



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 03:21 PM GMT

PDB ID : 4C5E
Title : Crystal structure of the minimal Pho-Sfmbt complex (P21 spacegroup)
Authors : Alfieri, C.; Glatt, S.; Mueller, C.W.
Deposited on : 2013-09-11
Resolution : 1.95 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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

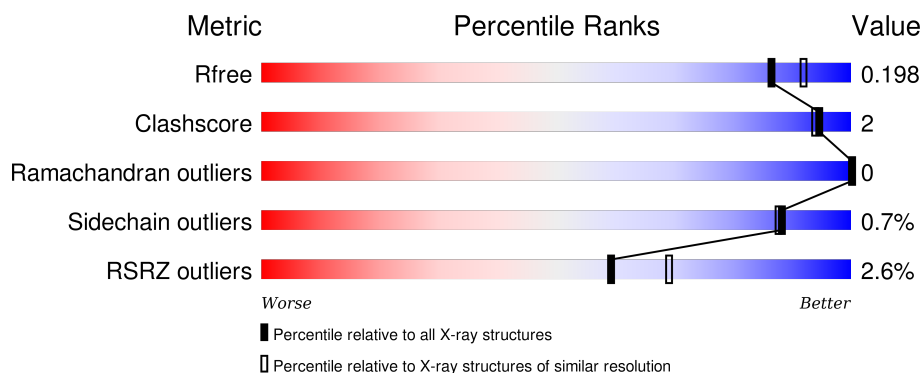
1 Overall quality at a glance ⓘ

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 $\leq 5\%$. 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	451	<div> <div>2%</div> <div>93%</div> <div>5%</div> <div>6%</div> </div>
1	B	451	<div> <div>2%</div> <div>93%</div> <div>5%</div> <div>6%</div> </div>
1	C	451	<div> <div>2%</div> <div>92%</div> <div>5%</div> <div>6%</div> </div>
1	D	451	<div> <div>5%</div> <div>92%</div> <div>5%</div> <div>6%</div> </div>
2	E	32	<div> <div>88%</div> <div>6%</div> <div>6%</div> </div>

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Mol	Chain	Length	Quality of chain
2	F	32	<div><div></div><div>91%</div><div></div><div>• 6%</div></div>
2	G	32	<div><div></div><div>94%</div><div></div><div>6%</div></div>
2	H	32	<div><div>3%</div><div></div><div>91%</div><div>• 6%</div></div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 16286 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 POLYCOMB PROTEIN SFMBT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	440	Total	C	N	O	S	1	2	0
			3479	2229	578	646	26			
1	B	439	Total	C	N	O	S	0	5	0
			3480	2229	578	647	26			
1	C	438	Total	C	N	O	S	0	2	0
			3456	2216	573	641	26			
1	D	437	Total	C	N	O	S	0	2	0
			3409	2186	568	630	25			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	530	MET	-	EXPRESSION TAG	UNP Q9VK33
B	530	MET	-	EXPRESSION TAG	UNP Q9VK33
C	530	MET	-	EXPRESSION TAG	UNP Q9VK33
D	530	MET	-	EXPRESSION TAG	UNP Q9VK33

