W O R L D W I D E

wwPDB

P R O T E I N   D A T A   B A N K

wwPDB X-ray Structure Validation Summary Report (i)

Nov 9, 2017 – 05:56 PM EST

PDB ID	:	4NAW
Title	:	Crystal Structure of Human ATG12 ATG5-ATG16N in complex with a fragment of ATG3
Authors	:	Metlagel, Z.; Otomo, C.; Takaesu, G.; Otomo, T.
Deposited on	:	unknown
Resolution	:	2.19 Å(reported)

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

|		
MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20030345
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	rb-20030345

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.19 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.
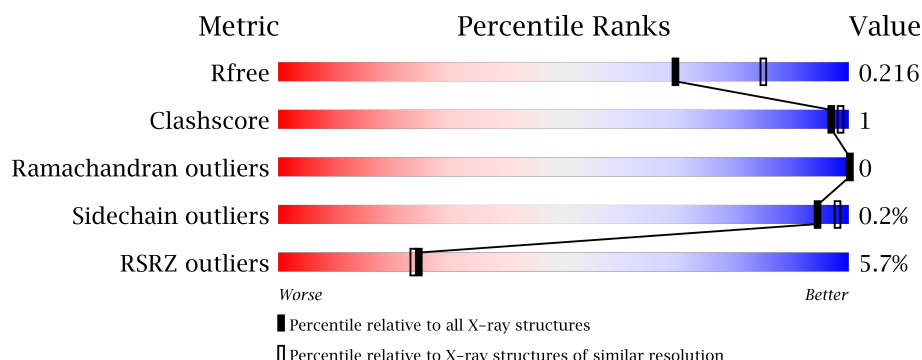
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	4002 (2.20-2.20)
Clashscore	112137	4730 (2.20-2.20)
Ramachandran outliers	110173	4656 (2.20-2.20)
Sidechain outliers	110143	4657 (2.20-2.20)
RSRZ outliers	101464	4033 (2.20-2.20)

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	91	
1	E	91	
1	I	91	
1	M	91	
2	B	275	

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	F	275	.% / 95%
2	J	275	3% / 93%
2	N	275	6% / 95%
3	C	36	86% / 8% / 6%
3	G	36	89% / 6% / 6%
3	K	36	8% / 86% / 8% / 6%
3	O	36	86% / 8% / 6%
4	D	34	18% / 32% / 6% / 62%
4	H	34	12% / 29% / 6% / 65%
4	L	34	6% / 32% / 65%
4	P	34	24% / 32% / 6% / 62%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	SO4	J	304	-	-	-	X
5	SO4	N	301	-	-	-	X
5	SO4	N	303	-	-	-	X

2 Entry composition ⓘ

There are 7 unique types of molecules in this entry. The entry contains 27188 atoms, of which 13255 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 Ubiquitin-like protein ATG12.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	88	Total 1435	C 461	H 731	N 115	O 125	S 3	0	0	0
1	E	88	Total 1435	C 461	H 731	N 115	O 125	S 3	0	0	0
1	I	88	Total 1435	C 461	H 731	N 115	O 125	S 3	0	0	0
1	M	88	Total 1435	C 461	H 731	N 115	O 125	S 3	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	50	GLY	-	EXPRESSION TAG	UNP O94817
A	51	SER	-	EXPRESSION TAG	UNP O94817
E	50	GLY	-	EXPRESSION TAG	UNP O94817
E	51	SER	-	EXPRESSION TAG	UNP O94817
I	50	GLY	-	EXPRESSION TAG	UNP O94817
I	51	SER	-	EXPRESSION TAG	UNP O94817
M	50	GLY	-	EXPRESSION TAG	UNP O94817
M	51	SER	-	EXPRESSION TAG	UNP O94817

- Molecule 2 is a protein called Autophagy protein 5.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	266	Total 4409	C 1440	H 2191	N 368	O 398	S 12	0	0	0
2	F	265	Total 4393	C 1436	H 2181	N 367	O 397	S 12	0	0	0
2	J	263	Total 4367	C 1427	H 2170	N 365	O 393	S 12	0	0	0
2	N	264	Total 4381	C 1432	H 2177	N 366	O 394	S 12	0	0	0

- Molecule 3 is a protein called Autophagy-related protein 16-1.

