Full wwPDB X-ray Structure Validation Report

Feb 1, 2016 – 07:15 AM GMT

PDB ID	:	3A36
Title	:	Structural insight into the membrane insertion of tail-anchored proteins by Get3
Authors	:	Yamagata, A.; Mimura, H.; Sato, Y.; Yamashita, M.; Yoshikawa, A.; Fukai, S.
Deposited on	:	2009-06-10
Resolution	:	2.80 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:

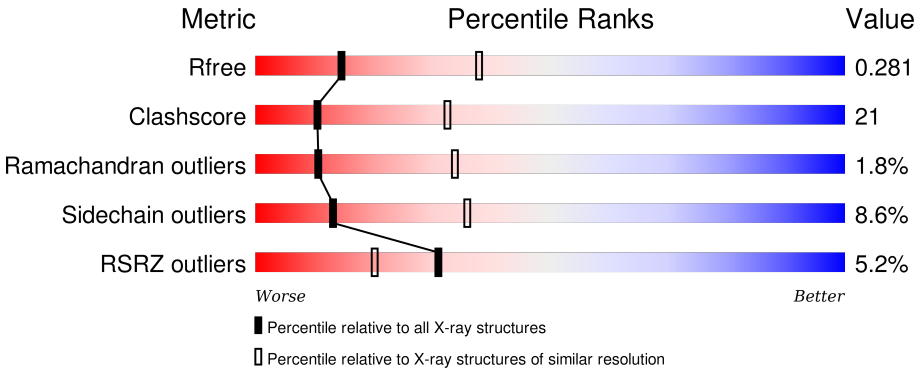
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.80 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	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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	362	6% 48% 33% 6% 13%
1	B	362	3% 56% 28% · 11%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4897 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 ATPase GET3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	314	Total	C	N	O	S	0	0	0
			2407	1519	402	470	16			
1	B	321	Total	C	N	O	S	0	0	0
			2489	1569	416	487	17			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	155	ASP	GLY	CONFLICT	UNP Q12154
A	355	LEU	-	EXPRESSION TAG	UNP Q12154
A	356	GLU	-	EXPRESSION TAG	UNP Q12154
A	357	HIS	-	EXPRESSION TAG	UNP Q12154
A	358	HIS	-	EXPRESSION TAG	UNP Q12154
A	359	HIS	-	EXPRESSION TAG	UNP Q12154
A	360	HIS	-	EXPRESSION TAG	UNP Q12154
A	361	HIS	-	EXPRESSION TAG	UNP Q12154
A	362	HIS	-	EXPRESSION TAG	UNP Q12154
B	155	ASP	GLY	CONFLICT	UNP Q12154
B	355	LEU	-	EXPRESSION TAG	UNP Q12154
B	356	GLU	-	EXPRESSION TAG	UNP Q12154
B	357	HIS	-	EXPRESSION TAG	UNP Q12154
B	358	HIS	-	EXPRESSION TAG	UNP Q12154
B	359	HIS	-	EXPRESSION TAG	UNP Q12154
B	360	HIS	-	EXPRESSION TAG	UNP Q12154
B	361	HIS	-	EXPRESSION TAG	UNP Q12154
B	362	HIS	-	EXPRESSION TAG	UNP Q12154

