



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 10:06 AM GMT

PDB ID : 3KO0
Title : Structure of the tfp-ca2+-bound activated form of the s100a4 Metastasis factor
Authors : Malashkevich, V.N.; Dulyaninova, N.G.; Knight, D.; Almo, S.C.; Bresnick, A.R.
Deposited on : 2009-11-12
Resolution : 2.30 Å(reported)

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

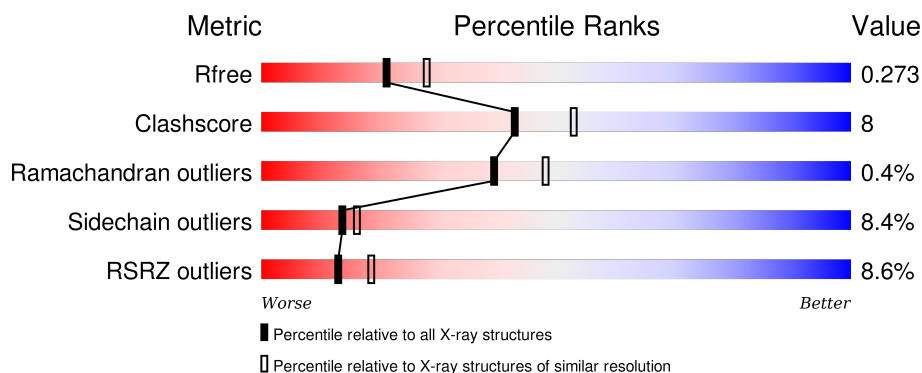
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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	101	<div> <div>5%</div> <div>72% 18% 8%</div> </div>
1	B	101	<div> <div>7%</div> <div>73% 17% 8%</div> </div>
1	C	101	<div> <div>3%</div> <div>66% 24% 8%</div> </div>
1	D	101	<div> <div>10%</div> <div>67% 20% 5% 8%</div> </div>
1	E	101	<div> <div>5%</div> <div>68% 19% 9%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	101	
1	G	101	
1	H	101	
1	I	101	
1	J	101	
1	K	101	
1	L	101	
1	M	101	
1	N	101	
1	O	101	
1	P	101	
1	Q	101	
1	R	101	
1	S	101	
1	T	101	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 16855 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 Protein S100-A4.

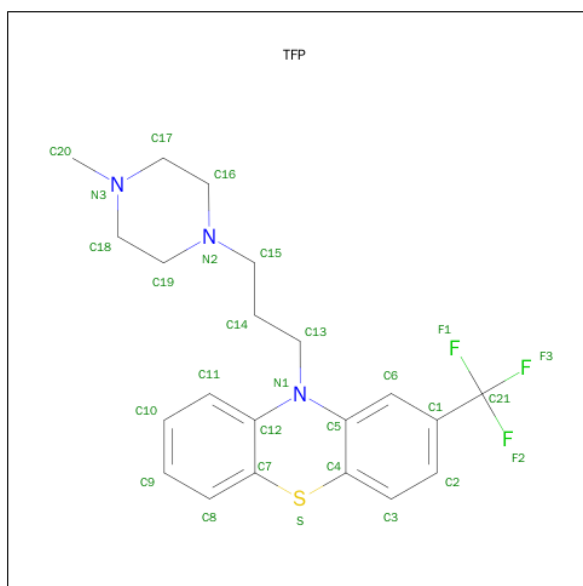
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	93	Total	C	N	O	S	0	1	0
			754	481	121	144	8			
1	B	93	Total	C	N	O	S	0	1	0
			740	471	118	142	9			
1	C	93	Total	C	N	O	S	0	1	0
			746	475	118	144	9			
1	D	93	Total	C	N	O	S	0	2	0
			752	479	119	144	10			
1	E	92	Total	C	N	O	S	0	0	0
			741	471	119	143	8			
1	F	90	Total	C	N	O	S	0	0	0
			709	451	110	140	8			
1	G	90	Total	C	N	O	S	0	0	0
			718	459	113	138	8			
1	H	94	Total	C	N	O	S	0	0	0
			752	477	120	147	8			
1	I	93	Total	C	N	O	S	0	0	0
			744	473	119	144	8			
1	J	93	Total	C	N	O	S	0	2	0
			756	482	120	144	10			
1	K	93	Total	C	N	O	S	0	0	0
			738	470	116	144	8			
1	L	93	Total	C	N	O	S	0	0	0
			744	473	119	144	8			
1	M	92	Total	C	N	O	S	0	0	0
			731	465	115	143	8			
1	N	92	Total	C	N	O	S	0	1	0
			743	473	118	143	9			
1	O	93	Total	C	N	O	S	0	0	0
			745	474	119	144	8			
1	P	92	Total	C	N	O	S	0	0	0
			733	465	117	143	8			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	88	Total	C	N	O	S	0	1	0
			702	450	107	136	9			
1	R	93	Total	C	N	O	S	0	1	0
			745	474	118	144	9			
1	S	93	Total	C	N	O	S	0	0	0
			748	476	120	144	8			
1	T	93	Total	C	N	O	S	0	1	0
			744	475	116	144	9			

