wwPDB X-ray Structure Validation Summary Report (i)

Aug 20, 2020 – 05:22 PM BST

PDB ID	:	5CDW
Title	:	Crystal Structure Analysis of a mutant Grb2 SH2 domain (W121G) with a pYVNV peptide
Authors	:	Papaioannou, D.; Geibel, S.; Kunze, M.; Kay, C.; Waksman, G.
Deposited on	:	2015-07-05
Resolution	:	2.60 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 following versions of software and data (see references (1)) were used in the production of this report:

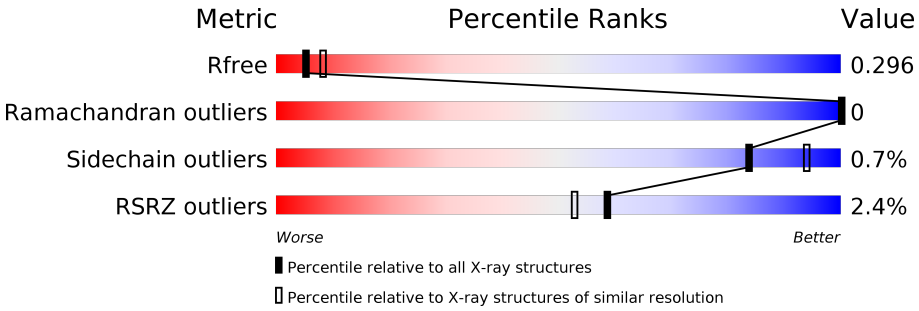
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13

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 2.60 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	3163 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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 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	100	2% 97%
1	B	100	% 100%
1	C	100	3% 99%
1	E	100	99%
1	G	100	3% 100%
1	H	100	4% 96%
1	K	100	6% 100%

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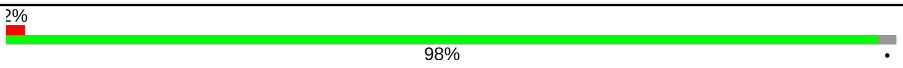
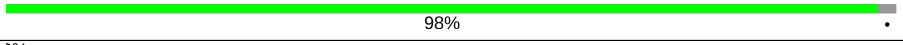
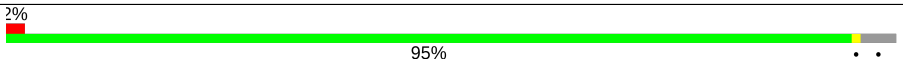
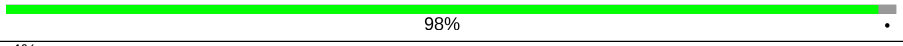
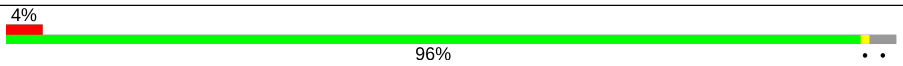
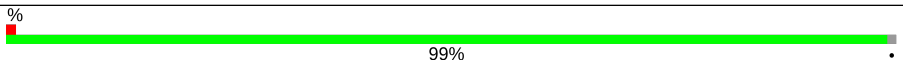
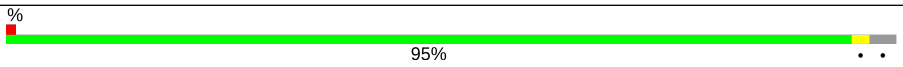
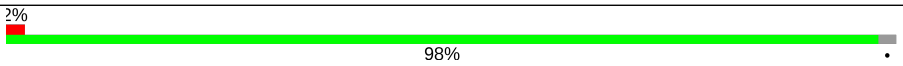
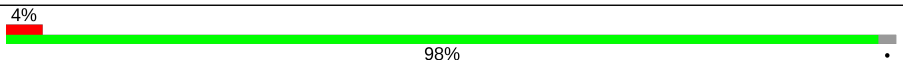
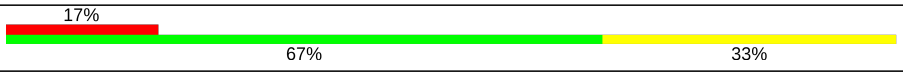
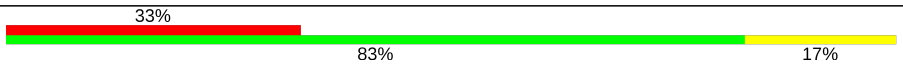
Mol	Chain	Length	Quality of chain
1	L	100	
1	O	100	
1	P	100	
1	U	100	
1	V	100	
1	Y	100	
1	Z	100	
1	c	100	
1	d	100	
2	D	6	
2	F	6	
2	I	6	
2	J	6	
2	M	6	
2	N	6	
2	Q	6	
2	R	6	
2	T	6	
2	X	6	
2	a	6	
2	b	6	
2	f	6	
2	h	6	
2	j	6	
2	s	6	