- Molecule 2 is a protein called POLYCOMB PROTEIN PHO.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	30	Total	C	N	O	S	0	0	0
			238	150	43	42	3			
2	F	30	Total	C	N	O	S	0	0	0
			232	147	40	42	3			
2	G	30	Total	C	N	O	S	1	0	0
			231	147	40	41	3			
2	H	30	Total	C	N	O	S	0	0	0
			233	148	40	42	3			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	141	GLY	-	EXPRESSION TAG	UNP Q8ST83
E	142	ALA	-	EXPRESSION TAG	UNP Q8ST83
E	143	MET	-	EXPRESSION TAG	UNP Q8ST83
E	144	ALA	-	EXPRESSION TAG	UNP Q8ST83
F	141	GLY	-	EXPRESSION TAG	UNP Q8ST83
F	142	ALA	-	EXPRESSION TAG	UNP Q8ST83
F	143	MET	-	EXPRESSION TAG	UNP Q8ST83
F	144	ALA	-	EXPRESSION TAG	UNP Q8ST83
G	141	GLY	-	EXPRESSION TAG	UNP Q8ST83
G	142	ALA	-	EXPRESSION TAG	UNP Q8ST83
G	143	MET	-	EXPRESSION TAG	UNP Q8ST83
G	144	ALA	-	EXPRESSION TAG	UNP Q8ST83
H	141	GLY	-	EXPRESSION TAG	UNP Q8ST83
H	142	ALA	-	EXPRESSION TAG	UNP Q8ST83
H	143	MET	-	EXPRESSION TAG	UNP Q8ST83
H	144	ALA	-	EXPRESSION TAG	UNP Q8ST83

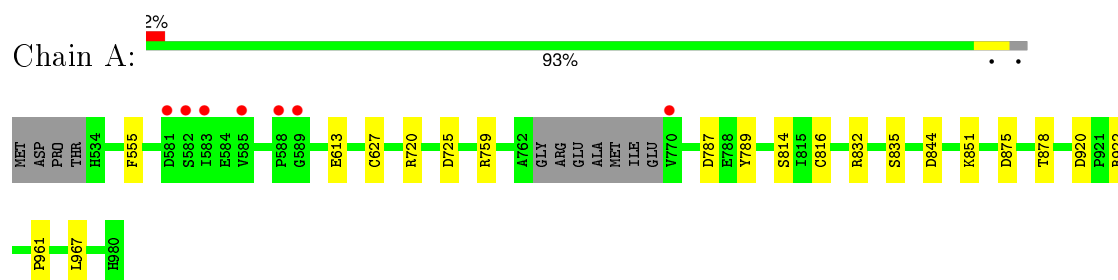
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	427	Total O 427 427	0	0
3	B	409	Total O 409 409	0	0
3	C	384	Total O 384 384	0	0
3	D	256	Total O 256 256	0	0
3	E	21	Total O 21 21	0	0
3	F	10	Total O 10 10	0	0
3	G	7	Total O 7 7	0	0
3	H	14	Total O 14 14	0	0

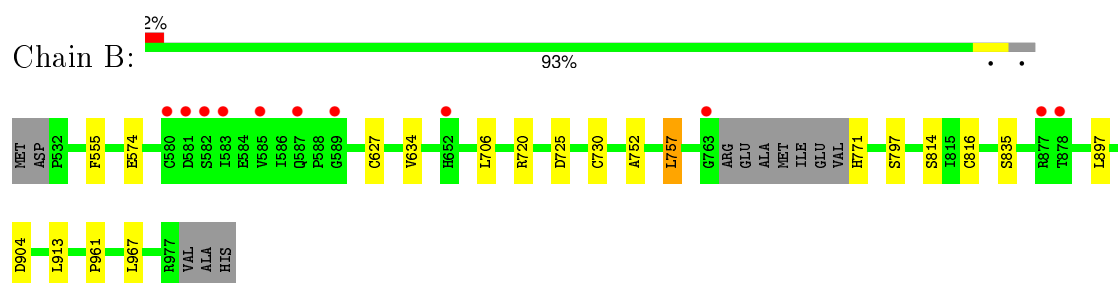
3 Residue-property plots [i](#)

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.