- Molecule 2 is 10-[3-(4-METHYL-PIPERAZIN-1-YL)-PROPYL]-2-TRIFLUOROMETHYL-10H-PHENOTHIAZINE (three-letter code: TFP) (formula: C₂₁H₂₄F₃N₃S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	F	N	S	0	0
			28	21	3	3	1		
2	J	1	Total	C	F	N	S	0	0
			28	21	3	3	1		
2	B	1	Total	C	F	N	S	0	0
			28	21	3	3	1		
2	C	1	Total	C	F	N	S	0	0
			28	21	3	3	1		
2	C	1	Total	C	F	N	S	0	0
			28	21	3	3	1		
2	E	1	Total	C	F	N	S	0	0
			28	21	3	3	1		
2	A	1	Total	C	F	N	S	0	0
			28	21	3	3	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	D	1	Total 28	C 21	F 3	N 3	S 1	0	0
2	E	1	Total 28	C 21	F 3	N 3	S 1	0	0
2	G	1	Total 28	C 21	F 3	N 3	S 1	0	0
2	D	1	Total 28	C 21	F 3	N 3	S 1	0	0
2	F	1	Total 28	C 21	F 3	N 3	S 1	0	0
2	G	1	Total 28	C 21	F 3	N 3	S 1	0	0
2	I	1	Total 28	C 21	F 3	N 3	S 1	0	0
2	F	1	Total 28	C 21	F 3	N 3	S 1	0	0
2	H	1	Total 28	C 21	F 3	N 3	S 1	0	0
2	B	1	Total 28	C 21	F 3	N 3	S 1	0	0
2	I	1	Total 28	C 21	F 3	N 3	S 1	0	0
2	H	1	Total 28	C 21	F 3	N 3	S 1	0	0
2	J	1	Total 28	C 21	F 3	N 3	S 1	0	0
2	K	1	Total 28	C 21	F 3	N 3	S 1	0	0
2	K	1	Total 28	C 21	F 3	N 3	S 1	0	0
2	N	1	Total 28	C 21	F 3	N 3	S 1	0	0
2	L	1	Total 28	C 21	F 3	N 3	S 1	0	0
2	S	1	Total 28	C 21	F 3	N 3	S 1	0	0
2	L	1	Total 28	C 21	F 3	N 3	S 1	0	0
2	M	1	Total 28	C 21	F 3	N 3	S 1	0	0
2	N	1	Total 28	C 21	F 3	N 3	S 1	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	P	1	Total 28	C 21	F 3	N 3	S 1	0	0
2	M	1	Total 28	C 21	F 3	N 3	S 1	0	0
2	O	1	Total 28	C 21	F 3	N 3	S 1	0	0
2	P	1	Total 28	C 21	F 3	N 3	S 1	0	0
2	Q	1	Total 28	C 21	F 3	N 3	S 1	0	0
2	Q	1	Total 28	C 21	F 3	N 3	S 1	0	0
2	T	1	Total 28	C 21	F 3	N 3	S 1	0	0
2	O	1	Total 28	C 21	F 3	N 3	S 1	0	0
2	R	1	Total 28	C 21	F 3	N 3	S 1	0	0
2	R	1	Total 28	C 21	F 3	N 3	S 1	0	0
2	S	1	Total 28	C 21	F 3	N 3	S 1	0	0
2	T	1	Total 28	C 21	F 3	N 3	S 1	0	0

