2.20	0.74
2:B:112:ARG:O	3:C:54:CYS:SG	2.47	0.72
3:C:109:ILE:CG2	3:C:121:LEU:HD13	2.20	0.69
3:C:96:GLN:HG2	3:C:134:ASP:OD1	1.92	0.69
3:C:393:TRP:CH2	3:F:345:VAL:HG22	2.28	0.68
2:E:21:ASN:HD22	2:E:22:VAL:N	1.92	0.67
1:A:2:ASN:O	1:A:4:GLU:N	2.29	0.66
3:C:113:ILE:O	3:C:113:ILE:HG23	1.95	0.66
3:F:109:ILE:HG21	3:F:121:LEU:HD12	1.80	0.64
3:C:75:LEU:HD22	3:C:80:TRP:CZ2	2.33	0.63
3:C:148:GLU:HA	3:C:151:THR:HG22	1.80	0.63
3:F:125:ILE:HD11	3:F:331:TYR:CD1	2.33	0.63
3:C:118:ASN:O	3:C:120:LYS:N	2.33	0.61
3:C:148:GLU:O	3:C:151:THR:HG22	2.01	0.61
2:B:101:ASP:OD1	2:B:101:ASP:N	2.31	0.60
2:B:128:VAL:HG22	3:C:300:ILE:HG21	1.83	0.60
3:C:250:ILE:HG21	4:G:398:PHE:CE1	2.37	0.59
3:C:96:GLN:CG	3:C:134:ASP:OD1	2.50	0.59
3:C:125:ILE:HD11	3:C:331:TYR:CD1	2.37	0.59
2:E:112:ARG:NH1	3:F:53:ASP:OD2	2.36	0.59
3:F:344:GLU:OE2	3:F:347:ARG:NH2	2.35	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2:ASN:O	1:D:4:GLU:N	2.37	0.58
3:F:95:TRP:CZ2	3:F:325:ARG:HD3	2.38	0.58
2:B:128:VAL:HG22	3:C:300:ILE:CG2	2.34	0.57
3:C:95:TRP:CZ2	3:C:325:ARG:HD3	2.39	0.57
3:F:147:VAL:O	3:F:151:THR:OG1	2.17	0.57
3:C:95:TRP:CE2	3:C:325:ARG:HD3	2.40	0.57
3:C:107:ASP:OD1	3:C:122:GLY:HA3	2.06	0.56
2:B:21:ASN:HD22	2:B:22:VAL:H	1.51	0.55
3:C:37:ARG:HB3	3:C:272:LEU:HD13	1.88	0.55
3:F:294:ARG:O	3:F:297:GLU:HG2	2.06	0.55
3:C:111:ASN:C	3:C:113:ILE:H	2.11	0.54
2:B:95:VAL:HG21	2:B:110:LEU:CD1	2.37	0.54
1:A:8:VAL:HG23	2:B:49:VAL:HG23	1.90	0.54
2:E:77:ASP:HB2	2:E:81:ARG:H	1.72	0.54
3:F:132:ILE:HD11	3:F:324:THR:OG1	2.08	0.54
2:E:77:ASP:HB2	2:E:81:ARG:HB2	1.90	0.53
3:C:195:PHE:CE2	3:C:268:VAL:HG22	2.44	0.53
3:C:278:ASP:O	3:C:279:LYS:C	2.45	0.53
3:C:107:ASP:OD1	3:C:127:ARG:NH2	2.43	0.52
2:B:77:ASP:HB2	2:B:81:ARG:H	1.74	0.52
3:F:95:TRP:CE2	3:F:325:ARG:HD3	2.44	0.52
3:F:118:ASN:O	3:F:120:LYS:N	2.40	0.52
2:B:112:ARG:O	2:B:113:PHE:CB	2.56	0.52
2:B:95:VAL:CG1	2:B:140:SER:HB3	2.40	0.52
3:C:62:LEU:HD11	3:C:157:MET:HE1	1.92	0.52
3:C:377:ARG:HG2	3:F:348:ARG:NH2	2.25	0.52
2:B:57:GLN:O	2:B:58:GLU:C	2.48	0.52
3:C:327:LEU:HD22	3:C:331:TYR:CZ	2.45	0.51
1:A:8:VAL:CG2	2:B:49:VAL:HA	2.41	0.51
3:C:122:GLY:O	3:C:125:ILE:HG22	2.11	0.51
2:E:49:VAL:HG22	2:E:51:TYR:CE1	2.46	0.51
3:F:109:ILE:HG21	3:F:121:LEU:CD1	2.39	0.51
1:A:11:ARG:HA	2:B:52:ILE:O	2.11	0.51
3:C:348:ARG:HH21	3:F:377:ARG:HG2	1.76	0.50
2:B:77:ASP:HB2	2:B:81:ARG:HB2	1.92	0.50
1:A:1:MET:HE1	2:B:17:VAL:HG21	1.92	0.50
3:C:6:ILE:HD11	3:C:223:LEU:HB3	1.94	0.50
3:C:72:GLY:O	3:C:76:ILE:HB	2.11	0.50
3:C:13:SER:HB2	3:C:216:HIS:CD2	2.47	0.50
2:E:138:LEU:HB3	3:F:290:LEU:HD21	1.93	0.50
3:C:75:LEU:HD22	3:C:80:TRP:CE2	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:68:ARG:NH2	3:C:158:LEU:HD21	2.28	0.49
