Full wwPDB X-ray Structure Validation Report (i)

Oct 11, 2021 – 06:33 PM EDT

PDB ID	:	2OEV
Title	:	Crystal structure of ALIX/AIP1
Authors	:	Fisher, R.D.; Zhai, Q.; Robinson, H.; Hill, C.P.
Deposited on	:	2007-01-01
Resolution	:	3.30 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 (i) symbol.

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

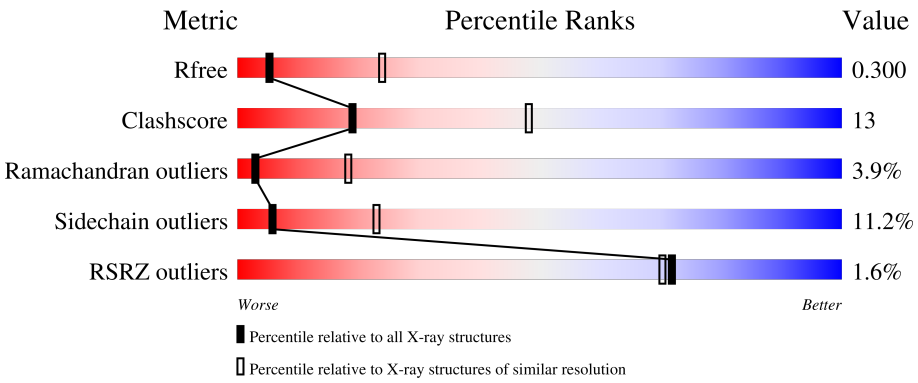
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

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 3.30 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	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

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	705	2% 63% 30% 6% •

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 5486 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 Programmed cell death 6-interacting protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	697	5486	3461	938	1069	18	0	0	0

There are 9 discrepancies between the modelled and reference sequences:

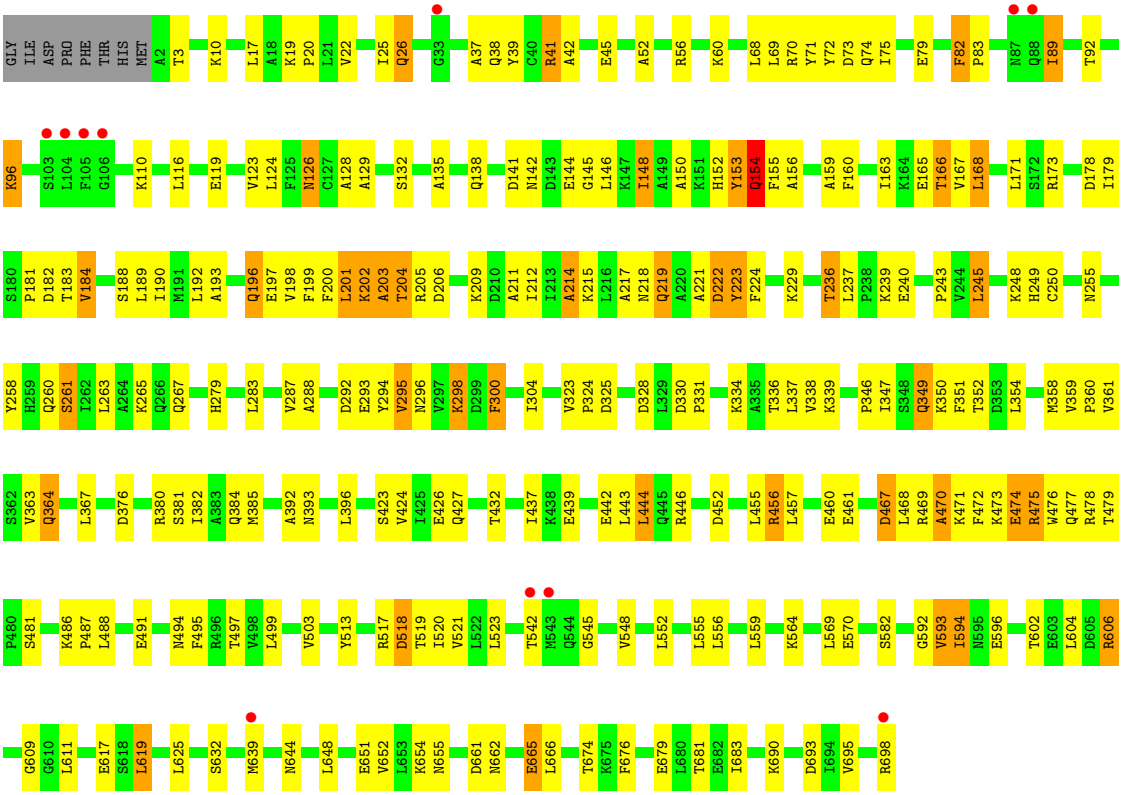
Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	GLY	-	cloning artifact	UNP Q8WUM4
A	-5	ILE	-	cloning artifact	UNP Q8WUM4
A	-4	ASP	-	cloning artifact	UNP Q8WUM4
A	-3	PRO	-	cloning artifact	UNP Q8WUM4
A	-2	PHE	-	cloning artifact	UNP Q8WUM4
A	-1	THR	-	cloning artifact	UNP Q8WUM4
A	0	HIS	-	cloning artifact	UNP Q8WUM4
A	268	TYR	LYS	engineered mutation	UNP Q8WUM4
A	269	TYR	LYS	engineered mutation	UNP Q8WUM4