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	P	2	Total 2	Ca 2	0	0
3	G	2	Total 2	Ca 2	0	0
3	J	2	Total 2	Ca 2	0	0
3	Q	2	Total 2	Ca 2	0	0
3	D	2	Total 2	Ca 2	0	0
3	K	2	Total 2	Ca 2	0	0
3	E	2	Total 2	Ca 2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	H	2	Total 2	Ca 2	0	0
3	B	2	Total 2	Ca 2	0	0
3	I	2	Total 2	Ca 2	0	0
3	C	2	Total 2	Ca 2	0	0
3	A	2	Total 2	Ca 2	0	0
3	T	2	Total 2	Ca 2	0	0
3	N	2	Total 2	Ca 2	0	0
3	O	2	Total 2	Ca 2	0	0
3	R	2	Total 2	Ca 2	0	0
3	L	2	Total 2	Ca 2	0	0
3	S	2	Total 2	Ca 2	0	0
3	F	2	Total 2	Ca 2	0	0
3	M	2	Total 2	Ca 2	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	57	Total 57	O 57	0	0
4	B	75	Total 75	O 75	0	0
4	C	56	Total 56	O 56	0	0
4	D	48	Total 48	O 48	0	0
4	E	47	Total 47	O 47	0	0
4	F	41	Total 41	O 41	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	G	28	Total 28	O 28	0	0
4	H	26	Total 26	O 26	0	0
4	I	51	Total 51	O 51	0	0
4	J	65	Total 65	O 65	0	0
4	K	52	Total 52	O 52	0	0
4	L	53	Total 53	O 53	0	0
4	M	35	Total 35	O 35	0	0
4	N	49	Total 49	O 49	0	0
4	O	33	Total 33	O 33	0	0
4	P	42	Total 42	O 42	0	0
4	Q	28	Total 28	O 28	0	0
4	R	32	Total 32	O 32	0	0
4	S	60	Total 60	O 60	0	0
4	T	32	Total 32	O 32	0	0

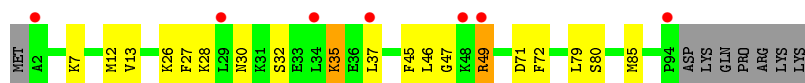
3 Residue-property plots [i](#)