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

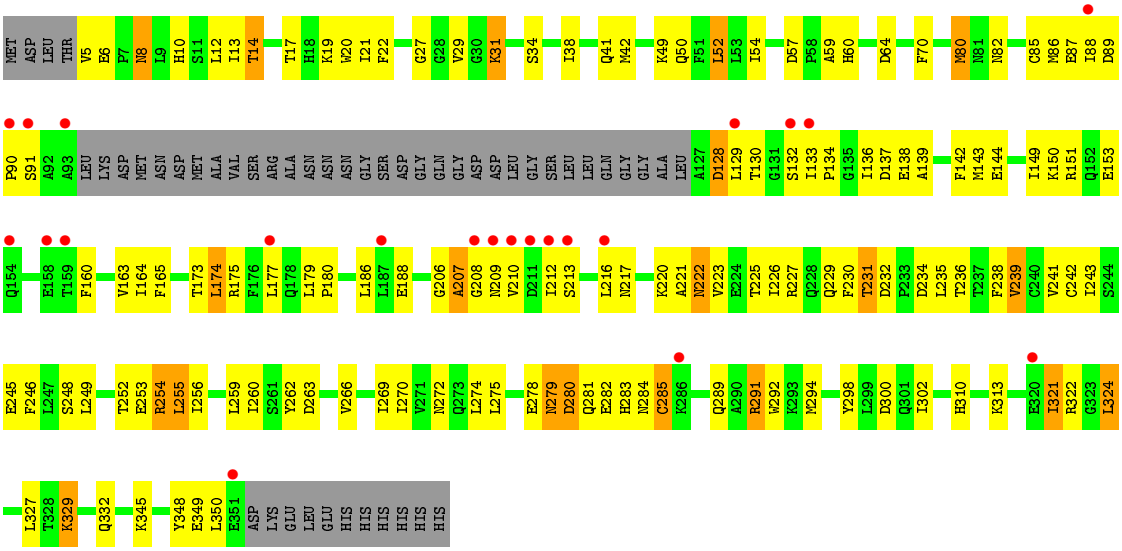
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Zn	0	0
			1	1		

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.

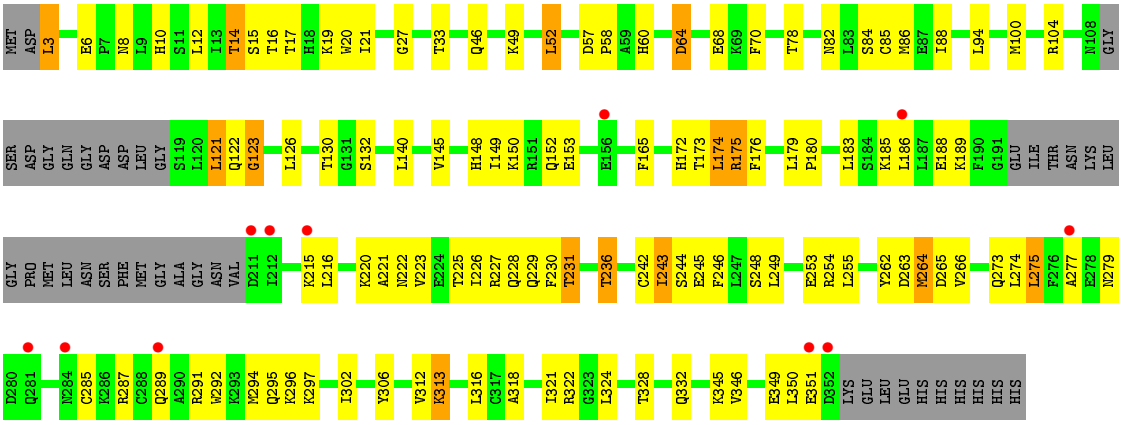
- Molecule 1: ATPase GET3

Chain A:



- Molecule 1: ATPase GET3

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	114.92Å 221.64Å 49.27Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.36 – 2.80 48.10 – 2.79	Depositor EDS
% Data completeness (in resolution range)	96.8 (45.36-2.80) 96.5 (48.10-2.79)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	3.83 (at 2.81Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.237 , 0.281 0.237 , 0.281	Depositor DCC
R_{free} test set	3116 reflections (10.06%)	DCC
Wilson B-factor (Å^2)	66.8	Xtriage
Anisotropy	0.528	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 65.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	0 of 31904 reflections	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	4897	wwPDB-VP
Average B, all atoms (Å^2)	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.60% 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: ZN

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	0.41	0/2447	0.63	0/3309
1	B	0.44	0/2527	0.64	0/3412
All	All	0.43	0/4974	0.64	0/6721

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	2407	0	2336	126	0
1	B	2489	0	2452	90	0
2	B	1	0	0	0	0
All	All	4897	0	4788	207	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 21.