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: Programmed cell death 6-interacting protein

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	143.99Å 98.51Å 72.16Å 90.00° 105.64° 90.00°	Depositor
Resolution (Å)	30.00 – 3.30 29.74 – 3.27	Depositor EDS
% Data completeness (in resolution range)	95.5 (30.00-3.30) 93.7 (29.74-3.27)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.38 (at 3.24Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.235 , 0.317 0.225 , 0.300	Depositor DCC
R_{free} test set	1000 reflections (7.02%)	wwPDB-VP
Wilson B-factor (Å^2)	103.1	Xtriage
Anisotropy	0.345	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.25 , 68.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	5486	wwPDB-VP
Average B, all atoms (Å^2)	140.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.23% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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	0.47	2/5570 (0.0%)	0.57	0/7523

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	617	GLU	CD-OE1	10.62	1.37	1.25
1	A	617	GLU	CD-OE2	7.93	1.34	1.25

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	237	LEU	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5486	0	5532	143	0
All	All	5486	0	5532	143	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 13.

All (143) 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:A:79:GLU:HB3	1:A:116:LEU:HD23	1.60	0.81
1:A:424:VAL:HG21	1:A:523:LEU:HD13	1.73	0.71
1:A:300:PHE:CE1	1:A:304:ILE:HD11	2.26	0.70
1:A:128:ALA:HB2	1:A:159:ALA:CB	2.22	0.68
1:A:82:PHE:HB2	1:A:83:PRO:HD3	1.75	0.68
1:A:22:VAL:HG12	1:A:26:GLN:HE22	1.59	0.68
1:A:198:VAL:O	1:A:201:LEU:N	2.27	0.68
1:A:193:ALA:HB2	1:A:223:TYR:HB3	1.76	0.68
1:A:96:LYS:HG3	1:A:110:LYS:HG2	1.75	0.67
1:A:662:ASN:O	1:A:666:LEU:HB2	1.95	0.67
1:A:651:GLU:O	1:A:655:ASN:ND2	2.29	0.66
1:A:288:ALA:O	1:A:292:ASP:HB3	1.97	0.65
1:A:145:GLY:O	1:A:148:ILE:HG13	1.96	0.64
1:A:190:ILE:HG12	1:A:245:LEU:HD21	1.79	0.64
1:A:38:GLN:HA	1:A:41:ARG:NH1	2.13	0.64
1:A:38:GLN:HA	1:A:41:ARG:HH11	1.64	0.62
1:A:135:ALA:HB2	1:A:152:HIS:HB2	1.82	0.62
1:A:202:LYS:O	1:A:204:THR:N	2.33	0.61
1:A:202:LYS:O	1:A:205:ARG:N	2.34	0.61
1:A:219:GLN:HE21	1:A:334:LYS:HB3	1.66	0.60
1:A:472:PHE:C	1:A:474:GLU:H	2.05	0.59
1:A:10:LYS:HB2	1:A:126:ASN:HD21	1.67	0.59
1:A:221:ALA:O	1:A:223:TYR:N	2.36	0.59
1:A:128:ALA:HB2	1:A:159:ALA:HB3	1.84	0.58
1:A:552:LEU:HD11	1:A:632:SER:HB3	1.85	0.58
1:A:461:GLU:HG3	1:A:695:VAL:HG13	1.86	0.58
1:A:163:ILE:HA	1:A:166:THR:HG22	1.86	0.58