Mol	Chain	Residues	Atoms							ZeroOcc	AltConf	Trace
3	C	34	Total	C	H	N	O	S		0	0	0
			637	196	326	65	49	1				
3	G	34	Total	C	H	N	O	S		0	0	0
			637	196	326	65	49	1				
3	K	34	Total	C	H	N	O	S		0	0	0
			637	196	326	65	49	1				
3	O	34	Total	C	H	N	O	S		0	0	0
			637	196	326	65	49	1				

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	8	SER	-	EXPRESSION TAG	UNP Q676U5
C	9	HIS	-	EXPRESSION TAG	UNP Q676U5
C	10	MET	-	EXPRESSION TAG	UNP Q676U5
G	8	SER	-	EXPRESSION TAG	UNP Q676U5
G	9	HIS	-	EXPRESSION TAG	UNP Q676U5
G	10	MET	-	EXPRESSION TAG	UNP Q676U5
K	8	SER	-	EXPRESSION TAG	UNP Q676U5
K	9	HIS	-	EXPRESSION TAG	UNP Q676U5
K	10	MET	-	EXPRESSION TAG	UNP Q676U5
O	8	SER	-	EXPRESSION TAG	UNP Q676U5
O	9	HIS	-	EXPRESSION TAG	UNP Q676U5
O	10	MET	-	EXPRESSION TAG	UNP Q676U5

- Molecule 4 is a protein called Ubiquitin-like-conjugating enzyme ATG3.

Mol	Chain	Residues	Atoms							ZeroOcc	AltConf	Trace
4	D	13	Total	C	H	N	O	S		0	0	0
			181	60	80	13	27	1				
4	H	12	Total	C	H	N	O	S		0	0	0
			166	55	74	12	24	1				
4	L	12	Total	C	H	N	O	S		0	0	0
			166	55	74	12	24	1				
4	P	13	Total	C	H	N	O	S		0	0	0
			181	60	80	13	27	1				

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	137	GLY	-	EXPRESSION TAG	UNP Q9NT62

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	138	HIS	-	EXPRESSION TAG	UNP Q9NT62
D	139	MET	-	EXPRESSION TAG	UNP Q9NT62
H	137	GLY	-	EXPRESSION TAG	UNP Q9NT62
H	138	HIS	-	EXPRESSION TAG	UNP Q9NT62
H	139	MET	-	EXPRESSION TAG	UNP Q9NT62
L	137	GLY	-	EXPRESSION TAG	UNP Q9NT62
L	138	HIS	-	EXPRESSION TAG	UNP Q9NT62
L	139	MET	-	EXPRESSION TAG	UNP Q9NT62
P	137	GLY	-	EXPRESSION TAG	UNP Q9NT62
P	138	HIS	-	EXPRESSION TAG	UNP Q9NT62
P	139	MET	-	EXPRESSION TAG	UNP Q9NT62

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O_4S).
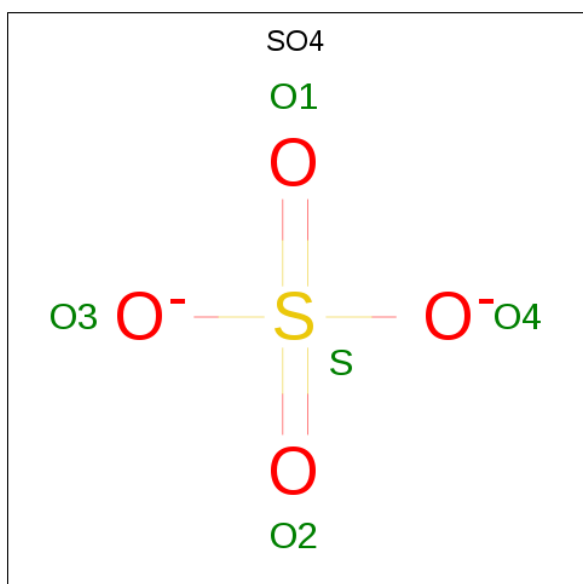
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total 5	O 4	S 1	0	0
5	B	1	Total 5	O 4	S 1	0	0
5	F	1	Total 5	O 4	S 1	0	0
5	F	1	Total 5	O 4	S 1	0	0
5	J	1	Total 5	O 4	S 1	0	0
5	J	1	Total 5	O 4	S 1	0	0

