wwPDB X-ray Structure Validation Summary Report (i)

Mar 5, 2026 – 10:30 PM UTC

PDB ID	:	4BWY / pdb_00004bwy
Title	:	P4 PROTEIN FROM BACTERIOPHAGE PHI8 (R32)
Authors	:	El Omari, K.; Meier, C.; Kainov, D.; Sutton, G.; Grimes, J.M.; Poranen, M.M.; Bamford, D.H.; Tuma, R.; Stuart, D.I.; Mancini, E.J.
Deposited on	:	2013-07-05
Resolution	:	3.10 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
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 (1)) were used in the production of this report:

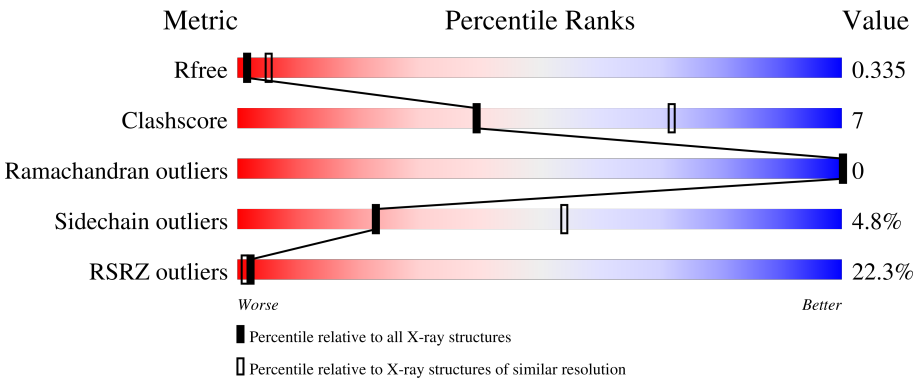
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

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 3.10 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}	180053	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

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	321	10% 76% 12% • 10%
1	B	321	17% 76% 13% • 10%
1	C	321	16% 75% 13% • 10%
1	D	321	31% 75% 13% • 10%
1	E	321	27% 69% 12% • 18%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	321	19% 75% 12% • 10%
1	G	321	12% 76% 12% • 10%
1	H	321	18% 74% 15% • 10%
1	I	321	13% 76% 13% • 10%
1	J	321	23% 77% 12% • 10%
1	K	321	33% 76% 12% • 10%
1	L	321	21% 76% 13% • 10%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 25719 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 P4.

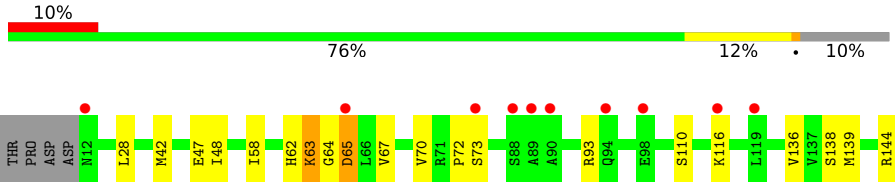
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	288	2158	1347	386	415	10	0	0	0
1	B	288	2158	1347	386	415	10	0	0	0
1	C	288	2158	1347	386	415	10	0	0	0
1	D	288	2158	1347	386	415	10	0	0	0
1	E	264	1981	1233	357	381	10	0	0	0
1	F	288	2158	1347	386	415	10	0	0	0
1	G	288	2158	1347	386	415	10	0	0	0
1	H	288	2158	1347	386	415	10	0	0	0
1	I	288	2158	1347	386	415	10	0	0	0
1	J	288	2158	1347	386	415	10	0	0	0
1	K	288	2158	1347	386	415	10	0	0	0
1	L	288	2158	1347	386	415	10	0	0	0

