Full wwPDB X-ray Structure Validation Report (i)

Sep 12, 2023 – 04:22 PM EDT

PDB ID	:	4O46
Title	:	14-3-3-gamma in complex with influenza NS1 C-terminal tail phosphorylated at S228
Authors	:	Qin, S.; Liu, Y.; Tempel, W.; Arrowsmith, C.H.; Bountra, C.; Edwards, A.M.; Min, J.; Structural Genomics Consortium (SGC)
Deposited on	:	2013-12-18
Resolution	:	2.90 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

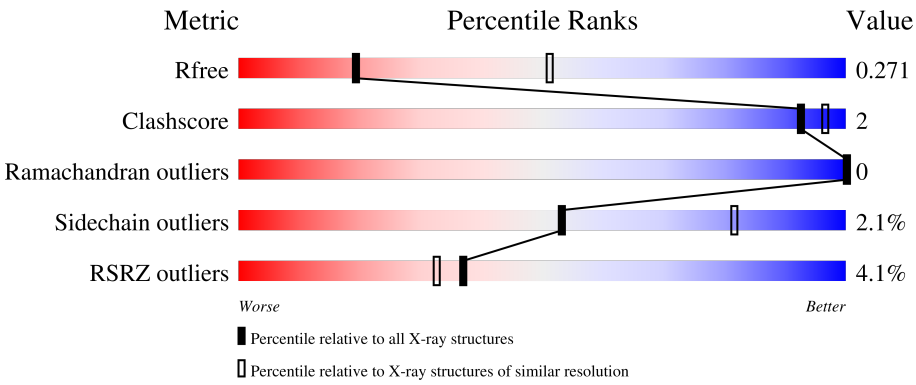
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 2.90 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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	256	2% 86% 6% 8%
1	B	256	87% • 9%
1	C	256	.% 86% 6% 8%
1	D	256	3% 86% 6% 8%
1	E	256	.% 86% 5% 8%

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Mol	Chain	Length	Quality of chain
1	F	256	14% 78% 20%
2	G	15	40% 60%
2	H	15	27% 13% 60%
2	I	15	7% 33% 7% 60%
2	J	15	20% 33% 7% 60%
2	K	15	7% 33% 7% 60%
2	L	15	7% 7% 87%
3	M	24	83% 17%
3	N	24	38% 63%
3	O	24	42% 58%
3	V	24	54% 46%

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
4	UNX	A	302	-	-	-	X
4	UNX	A	303	-	-	-	X
4	UNX	A	305	-	-	-	X
4	UNX	A	306	-	-	-	X
4	UNX	A	307	-	-	-	X
4	UNX	A	308	-	-	-	X
4	UNX	B	301	-	-	-	X
4	UNX	B	302	-	-	-	X
4	UNX	B	303	-	-	-	X
4	UNX	B	304	-	-	-	X
4	UNX	B	305	-	-	-	X
4	UNX	B	306	-	-	-	X
4	UNX	B	307	-	-	-	X
4	UNX	B	308	-	-	-	X
4	UNX	B	309	-	-	-	X
4	UNX	B	311	-	-	-	X
4	UNX	B	312	-	-	-	X
4	UNX	B	313	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	UNX	B	314	-	-	-	X
4	UNX	B	315	-	-	-	X
4	UNX	B	316	-	-	-	X
4	UNX	B	317	-	-	-	X
4	UNX	B	318	-	-	-	X
4	UNX	C	301	-	-	-	X
4	UNX	C	302	-	-	-	X
4	UNX	C	303	-	-	-	X
4	UNX	C	304	-	-	-	X
4	UNX	C	305	-	-	-	X
4	UNX	C	306	-	-	-	X
4	UNX	C	307	-	-	-	X
4	UNX	C	308	-	-	-	X
4	UNX	C	309	-	-	-	X
4	UNX	C	310	-	-	-	X
4	UNX	C	311	-	-	-	X
4	UNX	C	312	-	-	-	X
4	UNX	C	313	-	-	-	X
4	UNX	D	301	-	-	-	X
4	UNX	D	302	-	-	-	X
4	UNX	D	303	-	-	-	X
4	UNX	D	304	-	-	-	X
4	UNX	D	305	-	-	-	X
4	UNX	D	306	-	-	-	X
4	UNX	D	307	-	-	-	X
4	UNX	D	308	-	-	-	X
4	UNX	D	309	-	-	-	X
4	UNX	E	301	-	-	-	X
4	UNX	E	302	-	-	-	X
4	UNX	E	303	-	-	-	X
4	UNX	E	304	-	-	-	X
4	UNX	F	301	-	-	-	X