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 25334 atoms, of which 12144 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 Growth factor receptor-bound protein 2.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
1	A	98	Total C H N O S 1527 500 746 140 140 1	0	0	0
1	E	99	Total C H N O 1494 496 720 138 140	0	0	0
1	B	100	Total C H N O S 1585 516 775 145 147 2	0	0	0
1	C	99	Total C H N O S 1516 500 733 139 143 1	0	0	0
1	G	100	Total C H N O S 1531 504 739 142 144 2	0	0	0
1	H	97	Total C H N O 1475 489 714 134 138	0	0	0
1	K	100	Total C H N O S 1457 490 691 134 141 1	0	0	0
1	L	98	Total C H N O S 1457 489 698 132 137 1	0	0	0
1	O	98	Total C H N O S 1507 496 728 140 142 1	0	0	0
1	P	96	Total C H N O 1466 485 711 135 135	0	0	0
1	U	98	Total C H N O S 1505 496 728 138 142 1	0	0	0
1	V	97	Total C H N O S 1481 490 719 136 135 1	0	0	0
1	Y	99	Total C H N O S 1527 502 741 142 141 1	0	0	0
1	Z	97	Total C H N O S 1457 485 702 134 135 1	0	0	0
1	c	98	Total C H N O S 1413 479 669 127 137 1	0	0	0
1	d	98	Total C H N O 1430 482 681 130 137	0	0	0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	69	GLY	TRP	engineered mutation	UNP P62993
E	69	GLY	TRP	engineered mutation	UNP P62993
B	69	GLY	TRP	engineered mutation	UNP P62993
C	69	GLY	TRP	engineered mutation	UNP P62993
G	69	GLY	TRP	engineered mutation	UNP P62993
H	69	GLY	TRP	engineered mutation	UNP P62993
K	69	GLY	TRP	engineered mutation	UNP P62993
L	69	GLY	TRP	engineered mutation	UNP P62993
O	69	GLY	TRP	engineered mutation	UNP P62993
P	69	GLY	TRP	engineered mutation	UNP P62993
U	69	GLY	TRP	engineered mutation	UNP P62993
V	69	GLY	TRP	engineered mutation	UNP P62993
Y	69	GLY	TRP	engineered mutation	UNP P62993
Z	69	GLY	TRP	engineered mutation	UNP P62993
c	69	GLY	TRP	engineered mutation	UNP P62993
d	69	GLY	TRP	engineered mutation	UNP P62993

- Molecule 2 is a protein called SER-PTR-VAL-ASN-VAL-GLN.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	D	5	Total	C	H	N	O	P	0	0	0
			82	26	38	6	11	1			
2	M	5	Total	C	H	N	O	P	0	0	0
			82	26	38	6	11	1			
2	s	5	Total	C	H	N	O	P	0	0	0
			79	26	35	6	11	1			
2	a	6	Total	C	H	N	O	P	0	0	0
			98	31	46	8	12	1			
2	F	5	Total	C	H	N	O	P	0	0	0
			82	26	38	6	11	1			
2	J	6	Total	C	H	N	O	P	0	0	0
			99	31	46	8	13	1			
2	N	5	Total	C	H	N	O	P	0	0	0
			82	26	38	6	11	1			
2	R	6	Total	C	H	N	O	P	0	0	0
			99	31	46	8	13	1			
2	T	6	Total	C	H	N	O	P	0	0	0
			89	29	40	7	12	1			
2	X	6	Total	C	H	N	O	P	0	0	0
			89	29	40	7	12	1			
2	b	5	Total	C	H	N	O	P	0	0	0
			82	26	38	6	11	1			