All (207) 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:B:52:LEU:HD21	1:B:86:MET:HG2	1.49	0.94
1:B:230:PHE:HA	1:B:236:THR:HG21	1.54	0.89
1:B:324:LEU:O	1:B:328:THR:HG23	1.73	0.88
1:B:243:ILE:HD12	1:B:244:SER:H	1.38	0.86
1:A:291:ARG:NH1	1:B:291:ARG:HD3	1.93	0.81
1:A:242:CYS:HB3	1:A:252:THR:HG21	1.62	0.81
1:A:291:ARG:HD3	1:B:291:ARG:NH1	1.96	0.80
1:A:8:ASN:HD22	1:A:10:HIS:H	1.30	0.80
1:A:249:LEU:HD21	1:A:302:ILE:HD11	1.64	0.78
1:A:249:LEU:HD11	1:A:298:TYR:HB3	1.68	0.76
1:B:345:LYS:O	1:B:349:GLU:HG3	1.85	0.75
1:B:227:ARG:O	1:B:231:THR:HB	1.86	0.75
1:A:248:SER:O	1:A:252:THR:HG23	1.87	0.75
1:A:345:LYS:HA	1:A:345:LYS:HE2	1.69	0.74
1:A:54:ILE:HD11	1:A:88:ILE:HD12	1.68	0.73
1:A:291:ARG:HH11	1:B:291:ARG:HH11	1.37	0.73
1:B:253:GLU:HG2	1:B:306:TYR:OH	1.89	0.72
1:A:345:LYS:O	1:A:349:GLU:HG3	1.91	0.71
1:B:100:MET:HE1	1:B:104:ARG:HE	1.56	0.70
1:B:20:TRP:HB2	1:B:236:THR:HB	1.73	0.70
1:A:34:SER:OG	1:A:270:ILE:HD11	1.91	0.70
1:B:100:MET:CE	1:B:104:ARG:HE	2.05	0.70
1:A:129:LEU:HD12	1:A:129:LEU:H	1.57	0.69
1:B:318:ALA:O	1:B:351:GLU:HG3	1.92	0.69
1:A:52:LEU:HB3	1:A:163:VAL:HG22	1.75	0.67
1:A:282:GLU:C	1:A:284:ASN:H	1.96	0.67
1:B:10:HIS:O	1:B:14:THR:HB	1.95	0.67
1:A:221:ALA:O	1:A:225:THR:HG23	1.95	0.67
1:B:285:CYS:O	1:B:289:GLN:HG2	1.94	0.67
1:A:54:ILE:HD11	1:A:88:ILE:CD1	2.25	0.66
1:B:185:LYS:O	1:B:188:GLU:HG2	1.96	0.66
1:A:133:ILE:HB	1:A:136:ILE:CD1	2.26	0.66
1:B:121:LEU:HA	1:B:215:LYS:HD2	1.79	0.64
1:A:129:LEU:HD21	1:A:212:ILE:HG21	1.79	0.64
1:B:230:PHE:HA	1:B:236:THR:CG2	2.27	0.64
1:A:88:ILE:HG22	1:A:89:ASP:N	2.14	0.63
1:A:20:TRP:CD1	1:A:236:THR:HG22	2.34	0.63
1:B:179:LEU:HB3	1:B:180:PRO:HD3	1.80	0.63
1:B:19:LYS:NZ	1:B:229:GLN:NE2	2.47	0.62
1:A:291:ARG:HH11	1:B:291:ARG:NH1	1.97	0.62
1:B:318:ALA:HB3	1:B:351:GLU:CG	2.30	0.61
1:A:227:ARG:O	1:A:231:THR:HB	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:254:ARG:HH12	1:A:255:LEU:HA	1.65	0.61
1:A:207:ALA:O	1:A:209:ASN:N	2.33	0.61
1:A:88:ILE:HG22	1:A:89:ASP:H	1.65	0.61
1:B:275:LEU:HD23	1:B:295:GLN:OE1	2.01	0.60
1:A:6:GLU:O	1:A:310:HIS:HD2	1.84	0.60
1:A:133:ILE:HB	1:A:136:ILE:HD11	1.83	0.60
1:A:139:ALA:O	1:A:143:MET:HG2	2.01	0.59
1:B:249:LEU:HD13	1:B:302:ILE:HG12	1.84	0.59
1:B:172:HIS:HB2	1:B:175:ARG:HH21	1.68	0.59
1:B:19:LYS:NZ	1:B:229:GLN:HE22	2.00	0.59