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 10919 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 14-3-3 protein gamma.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	235	1811	1135	314	353	9	0	1	0
1	B	234	1818	1142	306	361	9	0	0	0
1	C	235	1804	1134	303	358	9	0	1	0
1	D	235	1777	1116	304	347	10	0	0	0
1	E	236	1814	1138	312	355	9	0	0	0
1	F	206	1354	841	243	265	5	0	0	0

There are 54 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	248	SER	-	expression tag	UNP P61981
A	249	LEU	-	expression tag	UNP P61981
A	250	GLU	-	expression tag	UNP P61981
A	251	HIS	-	expression tag	UNP P61981
A	252	HIS	-	expression tag	UNP P61981
A	253	HIS	-	expression tag	UNP P61981
A	254	HIS	-	expression tag	UNP P61981
A	255	HIS	-	expression tag	UNP P61981
A	256	HIS	-	expression tag	UNP P61981
B	248	SER	-	expression tag	UNP P61981
B	249	LEU	-	expression tag	UNP P61981
B	250	GLU	-	expression tag	UNP P61981
B	251	HIS	-	expression tag	UNP P61981
B	252	HIS	-	expression tag	UNP P61981
B	253	HIS	-	expression tag	UNP P61981
B	254	HIS	-	expression tag	UNP P61981
B	255	HIS	-	expression tag	UNP P61981

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Chain	Residue	Modelled	Actual	Comment	Reference
B	256	HIS	-	expression tag	UNP P61981
C	248	SER	-	expression tag	UNP P61981
C	249	LEU	-	expression tag	UNP P61981
C	250	GLU	-	expression tag	UNP P61981
C	251	HIS	-	expression tag	UNP P61981
C	252	HIS	-	expression tag	UNP P61981
C	253	HIS	-	expression tag	UNP P61981
C	254	HIS	-	expression tag	UNP P61981
C	255	HIS	-	expression tag	UNP P61981
C	256	HIS	-	expression tag	UNP P61981
D	248	SER	-	expression tag	UNP P61981
D	249	LEU	-	expression tag	UNP P61981
D	250	GLU	-	expression tag	UNP P61981
D	251	HIS	-	expression tag	UNP P61981
D	252	HIS	-	expression tag	UNP P61981
D	253	HIS	-	expression tag	UNP P61981
D	254	HIS	-	expression tag	UNP P61981
D	255	HIS	-	expression tag	UNP P61981
D	256	HIS	-	expression tag	UNP P61981
E	248	SER	-	expression tag	UNP P61981
E	249	LEU	-	expression tag	UNP P61981
E	250	GLU	-	expression tag	UNP P61981
E	251	HIS	-	expression tag	UNP P61981
E	252	HIS	-	expression tag	UNP P61981
E	253	HIS	-	expression tag	UNP P61981
E	254	HIS	-	expression tag	UNP P61981
E	255	HIS	-	expression tag	UNP P61981
E	256	HIS	-	expression tag	UNP P61981
F	248	SER	-	expression tag	UNP P61981
F	249	LEU	-	expression tag	UNP P61981
F	250	GLU	-	expression tag	UNP P61981
F	251	HIS	-	expression tag	UNP P61981
F	252	HIS	-	expression tag	UNP P61981
F	253	HIS	-	expression tag	UNP P61981
F	254	HIS	-	expression tag	UNP P61981
F	255	HIS	-	expression tag	UNP P61981
F	256	HIS	-	expression tag	UNP P61981

