wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 07:48 AM GMT

PDB ID	:	3C9I
Title	:	Structure of P22 Tail-Needle GP26 Bound to Xenon Gas
Authors	:	Cingolani, G.; Olia, A.S.
Deposited on	:	2008-02-15
Resolution	:	1.95 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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:

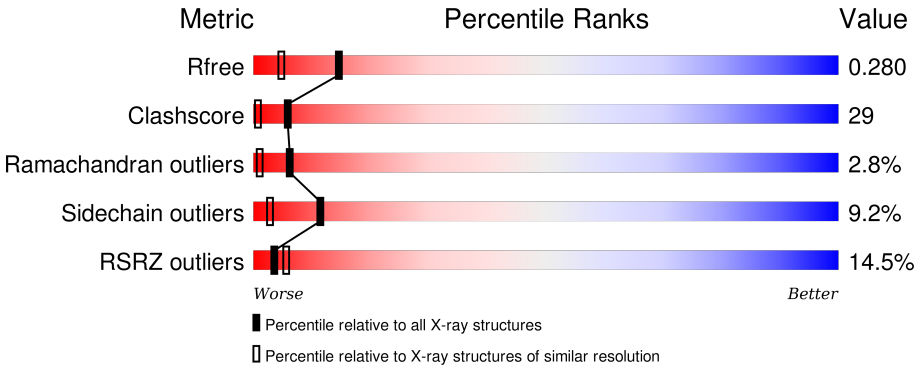
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 1.95 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	1833 (1.96-1.96)
Clashscore	102246	1953 (1.96-1.96)
Ramachandran outliers	100387	1936 (1.96-1.96)
Sidechain outliers	100360	1936 (1.96-1.96)
RSRZ outliers	91569	1835 (1.96-1.96)

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	242	7% 62% 26% 7%
1	B	242	9% 67% 29%
1	C	242	16% 55% 32% 6%
1	D	242	17% 50% 33% 8% 9%
1	E	242	17% 57% 31% 5% 7%

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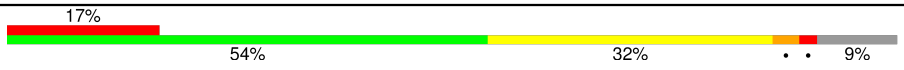
Mol	Chain	Length	Quality of chain
1	F	242	

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
2	XE	A	7	-	-	X	-
2	XE	D	11	-	-	X	-
2	XE	D	14	-	-	X	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 11851 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 Tail needle protein gp26.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	233	Total	C	N	O	S	0	0	0
			1738	1065	311	360	2			
1	B	242	Total	C	N	O	S	0	0	0
			1800	1103	325	370	2			
1	C	233	Total	C	N	O	S	0	0	0
			1735	1063	311	359	2			
1	D	221	Total	C	N	O	S	0	0	0
			1645	1009	297	337	2			
1	E	226	Total	C	N	O	S	0	0	0
			1681	1029	307	343	2			
1	F	221	Total	C	N	O	S	0	0	0
			1644	1005	298	339	2			

There are 66 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	992	GLY	-	EXPRESSION TAG	UNP P35837
A	993	ALA	-	EXPRESSION TAG	UNP P35837
A	994	LEU	-	EXPRESSION TAG	UNP P35837
A	995	VAL	-	EXPRESSION TAG	UNP P35837
A	996	PRO	-	EXPRESSION TAG	UNP P35837
A	997	ARG	-	EXPRESSION TAG	UNP P35837
A	998	GLY	-	EXPRESSION TAG	UNP P35837
A	999	SER	-	EXPRESSION TAG	UNP P35837
A	1000	HIS	-	EXPRESSION TAG	UNP P35837
A	1169	VAL	LEU	ENGINEERED	UNP P35837
A	1222	MET	LEU	ENGINEERED	UNP P35837
B	992	GLY	-	EXPRESSION TAG	UNP P35837
B	993	ALA	-	EXPRESSION TAG	UNP P35837
B	994	LEU	-	EXPRESSION TAG	UNP P35837
B	995	VAL	-	EXPRESSION TAG	UNP P35837
B	996	PRO	-	EXPRESSION TAG	UNP P35837
B	997	ARG	-	EXPRESSION TAG	UNP P35837

