



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 9, 2023 – 08:17 PM EDT

PDB ID : 6XM1
Title : SM Protein Vps45 in Complex with Qa SNARE Tlg2
Authors : Jeffrey, P.D.; Eisemann, T.J.; Hughson, F.M.
Deposited on : 2020-06-29
Resolution : 2.80 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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
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

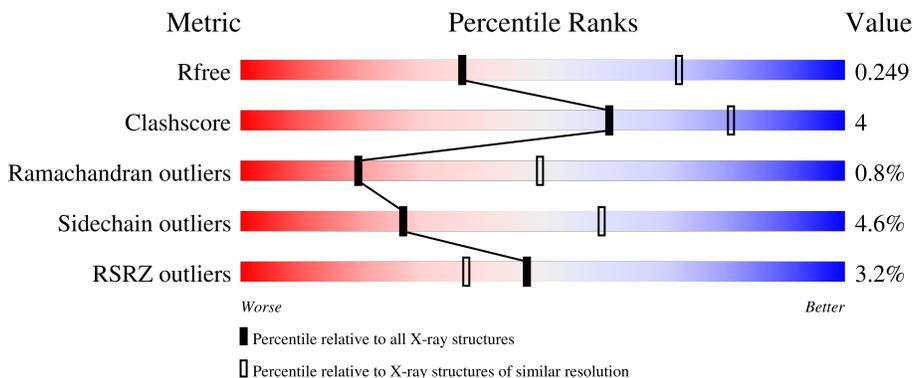
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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 $\leq 5\%$. 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	644	 76% 10% 14%
1	C	644	 78% 10% 11% 2%
2	B	284	 51% 11% 37% 6%
2	D	284	 52% 10% 36% 5%

2 Entry composition i

There are 3 unique types of molecules in this entry. The entry contains 11550 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 Vps45.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	556	4390	2789	769	814	18	0	0	0
1	C	570	4478	2844	784	832	18	0	0	0

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	625	GLY	-	expression tag	UNP G0S539
A	626	ALA	-	expression tag	UNP G0S539
A	627	ALA	-	expression tag	UNP G0S539
A	628	ALA	-	expression tag	UNP G0S539
A	629	LEU	-	expression tag	UNP G0S539
A	630	VAL	-	expression tag	UNP G0S539
A	631	PRO	-	expression tag	UNP G0S539
A	632	ARG	-	expression tag	UNP G0S539
A	633	GLY	-	expression tag	UNP G0S539
A	634	SER	-	expression tag	UNP G0S539
A	635	ARG	-	expression tag	UNP G0S539
A	636	SER	-	expression tag	UNP G0S539
A	637	VAL	-	expression tag	UNP G0S539
A	638	ASP	-	expression tag	UNP G0S539
A	639	HIS	-	expression tag	UNP G0S539
A	640	HIS	-	expression tag	UNP G0S539
A	641	HIS	-	expression tag	UNP G0S539
A	642	HIS	-	expression tag	UNP G0S539
A	643	HIS	-	expression tag	UNP G0S539
A	644	HIS	-	expression tag	UNP G0S539
C	625	GLY	-	expression tag	UNP G0S539
C	626	ALA	-	expression tag	UNP G0S539
C	627	ALA	-	expression tag	UNP G0S539
C	628	ALA	-	expression tag	UNP G0S539
C	629	LEU	-	expression tag	UNP G0S539

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Chain	Residue	Modelled	Actual	Comment	Reference
C	630	VAL	-	expression tag	UNP G0S539
C	631	PRO	-	expression tag	UNP G0S539
C	632	ARG	-	expression tag	UNP G0S539
C	633	GLY	-	expression tag	UNP G0S539
C	634	SER	-	expression tag	UNP G0S539
C	635	ARG	-	expression tag	UNP G0S539
C	636	SER	-	expression tag	UNP G0S539
C	637	VAL	-	expression tag	UNP G0S539
C	638	ASP	-	expression tag	UNP G0S539
C	639	HIS	-	expression tag	UNP G0S539
C	640	HIS	-	expression tag	UNP G0S539
C	641	HIS	-	expression tag	UNP G0S539
C	642	HIS	-	expression tag	UNP G0S539
C	643	HIS	-	expression tag	UNP G0S539
C	644	HIS	-	expression tag	UNP G0S539

- Molecule 2 is a protein called Tlg2 Qa SNARE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	180	1329	822	243	257	7	0	0	0
2	D	181	1335	824	244	260	7	0	0	0