1:A:452:ASP:O	1:A:456:ARG:HB2	2.04	0.58
1:A:548:VAL:HG21	1:A:639:MET:SD	2.43	0.57
1:A:128:ALA:HB2	1:A:159:ALA:HB1	1.85	0.57
1:A:258:TYR:HA	1:A:261:SER:OG	2.05	0.57
1:A:183:THR:HG23	1:A:236:THR:HG23	1.86	0.57
1:A:279:HIS:CD2	1:A:283:LEU:CD1	2.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:468:LEU:O	1:A:472:PHE:HB2	2.05	0.56
1:A:279:HIS:CD2	1:A:283:LEU:HD12	2.40	0.56
1:A:552:LEU:HA	1:A:555:LEU:HD12	1.89	0.55
1:A:221:ALA:C	1:A:223:TYR:H	2.11	0.54
1:A:283:LEU:O	1:A:287:VAL:HG23	2.07	0.54
1:A:679:GLU:O	1:A:683:ILE:HG12	2.07	0.54
1:A:42:ALA:HA	1:A:45:GLU:HB3	1.89	0.54
1:A:79:GLU:HB3	1:A:116:LEU:CD2	2.32	0.54
1:A:211:ALA:HB2	1:A:263:LEU:HD22	1.89	0.54
1:A:199:PHE:HD2	1:A:337:LEU:HD13	1.72	0.53
1:A:444:LEU:HD11	1:A:503:VAL:HG22	1.90	0.53
1:A:393:ASN:HA	1:A:396:LEU:HD12	1.90	0.53
1:A:423:SER:O	1:A:427:GLN:HB2	2.09	0.52
1:A:488:LEU:HD21	1:A:690:LYS:HD2	1.91	0.52
1:A:382:ILE:HG13	1:A:570:GLU:HG3	1.90	0.52
1:A:3:THR:HG21	1:A:294:TYR:O	2.10	0.52
1:A:96:LYS:HE2	1:A:110:LYS:HE3	1.93	0.51
1:A:160:PHE:O	1:A:163:ILE:N	2.42	0.51
1:A:72:TYR:HA	1:A:75:ILE:HD12	1.92	0.50
1:A:129:ALA:O	1:A:132:SER:OG	2.29	0.50
1:A:255:ASN:OD1	1:A:300:PHE:CE2	2.65	0.50
1:A:363:VAL:O	1:A:367:LEU:HB2	2.10	0.50
1:A:491:GLU:HB3	1:A:495:PHE:HE1	1.76	0.50
1:A:135:ALA:HB2	1:A:152:HIS:CB	2.41	0.50
1:A:593:VAL:HG12	1:A:594:ILE:H	1.76	0.50
1:A:439:GLU:O	1:A:442:GLU:HB2	2.11	0.50
1:A:499:LEU:O	1:A:503:VAL:HG23	2.12	0.50
1:A:604:LEU:C	1:A:606:ARG:H	2.14	0.50
1:A:197:GLU:O	1:A:200:PHE:HB3	2.11	0.49
1:A:19:LYS:HB3	1:A:20:PRO:HD3	1.94	0.49
1:A:37:ALA:O	1:A:41:ARG:HD3	2.13	0.49
1:A:467:ASP:O	1:A:471:LYS:HB2	2.12	0.49
1:A:518:ASP:O	1:A:521:VAL:HB	2.13	0.49
1:A:470:ALA:O	1:A:471:LYS:HG3	2.13	0.48
1:A:359:VAL:HB	1:A:364:GLN:HE22	1.78	0.48
1:A:648:LEU:O	1:A:652:VAL:HG23	2.14	0.48
1:A:39:TYR:CE1	1:A:358:MET:HG3	2.48	0.48
1:A:469:ARG:C	1:A:471:LYS:H	2.18	0.48
1:A:73:ASP:OD1	1:A:346:PRO:HA	2.14	0.48
1:A:651:GLU:HG3	1:A:654:LYS:HE3	1.95	0.48
1:A:279:HIS:HD2	1:A:283:LEU:HD12	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:52:ALA:HA	1:A:56:ARG:HH21	1.79	0.47
1:A:153:TYR:O	1:A:154:GLN:C	2.53	0.47
1:A:240:GLU:O	1:A:243:PRO:HD2	2.15	0.47
1:A:71:TYR:CE1	1:A:75:ILE:HD11	2.50	0.47
1:A:300:PHE:HE1	1:A:304:ILE:HD11	1.74	0.47
1:A:218:ASN:O	1:A:221:ALA:N	2.47	0.47
1:A:293:GLU:O	1:A:293:GLU:HG2	2.15	0.47
1:A:548:VAL:O	1:A:552:LEU:HD13	2.15	0.47
1:A:183:THR:HA	1:A:236:THR:CG2	2.44	0.47
1:A:178:ASP:OD1	1:A:179:ILE:HG23	2.14	0.47
1:A:279:HIS:CD2	1:A:283:LEU:HD11	2.50	0.46
1:A:376:ASP:O	1:A:380:ARG:HB2	2.15	0.46