1:A:291:ARG:NH1	1:B:291:ARG:HH11	2.00	0.59
1:A:20:TRP:HB2	1:A:236:THR:HG22	1.84	0.59
1:A:138:GLU:OE1	1:A:138:GLU:N	2.37	0.58
1:A:10:HIS:O	1:A:14:THR:HB	2.03	0.58
1:A:31:LYS:NZ	1:A:31:LYS:HB3	2.19	0.57
1:B:3:LEU:HD23	1:B:3:LEU:N	2.20	0.56
1:B:88:ILE:HD11	1:B:145:VAL:HG13	1.87	0.56
1:B:174:LEU:CD2	1:B:174:LEU:H	2.17	0.56
1:A:130:THR:HG23	1:A:137:ASP:HB2	1.88	0.56
1:A:348:TYR:C	1:A:350:LEU:H	2.10	0.56
1:A:20:TRP:HD1	1:A:236:THR:HG22	1.70	0.56
1:A:138:GLU:OE2	1:A:175:ARG:NH1	2.40	0.55
1:A:50:GLN:NE2	1:A:82:ASN:HA	2.22	0.55
1:B:243:ILE:HD12	1:B:244:SER:N	2.16	0.55
1:A:174:LEU:H	1:A:174:LEU:HD23	1.70	0.55
1:B:188:GLU:HG3	1:B:189:LYS:N	2.21	0.55
1:A:142:PHE:HE2	1:A:226:ILE:HD13	1.72	0.55
1:B:21:ILE:N	1:B:21:ILE:HD12	2.21	0.55
1:B:148:HIS:O	1:B:152:GLN:HG2	2.08	0.55
1:A:282:GLU:O	1:A:284:ASN:N	2.38	0.54
1:B:287:ARG:HH11	1:B:287:ARG:HG3	1.72	0.54
1:A:349:GLU:O	1:A:350:LEU:HD23	2.07	0.54
1:B:122:GLN:O	1:B:123:GLY:C	2.45	0.54
1:A:186:LEU:C	1:A:188:GLU:H	2.09	0.54
1:B:49:LYS:O	1:B:82:ASN:HB2	2.07	0.54
1:A:345:LYS:CA	1:A:345:LYS:HE2	2.37	0.54
1:A:150:LYS:HB2	1:A:150:LYS:HZ2	1.73	0.54
1:A:254:ARG:HG2	1:A:254:ARG:NH1	2.22	0.53
1:A:17:THR:HG23	1:A:234:ASP:O	2.09	0.53
1:B:318:ALA:HB3	1:B:351:GLU:CD	2.29	0.53
1:A:270:ILE:HG13	1:A:270:ILE:O	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:21:ILE:HD13	1:A:42:MET:HE1	1.91	0.53
1:A:149:ILE:O	1:A:153:GLU:HG3	2.08	0.53
1:A:291:ARG:CZ	1:B:291:ARG:HD3	2.38	0.53
1:B:100:MET:CE	1:B:104:ARG:NE	2.71	0.53
1:B:346:VAL:O	1:B:350:LEU:HD13	2.09	0.53
1:A:256:ILE:HG12	1:A:266:VAL:HG11	1.91	0.52
1:A:245:GLU:HG2	1:A:294:MET:HE3	1.92	0.52
1:B:264:MET:HG3	1:B:265:ASP:N	2.24	0.52
1:B:313:LYS:N	1:B:313:LYS:HD3	2.25	0.52
1:B:6:GLU:HB3	1:B:8:ASN:ND2	2.25	0.52
1:A:285:CYS:O	1:A:289:GLN:HG2	2.09	0.52
1:A:254:ARG:HG2	1:A:254:ARG:HH11	1.75	0.52
1:B:183:LEU:HD12	1:B:220:LYS:HB2	1.92	0.52
1:A:241:VAL:HG13	1:A:270:ILE:CG1	2.40	0.51
1:A:280:ASP:C	1:A:282:GLU:N	2.62	0.51
1:B:318:ALA:HB3	1:B:351:GLU:HG3	1.92	0.51
1:A:164:ILE:HD12	1:A:164:ILE:N	2.26	0.51
1:A:242:CYS:CB	1:A:252:THR:HG21	2.35	0.50
1:A:179:LEU:HB3	1:A:180:PRO:HD3	1.94	0.50
1:A:34:SER:OG	1:A:270:ILE:CD1	2.59	0.50
1:A:206:GLY:O	1:A:207:ALA:HB2	2.12	0.50
1:A:232:ASP:OD2	1:A:235:LEU:HG	2.12	0.50
1:B:94:LEU:HD11	1:B:140:LEU:HB3	1.93	0.50