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	J	1	Total 5	O 4	S 1	0	0
5	J	1	Total 5	O 4	S 1	0	0
5	N	1	Total 5	O 4	S 1	0	0
5	N	1	Total 5	O 4	S 1	0	0
5	N	1	Total 5	O 4	S 1	0	0

- Molecule 6 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	N	1	Total 1	Na 1	0	0
6	B	1	Total 1	Na 1	0	0
6	J	1	Total 1	Na 1	0	0
6	F	1	Total 1	Na 1	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	17	Total 17	O 17	0	0
7	B	132	Total 132	O 132	0	0
7	C	19	Total 19	O 19	0	0
7	E	23	Total 23	O 23	0	0
7	F	117	Total 117	O 117	0	0
7	G	17	Total 17	O 17	0	0
7	I	15	Total 15	O 15	0	0
7	J	130	Total 130	O 130	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	K	16	Total 16	O 16	0	0
7	L	1	Total 1	O 1	0	0
7	M	13	Total 13	O 13	0	0
7	N	82	Total 82	O 82	0	0
7	O	15	Total 15	O 15	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA 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.
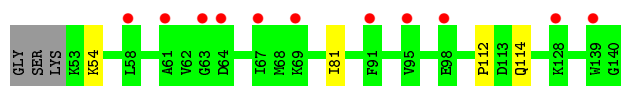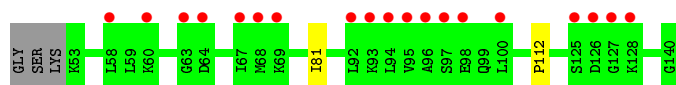
- Molecule 1: Ubiquitin-like protein ATG12
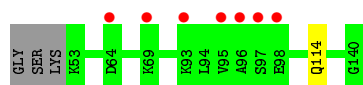
Chain A:
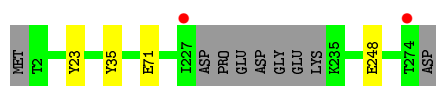
- Molecule 1: Ubiquitin-like protein ATG12

Chain E:
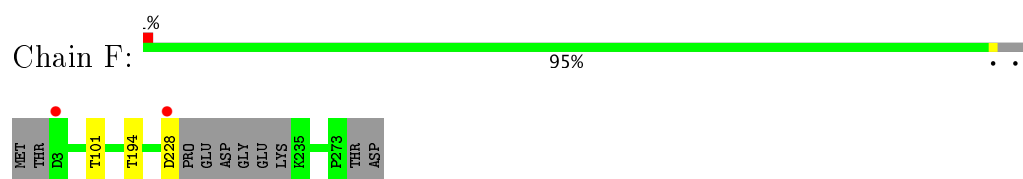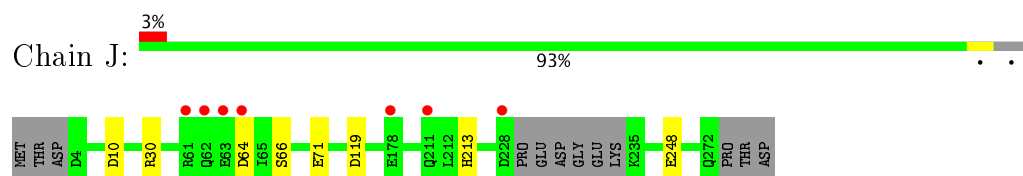
- Molecule 1: Ubiquitin-like protein ATG12

Chain I:

- Molecule 1: Ubiquitin-like protein ATG12

Chain M:

- Molecule 2: Autophagy protein 5

Chain B:

- Molecule 2: Autophagy protein 5

Chain F:

• Molecule 2: Autophagy protein 5

Chain J:

• Molecule 2: Autophagy protein 5

Chain N:

• Molecule 3: Autophagy-related protein 16-1

Chain C:

• Molecule 3: Autophagy-related protein 16-1

Chain G:

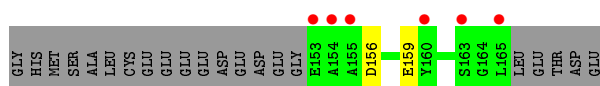• Molecule 3: Autophagy-related protein 16-1

Chain K:

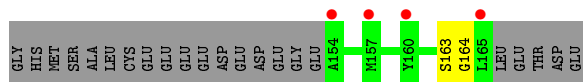• Molecule 3: Autophagy-related protein 16-1