1:A:196:GLN:HB2	1:A:338:VAL:HG11	1.98	0.45
1:A:491:GLU:HB3	1:A:495:PHE:CE1	2.51	0.45
1:A:75:ILE:CD1	1:A:123:VAL:HG21	2.47	0.45
1:A:178:ASP:HA	1:A:183:THR:HG21	1.99	0.45
1:A:294:TYR:O	1:A:295:VAL:HG13	2.16	0.45
1:A:150:ALA:O	1:A:154:GLN:HB2	2.16	0.45
1:A:69:LEU:HD22	1:A:347:ILE:HD12	2.00	0.44
1:A:381:SER:O	1:A:385:MET:HG2	2.17	0.44
1:A:475:ARG:H	1:A:475:ARG:HG2	1.43	0.44
1:A:661:ASP:O	1:A:665:GLU:HB2	2.18	0.44
1:A:349:GLN:O	1:A:351:PHE:N	2.51	0.44
1:A:183:THR:HA	1:A:236:THR:HG21	1.99	0.44
1:A:153:TYR:O	1:A:156:ALA:N	2.51	0.43
1:A:202:LYS:C	1:A:204:THR:N	2.71	0.43
1:A:263:LEU:HD11	1:A:267:GLN:HE21	1.83	0.43
1:A:279:HIS:NE2	1:A:283:LEU:HD11	2.33	0.43
1:A:74:GLN:HE22	1:A:354:LEU:N	2.16	0.43
1:A:154:GLN:HG3	1:A:339:LYS:O	2.19	0.43
1:A:202:LYS:O	1:A:203:ALA:C	2.57	0.43
1:A:323:VAL:HA	1:A:324:PRO:HD3	1.84	0.43
1:A:168:LEU:HD12	1:A:181:PRO:HG2	2.01	0.43
1:A:437:ILE:HG21	1:A:513:TYR:CE2	2.54	0.43
1:A:124:LEU:HD23	1:A:163:ILE:HG13	2.00	0.43
1:A:74:GLN:HE22	1:A:354:LEU:H	1.65	0.42
1:A:260:GLN:O	1:A:260:GLN:HG3	2.19	0.42
1:A:569:LEU:HD22	1:A:611:LEU:HD22	2.00	0.42
1:A:209:LYS:HB2	1:A:212:ILE:CD1	2.49	0.42
1:A:396:LEU:HD22	1:A:556:LEU:HD21	2.01	0.42
1:A:248:LYS:O	1:A:249:HIS:C	2.57	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:258:TYR:O	1:A:261:SER:OG	2.37	0.42
1:A:154:GLN:CG	1:A:339:LYS:O	2.67	0.42
1:A:481:SER:HA	1:A:698:ARG:HH21	1.84	0.42
1:A:206:ASP:N	1:A:206:ASP:OD1	2.51	0.42
1:A:296:ASN:HD21	1:A:298:LYS:HB2	1.84	0.42
1:A:559:LEU:HB2	1:A:625:LEU:HD13	2.01	0.42
1:A:119:GLU:O	1:A:123:VAL:HG23	2.19	0.41
1:A:325:ASP:O	1:A:328:ASP:HB2	2.21	0.41
1:A:469:ARG:HG3	1:A:476:TRP:CD1	2.54	0.41
1:A:193:ALA:CB	1:A:223:TYR:HB3	2.48	0.41
1:A:222:ASP:O	1:A:222:ASP:CG	2.58	0.41
1:A:154:GLN:HB2	1:A:154:GLN:HE21	1.46	0.41
1:A:674:THR:C	1:A:676:PHE:H	2.23	0.41
1:A:160:PHE:HB3	1:A:184:VAL:HG13	2.01	0.41
1:A:214:ALA:O	1:A:217:ALA:N	2.52	0.41
1:A:240:GLU:C	1:A:243:PRO:HD2	2.41	0.41
1:A:144:GLU:O	1:A:148:ILE:HG12	2.20	0.41
1:A:330:ASP:HA	1:A:331:PRO:HD2	1.90	0.41
1:A:520:ILE:O	1:A:521:VAL:C	2.58	0.41
1:A:82:PHE:HB2	1:A:83:PRO:CD	2.48	0.41
1:A:153:TYR:O	1:A:155:PHE:N	2.54	0.40
1:A:224:PHE:HD2	1:A:245:LEU:HD23	1.85	0.40
1:A:443:LEU:HD23	1:A:446:ARG:HD2	2.03	0.40
1:A:486:LYS:HB3	1:A:487:PRO:HD3	2.04	0.40
1:A:22:VAL:HA	1:A:25:ILE:HD12	2.03	0.40
1:A:392:ALA:O	1:A:396:LEU:HG	2.22	0.40
1:A:520:ILE:O	1:A:523:LEU:N	2.53	0.40
1:A:384:GLN:HB3	1:A:619:LEU:HD11	2.04	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	695/705 (99%)	581 (84%)	87 (12%)	27 (4%)	3 18