1:B:19:LYS:HZ1	1:B:229:GLN:NE2	2.10	0.50
1:A:49:LYS:O	1:A:82:ASN:HB2	2.12	0.50
1:A:210:VAL:C	1:A:212:ILE:H	2.15	0.50
1:A:254:ARG:HH11	1:A:254:ARG:CG	2.26	0.49
1:A:213:SER:O	1:A:217:ASN:ND2	2.46	0.49
1:A:270:ILE:HD12	1:A:272:ASN:OD1	2.13	0.49
1:A:150:LYS:NZ	1:A:150:LYS:HB2	2.28	0.49
1:A:177:LEU:HD12	1:A:262:TYR:HB3	1.94	0.49
1:A:246:PHE:CD2	1:B:27:GLY:HA2	2.48	0.48
1:A:70:PHE:CD2	1:A:85:CYS:HB2	2.48	0.48
1:A:52:LEU:HD12	1:A:163:VAL:HG22	1.94	0.48
1:A:52:LEU:HB2	1:A:160:PHE:CD2	2.49	0.48
1:A:21:ILE:HD13	1:A:42:MET:CE	2.44	0.48
1:B:15:SER:OG	1:B:17:THR:HG22	2.14	0.47
1:A:278:GLU:HG3	1:A:292:TRP:CD1	2.49	0.47
1:B:68:GLU:OE1	1:B:78:THR:N	2.42	0.47
1:A:280:ASP:C	1:A:282:GLU:H	2.16	0.47
1:B:174:LEU:CD2	1:B:174:LEU:N	2.77	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:209:ASN:O	1:A:212:ILE:HB	2.14	0.47
1:A:262:TYR:O	1:A:263:ASP:HB2	2.14	0.47
1:B:68:GLU:OE1	1:B:78:THR:HB	2.14	0.47
1:B:130:THR:C	1:B:132:SER:H	2.18	0.47
1:B:6:GLU:HB3	1:B:8:ASN:HD21	1.78	0.46
1:A:13:ILE:HD13	1:A:41:GLN:CG	2.45	0.46
1:A:90:PRO:HG2	1:A:91:SER:H	1.81	0.46
1:B:294:MET:O	1:B:297:LYS:HB3	2.15	0.46
1:A:31:LYS:HB3	1:A:31:LYS:HZ2	1.80	0.46
1:B:70:PHE:CD2	1:B:85:CYS:HB2	2.51	0.46
1:A:238:PHE:CD2	1:A:259:LEU:HD11	2.51	0.46
1:B:242:CYS:HB2	1:B:248:SER:OG	2.16	0.46
1:A:279:ASN:C	1:A:281:GLN:H	2.19	0.46
1:A:291:ARG:HD3	1:B:291:ARG:CZ	2.45	0.46
1:A:282:GLU:C	1:A:284:ASN:N	2.66	0.46
1:A:130:THR:C	1:A:132:SER:H	2.19	0.46
1:B:150:LYS:HD2	1:B:153:GLU:OE1	2.16	0.46
1:B:20:TRP:HE3	1:B:165:PHE:HE1	1.63	0.46
1:A:20:TRP:HD1	1:A:236:THR:CG2	2.28	0.46
1:A:38:ILE:HD11	1:A:239:VAL:HG21	1.98	0.45
1:A:254:ARG:NH1	1:A:255:LEU:HA	2.30	0.45
1:B:94:LEU:HD11	1:B:140:LEU:CB	2.47	0.45
1:B:20:TRP:HE3	1:B:165:PHE:CE1	2.35	0.45
1:A:242:CYS:HB3	1:A:252:THR:CG2	2.40	0.45
1:A:59:ALA:O	1:A:60:HIS:HB2	2.17	0.45
1:A:60:HIS:HA	1:A:87:GLU:OE1	2.17	0.45
1:A:144:GLU:HA	1:A:144:GLU:OE1	2.17	0.45
1:A:57:ASP:OD2	1:A:59:ALA:HB3	2.17	0.45
1:A:212:ILE:HG22	1:A:216:LEU:HG	1.98	0.45
1:A:279:ASN:O	1:A:281:GLN:N	2.40	0.45
1:A:19:LYS:NZ	1:A:229:GLN:NE2	2.65	0.44
1:B:292:TRP:NE1	1:B:296:LYS:HD2	2.32	0.44
1:A:27:GLY:HA2	1:B:246:PHE:CD2	2.52	0.44
1:A:20:TRP:CD1	1:A:236:THR:CG2	3.00	0.44
1:A:321:ILE:HG22	1:A:327:LEU:HD23	1.98	0.44
1:B:174:LEU:HA	1:B:176:PHE:CE1	2.52	0.44