Chain O:

• Molecule 4: Ubiquitin-like-conjugating enzyme ATG3

Chain D:

● Molecule 4: Ubiquitin-like-conjugating enzyme ATG3

Chain H:

● Molecule 4: Ubiquitin-like-conjugating enzyme ATG3

Chain L:

● Molecule 4: Ubiquitin-like-conjugating enzyme ATG3

Chain P:
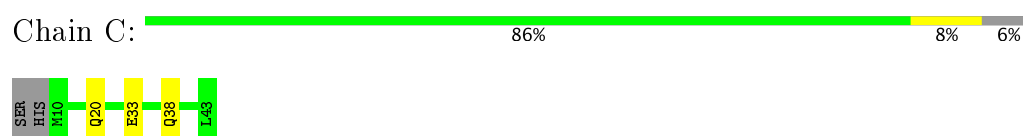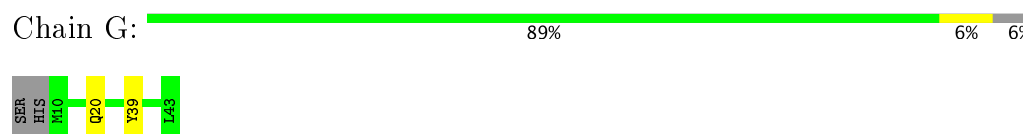
4   Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	93.58Å 120.10Å 189.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.83 – 2.19 48.83 – 2.19	Depositor EDS
% Data completeness (in resolution range)	99.6 (48.83-2.19) 99.6 (48.83-2.19)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	1.76 (at 2.20Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, R_{free}	0.172 , 0.215 0.171 , 0.216	Depositor DCC
R_{free} test set	1998 reflections (1.83%)	DCC
Wilson B-factor (Å²)	39.1	Xtriage
Anisotropy	0.316	Xtriage
Bulk solvent k_{sol}(e/Å³), B_{sol}(Å²)	0.36 , 41.3	EDS
L-test for twinning[2]	$<\|L\|>=0.50$, $<L^2>=0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	27188	wwPDB-VP
Average B, all atoms (Å²)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.17% 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)

Bond lengths and bond angles in the following residue types are not validated in this section: NA, SO4

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	0.24	0/719	0.39	0/968
1	E	0.23	0/719	0.42	0/968
1	I	0.24	0/719	0.41	0/968
1	M	0.23	0/719	0.40	0/968
2	B	0.25	0/2284	0.43	0/3098
2	F	0.25	0/2278	0.42	0/3089
2	J	0.25	0/2262	0.43	0/3066
2	N	0.24	0/2270	0.41	0/3078
3	C	0.26	0/316	0.44	0/420
3	G	0.25	0/316	0.43	0/420
3	K	0.24	0/316	0.39	0/420
3	O	0.25	0/316	0.46	0/420
4	D	0.21	0/101	0.34	0/134
4	H	0.21	0/92	0.34	0/122
4	L	0.22	0/92	0.35	0/122
4	P	0.22	0/101	0.32	0/134
All	All	0.24	0/13620	0.42	0/18395

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 (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	704	731	730	1	0
1	E	704	731	730	0	0
1	I	704	731	730	3	0
1	M	704	731	730	1	0
2	B	2218	2191	2181	3	0
2	F	2212	2181	2171	2	0
2	J	2197	2170	2160	8	0
2	N	2204	2177	2167	3	0
3	C	311	326	325	3	0
3	G	311	326	325	2	0
3	K	311	326	325	2	0
3	O	311	326	325	2	0
4	D	101	80	80	1	0
4	H	92	74	74	1	0
4	L	92	74	74	1	0
4	P	101	80	80	1	0
5	B	10	0	0	0	0
5	F	10	0	0	0	0
5	J	20	0	0	0	0
5	N	15	0	0	0	0
6	B	1	0	0	0	0
6	F	1	0	0	0	0
6	J	1	0	0	0	0
6	N	1	0	0	0	0
7	A	17	0	0	0	0
7	B	132	0	0	2	0
7	C	19	0	0	2	0
7	E	23	0	0	0	0
7	F	117	0	0	2	0
7	G	17	0	0	1	0
7	I	15	0	0	1	0
7	J	130	0	0	6	0
7	K	16	0	0	0	0
7	L	1	0	0	0	0
7	M	13	0	0	0	0
7	N	82	0	0	2	0
7	O	15	0	0	0	0
All	All	13933	13255	13207	30	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 1.