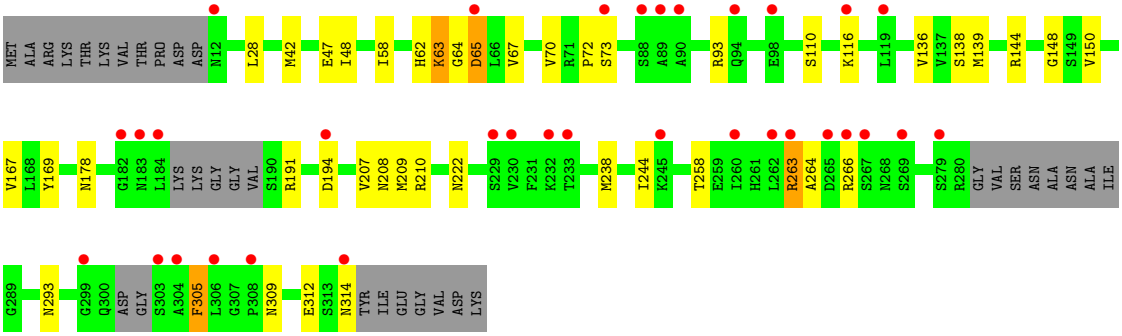
3 Residue-property plots (i)

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: P4

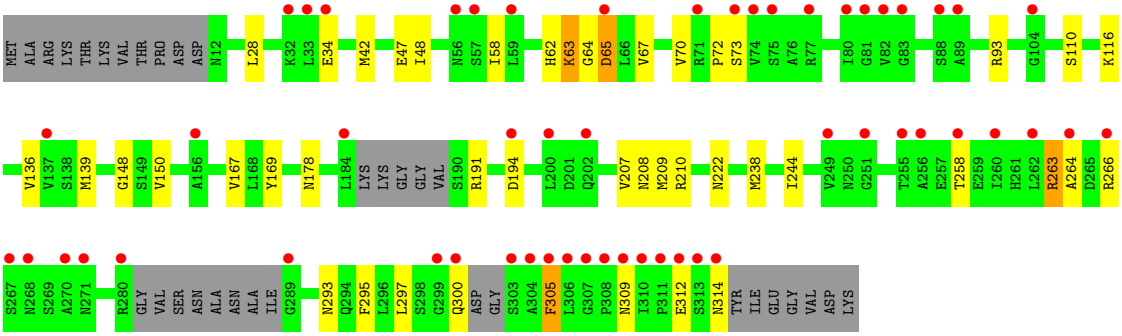
Chain A:





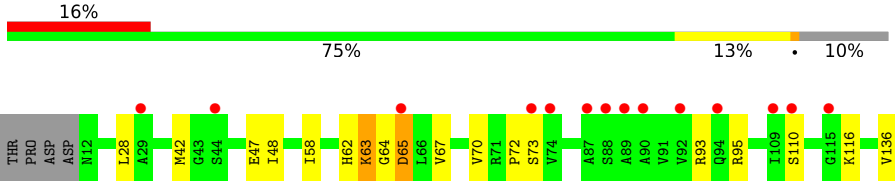
- Molecule 1: P4

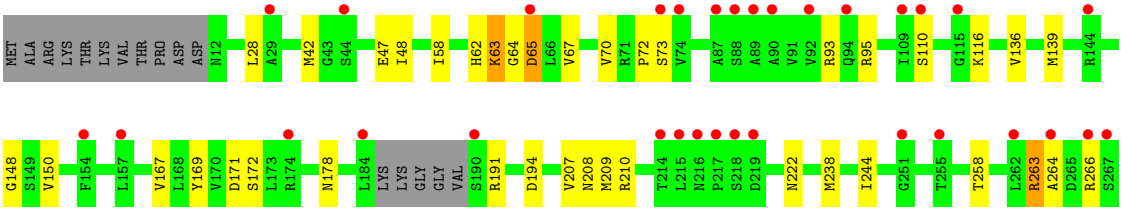
Chain B:

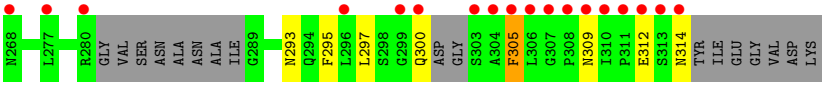


- Molecule 1: P4

Chain C:

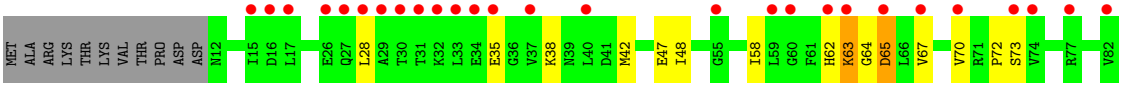


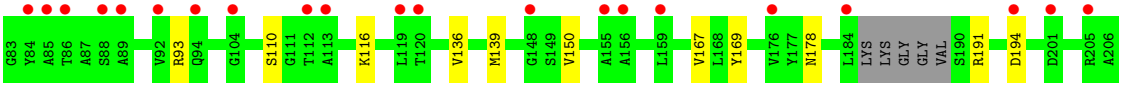


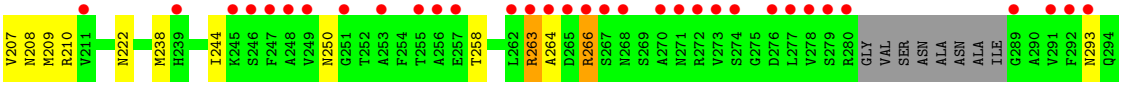


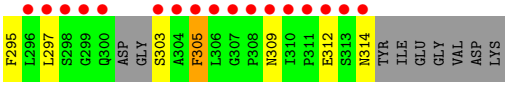
- Molecule 1: P4

Chain D:



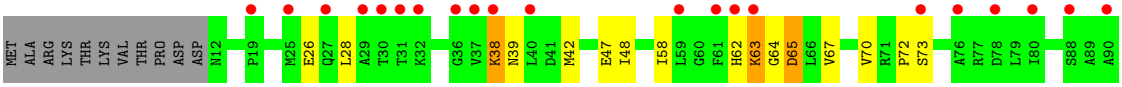


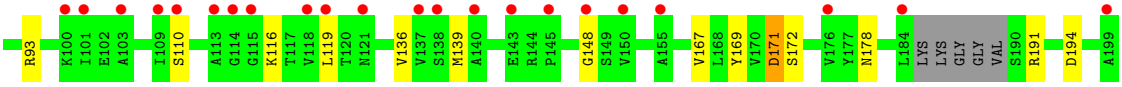


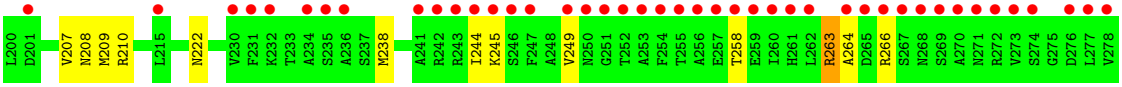


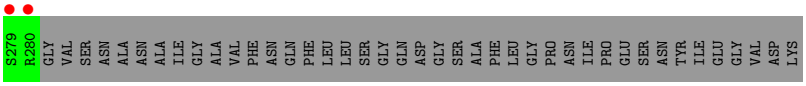
- Molecule 1: P4

Chain E:



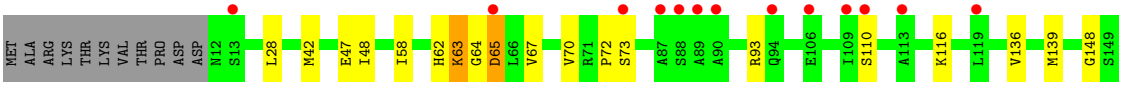


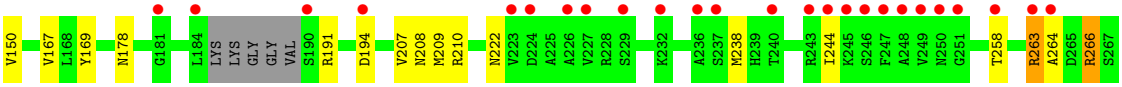


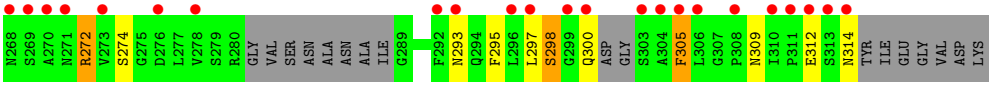


- Molecule 1: P4

Chain F:

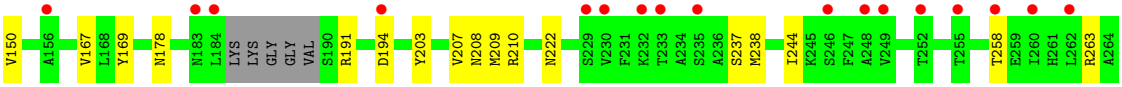


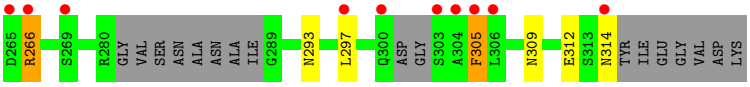




• Molecule 1: P4

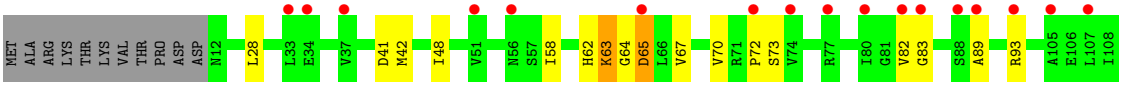
Chain G:

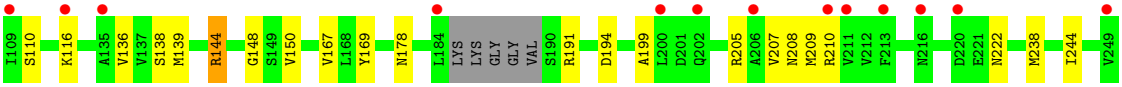


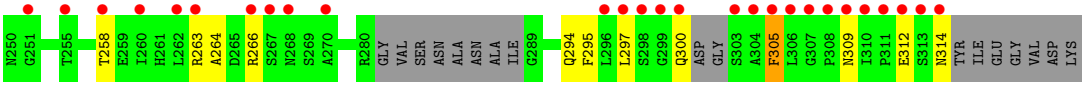


• Molecule 1: P4

Chain H:

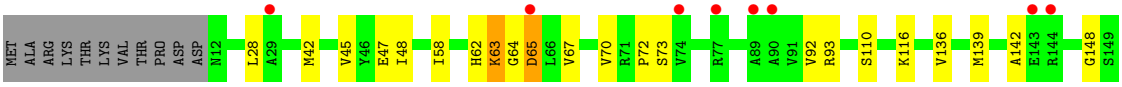


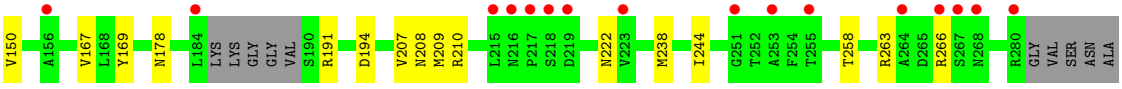


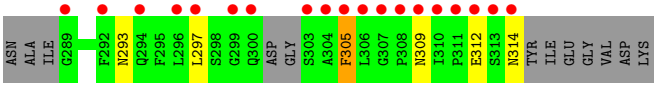


• Molecule 1: P4

Chain I:

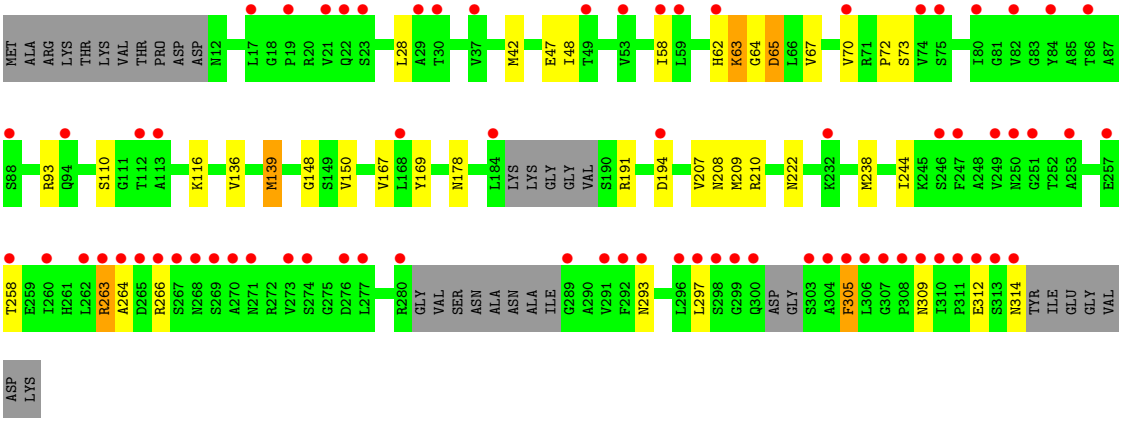






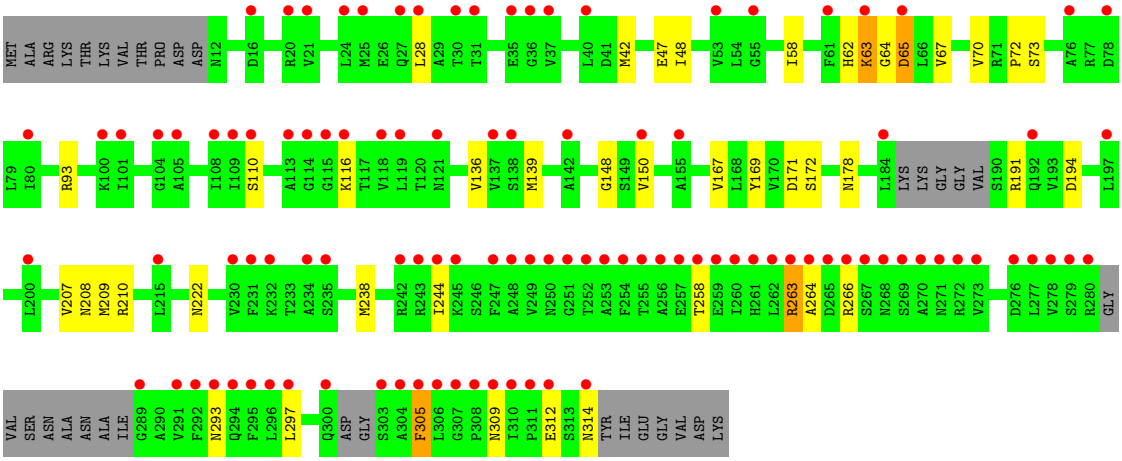
• Molecule 1: P4

Chain J:



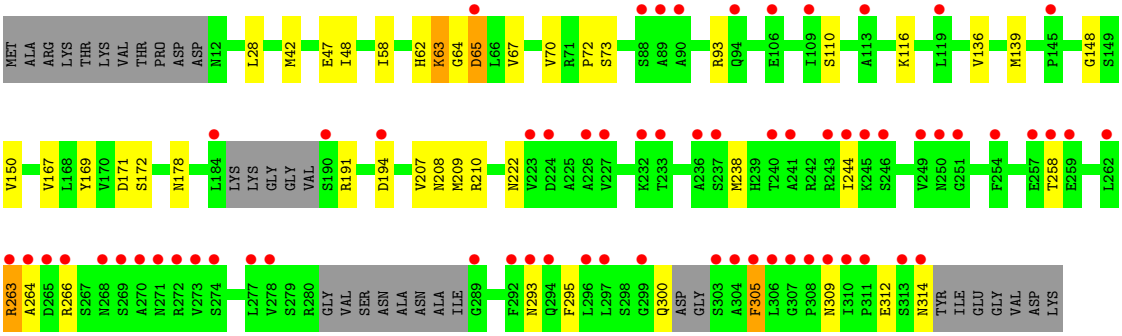
- Molecule 1: P4

Chain K:



- Molecule 1: P4

Chain L:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α, β, γ	197.72Å 197.72Å 562.58Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	45.39 – 3.10 45.39 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.9 (45.39-3.10) 99.8 (45.39-3.10)	Depositor EDS
R_{merge}	0.31	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.61 (at 3.12Å)	Xtriage
Refinement program	BUSTER 2.11.4	Depositor
R, R_{free}	0.295 , 0.309 0.319 , 0.335	Depositor DCC
R_{free} test set	3870 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	60.1	Xtriage
Anisotropy	0.040	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 41.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.82	EDS
Total number of atoms	25719	wwPDB-VP
Average B, all atoms (Å^2)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 27.16 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.3095e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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	0.73	0/2183	1.32	9/2951 (0.3%)
1	B	0.74	0/2183	1.33	9/2951 (0.3%)
1	C	0.74	0/2183	1.32	9/2951 (0.3%)
1	D	0.75	0/2183	1.33	11/2951 (0.4%)
1	E	0.76	1/2003 (0.0%)	1.33	7/2709 (0.3%)
1	F	0.74	0/2183	1.32	9/2951 (0.3%)
1	G	0.73	0/2183	1.33	9/2951 (0.3%)
1	H	0.74	0/2183	1.33	7/2951 (0.2%)
1	I	0.74	0/2183	1.33	9/2951 (0.3%)
1	J	0.75	0/2183	1.32	11/2951 (0.4%)
1	K	0.75	0/2183	1.33	9/2951 (0.3%)
1	L	0.74	0/2183	1.32	9/2951 (0.3%)
All	All	0.74	1/26016 (0.0%)	1.33	108/35170 (0.3%)

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
1	B	0	1
1	C	0	1
1	D	0	1
1	E	0	1
1	F	0	1
1	G	0	1
1	H	0	1
1	I	0	1
1	J	0	1
1	K	0	1
1	L	0	1
All	All	0	12

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	249	VAL	C-N	5.54	1.44	1.34

The worst 5 of 108 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	J	305	PHE	CA-CB-CG	6.81	120.61	113.80
1	I	305	PHE	CA-CB-CG	6.77	120.57	113.80
1	A	305	PHE	CA-CB-CG	6.76	120.56	113.80
1	C	305	PHE	CA-CB-CG	6.75	120.55	113.80
1	K	305	PHE	CA-CB-CG	6.73	120.53	113.80

There are no chirality outliers.

5 of 12 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	65	ASP	Peptide
1	B	65	ASP	Peptide
1	C	65	ASP	Peptide
1	D	65	ASP	Peptide
1	E	65	ASP	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	2158	0	2181	26	0
1	B	2158	0	2181	29	0
1	C	2158	0	2181	29	1
1	D	2158	0	2181	31	5
1	E	1981	0	2015	29	2
1	F	2158	0	2181	32	3
1	G	2158	0	2181	31	0
1	H	2158	0	2181	50	1
1	I	2158	0	2181	32	0
1	J	2158	0	2181	26	0
1	K	2158	0	2181	27	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	L	2158	0	2181	27	0
All	All	25719	0	26006	347	6

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 7.

The worst 5 of 347 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:H:205:ARG:NH1	1:H:263:ARG:NH2	1.80	1.27
1:H:82:VAL:HG21	1:H:199:ALA:HB2	1.36	1.04
1:H:205:ARG:HH12	1:H:263:ARG:HH22	1.00	0.99
1:H:82:VAL:HG21	1:H:199:ALA:CB	1.94	0.97
1:A:138:SER:HB3	1:A:144:ARG:HG2	1.48	0.96

The worst 5 of 6 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:250:ASN:ND2	1:F:272:ARG:NH2[4_555]	0.76	1.44
1:D:266:ARG:NH1	1:E:245:LYS:NZ[4_555]	1.49	0.71
1:D:250:ASN:CG	1:F:272:ARG:NH2[4_555]	1.65	0.55
1:D:250:ASN:ND2	1:F:272:ARG:CZ[4_555]	1.89	0.31
1:D:266:ARG:CZ	1:E:245:LYS:NZ[4_555]	1.99	0.21