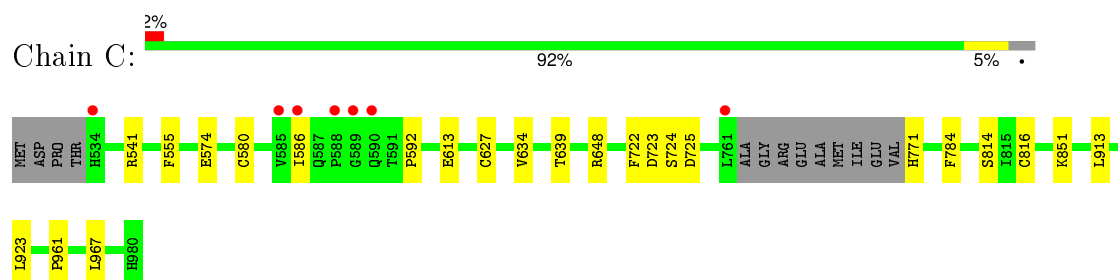
• Molecule 1: POLYCOMB PROTEIN SFMBT



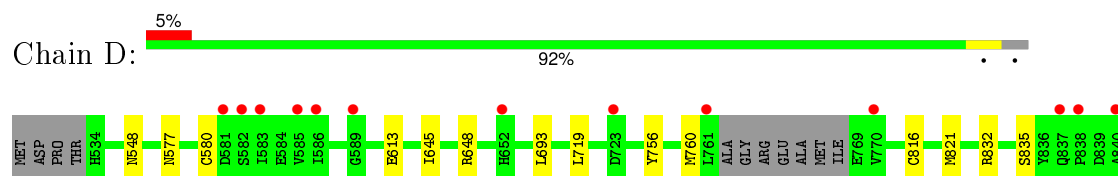
• Molecule 1: POLYCOMB PROTEIN SFMBT

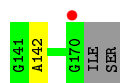


• Molecule 1: POLYCOMB PROTEIN SFMBT



• Molecule 1: POLYCOMB PROTEIN SFMBT





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	87.51Å 147.88Å 97.88Å 90.00° 112.26° 90.00°	Depositor
Resolution (Å)	48.60 – 1.95 49.29 – 1.95	Depositor EDS
% Data completeness (in resolution range)	99.8 (48.60-1.95) 99.8 (49.29-1.95)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.66 (at 1.95Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.179 , 0.198 0.178 , 0.198	Depositor DCC
R_{free} test set	8323 reflections (5.00%)	DCC
Wilson B-factor (Å ²)	28.8	Xtriage
Anisotropy	0.256	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 52.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 166532 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	16286	wwPDB-VP
Average B, all atoms (Å ²)	33.0	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 30.08 % 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 1.3892e-03. 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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.23	0/3582	0.43	0/4880
1	B	0.23	0/3583	0.43	0/4883
1	C	0.22	0/3556	0.42	0/4843
1	D	0.22	0/3509	0.42	0/4783
2	E	0.25	0/243	0.40	0/324
2	F	0.26	0/237	0.40	0/317
2	G	0.22	0/236	0.38	0/316
2	H	0.24	0/238	0.40	0/318
All	All	0.23	0/15184	0.42	0/20664