The worst 5 of 30 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:J:64:ASP:O	7:J:526:HOH:O	1.84	0.93
2:N:164:GLN:OE1	7:N:465:HOH:O	1.90	0.89
2:J:66:SER:O	7:J:479:HOH:O	1.96	0.81
2:J:10:ASP:OD2	7:J:529:HOH:O	2.03	0.77
2:J:213:HIS:O	7:J:465:HOH:O	2.02	0.76

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	86/91 (94%)	84 (98%)	2 (2%)	0	100	100
1	E	86/91 (94%)	84 (98%)	2 (2%)	0	100	100
1	I	86/91 (94%)	84 (98%)	2 (2%)	0	100	100
1	M	86/91 (94%)	83 (96%)	3 (4%)	0	100	100
2	B	262/275 (95%)	257 (98%)	5 (2%)	0	100	100
2	F	261/275 (95%)	253 (97%)	8 (3%)	0	100	100
2	J	259/275 (94%)	255 (98%)	4 (2%)	0	100	100
2	N	260/275 (94%)	257 (99%)	3 (1%)	0	100	100
3	C	32/36 (89%)	31 (97%)	1 (3%)	0	100	100
3	G	32/36 (89%)	32 (100%)	0	0	100	100
3	K	32/36 (89%)	32 (100%)	0	0	100	100
3	O	32/36 (89%)	32 (100%)	0	0	100	100
4	D	11/34 (32%)	10 (91%)	1 (9%)	0	100	100
4	H	10/34 (29%)	7 (70%)	3 (30%)	0	100	100
4	L	10/34 (29%)	8 (80%)	2 (20%)	0	100	100
4	P	11/34 (32%)	9 (82%)	2 (18%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1556/1744 (89%)	1518 (98%)	38 (2%)	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	77/79 (98%)	77 (100%)	0	100 100
1	E	77/79 (98%)	76 (99%)	1 (1%)	73 85
1	I	77/79 (98%)	77 (100%)	0	100 100
1	M	77/79 (98%)	77 (100%)	0	100 100
2	B	246/254 (97%)	245 (100%)	1 (0%)	93 97
2	F	245/254 (96%)	244 (100%)	1 (0%)	93 97
2	J	243/254 (96%)	243 (100%)	0	100 100
2	N	244/254 (96%)	244 (100%)	0	100 100
3	C	33/35 (94%)	33 (100%)	0	100 100
3	G	33/35 (94%)	33 (100%)	0	100 100
3	K	33/35 (94%)	33 (100%)	0	100 100
3	O	33/35 (94%)	33 (100%)	0	100 100
4	D	10/28 (36%)	10 (100%)	0	100 100
4	H	9/28 (32%)	9 (100%)	0	100 100
4	L	9/28 (32%)	9 (100%)	0	100 100
4	P	10/28 (36%)	10 (100%)	0	100 100
All	All	1456/1584 (92%)	1453 (100%)	3 (0%)	94 98

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	71	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	114	GLN
2	F	228	ASP

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

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 carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 15 ligands modelled in this entry, 4 are monoatomic - leaving 11 for Mogul analysis.