3:C:136:LYS:HD2	3:C:317:CYS:SG	2.53	0.49
3:F:113:ILE:HG23	3:F:113:ILE:O	2.12	0.49
2:E:95:VAL:CG1	2:E:140:SER:HB3	2.43	0.49
2:E:112:ARG:O	2:E:113:PHE:O	2.30	0.49
2:B:95:VAL:HG11	2:B:140:SER:HB3	1.95	0.49
2:E:85:VAL:HG22	2:E:97:TYR:CG	2.48	0.49
3:F:109:ILE:HG21	3:F:121:LEU:CG	2.42	0.48
3:F:136:LYS:HD2	3:F:317:CYS:SG	2.53	0.48
3:F:111:ASN:C	3:F:113:ILE:H	2.17	0.48
2:E:99:VAL:HG23	2:E:105:VAL:HG12	1.96	0.48
1:A:30:LEU:O	1:A:30:LEU:HD23	2.14	0.48
3:C:347:ARG:HH22	3:F:377:ARG:HG3	1.78	0.48
2:E:87:LEU:HD12	2:E:107:ILE:HG21	1.96	0.48
2:B:52:ILE:HD13	2:B:61:PRO:HA	1.96	0.47
2:E:87:LEU:CD1	2:E:107:ILE:HG21	2.44	0.47
3:C:113:ILE:O	3:C:113:ILE:CG2	2.63	0.47
3:C:345:VAL:HG23	3:F:393:TRP:CH2	2.49	0.47
3:C:267:LYS:HG3	3:C:268:VAL:N	2.28	0.47
3:C:294:ARG:O	3:C:297:GLU:HG2	2.14	0.47
3:C:387:TYR:O	3:F:334:PHE:HD2	1.98	0.47
3:C:377:ARG:HG3	3:F:347:ARG:HH22	1.79	0.47
3:C:27:SER:HB3	3:C:261:VAL:HG11	1.95	0.47
3:F:110:THR:O	3:F:111:ASN:CB	2.63	0.47
2:B:110:LEU:HD13	2:B:141:LEU:HD21	1.96	0.47
2:E:126:LYS:HE3	2:E:130:LEU:HD21	1.96	0.47
1:A:20:PHE:CD1	1:A:21:VAL:N	2.83	0.46
3:C:237:PHE:CD1	3:C:237:PHE:C	2.89	0.46
3:C:195:PHE:CD2	3:C:268:VAL:HG22	2.50	0.46
3:C:347:ARG:NH1	3:F:373:ASP:OD1	2.40	0.46
3:C:3:GLU:O	3:C:6:ILE:HG22	2.16	0.46
3:C:228:VAL:O	3:C:229:SER:CB	2.64	0.46
2:E:22:VAL:HG11	2:E:130:LEU:HD22	1.96	0.46
3:C:62:LEU:HD11	3:C:157:MET:CE	2.45	0.46
3:C:405:THR:O	3:F:408:TYR:HA	2.15	0.46
1:A:27:TYR:CE2	1:A:29:ASP:HB2	2.51	0.46
3:F:111:ASN:C	3:F:113:ILE:N	2.68	0.46
2:E:112:ARG:O	2:E:113:PHE:C	2.53	0.46
3:C:358:ILE:HD13	3:F:365:GLN:CG	2.46	0.45
3:F:111:ASN:O	3:F:113:ILE:N	2.50	0.45
3:C:250:ILE:HG21	4:G:398:PHE:CD1	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:21:ASN:HD22	2:E:22:VAL:H	1.63	0.45
3:F:109:ILE:HG21	3:F:121:LEU:HG	1.99	0.45
3:F:23:ILE:HG21	3:F:254:LEU:HD13	1.99	0.45
2:B:85:VAL:HG22	2:B:97:TYR:CG	2.52	0.45
1:A:26:PHE:CD2	2:B:47:THR:HG21	2.51	0.45
2:B:95:VAL:HG21	2:B:110:LEU:HD12	1.99	0.45
1:D:11:ARG:HA	2:E:52:ILE:O	2.16	0.45
3:C:111:ASN:C	3:C:113:ILE:N	2.69	0.45
3:C:147:VAL:HA	3:C:150:ILE:HG22	1.98	0.45
3:C:125:ILE:HG23	3:C:127:ARG:HG3	1.99	0.45
3:F:41:TRP:CH2	3:F:45:GLN:OE1	2.70	0.44
3:C:258:ALA:HA	3:C:261:VAL:HG12	2.00	0.44
3:F:344:GLU:CD	3:F:347:ARG:HH21	2.21	0.44
3:F:287:SER:O	3:F:291:THR:OG1	2.33	0.44
2:B:110:LEU:HD21	2:B:137:GLN:HB3	1.99	0.44
3:C:327:LEU:CD2	3:C:331:TYR:CE1	3.00	0.44
3:C:393:TRP:CZ3	3:F:345:VAL:HG22	2.52	0.44
3:F:52:LEU:O	3:F:53:ASP:C	2.56	0.44
2:E:128:VAL:HG22	3:F:300:ILE:HG21	1.99	0.43
3:C:118:ASN:C	3:C:118:ASN:ND2	2.72	0.43