- Molecule 2 is a protein called Nonstructural protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	G	6	42	24	7	10	1	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	H	6	42	24	6	11	1	0	0	0
2	I	6	44	25	7	11	1	0	0	0
2	J	6	40	23	6	10	1	0	0	0
2	K	6	41	24	6	10	1	0	0	0
2	L	2	15	6	2	6	1	0	0	0

- Molecule 3 is a protein called Unidentified polymer.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
3	M	20	100	60	20	20	0	0	0
3	N	9	45	27	9	9	0	0	0
3	O	10	50	30	10	10	0	0	0
3	V	13	65	39	13	13	0	0	0

- Molecule 4 is UNKNOWN ATOM OR ION (three-letter code: UNX) (formula: X).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	X		
4	A	10	10	10	0	0
4	B	18	18	18	0	0
4	C	14	14	14	0	0
4	D	9	9	9	0	0
4	E	5	5	5	0	0
4	F	1	1	1	0	0

3 Residue-property plots (i)

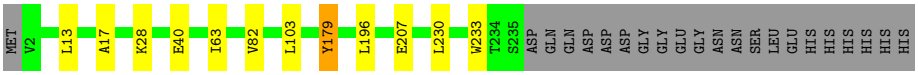
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: 14-3-3 protein gamma

Chain A:

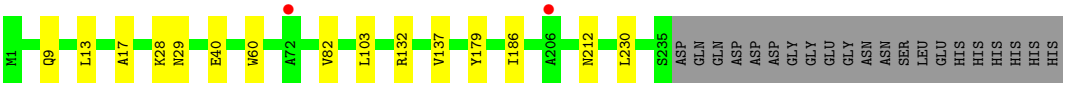
• Molecule 1: 14-3-3 protein gamma

Chain B:



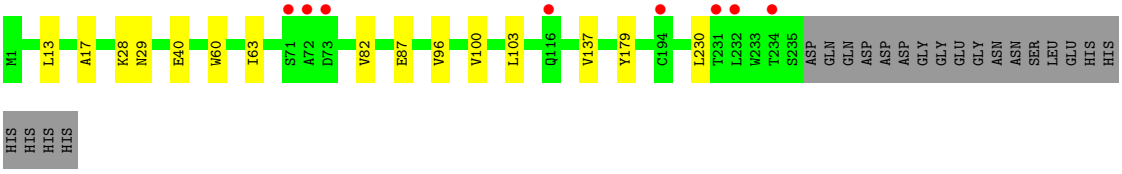
• Molecule 1: 14-3-3 protein gamma

Chain C:



• Molecule 1: 14-3-3 protein gamma

Chain D:

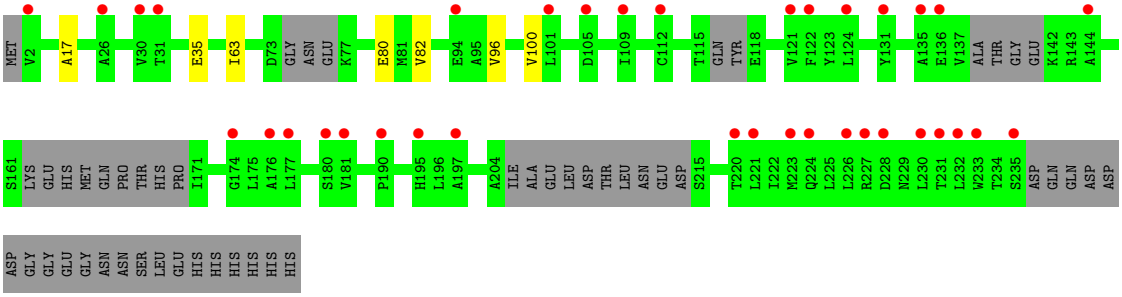


• Molecule 1: 14-3-3 protein gamma

Chain E:

• Molecule 1: 14-3-3 protein gamma

Chain F:



• Molecule 2: Nonstructural protein 1

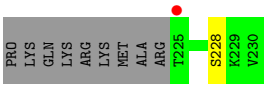
Chain G:

• Molecule 2: Nonstructural protein 1

Chain H:

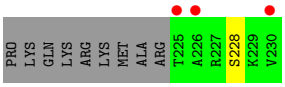
• Molecule 2: Nonstructural protein 1

Chain I:



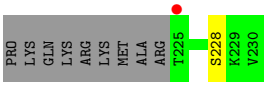
• Molecule 2: Nonstructural protein 1

Chain J:



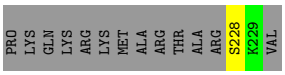
• Molecule 2: Nonstructural protein 1

Chain K:



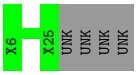
• Molecule 2: Nonstructural protein 1

Chain L: 7% 7% 87%



• Molecule 3: Unidentified polymer

Chain M: 83% 17%



• Molecule 3: Unidentified polymer

Chain N: 38% 63%

• Molecule 3: Unidentified polymer

Chain O: 42% 58%

• Molecule 3: Unidentified polymer

Chain V: 54% 46%

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	121.83Å 121.83Å 314.22Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.53 – 2.90 38.53 – 2.90	Depositor EDS
% Data completeness (in resolution range)	100.0 (38.53-2.90) 100.0 (38.53-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.14	Depositor
$< I/\sigma(I) >$ [1]	3.31 (at 2.90Å)	Xtriage
Refinement program	BUSTER-TNT BUSTER 2.10.0, BUSTER 2.10.0	Depositor
R, R_{free}	0.226 , 0.249 0.249 , 0.271	Depositor DCC
R_{free} test set	1510 reflections (2.83%)	wwPDB-VP
Wilson B-factor (Å^2)	56.7	Xtriage
Anisotropy	0.313	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 60.3	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	0.90	EDS
Total number of atoms	10919	wwPDB-VP
Average B, all atoms (Å^2)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.25% 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: UNX, SEP

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	0/1844	0.55	0/2501
1	B	0.40	0/1846	0.55	0/2503
1	C	0.41	0/1837	0.56	0/2496
1	D	0.40	0/1803	0.54	0/2446
1	E	0.40	0/1841	0.55	0/2497
1	F	0.42	0/1363	0.56	0/1855
2	G	0.32	0/30	0.48	0/37
2	H	0.36	0/30	0.49	0/38
2	I	0.35	0/32	0.51	0/40
2	J	0.32	0/28	0.53	0/35
2	K	0.36	0/29	0.51	0/36
2	L	0.18	0/4	0.15	0/4
All	All	0.40	0/10687	0.55	0/14488

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	1811	0	1694	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1818	0	1710	7	0
1	C	1804	0	1675	7	0
1	D	1777	0	1642	7	0
1	E	1814	0	1710	9	0
1	F	1354	0	1052	4	0
2	G	42	0	35	0	0
2	H	42	0	33	1	0
2	I	44	0	40	0	0
2	J	40	0	28	0	0
2	K	41	0	30	0	0
2	L	15	0	7	0	0
3	M	100	0	22	0	0
3	N	45	0	11	0	0
3	O	50	0	12	0	0
3	V	65	0	15	0	0
4	A	10	0	0	0	0
4	B	18	0	0	0	0
4	C	14	0	0	0	0
4	D	9	0	0	0	0
4	E	5	0	0	0	0
4	F	1	0	0	0	0
All	All	10919	0	9716	31	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 2.