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	$\#|Z| > 2$
5	SO4	B	301	-	4,4,4	0.15	0	6,6,6	0.12	0
5	SO4	B	302	-	4,4,4	0.15	0	6,6,6	0.10	0
5	SO4	F	301	-	4,4,4	0.14	0	6,6,6	0.05	0
5	SO4	F	302	-	4,4,4	0.14	0	6,6,6	0.05	0
5	SO4	J	301	-	4,4,4	0.14	0	6,6,6	0.07	0
5	SO4	J	302	-	4,4,4	0.14	0	6,6,6	0.07	0
5	SO4	J	303	-	4,4,4	0.15	0	6,6,6	0.06	0
5	SO4	J	304	-	4,4,4	0.15	0	6,6,6	0.07	0
5	SO4	N	301	-	4,4,4	0.16	0	6,6,6	0.06	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\lvert Z\rvert>2$	Counts	RMSZ	$\#\lvert Z\rvert>2$
5	SO4	N	302	-	4,4,4	0.14	0	6,6,6	0.05	0
5	SO4	N	303	-	4,4,4	0.16	0	6,6,6	0.07	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
5	SO4	B	301	-	-	0/0/0/0	0/0/0/0
5	SO4	B	302	-	-	0/0/0/0	0/0/0/0
5	SO4	F	301	-	-	0/0/0/0	0/0/0/0
5	SO4	F	302	-	-	0/0/0/0	0/0/0/0
5	SO4	J	301	-	-	0/0/0/0	0/0/0/0
5	SO4	J	302	-	-	0/0/0/0	0/0/0/0
5	SO4	J	303	-	-	0/0/0/0	0/0/0/0
5	SO4	J	304	-	-	0/0/0/0	0/0/0/0
5	SO4	N	301	-	-	0/0/0/0	0/0/0/0
5	SO4	N	302	-	-	0/0/0/0	0/0/0/0
5	SO4	N	303	-	-	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 (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(Å²)	Q<0.9
1	A	88/91 (96%)	0.51	4 (4%)	34	32	49, 74, 104, 109	0
1	E	88/91 (96%)	0.48	7 (7%)	13	12	44, 71, 110, 127	0
1	I	88/91 (96%)	0.76	11 (12%)	4	4	44, 74, 106, 126	0
1	M	88/91 (96%)	1.01	19 (21%)	1	1	55, 80, 110, 119	0
2	B	266/275 (96%)	0.05	2 (0%)	86	85	31, 45, 79, 105	0
2	F	265/275 (96%)	0.11	2 (0%)	86	85	32, 48, 86, 104	0
2	J	263/275 (95%)	0.06	7 (2%)	55	52	31, 50, 95, 127	0
2	N	264/275 (96%)	0.32	16 (6%)	22	21	36, 59, 102, 118	0
3	C	34/36 (94%)	0.02	0	100	100	32, 47, 77, 85	0
3	G	34/36 (94%)	-0.10	0	100	100	36, 51, 74, 88	0
3	K	34/36 (94%)	0.31	3 (8%)	11	9	37, 54, 92, 106	0
3	O	34/36 (94%)	0.06	0	100	100	35, 48, 86, 105	0
4	D	13/34 (38%)	2.48	6 (46%)	0	0	83, 94, 115, 128	0
4	H	12/34 (35%)	1.84	4 (33%)	0	0	85, 90, 105, 107	0
4	L	12/34 (35%)	1.37	2 (16%)	2	2	77, 86, 101, 104	0
4	P	13/34 (38%)	2.09	8 (61%)	0	0	89, 95, 106, 123	0
All	All	1596/1744 (91%)	0.31	91 (5%)	24	24	31, 56, 101, 128	0

The worst 5 of 91 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	153	GLU	5.5
1	M	94	LEU	4.3
4	H	160	TYR	4.2
4	D	154	ALA	4.2
1	I	64	ASP	4.1

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 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, 95th 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
5	SO4	N	301	5/5	0.94	0.21	3.50	58,74,79,85	0
5	SO4	N	303	5/5	0.86	0.18	2.88	70,79,101,116	0
5	SO4	J	304	5/5	0.89	0.17	2.52	80,99,122,135	0
6	NA	N	304	1/1	0.77	0.15	1.89	69,69,69,69	0
5	SO4	J	301	5/5	0.95	0.14	1.28	79,92,104,105	0
5	SO4	B	302	5/5	0.99	0.13	1.18	42,48,52,56	0
6	NA	B	303	1/1	0.96	0.13	0.24	41,41,41,41	0
5	SO4	B	301	5/5	0.97	0.11	-0.15	52,61,73,74	0
6	NA	F	303	1/1	0.99	0.07	-4.27	39,39,39,39	0
6	NA	J	305	1/1	0.52	0.20	-	72,72,72,72	0
5	SO4	J	302	5/5	0.81	0.23	-	110,117,125,135	0
5	SO4	F	302	5/5	0.97	0.13	-	76,78,92,93	0
5	SO4	N	302	5/5	0.92	0.13	-	100,110,111,116	0
5	SO4	F	301	5/5	0.89	0.26	-	110,113,126,127	0
5	SO4	J	303	5/5	0.92	0.19	-	103,112,116,117	0

6.5 Other polymers (i)

There are no such residues in this entry.