3:C:147:VAL:O	3:C:151:THR:HB	2.17	0.43
2:E:128:VAL:HG22	3:F:300:ILE:CG2	2.48	0.43
2:E:125:GLU:HG3	2:E:126:LYS:N	2.34	0.43
2:E:124:LEU:HD23	2:E:128:VAL:HG23	2.00	0.43
2:B:81:ARG:O	2:B:82:VAL:HB	2.19	0.43
3:C:6:ILE:HG23	3:C:7:GLU:N	2.34	0.43
3:F:384:ASN:O	3:F:386:ASN:N	2.52	0.43
3:F:72:GLY:O	3:F:76:ILE:HB	2.18	0.43
3:F:76:ILE:HD12	3:F:151:THR:HG23	2.01	0.43
3:C:373:ASP:OD1	3:F:347:ARG:NH1	2.44	0.43
2:E:85:VAL:HG22	2:E:97:TYR:CD2	2.53	0.43
1:A:8:VAL:HG23	2:B:49:VAL:HA	2.01	0.42
3:C:23:ILE:HG21	3:C:254:LEU:HD13	2.01	0.42
3:F:162:GLN:O	3:F:166:VAL:HG23	2.19	0.42
3:C:385:GLY:O	3:C:388:LEU:N	2.49	0.42
3:F:278:ASP:O	3:F:279:LYS:C	2.58	0.42
1:D:8:VAL:HG23	2:E:49:VAL:HG23	2.01	0.42
2:E:95:VAL:HG11	2:E:140:SER:HB3	2.02	0.42
3:C:52:LEU:O	3:C:53:ASP:C	2.56	0.42
1:D:8:VAL:CG2	2:E:49:VAL:HA	2.50	0.42
3:C:296:HIS:O	3:C:297:GLU:C	2.57	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:125:ILE:HG13	3:C:331:TYR:CE1	2.54	0.42
2:E:22:VAL:CG1	2:E:130:LEU:HD22	2.50	0.41
2:E:113:PHE:O	3:F:57:GLN:HG2	2.20	0.41
3:C:358:ILE:HD13	3:F:365:GLN:HG3	2.01	0.41
2:B:59:LEU:O	2:B:60:LEU:O	2.38	0.41
2:B:113:PHE:O	3:C:57:GLN:HG3	2.21	0.41
3:F:125:ILE:HG13	3:F:331:TYR:CE1	2.54	0.41
3:C:6:ILE:CD1	3:C:223:LEU:HB3	2.50	0.41
3:C:294:ARG:O	3:C:295:LYS:C	2.59	0.41
3:C:369:ILE:HG21	3:F:355:LEU:HD13	2.01	0.41
3:C:287:SER:O	3:C:291:THR:OG1	2.37	0.41
2:B:22:VAL:HG11	2:B:130:LEU:HD22	2.01	0.41
2:E:81:ARG:O	2:E:82:VAL:HB	2.21	0.41
3:F:195:PHE:CE2	3:F:268:VAL:HG22	2.56	0.41
3:F:122:GLY:O	3:F:125:ILE:HG22	2.21	0.41
2:B:138:LEU:HB3	3:C:290:LEU:HD11	2.03	0.41
3:C:150:ILE:HD13	3:C:150:ILE:O	2.21	0.41
3:F:327:LEU:CD2	3:F:331:TYR:CZ	3.04	0.41
3:F:52:LEU:O	3:F:55:ILE:N	2.54	0.41
2:B:95:VAL:HG21	2:B:110:LEU:HD13	2.03	0.41
2:E:80:LEU:N	2:E:80:LEU:CD1	2.84	0.41
3:F:366:LEU:HB3	3:F:404:TYR:CZ	2.56	0.40
3:F:375:ARG:O	3:F:379:MET:HB2	2.21	0.40
3:F:149:ASN:HA	3:F:152:ARG:NH1	2.37	0.40
2:E:119:LEU:HD13	3:F:65:ILE:HG21	2.04	0.40
1:D:37:TRP:O	1:D:41:SER:N	2.52	0.40
1:A:8:VAL:HG22	2:B:49:VAL:HA	2.03	0.40
2:E:52:ILE:HD13	2:E:61:PRO:HA	2.03	0.40
3:C:337:SER:OG	3:F:384:ASN:HB3	2.22	0.40
3:F:220:CYS:SG	3:F:240:VAL:HG11	2.61	0.40
3:C:125:ILE:HD12	3:C:125:ILE:HA	1.97	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	37/74 (50%)	32 (86%)	2 (5%)	3 (8%)	1 7
1	D	33/74 (45%)	29 (88%)	2 (6%)	2 (6%)	2 15
2	B	131/151 (87%)	108 (82%)	13 (10%)	10 (8%)	1 9
2	E	120/151 (80%)	98 (82%)	12 (10%)	10 (8%)	1 7
3	C	395/413 (96%)	352 (89%)	35 (9%)	8 (2%)	9 48
3	F	383/413 (93%)	352 (92%)	22 (6%)	9 (2%)	8 44
4	G	4/13 (31%)	2 (50%)	2 (50%)	0	100 100
All	All	1103/1289 (86%)	973 (88%)	88 (8%)	42 (4%)	4 28