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-1	GLY	-	expression tag	UNP G0SGW7
B	0	SER	-	expression tag	UNP G0SGW7
B	?	-	ASP	deletion	UNP G0SGW7
B	?	-	MET	deletion	UNP G0SGW7
B	?	-	ALA	deletion	UNP G0SGW7
B	?	-	GLY	deletion	UNP G0SGW7
B	?	-	VAL	deletion	UNP G0SGW7
B	?	-	ALA	deletion	UNP G0SGW7
B	?	-	SER	deletion	UNP G0SGW7
B	?	-	ASP	deletion	UNP G0SGW7
B	?	-	ILE	deletion	UNP G0SGW7
B	?	-	GLU	deletion	UNP G0SGW7
B	?	-	ARG	deletion	UNP G0SGW7
B	?	-	ALA	deletion	UNP G0SGW7
B	?	-	ALA	deletion	UNP G0SGW7

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Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	SER	deletion	UNP G0SGW7
B	?	-	PRO	deletion	UNP G0SGW7
B	?	-	PHE	deletion	UNP G0SGW7
B	?	-	PRO	deletion	UNP G0SGW7
B	?	-	GLY	deletion	UNP G0SGW7
B	?	-	SER	deletion	UNP G0SGW7
B	?	-	SER	deletion	UNP G0SGW7
B	?	-	TYR	deletion	UNP G0SGW7
B	?	-	SER	deletion	UNP G0SGW7
B	?	-	ASN	deletion	UNP G0SGW7
B	?	-	ASN	deletion	UNP G0SGW7
B	?	-	PRO	deletion	UNP G0SGW7
B	?	-	SER	deletion	UNP G0SGW7
B	?	-	LEU	deletion	UNP G0SGW7
B	?	-	LEU	deletion	UNP G0SGW7
D	-1	GLY	-	expression tag	UNP G0SGW7
D	0	SER	-	expression tag	UNP G0SGW7
D	?	-	ASP	deletion	UNP G0SGW7
D	?	-	MET	deletion	UNP G0SGW7
D	?	-	ALA	deletion	UNP G0SGW7
D	?	-	GLY	deletion	UNP G0SGW7
D	?	-	VAL	deletion	UNP G0SGW7
D	?	-	ALA	deletion	UNP G0SGW7
D	?	-	SER	deletion	UNP G0SGW7
D	?	-	ASP	deletion	UNP G0SGW7
D	?	-	ILE	deletion	UNP G0SGW7
D	?	-	GLU	deletion	UNP G0SGW7
D	?	-	ARG	deletion	UNP G0SGW7
D	?	-	ALA	deletion	UNP G0SGW7
D	?	-	ALA	deletion	UNP G0SGW7
D	?	-	SER	deletion	UNP G0SGW7
D	?	-	PRO	deletion	UNP G0SGW7
D	?	-	PHE	deletion	UNP G0SGW7
D	?	-	PRO	deletion	UNP G0SGW7
D	?	-	GLY	deletion	UNP G0SGW7
D	?	-	SER	deletion	UNP G0SGW7
D	?	-	SER	deletion	UNP G0SGW7
D	?	-	TYR	deletion	UNP G0SGW7
D	?	-	SER	deletion	UNP G0SGW7
D	?	-	ASN	deletion	UNP G0SGW7
D	?	-	ASN	deletion	UNP G0SGW7
D	?	-	PRO	deletion	UNP G0SGW7

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Chain	Residue	Modelled	Actual	Comment	Reference
D	?	-	SER	deletion	UNP G0SGW7
D	?	-	LEU	deletion	UNP G0SGW7
D	?	-	LEU	deletion	UNP G0SGW7

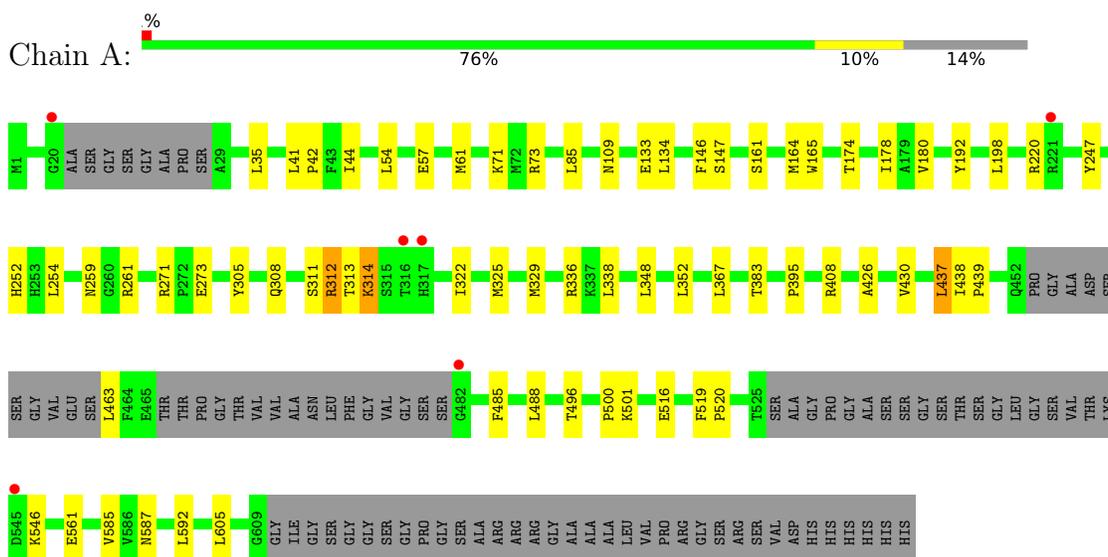
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	5	Total O 5 5	0	0
3	C	12	Total O 12 12	0	0
3	D	1	Total O 1 1	0	0