1:A:70:PHE:HB2	1:A:87:GLU:HG3	2.00	0.44
1:A:222:ASN:HD22	1:A:222:ASN:HA	1.50	0.44
1:B:291:ARG:O	1:B:294:MET:HB3	2.18	0.44
1:B:225:THR:O	1:B:228:GLN:HB3	2.18	0.44
1:B:19:LYS:HZ3	1:B:229:GLN:NE2	2.16	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:180:PRO:HD3	1:A:223:VAL:HG11	1.99	0.43
1:A:22:PHE:CD1	1:A:165:PHE:HB2	2.53	0.43
1:B:254:ARG:HG2	1:B:254:ARG:HH11	1.83	0.43
1:A:230:PHE:HA	1:A:236:THR:HG21	1.99	0.43
1:B:64:ASP:OD1	1:B:322:ARG:NH2	2.49	0.43
1:B:273:GLN:HA	1:B:316:LEU:HA	2.00	0.43
1:A:21:ILE:CD1	1:A:42:MET:CE	2.97	0.43
1:A:243:ILE:HG12	1:A:245:GLU:HG3	2.00	0.43
1:A:80:MET:HG2	1:A:324:LEU:HD11	2.01	0.43
1:B:275:LEU:HD23	1:B:275:LEU:H	1.84	0.42
1:B:19:LYS:HZ1	1:B:229:GLN:HE22	1.65	0.42
1:B:262:TYR:O	1:B:263:ASP:HB2	2.19	0.42
1:A:64:ASP:O	1:A:322:ARG:HD3	2.20	0.42
1:B:180:PRO:HD3	1:B:223:VAL:HG11	2.02	0.42
1:A:5:VAL:HG12	1:A:310:HIS:CD2	2.54	0.42
1:A:86:MET:SD	1:A:88:ILE:HD11	2.59	0.42
1:B:19:LYS:HZ3	1:B:229:GLN:HE22	1.67	0.42
1:A:246:PHE:C	1:A:246:PHE:CD2	2.93	0.42
1:B:188:GLU:CG	1:B:189:LYS:N	2.83	0.42
1:A:133:ILE:HA	1:A:134:PRO:HD3	1.91	0.42
1:A:180:PRO:HA	1:A:220:LYS:HG3	2.02	0.42
1:B:222:ASN:O	1:B:226:ILE:HG13	2.20	0.41
1:B:277:ALA:HB1	1:B:289:GLN:OE1	2.20	0.41
1:A:29:VAL:HG12	1:A:243:ILE:HG22	2.02	0.41
1:B:16:THR:HG22	1:B:46:GLN:NE2	2.35	0.41
1:A:151:ARG:HH11	1:A:151:ARG:HG2	1.86	0.41
1:B:245:GLU:HG2	1:B:294:MET:CE	2.50	0.41
1:A:129:LEU:HD12	1:A:129:LEU:N	2.30	0.41
1:A:256:ILE:O	1:A:260:ILE:HG13	2.20	0.41
1:A:329:LYS:O	1:A:332:GLN:HG2	2.20	0.41
1:A:249:LEU:CD1	1:A:298:TYR:HB3	2.45	0.41
1:A:186:LEU:C	1:A:188:GLU:N	2.73	0.41
1:B:221:ALA:O	1:B:225:THR:HG23	2.19	0.41
1:B:57:ASP:HA	1:B:58:PRO:HD3	1.90	0.41
1:A:210:VAL:C	1:A:212:ILE:N	2.74	0.41
1:B:174:LEU:H	1:B:174:LEU:HD22	1.84	0.41
1:A:227:ARG:HG2	1:A:227:ARG:HH11	1.84	0.41
1:B:145:VAL:O	1:B:149:ILE:HG13	2.21	0.41
1:A:128:ASP:C	1:A:130:THR:H	2.23	0.41
1:B:126:LEU:HD11	1:B:216:LEU:HD23	2.03	0.40
1:B:243:ILE:HD13	1:B:273:GLN:HB2	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:275:LEU:O	1:B:277:ALA:N	2.52	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	310/362 (86%)	282 (91%)	21 (7%)	7 (2%)	8 26
1	B	315/362 (87%)	287 (91%)	24 (8%)	4 (1%)	15 44
All	All	625/724 (86%)	569 (91%)	45 (7%)	11 (2%)	11 34