All (42) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3	SER
1	A	21	VAL
2	B	57	GLN
2	B	64	GLU
2	B	113	PHE
3	C	115	GLN
3	C	119	SER
3	C	120	LYS
3	C	229	SER
3	C	386	ASN
2	E	97	TYR
3	F	119	SER
3	F	120	LYS
3	F	394	PRO
2	B	58	GLU
2	B	97	TYR
3	C	396	GLU
1	D	3	SER
2	E	64	GLU
2	E	113	PHE
3	F	110	THR
1	A	2	ASN
2	B	60	LEU
1	D	2	ASN
2	E	10	LEU
2	E	22	VAL

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Mol	Chain	Res	Type
2	E	37	ASP
2	E	112	ARG
3	F	111	ASN
3	F	112	GLU
3	F	400	LEU
2	B	28	GLY
3	C	226	ARG
3	F	115	GLN
2	B	10	LEU
2	B	82	VAL
2	B	22	VAL
3	C	400	LEU
2	E	82	VAL
3	F	385	GLY
2	E	42	GLY
2	E	61	PRO

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	23/39 (59%)	22 (96%)	1 (4%)	35 75
1	D	17/39 (44%)	16 (94%)	1 (6%)	24 65
2	B	103/140 (74%)	89 (86%)	14 (14%)	5 22
2	E	98/140 (70%)	88 (90%)	10 (10%)	9 36
3	C	316/383 (82%)	283 (90%)	33 (10%)	9 35
3	F	300/383 (78%)	268 (89%)	32 (11%)	8 34
4	G	5/12 (42%)	5 (100%)	0	100 100
All	All	862/1136 (76%)	771 (89%)	91 (11%)	8 34