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Chain	Residue	Modelled	Actual	Comment	Reference
B	998	GLY	-	EXPRESSION TAG	UNP P35837
B	999	SER	-	EXPRESSION TAG	UNP P35837
B	1000	HIS	-	EXPRESSION TAG	UNP P35837
B	1169	VAL	LEU	ENGINEERED	UNP P35837
B	1222	MET	LEU	ENGINEERED	UNP P35837
C	992	GLY	-	EXPRESSION TAG	UNP P35837
C	993	ALA	-	EXPRESSION TAG	UNP P35837
C	994	LEU	-	EXPRESSION TAG	UNP P35837
C	995	VAL	-	EXPRESSION TAG	UNP P35837
C	996	PRO	-	EXPRESSION TAG	UNP P35837
C	997	ARG	-	EXPRESSION TAG	UNP P35837
C	998	GLY	-	EXPRESSION TAG	UNP P35837
C	999	SER	-	EXPRESSION TAG	UNP P35837
C	1000	HIS	-	EXPRESSION TAG	UNP P35837
C	1169	VAL	LEU	ENGINEERED	UNP P35837
C	1222	MET	LEU	ENGINEERED	UNP P35837
D	992	GLY	-	EXPRESSION TAG	UNP P35837
D	993	ALA	-	EXPRESSION TAG	UNP P35837
D	994	LEU	-	EXPRESSION TAG	UNP P35837
D	995	VAL	-	EXPRESSION TAG	UNP P35837
D	996	PRO	-	EXPRESSION TAG	UNP P35837
D	997	ARG	-	EXPRESSION TAG	UNP P35837
D	998	GLY	-	EXPRESSION TAG	UNP P35837
D	999	SER	-	EXPRESSION TAG	UNP P35837
D	1000	HIS	-	EXPRESSION TAG	UNP P35837
D	1169	VAL	LEU	ENGINEERED	UNP P35837
D	1222	MET	LEU	ENGINEERED	UNP P35837
E	992	GLY	-	EXPRESSION TAG	UNP P35837
E	993	ALA	-	EXPRESSION TAG	UNP P35837
E	994	LEU	-	EXPRESSION TAG	UNP P35837
E	995	VAL	-	EXPRESSION TAG	UNP P35837
E	996	PRO	-	EXPRESSION TAG	UNP P35837
E	997	ARG	-	EXPRESSION TAG	UNP P35837
E	998	GLY	-	EXPRESSION TAG	UNP P35837
E	999	SER	-	EXPRESSION TAG	UNP P35837
E	1000	HIS	-	EXPRESSION TAG	UNP P35837
E	1169	VAL	LEU	ENGINEERED	UNP P35837
E	1222	MET	LEU	ENGINEERED	UNP P35837
F	992	GLY	-	EXPRESSION TAG	UNP P35837
F	993	ALA	-	EXPRESSION TAG	UNP P35837
F	994	LEU	-	EXPRESSION TAG	UNP P35837
F	995	VAL	-	EXPRESSION TAG	UNP P35837

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Chain	Residue	Modelled	Actual	Comment	Reference
F	996	PRO	-	EXPRESSION TAG	UNP P35837
F	997	ARG	-	EXPRESSION TAG	UNP P35837
F	998	GLY	-	EXPRESSION TAG	UNP P35837
F	999	SER	-	EXPRESSION TAG	UNP P35837
F	1000	HIS	-	EXPRESSION TAG	UNP P35837
F	1169	VAL	LEU	ENGINEERED	UNP P35837
F	1222	MET	LEU	ENGINEERED	UNP P35837

- Molecule 2 is XENON (three-letter code: XE) (formula: Xe).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	6	Total Xe 6 6	0	0
2	D	6	Total Xe 6 6	0	0
2	C	1	Total Xe 1 1	0	0
2	F	1	Total Xe 1 1	0	0

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Ca 1 1	0	0
3	D	1	Total Ca 1 1	0	0

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Cl 1 1	0	0
4	D	1	Total Cl 1 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	266	Total O 266 266	0	0