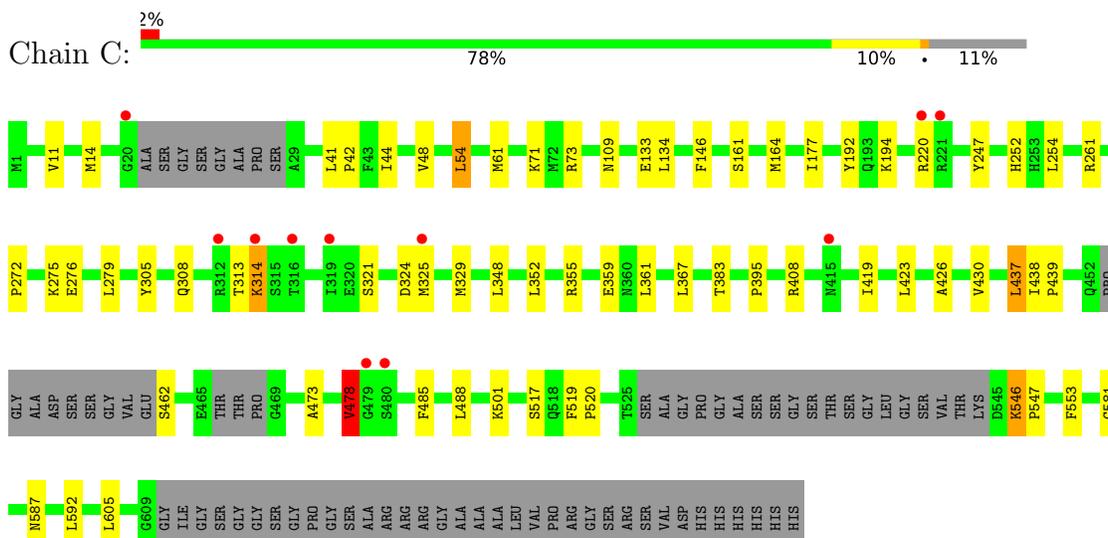
3 Residue-property plots [i](#)