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	3479	0	3272	13	0
1	B	3480	0	3267	12	0
1	C	3456	0	3245	13	0
1	D	3409	0	3182	10	0
2	E	238	0	233	1	0
2	F	232	0	222	1	0
2	G	231	0	219	0	0
2	H	233	0	224	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	427	0	0	2	0
3	B	409	0	0	0	0
3	C	384	0	0	2	0
3	D	256	0	0	2	0
3	E	21	0	0	0	0
3	F	10	0	0	1	0
3	G	7	0	0	0	0
3	H	14	0	0	0	0
All	All	16286	0	13864	49	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (49) 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:722:PHE:CG	1:C:722:PHE:CE2	2.41	0.99
1:B:814:SER:OG	1:B:816[B]:CYS:SG	2.51	0.69
1:B:720:ARG:NH1	1:B:725:ASP:O	2.27	0.67
1:A:832:ARG:NH1	1:A:844:ASP:OD2	2.26	0.67
1:D:853:PRO:O	1:D:900:ARG:NH2	2.27	0.67
2:F:143:MET:O	3:F:2001:HOH:O	2.16	0.62
1:A:720:ARG:NH1	1:A:725:ASP:O	2.32	0.62
1:B:814:SER:HG	1:B:816[B]:CYS:HG	1.46	0.62
1:A:875:ASP:HB3	1:A:878:THR:H	1.65	0.62
1:D:613:GLU:OE2	3:D:2055:HOH:O	2.16	0.61
1:A:814:SER:OG	1:A:816[B]:CYS:SG	2.58	0.61
1:C:613:GLU:OE1	3:C:2059:HOH:O	2.17	0.59
1:C:580:CYS:HA	1:C:648:ARG:HG3	1.87	0.55
1:B:904[A]:ASP:OD1	1:B:904[A]:ASP:N	2.40	0.54
1:A:789:TYR:OH	1:A:851:LYS:NZ	2.41	0.54
1:C:814:SER:OG	1:C:816[B]:CYS:SG	2.67	0.53
1:A:627:CYS:HB2	1:A:967:LEU:HD13	1.91	0.53
1:A:759:ARG:NH2	3:A:2222:HOH:O	2.44	0.51
1:A:787:ASP:OD1	1:C:639:THR:OG1	2.26	0.49
1:B:816[A]:CYS:SG	1:B:835:SER:HB3	2.53	0.48
1:B:574:GLU:HG3	1:B:634:VAL:HA	1.97	0.47
1:C:627:CYS:HB2	1:C:967:LEU:HD13	1.97	0.46
1:C:724:SER:OG	1:C:725:ASP:N	2.49	0.46
1:A:613:GLU:OE1	3:A:2064:HOH:O	2.20	0.46
1:D:548:ASN:ND2	3:D:2015:HOH:O	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:152:LEU:HD11	2:E:163:SER:HB2	1.98	0.45
1:D:577:ASN:ND2	1:D:645:ILE:O	2.49	0.45
1:B:752:ALA:HB3	1:B:757:LEU:HD13	1.99	0.44
1:A:816[A]:CYS:SG	1:A:835:SER:HB3	2.58	0.43
1:D:756:TYR:O	1:D:760:MET:HG2	2.18	0.43
1:C:784:PHE:HB3	1:C:851:LYS:HD2	2.01	0.43
1:B:627:CYS:HB2	1:B:967:LEU:HD13	2.00	0.43
1:C:555:PHE:CD1	1:C:961:PRO:HG3	2.54	0.43
1:A:555:PHE:CD1	1:A:961:PRO:HG3	2.54	0.42
1:D:904:ASP:OD1	1:D:904:ASP:N	2.44	0.42
1:D:580:CYS:HA	1:D:648:ARG:HG3	2.01	0.42
1:C:541:ARG:NH2	3:C:2015:HOH:O	2.46	0.42
1:C:722:PHE:CE2	1:C:723:ASP:HB3	2.55	0.42
1:B:797:SER:HB3	1:B:897:LEU:HD22	2.02	0.42
1:D:693:LEU:HD11	1:D:719:LEU:HD22	2.01	0.41
1:D:821:MET:SD	1:D:832:ARG:HG2	2.60	0.41
1:A:920:ASP:OD2	1:A:922:ARG:NH2	2.53	0.41
1:C:574:GLU:HG3	1:C:634:VAL:HA	2.02	0.41
1:B:555:PHE:CD1	1:B:961:PRO:HG3	2.56	0.41
1:D:816:CYS:SG	1:D:835:SER:HB3	2.60	0.41
1:C:586:ILE:HG21	1:C:592:PRO:HA	2.04	0.41
1:B:904[A]:ASP:OD2	2:H:142:ALA:N	2.49	0.40
1:B:757:LEU:HD12	1:B:757:LEU:HA	1.91	0.40
1:A:844:ASP:OD1	1:A:844:ASP:N	2.54	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	438/451 (97%)	426 (97%)	12 (3%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	440/451 (98%)	431 (98%)	9 (2%)	0	100	100
1	C	436/451 (97%)	426 (98%)	10 (2%)	0	100	100
1	D	435/451 (96%)	424 (98%)	11 (2%)	0	100	100
2	E	28/32 (88%)	27 (96%)	1 (4%)	0	100	100
2	F	28/32 (88%)	26 (93%)	2 (7%)	0	100	100
2	G	28/32 (88%)	27 (96%)	1 (4%)	0	100	100
2	H	28/32 (88%)	27 (96%)	1 (4%)	0	100	100
All	All	1861/1932 (96%)	1814 (98%)	47 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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	372/392 (95%)	372 (100%)	0	100	100
1	B	372/392 (95%)	367 (99%)	5 (1%)	76	72
1	C	368/392 (94%)	365 (99%)	3 (1%)	86	85
1	D	358/392 (91%)	355 (99%)	3 (1%)	86	85
2	E	24/26 (92%)	24 (100%)	0	100	100
2	F	23/26 (88%)	23 (100%)	0	100	100
2	G	22/26 (85%)	22 (100%)	0	100	100
2	H	23/26 (88%)	23 (100%)	0	100	100
All	All	1562/1672 (93%)	1551 (99%)	11 (1%)	88	88