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	f	5	Total	C	H	N	O	P	0	0	0
			82	26	38	6	11	1			
2	h	6	Total	C	H	N	O	P	0	0	0
			99	31	46	8	13	1			
2	j	5	Total	C	H	N	O	P	0	0	0
			82	26	38	6	11	1			
2	I	6	Total	C	H	N	O	P	0	0	0
			99	31	46	8	13	1			
2	Q	5	Total	C	H	N	O	P	0	0	0
			82	26	38	6	11	1			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	4	Total	O	0	0
			4	4		
3	E	9	Total	O	0	0
			9	9		
3	B	5	Total	O	0	0
			5	5		
3	C	10	Total	O	0	0
			10	10		
3	G	3	Total	O	0	0
			3	3		
3	H	4	Total	O	0	0
			4	4		
3	K	3	Total	O	0	0
			3	3		
3	L	5	Total	O	0	0
			5	5		
3	O	7	Total	O	0	0
			7	7		
3	P	12	Total	O	0	0
			12	12		
3	U	6	Total	O	0	0
			6	6		
3	V	6	Total	O	0	0
			6	6		
3	Y	7	Total	O	0	0
			7	7		
3	Z	7	Total	O	0	0
			7	7		

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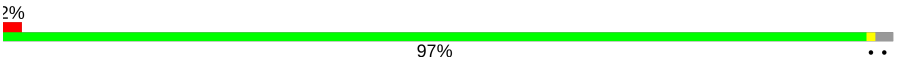
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	c	4	Total O 4 4	0	0
3	d	4	Total O 4 4	0	0
3	b	1	Total O 1 1	0	0
3	f	1	Total O 1 1	0	0
3	j	1	Total O 1 1	0	0

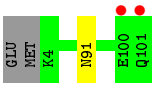
3 Residue-property plots

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: Growth factor receptor-bound protein 2

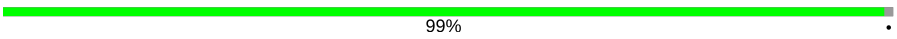
Chain A:





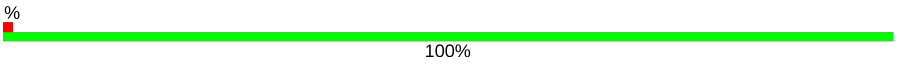
- Molecule 1: Growth factor receptor-bound protein 2

Chain E:



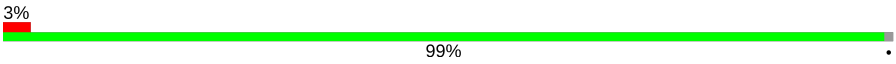
- Molecule 1: Growth factor receptor-bound protein 2

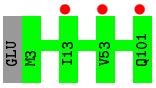
Chain B:



- Molecule 1: Growth factor receptor-bound protein 2

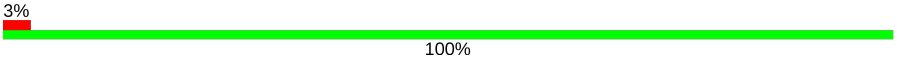
Chain C:

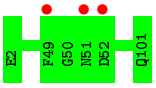




- Molecule 1: Growth factor receptor-bound protein 2

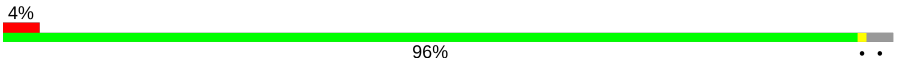
Chain G:

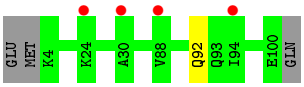




- Molecule 1: Growth factor receptor-bound protein 2

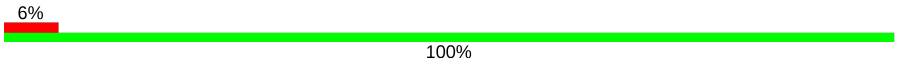
Chain H:

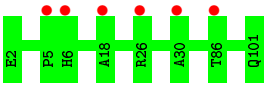




• Molecule 1: Growth factor receptor-bound protein 2

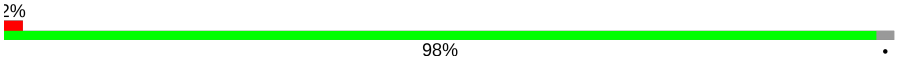
Chain K:

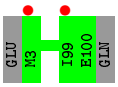




• Molecule 1: Growth factor receptor-bound protein 2

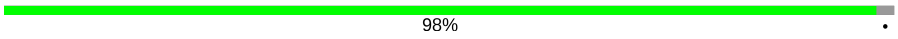
Chain L:





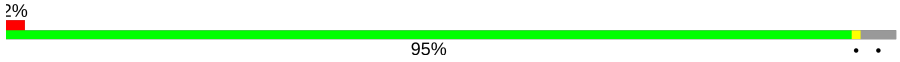
• Molecule 1: Growth factor receptor-bound protein 2

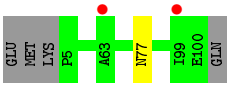
Chain O:



• Molecule 1: Growth factor receptor-bound protein 2

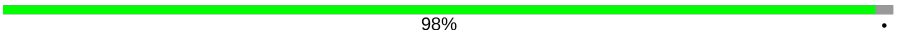
Chain P:





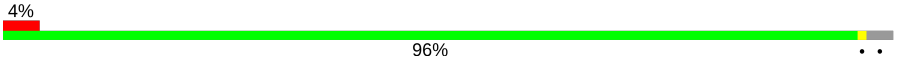
• Molecule 1: Growth factor receptor-bound protein 2

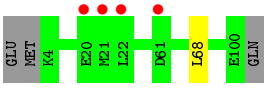
Chain U:



• Molecule 1: Growth factor receptor-bound protein 2

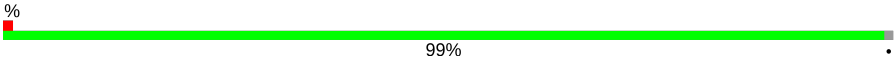
Chain V:

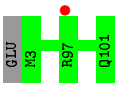




• Molecule 1: Growth factor receptor-bound protein 2

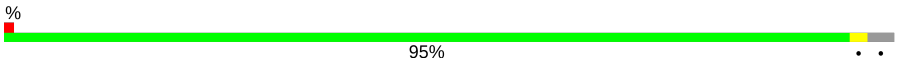
Chain Y:

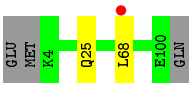




• Molecule 1: Growth factor receptor-bound protein 2

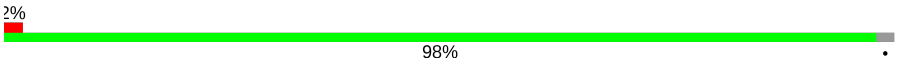
Chain Z:

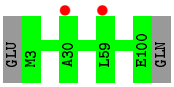




• Molecule 1: Growth factor receptor-bound protein 2

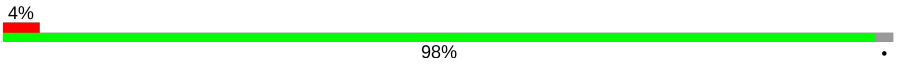
Chain c:





• Molecule 1: Growth factor receptor-bound protein 2

Chain d:



• Molecule 2: SER-PTR-VAL-ASN-VAL-GLN

Chain D:

• Molecule 2: SER-PTR-VAL-ASN-VAL-GLN

Chain M:

• Molecule 2: SER-PTR-VAL-ASN-VAL-GLN

Chain s:

• Molecule 2: SER-PTR-VAL-ASN-VAL-GLN

Chain a:

• Molecule 2: SER-PTR-VAL-ASN-VAL-GLN

Chain F:

• Molecule 2: SER-PTR-VAL-ASN-VAL-GLN

Chain J:

• Molecule 2: SER-PTR-VAL-ASN-VAL-GLN

Chain N:

• Molecule 2: SER-PTR-VAL-ASN-VAL-GLN

Chain R:

• Molecule 2: SER-PTR-VAL-ASN-VAL-GLN

Chain T:

• Molecule 2: SER-PTR-VAL-ASN-VAL-GLN

Chain X:

• Molecule 2: SER-PTR-VAL-ASN-VAL-GLN

Chain b:

• Molecule 2: SER-PTR-VAL-ASN-VAL-GLN

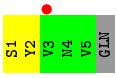
Chain f:

• Molecule 2: SER-PTR-VAL-ASN-VAL-GLN

Chain h:

• Molecule 2: SER-PTR-VAL-ASN-VAL-GLN

Chain j:



• Molecule 2: SER-PTR-VAL-ASN-VAL-GLN

Chain I:

• Molecule 2: SER-PTR-VAL-ASN-VAL-GLN

Chain Q:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	82.65Å 72.14Å 172.14Å 90.00° 93.31° 90.00°	Depositor
Resolution (Å)	41.26 – 2.60 41.26 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.0 (41.26-2.60) 99.2 (41.26-2.60)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.56 (at 2.61Å)	Xtriage
Refinement program	PHENIX 1.8.4_1496	Depositor
R, R_{free}	0.236 , 0.294 0.245 , 0.296	Depositor DCC
R_{free} test set	3103 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	46.0	Xtriage
Anisotropy	1.023	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.40 , 46.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	25334	wwPDB-VP
Average B, all atoms (Å^2)	63.0	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 26.64 % 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 2.5401e-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

5.1 Standard geometry

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

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	0.22	0/801	0.36	0/1078
1	B	0.22	0/830	0.36	0/1115
1	C	0.22	0/803	0.35	0/1083
1	E	0.22	0/794	0.35	0/1072
1	G	0.22	0/812	0.36	0/1095
1	H	0.22	0/781	0.36	0/1054
1	K	0.22	0/786	0.35	0/1065
1	L	0.21	0/779	0.34	0/1053
1	O	0.22	0/799	0.34	0/1078
1	P	0.22	0/775	0.36	0/1045
1	U	0.21	0/797	0.35	0/1075
1	V	0.23	0/782	0.35	0/1054
1	Y	0.22	0/806	0.36	0/1086
1	Z	0.23	0/775	0.39	0/1047
1	c	0.21	0/764	0.35	0/1036
1	d	0.22	0/769	0.35	0/1042
2	D	0.37	0/26	0.38	0/33
2	F	0.42	0/26	0.44	0/33
2	I	0.33	0/35	0.41	0/45
2	J	0.35	0/35	0.42	0/45
2	M	0.41	0/26	0.54	0/33
2	N	0.37	0/26	0.41	0/33
2	Q	0.38	0/26	0.45	0/33
2	R	0.33	0/35	0.36	0/45
2	T	0.36	0/31	0.36	0/40
2	X	0.35	0/31	0.38	0/40
2	a	0.36	0/34	0.39	0/44
2	b	0.37	0/26	0.40	0/33
2	f	0.37	0/26	0.41	0/33
2	h	0.33	0/35	0.41	0/45
2	j	0.36	0/26	0.43	0/33
2	s	0.23	0/26	0.48	0/33

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
All	All	0.23	0/13123	0.36	0/17679