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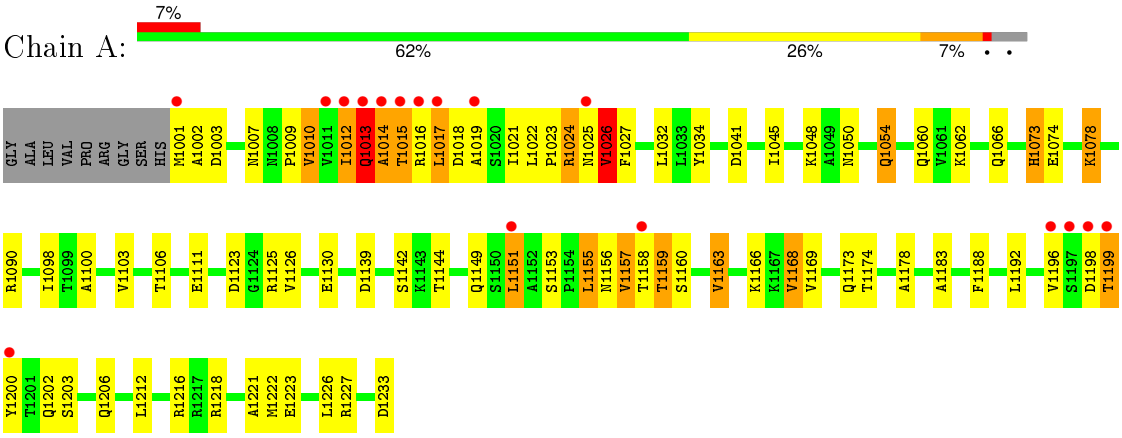
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	272	Total O 272 272	0	0
5	C	277	Total O 277 277	0	0
5	D	211	Total O 211 211	0	0
5	E	275	Total O 275 275	0	0
5	F	289	Total O 289 289	0	0

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.

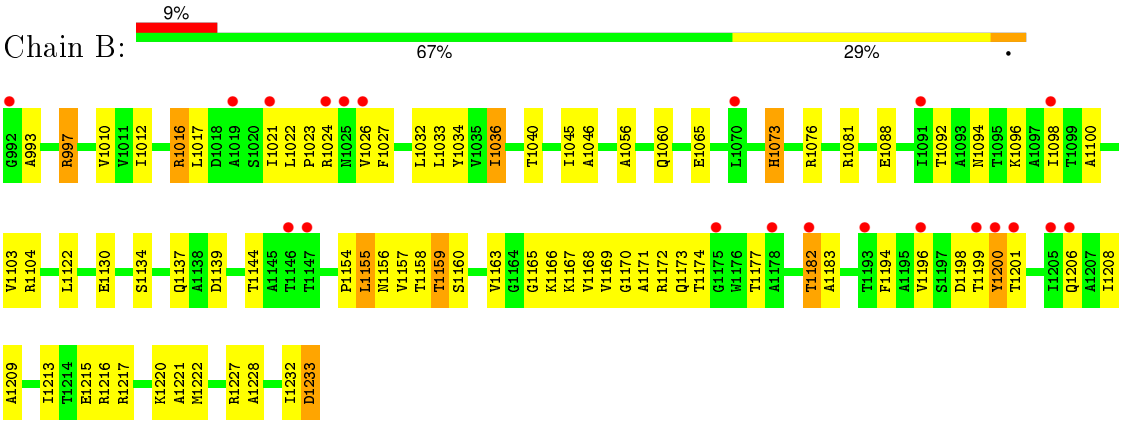
- Molecule 1: Tail needle protein gp26

Chain A:



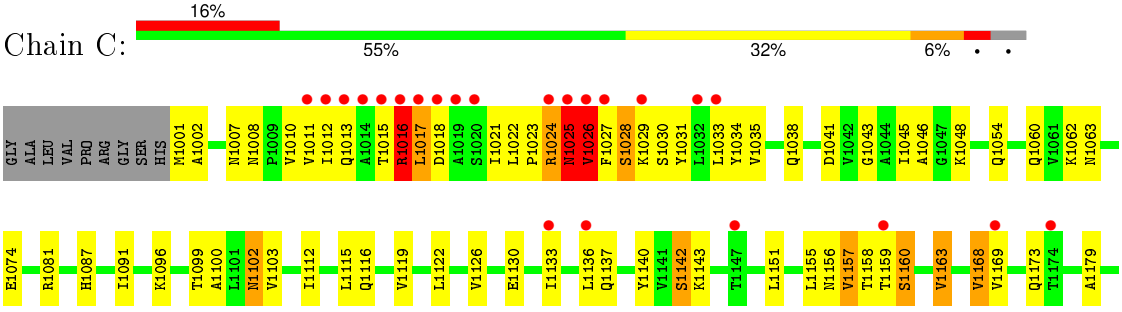
- Molecule 1: Tail needle protein gp26

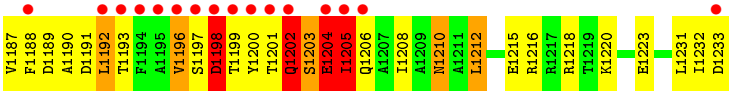
Chain B:



- Molecule 1: Tail needle protein gp26

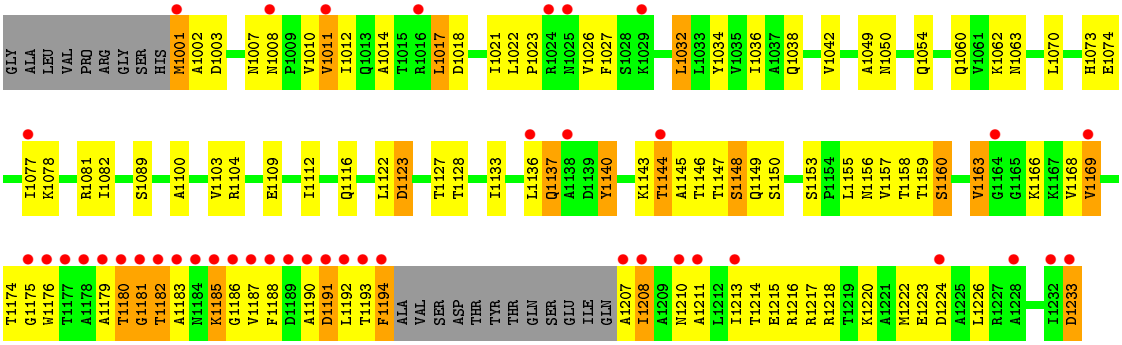
Chain C:





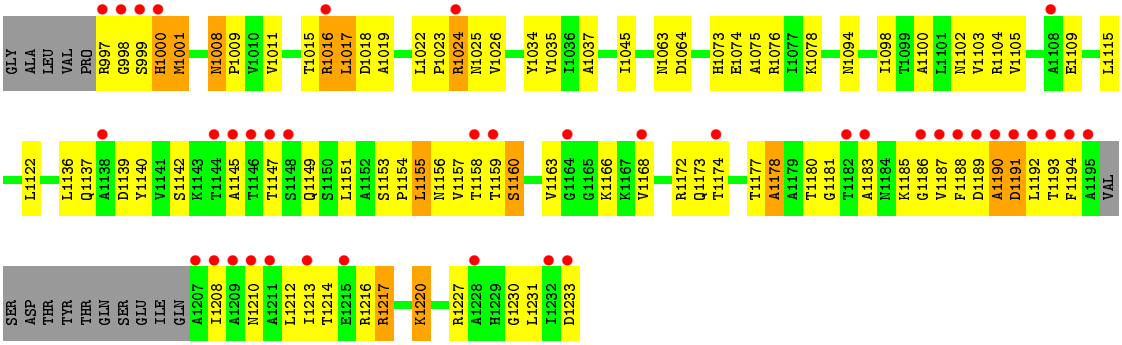
- Molecule 1: Tail needle protein gp26

Chain D:



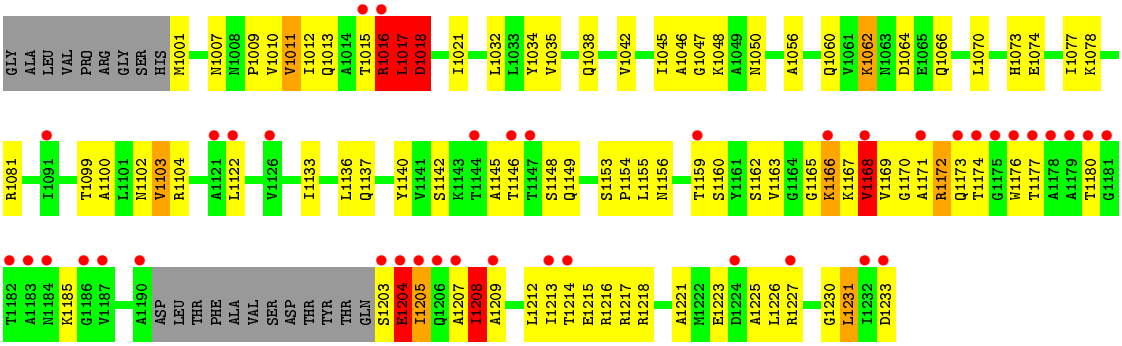
- Molecule 1: Tail needle protein gp26

Chain E:



- Molecule 1: Tail needle protein gp26

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	40.54Å 114.53Å 172.04Å 90.00° 91.01° 90.00°	Depositor
Resolution (Å)	20.00 – 1.95 14.99 – 1.95	Depositor EDS
% Data completeness (in resolution range)	92.5 (20.00-1.95) 91.5 (14.99-1.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	2.17 (at 1.95Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.234 , 0.269 0.247 , 0.280	Depositor DCC
R_{free} test set	5233 reflections (5.31%)	DCC
Wilson B-factor (Å^2)	21.8	Xtriage
Anisotropy	0.828	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 67.0	EDS
Estimated twinning fraction	0.028 for h,-k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Outliers	0 of 103760 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	11851	wwPDB-VP
Average B, all atoms (Å^2)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.95% 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: CA, CL, XE

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	0.34	0/1755	0.57	0/2387
1	B	0.34	0/1819	0.61	0/2474
1	C	0.33	0/1752	0.69	2/2382 (0.1%)
1	D	0.43	2/1660 (0.1%)	0.62	1/2255 (0.0%)
1	E	0.31	0/1697	0.59	0/2304
1	F	0.32	0/1658	0.58	0/2250
All	All	0.35	2/10341 (0.0%)	0.61	3/14052 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	1169	VAL	CA-CB	8.12	1.71	1.54
1	D	1169	VAL	C-O	5.01	1.32	1.23

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	1205	ILE	N-CA-C	-7.39	91.05	111.00
1	C	1198	ASP	CB-CA-C	6.78	123.95	110.40
1	D	1180	THR	N-CA-C	5.60	126.12	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1738	0	1728	122	0
1	B	1800	0	1791	102	0
1	C	1735	0	1722	145	0
1	D	1645	0	1643	145	0
1	E	1681	0	1676	108	0
1	F	1644	0	1642	124	0
2	A	6	0	0	2	0
2	C	1	0	0	1	0
2	D	6	0	0	4	0
2	F	1	0	0	0	0
3	A	1	0	0	0	0
3	D	1	0	0	0	0
4	A	1	0	0	0	0
4	D	1	0	0	0	0
5	A	266	0	0	13	0
5	B	272	0	0	7	0
5	C	277	0	0	16	0
5	D	211	0	0	12	0
5	E	275	0	0	15	0
5	F	289	0	0	19	0
All	All	11851	0	10202	590	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 29.

The worst 5 of 590 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:D:1193:THR:HG21	1:F:1216:ARG:CD	1.60	1.32
1:A:1199:THR:HB	5:A:1472:HOH:O	1.45	1.16
1:C:1024:ARG:H	1:C:1024:ARG:CD	1.64	1.07
1:D:1193:THR:CG2	1:F:1216:ARG:HD2	1.86	1.06
1:C:1024:ARG:H	1:C:1024:ARG:HD2	1.00	1.05