All (31) 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:13:LEU:HD11	1:D:82:VAL:HG22	1.84	0.58
1:D:28:LYS:HG3	1:D:103:LEU:HD21	1.87	0.56
1:A:13:LEU:HD11	1:C:82:VAL:HG22	1.89	0.54
1:A:28:LYS:HG3	1:A:103:LEU:HD21	1.91	0.52
1:D:96:VAL:O	1:D:100:VAL:HG23	2.10	0.52
1:B:63:ILE:HD11	1:D:17:ALA:HB2	1.92	0.52
1:B:28:LYS:HG3	1:B:103:LEU:HD21	1.92	0.52
1:E:28:LYS:HG3	1:E:103:LEU:HD21	1.93	0.51
1:C:28:LYS:HG3	1:C:103:LEU:HD21	1.91	0.51
1:E:63:ILE:HD11	1:F:17:ALA:HB2	1.93	0.51
1:B:82:VAL:HG22	1:D:13:LEU:HD11	1.92	0.50
1:E:96:VAL:O	1:E:100:VAL:HG23	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:17:ALA:HB2	1:D:63:ILE:HD11	1.95	0.48
1:E:17:ALA:HB2	1:F:63:ILE:HD11	1.96	0.48
1:A:63:ILE:HD11	1:C:17:ALA:HB2	1.96	0.47
1:A:96:VAL:O	1:A:100:VAL:HG23	2.14	0.47
1:A:82:VAL:HG22	1:C:13:LEU:HD11	1.98	0.46
1:E:132:ARG:HG3	1:E:186:ILE:HG13	2.01	0.43
1:E:60:TRP:CE2	1:E:137:VAL:HG12	2.55	0.42
1:A:132:ARG:HG3	1:A:186:ILE:HG13	2.02	0.41
1:B:179:TYR:HB3	1:B:196:LEU:HD21	2.02	0.41
1:C:132:ARG:HG3	1:C:186:ILE:HG13	2.02	0.41
1:D:60:TRP:CE2	1:D:137:VAL:HG12	2.55	0.41
1:E:13:LEU:HD11	1:F:82:VAL:HG22	2.02	0.41
1:E:179:TYR:HB3	1:E:196:LEU:HD21	2.03	0.41
1:E:78:LYS:O	1:E:82:VAL:HG23	2.21	0.41
1:A:60:TRP:CE2	1:A:137:VAL:HG12	2.57	0.40
1:B:233:TRP:HE1	2:H:226:ALA:HB2	1.86	0.40
1:F:96:VAL:O	1:F:100:VAL:HG23	2.22	0.40
1:A:81:MET:HE1	1:C:9:GLN:HG3	2.04	0.40
1:C:60:TRP:CE2	1:C:137:VAL:HG12	2.56	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	234/256 (91%)	232 (99%)	2 (1%)	0	100	100
1	B	232/256 (91%)	230 (99%)	2 (1%)	0	100	100
1	C	234/256 (91%)	231 (99%)	3 (1%)	0	100	100
1	D	233/256 (91%)	230 (99%)	3 (1%)	0	100	100
1	E	234/256 (91%)	231 (99%)	3 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	194/256 (76%)	191 (98%)	3 (2%)	0	100	100
2	G	3/15 (20%)	3 (100%)	0	0	100	100
2	H	3/15 (20%)	3 (100%)	0	0	100	100
2	I	3/15 (20%)	3 (100%)	0	0	100	100
2	J	3/15 (20%)	3 (100%)	0	0	100	100
2	K	3/15 (20%)	3 (100%)	0	0	100	100
All	All	1376/1611 (85%)	1360 (99%)	16 (1%)	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	177/225 (79%)	174 (98%)	3 (2%)	60	86
1	B	181/225 (80%)	177 (98%)	4 (2%)	52	81
1	C	176/225 (78%)	171 (97%)	5 (3%)	43	76
1	D	167/225 (74%)	162 (97%)	5 (3%)	41	75
1	E	179/225 (80%)	178 (99%)	1 (1%)	86	96
1	F	86/225 (38%)	84 (98%)	2 (2%)	50	80
2	G	2/12 (17%)	2 (100%)	0	100	100
2	H	2/12 (17%)	2 (100%)	0	100	100
2	I	3/12 (25%)	3 (100%)	0	100	100
2	J	1/12 (8%)	1 (100%)	0	100	100
2	K	1/12 (8%)	1 (100%)	0	100	100
All	All	975/1410 (69%)	955 (98%)	20 (2%)	53	81