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)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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	96/100 (96%)	94 (98%)	2 (2%)	0	100	100
1	B	98/100 (98%)	96 (98%)	2 (2%)	0	100	100
1	C	97/100 (97%)	94 (97%)	3 (3%)	0	100	100
1	E	97/100 (97%)	96 (99%)	1 (1%)	0	100	100
1	G	98/100 (98%)	92 (94%)	6 (6%)	0	100	100
1	H	95/100 (95%)	92 (97%)	3 (3%)	0	100	100
1	K	98/100 (98%)	91 (93%)	7 (7%)	0	100	100
1	L	96/100 (96%)	92 (96%)	4 (4%)	0	100	100
1	O	96/100 (96%)	93 (97%)	3 (3%)	0	100	100
1	P	94/100 (94%)	92 (98%)	2 (2%)	0	100	100
1	U	96/100 (96%)	96 (100%)	0	0	100	100
1	V	95/100 (95%)	95 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Y	97/100 (97%)	94 (97%)	3 (3%)	0	100	100
1	Z	95/100 (95%)	91 (96%)	4 (4%)	0	100	100
1	c	96/100 (96%)	92 (96%)	4 (4%)	0	100	100
1	d	96/100 (96%)	91 (95%)	5 (5%)	0	100	100
2	D	2/6 (33%)	1 (50%)	1 (50%)	0	100	100
2	F	2/6 (33%)	1 (50%)	1 (50%)	0	100	100
2	I	3/6 (50%)	3 (100%)	0	0	100	100
2	J	3/6 (50%)	3 (100%)	0	0	100	100
2	M	2/6 (33%)	1 (50%)	1 (50%)	0	100	100
2	N	2/6 (33%)	2 (100%)	0	0	100	100
2	Q	2/6 (33%)	2 (100%)	0	0	100	100
2	R	3/6 (50%)	3 (100%)	0	0	100	100
2	T	3/6 (50%)	3 (100%)	0	0	100	100
2	X	3/6 (50%)	3 (100%)	0	0	100	100
2	a	3/6 (50%)	2 (67%)	1 (33%)	0	100	100
2	b	2/6 (33%)	1 (50%)	1 (50%)	0	100	100
2	f	2/6 (33%)	1 (50%)	1 (50%)	0	100	100
2	h	3/6 (50%)	2 (67%)	1 (33%)	0	100	100
2	j	2/6 (33%)	1 (50%)	1 (50%)	0	100	100
2	s	2/6 (33%)	1 (50%)	1 (50%)	0	100	100
All	All	1579/1696 (93%)	1521 (96%)	58 (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	81/88 (92%)	80 (99%)	1 (1%)	71	87

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	85/88 (97%)	85 (100%)	0	100 100
1	C	81/88 (92%)	81 (100%)	0	100 100
1	E	78/88 (89%)	78 (100%)	0	100 100
1	G	81/88 (92%)	81 (100%)	0	100 100
1	H	78/88 (89%)	77 (99%)	1 (1%)	69 86
1	K	75/88 (85%)	75 (100%)	0	100 100
1	L	75/88 (85%)	75 (100%)	0	100 100
1	O	80/88 (91%)	80 (100%)	0	100 100
1	P	77/88 (88%)	76 (99%)	1 (1%)	69 86
1	U	80/88 (91%)	80 (100%)	0	100 100
1	V	78/88 (89%)	77 (99%)	1 (1%)	69 86
1	Y	80/88 (91%)	80 (100%)	0	100 100
1	Z	76/88 (86%)	74 (97%)	2 (3%)	46 72
1	c	72/88 (82%)	72 (100%)	0	100 100
1	d	74/88 (84%)	74 (100%)	0	100 100
2	D	4/5 (80%)	4 (100%)	0	100 100
2	F	4/5 (80%)	4 (100%)	0	100 100
2	I	5/5 (100%)	4 (80%)	1 (20%)	1 2
2	J	5/5 (100%)	5 (100%)	0	100 100
2	M	4/5 (80%)	4 (100%)	0	100 100
2	N	4/5 (80%)	4 (100%)	0	100 100
2	Q	4/5 (80%)	3 (75%)	1 (25%)	0 1
2	R	5/5 (100%)	5 (100%)	0	100 100
2	T	4/5 (80%)	4 (100%)	0	100 100
2	X	4/5 (80%)	4 (100%)	0	100 100
2	a	5/5 (100%)	5 (100%)	0	100 100
2	b	4/5 (80%)	4 (100%)	0	100 100
2	f	4/5 (80%)	4 (100%)	0	100 100
2	h	5/5 (100%)	5 (100%)	0	100 100
2	j	4/5 (80%)	3 (75%)	1 (25%)	0 1
2	s	4/5 (80%)	4 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1320/1488 (89%)	1311 (99%)	9 (1%)	84 94

5 of 9 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	Z	25	GLN
2	Q	5	VAL
2	j	1	SER
1	P	77	ASN
1	Z	68	LEU