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	89	ILE
1	A	203	ALA
1	A	222	ASP
1	A	60	LYS
1	A	171	LEU
1	A	219	GLN
1	A	350	LYS
1	A	592	GLY
1	A	82	PHE
1	A	154	GLN
1	A	196	GLN
1	A	202	LYS
1	A	214	ALA
1	A	349	GLN
1	A	470	ALA
1	A	473	LYS
1	A	479	THR
1	A	138	GLN
1	A	229	LYS
1	A	236	THR
1	A	245	LEU
1	A	545	GLY
1	A	153	TYR
1	A	215	LYS
1	A	360	PRO
1	A	609	GLY
1	A	593	VAL

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	600/607 (99%)	533 (89%)	67 (11%)	6 23

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	LEU
1	A	26	GLN
1	A	41	ARG
1	A	68	LEU
1	A	70	ARG
1	A	89	ILE
1	A	92	THR
1	A	96	LYS
1	A	126	ASN
1	A	141	ASP
1	A	142	ASN
1	A	146	LEU
1	A	148	ILE
1	A	154	GLN
1	A	165	GLU
1	A	166	THR
1	A	167	VAL
1	A	168	LEU
1	A	173	ARG
1	A	182	ASP
1	A	184	VAL
1	A	188	SER
1	A	189	LEU
1	A	192	LEU
1	A	201	LEU
1	A	204	THR
1	A	223	TYR
1	A	239	LYS
1	A	250	CYS
1	A	261	SER
1	A	265	LYS
1	A	295	VAL
1	A	298	LYS
1	A	300	PHE
1	A	336	THR
1	A	352	THR
1	A	361	VAL
1	A	364	GLN

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Mol	Chain	Res	Type
1	A	426	GLU
1	A	432	THR
1	A	444	LEU
1	A	455	LEU
1	A	456	ARG
1	A	457	LEU
1	A	460	GLU
1	A	467	ASP
1	A	474	GLU
1	A	475	ARG
1	A	477	GLN
1	A	478	ARG
1	A	494	ASN
1	A	497	THR
1	A	517	ARG
1	A	518	ASP
1	A	519	THR
1	A	542	THR
1	A	564	LYS
1	A	582	SER
1	A	594	ILE
1	A	596	GLU
1	A	602	THR
1	A	606	ARG
1	A	619	LEU
1	A	644	ASN
1	A	665	GLU
1	A	681	THR
1	A	693	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	GLN
1	A	74	GLN
1	A	126	ASN
1	A	219	GLN
1	A	267	GLN
1	A	279	HIS
1	A	296	ASN
1	A	364	GLN
1	A	415	GLN

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Mol	Chain	Res	Type
1	A	477	GLN
1	A	504	GLN
1	A	531	ASN
1	A	644	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	697/705 (98%)	-0.19	11 (1%)	72	70	64, 146, 196, 232	4 (0%)

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	106	GLY	5.9
1	A	543	MET	5.8
1	A	105	PHE	5.7
1	A	88	GLN	4.0
1	A	542	THR	3.5
1	A	103	SER	2.7
1	A	698	ARG	2.5
1	A	639	MET	2.5
1	A	33	GLY	2.4
1	A	104	LEU	2.2
1	A	87	ASN	2.2

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.