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	GLU
1	A	179	TYR
1	A	230	LEU
1	B	40	GLU
1	B	179	TYR
1	B	207	GLU
1	B	230	LEU
1	C	29	ASN
1	C	40	GLU
1	C	179	TYR
1	C	212	ASN
1	C	230	LEU
1	D	29	ASN
1	D	40	GLU
1	D	87	GLU
1	D	179	TYR
1	D	230	LEU
1	E	179	TYR
1	F	35	GLU
1	F	80	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	6	GLN
1	C	106	ASN
1	D	106	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)

6 non-standard protein/DNA/RNA residues are modelled in this entry.

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	$\#\|Z\| > 2$
2	SEP	K	228	2	8,9,10	0.80	0	8,12,14	1.28	1 (12%)
2	SEP	H	228	2	8,9,10	0.95	0	8,12,14	1.21	1 (12%)
2	SEP	I	228	2	8,9,10	0.78	0	8,12,14	1.31	1 (12%)
2	SEP	J	228	2	8,9,10	0.98	0	8,12,14	1.49	1 (12%)
2	SEP	G	228	2	8,9,10	0.93	0	8,12,14	1.14	0
2	SEP	L	228	2	8,9,10	0.97	0	8,12,14	2.91	2 (25%)

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
2	SEP	K	228	2	-	0/5/8/10	-
2	SEP	H	228	2	-	0/5/8/10	-
2	SEP	I	228	2	-	0/5/8/10	-
2	SEP	J	228	2	-	0/5/8/10	-
2	SEP	G	228	2	-	0/5/8/10	-
2	SEP	L	228	2	-	1/5/8/10	-

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	L	228	SEP	OG-CB-CA	7.19	115.14	108.14
2	J	228	SEP	OG-CB-CA	2.69	110.76	108.14
2	L	228	SEP	P-OG-CB	-2.64	111.03	118.30
2	K	228	SEP	OG-CB-CA	2.62	110.69	108.14
2	H	228	SEP	OG-CB-CA	2.50	110.58	108.14
2	I	228	SEP	OG-CB-CA	2.27	110.35	108.14

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	L	228	SEP	N-CA-CB-OG

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 57 ligands modelled in this entry, 57 are unknown - 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 (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	235/256 (91%)	0.02	4 (1%) 70 69	30, 55, 100, 121	1 (0%)
1	B	234/256 (91%)	-0.12	0 100 100	30, 48, 77, 113	1 (0%)
1	C	235/256 (91%)	-0.07	2 (0%) 84 84	31, 55, 93, 123	1 (0%)
1	D	235/256 (91%)	0.04	8 (3%) 45 40	36, 66, 108, 131	0
1	E	236/256 (92%)	-0.02	2 (0%) 86 86	45, 68, 112, 149	0
1	F	206/256 (80%)	0.81	36 (17%) 1 1	65, 114, 156, 187	0
2	G	5/15 (33%)	-0.17	0 100 100	67, 68, 73, 75	0
2	H	5/15 (33%)	0.16	0 100 100	56, 58, 66, 71	0
2	I	5/15 (33%)	0.33	1 (20%) 1 0	57, 61, 73, 84	0
2	J	5/15 (33%)	1.62	3 (60%) 0 0	65, 69, 77, 89	0
2	K	5/15 (33%)	0.83	1 (20%) 1 0	63, 63, 73, 76	0
2	L	1/15 (6%)	0.05	0 100 100	125, 125, 125, 125	0
3	M	0/24	-	-	-	-
3	N	0/24	-	-	-	-
3	O	0/24	-	-	-	-
3	V	0/24	-	-	-	-
All	All	1407/1722 (81%)	0.10	57 (4%) 37 32	30, 63, 128, 187	3 (0%)