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	208	GLY
1	A	173	THR
1	A	207	ALA
1	A	280	ASP
1	A	283	HIS
1	B	123	GLY
1	B	173	THR
1	A	285	CYS
1	B	279	ASN
1	B	321	ILE
1	A	321	ILE

5.3.2 Protein sidechains

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	261/318 (82%)	238 (91%)	23 (9%)	12 35
1	B	276/318 (87%)	253 (92%)	23 (8%)	14 38
All	All	537/636 (84%)	491 (91%)	46 (9%)	13 36

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	ASN
1	A	12	LEU
1	A	14	THR
1	A	31	LYS
1	A	52	LEU
1	A	80	MET
1	A	128	ASP
1	A	174	LEU
1	A	222	ASN
1	A	231	THR
1	A	239	VAL
1	A	253	GLU
1	A	254	ARG
1	A	255	LEU
1	A	269	ILE
1	A	274	LEU
1	A	275	LEU
1	A	279	ASN
1	A	291	ARG
1	A	300	ASP
1	A	313	LYS
1	A	324	LEU
1	A	329	LYS
1	B	3	LEU
1	B	12	LEU
1	B	14	THR
1	B	33	THR
1	B	52	LEU
1	B	60	HIS
1	B	64	ASP
1	B	84	SER
1	B	121	LEU
1	B	174	LEU

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Mol	Chain	Res	Type
1	B	175	ARG
1	B	186	LEU
1	B	231	THR
1	B	236	THR
1	B	243	ILE
1	B	255	LEU
1	B	264	MET
1	B	266	VAL
1	B	274	LEU
1	B	275	LEU
1	B	312	VAL
1	B	313	LYS
1	B	332	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	ASN
1	A	50	GLN
1	A	148	HIS
1	A	178	GLN
1	A	222	ASN
1	A	229	GLN
1	A	279	ASN
1	A	310	HIS
1	B	46	GLN
1	B	98	ASN
1	B	122	GLN
1	B	178	GLN
1	B	222	ASN
1	B	229	GLN
1	B	310	HIS
1	B	332	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

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	314/362 (86%)	0.39	22 (7%)	19	11	46, 80, 153, 160	0
1	B	321/362 (88%)	0.22	11 (3%)	49	36	42, 68, 113, 140	0
All	All	635/724 (87%)	0.31	33 (5%)	31	20	42, 74, 141, 160	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	210	VAL	10.2
1	A	90	PRO	5.0
1	A	209	ASN	4.9
1	B	215	LYS	4.4
1	A	91	SER	4.0
1	A	213	SER	3.9
1	A	216	LEU	3.7
1	A	93	ALA	3.7
1	A	211	ASP	3.5
1	B	277	ALA	3.5
1	B	212	ILE	3.4
1	A	177	LEU	3.4
1	A	187	LEU	3.4
1	B	289	GLN	3.3
1	A	133	ILE	3.3
1	B	284	ASN	3.1
1	B	352	ASP	2.9
1	A	132	SER	2.9
1	B	351	GLU	2.8
1	A	212	ILE	2.7
1	A	208	GLY	2.6
1	A	129	LEU	2.5
1	B	186	LEU	2.2
1	A	158	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	351	GLU	2.2
1	B	281	GLN	2.2
1	B	156	GLU	2.2
1	A	154	GLN	2.1
1	A	320	GLU	2.1
1	A	88	ILE	2.1
1	A	159	THR	2.0
1	B	211	ASP	2.0
1	A	286	LYS	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
2	ZN	B	500	1/1	0.99	0.09	-2.07	81,81,81,81	0

6.5 Other polymers (i)

There are no such residues in this entry.