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: Vps45

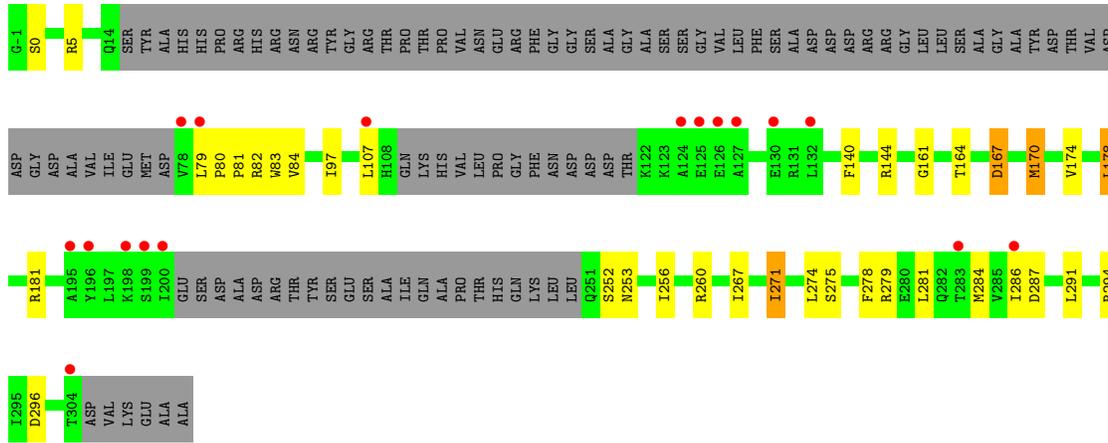


- Molecule 1: Vps45

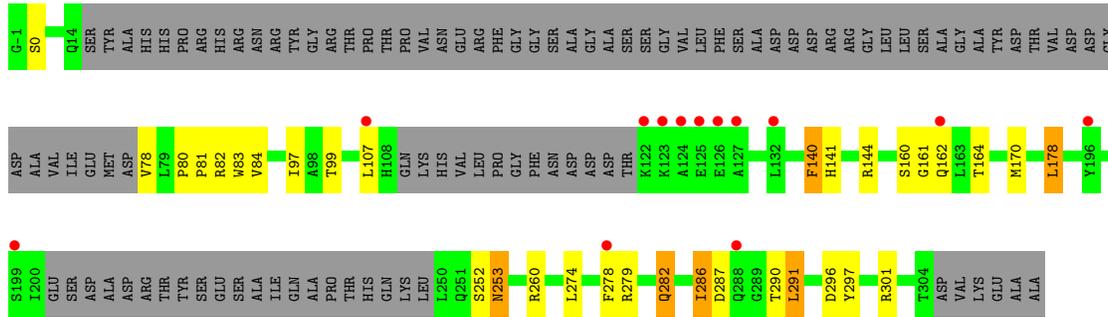


- Molecule 2: Tlg2 Qa SNARE





• Molecule 2: Tlg2 Qa SNARE



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	58.73Å 180.06Å 202.09Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.68 – 2.80 29.68 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.9 (29.68-2.80) 100.0 (29.68-2.80)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.65 (at 2.80Å)	Xtrriage
Refinement program	PHENIX 1.17_3644	Depositor
R, R_{free}	0.194 , 0.248 0.194 , 0.249	Depositor DCC
R_{free} test set	2679 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	72.7	Xtrriage
Anisotropy	0.268	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 52.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	11550	wwPDB-VP
Average B, all atoms (Å ²)	93.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 44.69 % 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 1.4712e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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	0.33	0/4471	0.53	0/6048
1	C	0.33	0/4560	0.53	0/6169
2	B	0.25	0/1337	0.44	0/1808
2	D	0.27	0/1343	0.46	0/1816
All	All	0.31	0/11711	0.51	0/15841

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	4390	0	4436	35	0
1	C	4478	0	4520	36	0
2	B	1329	0	1245	25	0
2	D	1335	0	1242	19	0
3	A	5	0	0	1	0
3	C	12	0	0	0	0
3	D	1	0	0	0	0
All	All	11550	0	11443	103	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 4.

The worst 5 of 103 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:C:261:ARG:HH21	2:D:296:ASP:CG	1.75	0.89
1:A:312:ARG:HH11	1:A:312:ARG:HG3	1.50	0.76
2:B:281:LEU:HA	2:B:284:MET:HB2	1.73	0.69
1:C:473:ALA:HB1	1:C:478:VAL:HB	1.75	0.68
1:A:485:PHE:HB2	1:A:488:LEU:HD22	1.78	0.66

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	546/644 (85%)	529 (97%)	14 (3%)	3 (0%)	29	61
1	C	560/644 (87%)	537 (96%)	19 (3%)	4 (1%)	22	53
2	B	172/284 (61%)	160 (93%)	10 (6%)	2 (1%)	13	39
2	D	173/284 (61%)	160 (92%)	10 (6%)	3 (2%)	9	29
All	All	1451/1856 (78%)	1386 (96%)	53 (4%)	12 (1%)	19	49

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	82	ARG
2	D	82	ARG
2	D	161	GLY
1	A	426	ALA
2	B	161	GLY

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	485/549 (88%)	467 (96%)	18 (4%)	34 68
1	C	494/549 (90%)	480 (97%)	14 (3%)	43 77
2	B	124/241 (52%)	113 (91%)	11 (9%)	9 28
2	D	124/241 (52%)	110 (89%)	14 (11%)	6 18
All	All	1227/1580 (78%)	1170 (95%)	57 (5%)	27 60

5 of 57 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	291	LEU
2	D	291	LEU
1	C	220	ARG
2	D	290	THR
2	D	178	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	D	282	GLN

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 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 [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	556/644 (86%)	-0.39	6 (1%) 80 75	42, 75, 136, 208	0
1	C	570/644 (88%)	-0.40	11 (1%) 66 59	38, 70, 141, 213	0
2	B	180/284 (63%)	0.10	17 (9%) 8 4	60, 141, 220, 243	0
2	D	181/284 (63%)	0.05	13 (7%) 15 8	60, 144, 217, 258	0
All	All	1487/1856 (80%)	-0.28	47 (3%) 47 37	38, 80, 186, 258	0

The worst 5 of 47 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	317	HIS	6.1
1	C	221	ARG	5.4
2	B	199	SER	4.7
1	C	415	ASN	4.6
1	A	316	THR	4.6

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 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.