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	706	LEU
1	B	730	CYS

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Mol	Chain	Res	Type
1	B	757	LEU
1	B	771	HIS
1	B	913	LEU
1	C	771	HIS
1	C	913	LEU
1	C	923	LEU
1	D	882	GLU
1	D	913	LEU
1	D	968	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	566	ASN
1	D	692	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 carbohydrates 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 ⓘ

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, 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	440/451 (97%)	-0.17	7 (1%) 74 83	13, 25, 50, 67	1 (0%)
1	B	439/451 (97%)	-0.24	11 (2%) 61 71	15, 27, 56, 73	0
1	C	438/451 (97%)	-0.18	7 (1%) 74 83	18, 30, 52, 75	0
1	D	437/451 (96%)	0.00	22 (5%) 32 44	18, 39, 65, 77	0
2	E	30/32 (93%)	-0.32	0 100 100	14, 25, 46, 53	0
2	F	30/32 (93%)	0.08	0 100 100	18, 33, 61, 77	0
2	G	30/32 (93%)	-0.04	0 100 100	24, 36, 55, 62	1 (3%)
2	H	30/32 (93%)	0.01	1 (3%) 50 61	17, 29, 52, 58	0
All	All	1874/1932 (96%)	-0.14	48 (2%) 59 69	13, 30, 58, 77	2 (0%)

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	583	ILE	4.9
1	D	589	GLY	4.6
1	B	585	VAL	4.5
1	D	582	SER	4.0
1	B	582	SER	3.9
1	B	763	GLY	3.6
1	C	588	PRO	3.5
1	A	585	VAL	3.4
1	D	838	PRO	3.4
1	A	588	PRO	3.4
1	B	587	GLN	3.3
1	D	581	ASP	3.2
1	C	534	HIS	3.2
1	D	888	THR	3.1
1	D	770	VAL	3.1
1	A	582	SER	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	586	ILE	3.0
1	C	585	VAL	3.0
1	A	770	VAL	2.9
1	B	581	ASP	2.9
1	A	589	GLY	2.9
1	D	873	GLY	2.8
1	B	580	CYS	2.8
1	A	581	ASP	2.8
1	C	589	GLY	2.8
1	D	723	ASP	2.7
1	D	840	ALA	2.6
1	D	891	VAL	2.6
1	D	652	HIS	2.6
1	D	890	ALA	2.5
1	A	583	ILE	2.5
1	B	652	HIS	2.5
1	B	878	THR	2.5
1	D	586	ILE	2.4
1	B	589	GLY	2.4
1	C	761	LEU	2.4
1	D	761	LEU	2.4
1	D	843	SER	2.4
1	D	585	VAL	2.3
1	D	583	ILE	2.3
1	D	886	ARG	2.3
1	D	837	GLN	2.1
1	D	878	THR	2.1
1	B	877	ARG	2.0
1	D	876	SER	2.0
1	C	590	GLN	2.0
1	D	872	ASN	2.0
2	H	170	GLY	2.0

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 carbohydrates 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.