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	176	ALA	6.7
1	F	135	ALA	6.5
1	D	72	ALA	5.0
1	F	230	LEU	4.5
1	F	220	THR	4.0
1	D	73	ASP	3.8
1	F	235	SER	3.8

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Mol	Chain	Res	Type	RSRZ
1	F	224	GLN	3.6
1	F	124	LEU	3.6
1	F	180	SER	3.5
1	F	231	THR	3.5
1	F	221	LEU	3.5
1	F	26	ALA	3.4
1	F	109	ILE	3.3
1	F	174	GLY	3.3
2	J	226	ALA	3.2
1	F	136	GLU	3.2
1	F	226	LEU	3.1
1	F	232	LEU	3.1
2	J	225	THR	3.1
1	C	72	ALA	3.1
1	A	72	ALA	3.0
1	F	101	LEU	2.9
1	F	233	TRP	2.9
1	D	71	SER	2.8
1	F	30	VAL	2.8
1	A	212	ASN	2.7
2	K	225	THR	2.7
1	A	70	THR	2.7
1	F	94	GLU	2.6
1	A	68	GLN	2.6
1	F	197	ALA	2.5
1	F	121	VAL	2.5
1	F	190	PRO	2.5
1	D	234	THR	2.4
1	F	112	CYS	2.4
1	F	223	MET	2.4
1	F	122	PHE	2.3
1	D	231	THR	2.3
1	F	228	ASP	2.3
1	E	236	ASP	2.3
1	F	105	ASP	2.3
2	I	225	THR	2.2
1	F	195	HIS	2.2
1	F	177	LEU	2.2
1	C	206	ALA	2.2
1	F	144	ALA	2.2
2	J	230	VAL	2.2
1	F	227	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	F	31	THR	2.1
1	F	2	VAL	2.1
1	E	195	HIS	2.1
1	D	194	CYS	2.1
1	D	116	GLN	2.0
1	D	232	LEU	2.0
1	F	181	VAL	2.0
1	F	131	TYR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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. 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	B-factors(Å^2)	Q<0.9
2	SEP	L	228	10/11	0.83	0.26	119,121,122,122	0
2	SEP	J	228	10/11	0.96	0.20	59,61,66,66	0
2	SEP	K	228	10/11	0.96	0.14	49,52,58,58	0
2	SEP	G	228	10/11	0.96	0.15	55,58,61,62	0
2	SEP	H	228	10/11	0.97	0.16	45,48,55,55	0
2	SEP	I	228	10/11	0.98	0.15	49,52,53,54	0