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	231/242 (96%)	219 (95%)	7 (3%)	5 (2%)	8 2
1	B	240/242 (99%)	231 (96%)	5 (2%)	4 (2%)	11 3
1	C	231/242 (96%)	206 (89%)	13 (6%)	12 (5%)	2 0
1	D	217/242 (90%)	197 (91%)	14 (6%)	6 (3%)	6 1
1	E	222/242 (92%)	208 (94%)	9 (4%)	5 (2%)	8 1
1	F	217/242 (90%)	205 (94%)	6 (3%)	6 (3%)	6 1
All	All	1358/1452 (94%)	1266 (93%)	54 (4%)	38 (3%)	6 1

5 of 38 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1014	ALA
1	A	1159	THR
1	A	1199	THR
1	B	1200	TYR
1	C	1016	ARG

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	184/190 (97%)	164 (89%)	20 (11%)	8 1
1	B	190/190 (100%)	180 (95%)	10 (5%)	28 13
1	C	183/190 (96%)	163 (89%)	20 (11%)	8 1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	D	173/190 (91%)	155 (90%)	18 (10%)	9 2
1	E	176/190 (93%)	160 (91%)	16 (9%)	12 3
1	F	173/190 (91%)	158 (91%)	15 (9%)	13 3
All	All	1079/1140 (95%)	980 (91%)	99 (9%)	11 3

5 of 99 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	1192	LEU
1	D	1140	TYR
1	F	1166	LYS
1	C	1204	GLU
1	D	1001	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 51 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	1156	ASN
1	D	1060	GLN
1	F	1118	ASN
1	C	1206	GLN
1	D	1073	HIS

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

Of 18 ligands modelled in this entry, 18 are 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	233/242 (96%)	0.63	17 (7%) 18 28	15, 33, 63, 99	0
1	B	242/242 (100%)	0.68	21 (8%) 13 20	10, 34, 60, 88	0
1	C	233/242 (96%)	0.97	39 (16%) 2 3	13, 33, 86, 112	0
1	D	221/242 (91%)	1.17	42 (19%) 2 2	18, 38, 80, 97	0
1	E	226/242 (93%)	1.05	40 (17%) 2 3	10, 37, 78, 98	0
1	F	221/242 (91%)	0.94	40 (18%) 2 2	18, 35, 73, 91	0
All	All	1376/1452 (94%)	0.90	199 (14%) 3 5	10, 35, 75, 112	0

The worst 5 of 199 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	998	GLY	11.0
1	D	1183	ALA	10.0
1	C	1201	THR	7.9
1	A	1013	GLN	7.8
1	F	1204	GLU	7.7

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

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands (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
4	CL	A	2	1/1	0.99	0.13	-0.67	28,28,28,28	0
4	CL	D	4	1/1	0.97	0.11	-0.88	33,33,33,33	0
2	XE	D	11	1/1	0.77	0.12	-1.06	121,121,121,121	0
3	CA	D	3	1/1	1.00	0.10	-1.12	23,23,23,23	0
3	CA	A	1	1/1	0.98	0.07	-2.55	21,21,21,21	0
2	XE	D	13	1/1	0.99	0.05	-2.68	35,35,35,35	0
2	XE	C	4	1/1	0.99	0.06	-2.89	73,73,73,73	0
2	XE	A	6	1/1	1.00	0.04	-3.08	31,31,31,31	0
2	XE	D	9	1/1	1.00	0.04	-3.11	32,32,32,32	0
2	XE	A	7	1/1	0.92	0.06	-3.39	96,96,96,96	0
2	XE	A	5	1/1	1.00	0.05	-3.55	33,33,33,33	0
2	XE	A	1234	1/1	0.99	0.05	-5.01	59,59,59,59	0
2	XE	F	10	1/1	0.94	0.04	-5.68	65,65,65,65	0
2	XE	D	8	1/1	0.99	0.02	-6.47	33,33,33,33	0
2	XE	A	1235	1/1	1.00	0.05	-6.85	34,34,34,34	0
2	XE	D	12	1/1	0.99	0.02	-7.67	35,35,35,35	0
2	XE	A	3	1/1	1.00	0.03	-9.10	39,39,39,39	0
2	XE	D	14	1/1	0.75	0.12	-	122,122,122,122	0

6.5 Other polymers (i)

There are no such residues in this entry.