All (91) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	ARG

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Mol	Chain	Res	Type
2	B	14	THR
2	B	21	ASN
2	B	38	HIS
2	B	43	VAL
2	B	59	LEU
2	B	65	ASP
2	B	80	LEU
2	B	94	GLN
2	B	97	TYR
2	B	101	ASP
2	B	110	LEU
2	B	119	LEU
2	B	124	LEU
2	B	126	LYS
3	C	23	ILE
3	C	36	LEU
3	C	37	ARG
3	C	47	LYS
3	C	64	GLU
3	C	66	LEU
3	C	81	SER
3	C	93	LYS
3	C	116	GLN
3	C	118	ASN
3	C	129	SER
3	C	137	LEU
3	C	142	THR
3	C	149	ASN
3	C	150	ILE
3	C	189	LEU
3	C	204	GLN
3	C	223	LEU
3	C	251	ASN
3	C	289	LEU
3	C	290	LEU
3	C	301	SER
3	C	306	ILE
3	C	324	THR
3	C	327	LEU
3	C	344	GLU
3	C	345	VAL
3	C	356	SER

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Mol	Chain	Res	Type
3	C	357	GLN
3	C	360	LYS
3	C	362	CYS
3	C	382	LEU
3	C	407	ASN
1	D	11	ARG
2	E	21	ASN
2	E	43	VAL
2	E	59	LEU
2	E	65	ASP
2	E	80	LEU
2	E	94	GLN
2	E	97	TYR
2	E	110	LEU
2	E	119	LEU
2	E	141	LEU
3	F	14	ARG
3	F	22	LEU
3	F	23	ILE
3	F	39	ARG
3	F	57	GLN
3	F	63	SER
3	F	66	LEU
3	F	118	ASN
3	F	126	SER
3	F	132	ILE
3	F	137	LEU
3	F	165	LEU
3	F	173	LEU
3	F	198	GLU
3	F	240	VAL
3	F	251	ASN
3	F	255	GLN
3	F	263	SER
3	F	289	LEU
3	F	314	LYS
3	F	324	THR
3	F	327	LEU
3	F	344	GLU
3	F	351	THR
3	F	357	GLN
3	F	363	GLU

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Mol	Chain	Res	Type
3	F	365	GLN
3	F	367	GLU
3	F	381	LEU
3	F	382	LEU
3	F	391	THR
3	F	411	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	21	ASN
2	B	24	HIS
2	B	38	HIS
2	B	91	GLN
3	C	49	HIS
3	C	56	GLN
3	C	57	GLN
3	C	96	GLN
3	C	118	ASN
3	C	149	ASN
3	C	153	GLN
3	C	162	GLN
3	C	216	HIS
3	C	251	ASN
3	C	255	GLN
3	C	384	ASN
3	C	386	ASN
3	C	407	ASN
2	E	21	ASN
2	E	24	HIS
2	E	91	GLN
2	E	129	GLN
3	F	49	HIS
3	F	56	GLN
3	F	57	GLN
3	F	74	ASN
3	F	118	ASN
3	F	251	ASN
3	F	311	GLN
3	F	357	GLN
3	F	384	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 carbohydrates 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

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1
1	D	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	43:LEU	C	52:UNK	N	12.71
1	A	43:LEU	C	52:UNK	N	11.09

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	41/74 (55%)	-0.02	1 (2%) 62 47	102, 122, 150, 152	0
1	D	37/74 (50%)	-0.27	1 (2%) 58 44	118, 137, 150, 152	0
2	B	135/151 (89%)	-0.31	0 100 100	69, 104, 169, 183	0
2	E	126/151 (83%)	-0.18	2 (1%) 74 62	79, 124, 165, 185	0
3	C	399/413 (96%)	-0.28	2 (0%) 91 87	61, 100, 165, 195	0
3	F	389/413 (94%)	-0.20	1 (0%) 94 93	80, 118, 181, 240	0
4	G	6/13 (46%)	0.16	0 100 100	116, 137, 147, 156	0
All	All	1133/1289 (87%)	-0.23	7 (0%) 90 84	61, 113, 174, 240	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	236	LEU	2.9
2	E	13	PHE	2.4
3	C	110	THR	2.3
1	D	37	TRP	2.3
3	F	119	SER	2.3
2	E	65	ASP	2.1
1	A	28	TRP	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.