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)

16 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	PTR	J	2	2	15,16,17	1.33	1 (6%)	19,22,24	0.53	0
2	PTR	j	2	2	15,16,17	1.37	1 (6%)	19,22,24	0.49	0
2	PTR	N	2	2	15,16,17	1.24	1 (6%)	19,22,24	0.58	0
2	PTR	M	2	2	15,16,17	1.35	1 (6%)	19,22,24	0.52	0
2	PTR	I	2	2	15,16,17	1.27	1 (6%)	19,22,24	0.56	0
2	PTR	b	2	2	15,16,17	1.35	1 (6%)	19,22,24	0.53	0
2	PTR	a	2	2	15,16,17	1.34	1 (6%)	19,22,24	0.52	0
2	PTR	D	2	2	15,16,17	1.36	1 (6%)	19,22,24	0.46	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	PTR	F	2	2	15,16,17	1.37	1 (6%)	19,22,24	0.61	0
2	PTR	X	2	2	15,16,17	1.25	1 (6%)	19,22,24	0.54	0
2	PTR	f	2	2	15,16,17	1.24	1 (6%)	19,22,24	0.57	0
2	PTR	R	2	2	15,16,17	1.35	1 (6%)	19,22,24	0.52	0
2	PTR	Q	2	2	15,16,17	1.27	1 (6%)	19,22,24	0.63	0
2	PTR	T	2	2	15,16,17	1.24	1 (6%)	19,22,24	0.54	0
2	PTR	s	1003	2	15,16,17	1.36	1 (6%)	19,22,24	0.51	0
2	PTR	h	2	2	15,16,17	1.38	1 (6%)	19,22,24	0.53	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
2	PTR	J	2	2	-	0/10/11/13	0/1/1/1
2	PTR	j	2	2	-	2/10/11/13	0/1/1/1
2	PTR	N	2	2	-	2/10/11/13	0/1/1/1
2	PTR	M	2	2	-	0/10/11/13	0/1/1/1
2	PTR	I	2	2	-	1/10/11/13	0/1/1/1
2	PTR	b	2	2	-	0/10/11/13	0/1/1/1
2	PTR	a	2	2	-	0/10/11/13	0/1/1/1
2	PTR	D	2	2	-	0/10/11/13	0/1/1/1
2	PTR	F	2	2	-	0/10/11/13	0/1/1/1
2	PTR	X	2	2	-	1/10/11/13	0/1/1/1
2	PTR	f	2	2	-	1/10/11/13	0/1/1/1
2	PTR	R	2	2	-	1/10/11/13	0/1/1/1
2	PTR	Q	2	2	-	2/10/11/13	0/1/1/1
2	PTR	T	2	2	-	1/10/11/13	0/1/1/1
2	PTR	s	1003	2	-	0/10/11/13	0/1/1/1
2	PTR	h	2	2	-	1/10/11/13	0/1/1/1

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	2	PTR	OH-CZ	-4.59	1.30	1.40
2	h	2	PTR	OH-CZ	-4.59	1.30	1.40
2	Q	2	PTR	OH-CZ	-4.55	1.30	1.40
2	I	2	PTR	OH-CZ	-4.52	1.30	1.40
2	j	2	PTR	OH-CZ	-4.49	1.30	1.40

There are no bond angle outliers.

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	j	2	PTR	O-C-CA-CB
2	N	2	PTR	O-C-CA-CB
2	R	2	PTR	O-C-CA-CB
2	h	2	PTR	O-C-CA-CB
2	I	2	PTR	CZ-OH-P-O1P

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)