6.3 Carbohydrates (i)

There are no monosaccharides 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. 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	B-factors(Å^2)	Q<0.9
4	UNX	A	303	1/1	-0.30	3.69	30,30,30,30	1
4	UNX	C	313	1/1	-0.21	3.54	30,30,30,30	1
4	UNX	A	307	1/1	-0.11	2.59	30,30,30,30	1
4	UNX	E	301	1/1	-0.11	3.16	30,30,30,30	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	UNX	A	308	1/1	-0.10	4.28	30,30,30,30	1
4	UNX	B	305	1/1	-0.06	2.76	30,30,30,30	1
4	UNX	C	304	1/1	-0.05	2.02	30,30,30,30	1
4	UNX	B	314	1/1	-0.02	2.76	30,30,30,30	1
4	UNX	B	317	1/1	-0.01	4.33	30,30,30,30	1
4	UNX	D	309	1/1	0.05	1.01	30,30,30,30	1
4	UNX	D	305	1/1	0.06	3.92	30,30,30,30	1
4	UNX	B	316	1/1	0.10	2.99	30,30,30,30	1
4	UNX	B	315	1/1	0.11	3.01	30,30,30,30	1
4	UNX	E	303	1/1	0.12	1.02	30,30,30,30	1
4	UNX	C	305	1/1	0.14	1.75	30,30,30,30	1
4	UNX	E	302	1/1	0.15	1.83	30,30,30,30	1
4	UNX	B	306	1/1	0.18	1.45	30,30,30,30	1
4	UNX	C	312	1/1	0.25	1.29	30,30,30,30	1
4	UNX	A	306	1/1	0.30	2.58	30,30,30,30	1
4	UNX	C	307	1/1	0.32	5.84	30,30,30,30	1
4	UNX	C	309	1/1	0.32	1.97	30,30,30,30	1
4	UNX	A	305	1/1	0.32	3.21	30,30,30,30	1
4	UNX	B	307	1/1	0.35	2.59	30,30,30,30	1
4	UNX	C	310	1/1	0.39	1.83	30,30,30,30	1
4	UNX	D	306	1/1	0.39	1.39	30,30,30,30	1
4	UNX	C	301	1/1	0.41	2.96	30,30,30,30	1
4	UNX	D	303	1/1	0.41	2.30	30,30,30,30	1
4	UNX	C	306	1/1	0.43	2.60	30,30,30,30	1
4	UNX	F	301	1/1	0.43	2.43	30,30,30,30	1
4	UNX	B	313	1/1	0.45	1.39	30,30,30,30	1
4	UNX	B	301	1/1	0.45	0.98	30,30,30,30	1
4	UNX	B	302	1/1	0.47	1.34	30,30,30,30	1
4	UNX	B	309	1/1	0.51	1.15	30,30,30,30	1
4	UNX	B	312	1/1	0.51	1.67	30,30,30,30	1
4	UNX	C	308	1/1	0.51	1.08	30,30,30,30	1
4	UNX	E	304	1/1	0.55	2.15	30,30,30,30	1
4	UNX	C	302	1/1	0.56	0.76	30,30,30,30	1
4	UNX	D	308	1/1	0.56	1.24	30,30,30,30	1
4	UNX	D	301	1/1	0.59	2.52	30,30,30,30	1
4	UNX	C	311	1/1	0.60	1.42	30,30,30,30	1
4	UNX	B	311	1/1	0.62	0.61	30,30,30,30	1
4	UNX	D	302	1/1	0.66	1.55	30,30,30,30	1
4	UNX	A	302	1/1	0.67	1.65	30,30,30,30	1
4	UNX	B	303	1/1	0.69	1.03	30,30,30,30	1
4	UNX	B	318	1/1	0.69	1.54	30,30,30,30	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	UNX	D	307	1/1	0.72	1.26	30,30,30,30	1
4	UNX	B	308	1/1	0.73	0.69	30,30,30,30	1
4	UNX	A	310	1/1	0.75	0.18	30,30,30,30	0
4	UNX	A	309	1/1	0.77	0.38	30,30,30,30	0
4	UNX	D	304	1/1	0.77	1.25	30,30,30,30	1
4	UNX	C	303	1/1	0.78	2.23	30,30,30,30	1
4	UNX	B	304	1/1	0.80	1.22	30,30,30,30	1
4	UNX	A	301	1/1	0.83	1.61	30,30,30,30	1
4	UNX	A	304	1/1	0.86	1.85	30,30,30,30	1
4	UNX	E	305	1/1	0.87	0.25	30,30,30,30	0
4	UNX	B	310	1/1	0.92	2.23	30,30,30,30	1
4	UNX	C	314	1/1	0.95	0.28	30,30,30,30	0

6.5 Other polymers (i)

There are no such residues in this entry.