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	280/321 (87%)	269 (96%)	11 (4%)	0	100	100
1	B	280/321 (87%)	269 (96%)	11 (4%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	280/321 (87%)	269 (96%)	11 (4%)	0	100	100
1	D	280/321 (87%)	269 (96%)	11 (4%)	0	100	100
1	E	260/321 (81%)	250 (96%)	10 (4%)	0	100	100
1	F	280/321 (87%)	269 (96%)	11 (4%)	0	100	100
1	G	280/321 (87%)	269 (96%)	11 (4%)	0	100	100
1	H	280/321 (87%)	269 (96%)	11 (4%)	0	100	100
1	I	280/321 (87%)	269 (96%)	11 (4%)	0	100	100
1	J	280/321 (87%)	269 (96%)	11 (4%)	0	100	100
1	K	280/321 (87%)	269 (96%)	11 (4%)	0	100	100
1	L	280/321 (87%)	269 (96%)	11 (4%)	0	100	100
All	All	3340/3852 (87%)	3209 (96%)	131 (4%)	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	232/257 (90%)	221 (95%)	11 (5%)	23	55
1	B	232/257 (90%)	221 (95%)	11 (5%)	23	55
1	C	232/257 (90%)	221 (95%)	11 (5%)	23	55
1	D	232/257 (90%)	221 (95%)	11 (5%)	23	55
1	E	213/257 (83%)	203 (95%)	10 (5%)	23	55
1	F	232/257 (90%)	219 (94%)	13 (6%)	19	49
1	G	232/257 (90%)	221 (95%)	11 (5%)	23	55
1	H	232/257 (90%)	221 (95%)	11 (5%)	23	55
1	I	232/257 (90%)	221 (95%)	11 (5%)	23	55
1	J	232/257 (90%)	221 (95%)	11 (5%)	23	55
1	K	232/257 (90%)	221 (95%)	11 (5%)	23	55

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	L	232/257 (90%)	221 (95%)	11 (5%)	23	55
All	All	2765/3084 (90%)	2632 (95%)	133 (5%)	23	54

5 of 133 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	K	194	ASP
1	K	305	PHE
1	L	305	PHE
1	E	116	LYS
1	E	73	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 47 such sidechains are listed below:

Mol	Chain	Res	Type
1	H	39	ASN
1	I	271	ASN
1	H	122	HIS
1	H	309	ASN
1	I	314	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 oligosaccharides 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	288/321 (89%)	0.93	33 (11%)	9	5	34, 53, 78, 109	0
1	B	288/321 (89%)	1.33	54 (18%)	3	1	39, 61, 99, 124	0
1	C	288/321 (89%)	1.19	50 (17%)	4	2	29, 54, 102, 137	0
1	D	288/321 (89%)	1.72	98 (34%)	1	0	40, 69, 120, 155	0
1	E	264/321 (82%)	1.69	88 (33%)	1	0	44, 70, 109, 135	0
1	F	288/321 (89%)	1.26	61 (21%)	2	1	41, 59, 100, 137	0
1	G	288/321 (89%)	0.97	38 (13%)	7	4	32, 53, 85, 127	0
1	H	288/321 (89%)	1.32	57 (19%)	3	1	36, 58, 102, 149	0
1	I	288/321 (89%)	1.20	43 (14%)	5	3	35, 55, 112, 156	0
1	J	288/321 (89%)	1.56	73 (25%)	1	1	36, 68, 119, 152	0
1	K	288/321 (89%)	1.85	106 (36%)	1	0	44, 75, 123, 162	0
1	L	288/321 (89%)	1.26	66 (22%)	2	1	40, 61, 119, 147	0
All	All	3432/3852 (89%)	1.35	767 (22%)	2	1	29, 61, 110, 162	0

The worst 5 of 767 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	310	ILE	7.5
1	C	310	ILE	7.0
1	K	314	ASN	6.8
1	I	306	LEU	6.6
1	J	303	SER	6.5

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 oligosaccharides 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.