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

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	98/100 (98%)	0.30	2 (2%) 65 60	46, 54, 62, 67	0
1	B	100/100 (100%)	0.38	1 (1%) 82 80	45, 52, 66, 106	0
1	C	99/100 (99%)	0.39	3 (3%) 50 43	45, 55, 68, 71	0
1	E	99/100 (99%)	0.26	0 100 100	44, 54, 67, 75	0
1	G	100/100 (100%)	0.46	3 (3%) 50 43	46, 63, 78, 85	0
1	H	97/100 (97%)	0.32	4 (4%) 37 30	46, 60, 74, 76	0
1	K	100/100 (100%)	0.67	6 (6%) 21 16	53, 62, 83, 93	0
1	L	98/100 (98%)	0.39	2 (2%) 65 60	51, 60, 72, 79	0
1	O	98/100 (98%)	0.23	0 100 100	43, 53, 59, 71	0
1	P	96/100 (96%)	0.36	2 (2%) 63 58	45, 52, 60, 64	0
1	U	98/100 (98%)	0.33	0 100 100	49, 60, 72, 80	0
1	V	97/100 (97%)	0.41	4 (4%) 37 30	48, 62, 72, 75	0
1	Y	99/100 (99%)	0.44	1 (1%) 82 80	48, 55, 69, 73	0
1	Z	97/100 (97%)	0.35	1 (1%) 82 80	49, 58, 72, 77	0
1	c	98/100 (98%)	0.31	2 (2%) 65 60	53, 63, 76, 80	0
1	d	98/100 (98%)	0.49	4 (4%) 37 30	51, 60, 73, 78	0
2	D	4/6 (66%)	0.94	0 100 100	53, 53, 54, 56	0
2	F	4/6 (66%)	0.54	0 100 100	56, 57, 59, 63	0
2	I	5/6 (83%)	1.46	1 (20%) 1 0	60, 60, 69, 79	0
2	J	5/6 (83%)	0.50	0 100 100	54, 55, 62, 64	0
2	M	4/6 (66%)	0.46	0 100 100	67, 68, 71, 75	0
2	N	4/6 (66%)	0.16	0 100 100	55, 56, 57, 69	0
2	Q	4/6 (66%)	0.22	0 100 100	62, 65, 65, 70	0
2	R	5/6 (83%)	0.54	0 100 100	54, 56, 62, 63	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
2	T	5/6 (83%)	0.33	0 100 100	53, 57, 62, 64	0
2	X	5/6 (83%)	0.06	0 100 100	55, 57, 62, 67	0
2	a	5/6 (83%)	0.47	0 100 100	52, 52, 54, 57	0
2	b	4/6 (66%)	0.50	0 100 100	51, 53, 57, 60	0
2	f	4/6 (66%)	0.11	0 100 100	49, 52, 54, 58	0
2	h	5/6 (83%)	1.48	2 (40%) 0 0	66, 67, 76, 87	0
2	j	4/6 (66%)	0.99	1 (25%) 0 0	64, 65, 67, 68	0
2	s	4/6 (66%)	0.27	0 100 100	53, 53, 59, 59	0
All	All	1643/1696 (96%)	0.39	39 (2%) 59 53	43, 57, 73, 106	0

The worst 5 of 39 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	51	ASN	5.6
2	I	6	GLN	5.1
1	B	2	GLU	4.5
1	K	26	ARG	4.0
2	h	6	GLN	3.8

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	PTR	M	2	16/17	0.92	0.19	62,70,84,86	0
2	PTR	F	2	16/17	0.92	0.20	58,60,72,72	0
2	PTR	Q	2	16/17	0.92	0.18	64,66,78,81	0
2	PTR	h	2	16/17	0.92	0.21	61,66,79,81	0
2	PTR	a	2	16/17	0.94	0.21	50,52,62,64	0
2	PTR	D	2	16/17	0.94	0.21	47,51,61,63	0
2	PTR	J	2	16/17	0.94	0.19	56,59,70,71	0
2	PTR	I	2	16/17	0.94	0.20	53,58,70,71	0
2	PTR	b	2	16/17	0.94	0.19	54,57,69,69	0
2	PTR	R	2	16/17	0.95	0.15	53,57,68,69	0
2	PTR	N	2	16/17	0.95	0.18	58,63,74,76	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	PTR	T	2	16/17	0.95	0.22	52,55,67,68	0
2	PTR	s	1003	16/17	0.95	0.17	50,53,64,64	0
2	PTR	f	2	16/17	0.95	0.19	51,55,65,65	0
2	PTR	j	2	16/17	0.96	0.19	60,63,75,76	0
2	PTR	X	2	16/17	0.96	0.18	55,57,69,69	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.