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: Protein S100-A4



- Molecule 1: Protein S100-A4



- Molecule 1: Protein S100-A4



- Molecule 1: Protein S100-A4



- Molecule 1: Protein S100-A4

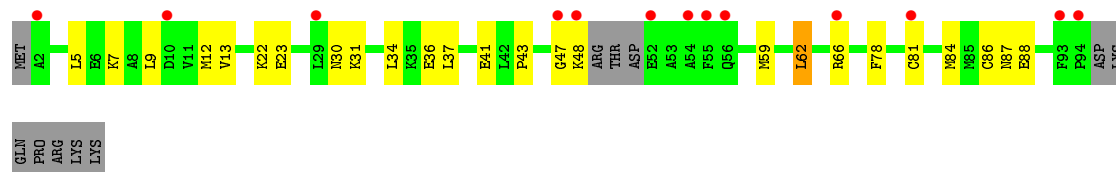


- Molecule 1: Protein S100-A4

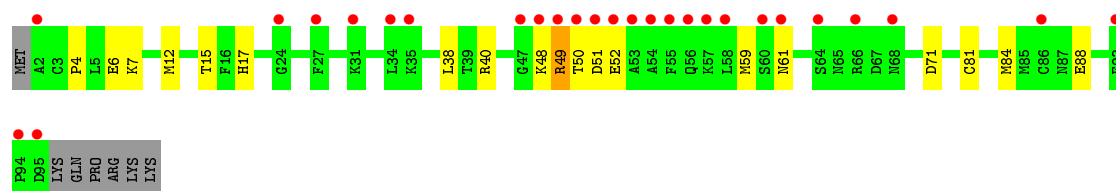




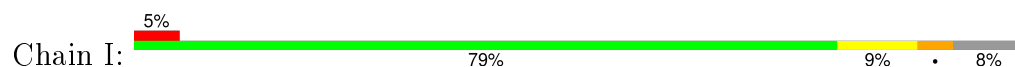
- Molecule 1: Protein S100-A4



- Molecule 1: Protein S100-A4



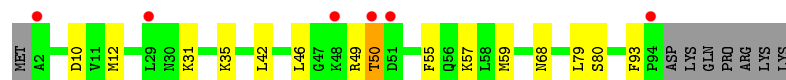
- Molecule 1: Protein S100-A4



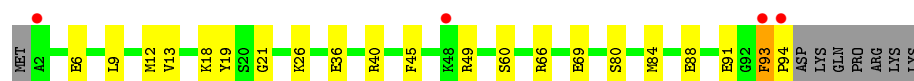
- Molecule 1: Protein S100-A4



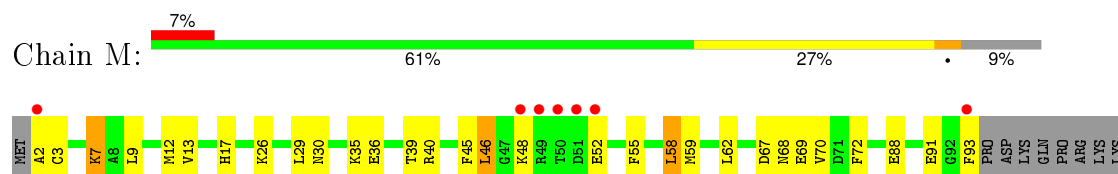
- Molecule 1: Protein S100-A4



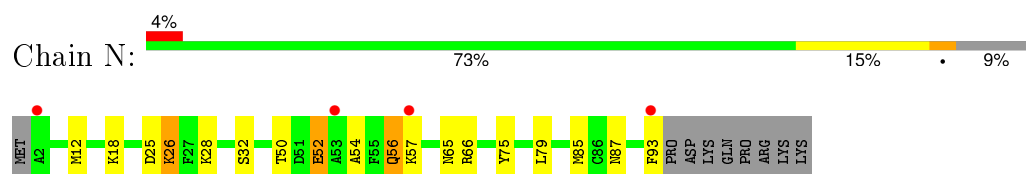
- Molecule 1: Protein S100-A4



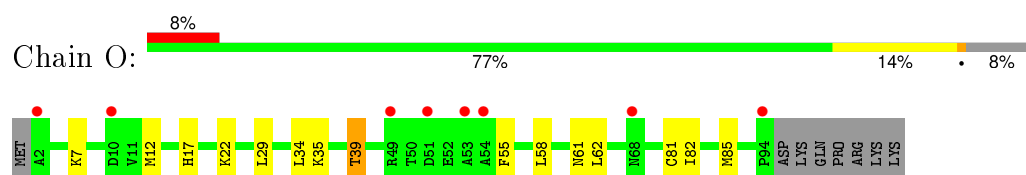
- Molecule 1: Protein S100-A4



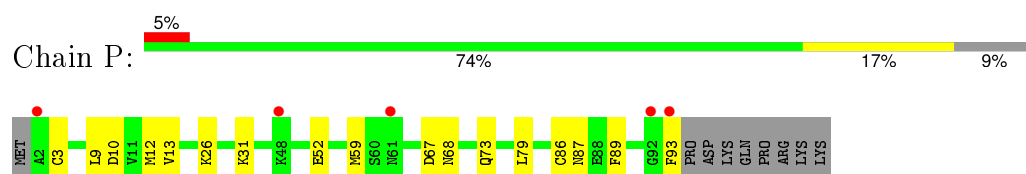
- Molecule 1: Protein S100-A4



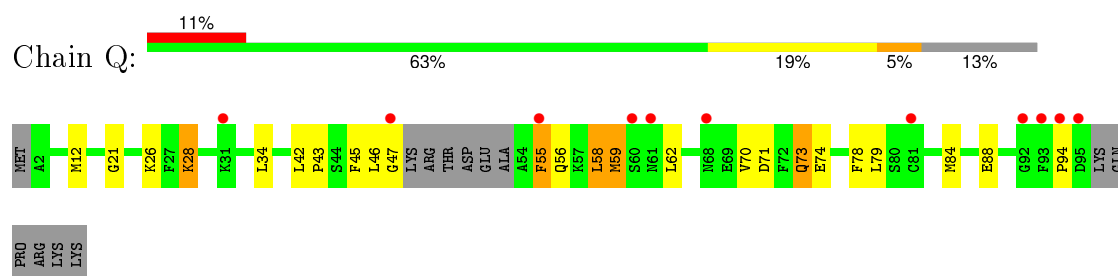
- Molecule 1: Protein S100-A4



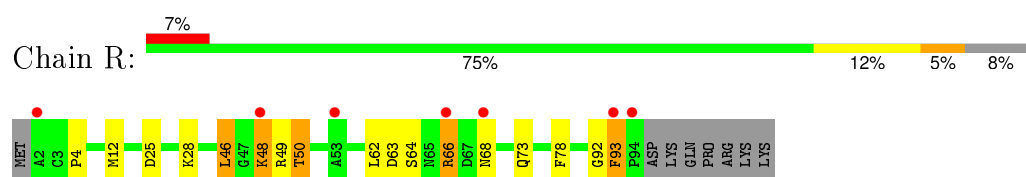
- Molecule 1: Protein S100-A4



- Molecule 1: Protein S100-A4

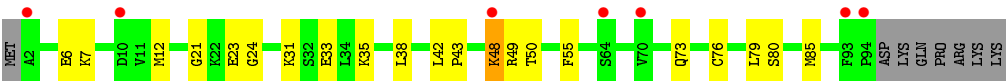


- Molecule 1: Protein S100-A4

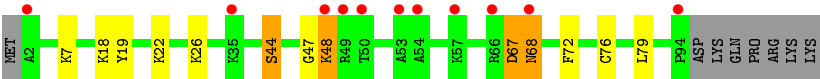
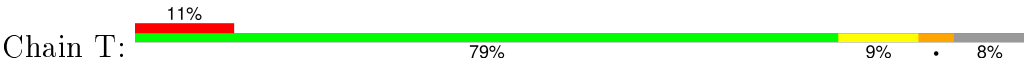


- Molecule 1: Protein S100-A4





● Molecule 1: Protein S100-A4



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	108.79Å 102.49Å 116.63Å 90.00° 92.59° 90.00°	Depositor
Resolution (Å)	19.94 – 2.30 19.88 – 2.30	Depositor EDS
% Data completeness (in resolution range)	97.7 (19.94-2.30) 97.7 (19.88-2.30)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.48 (at 2.30Å)	Xtriage
Refinement program	REFMAC 5.5.0089	Depositor
R, R_{free}	0.206 , 0.259 0.226 , 0.273	Depositor DCC
R_{free} test set	5579 reflections (5.30%)	DCC
Wilson B-factor (Å ²)	38.8	Xtriage
Anisotropy	0.039	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 47.5	EDS
Estimated twinning fraction	0.002 for h,-k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Outliers	4 of 110850 reflections (0.004%)	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	16855	wwPDB-VP
Average B, all atoms (Å ²)	28.0	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 66.75 % 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 5.7495e-06. 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](#)

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

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	1.01	0/771	0.90	1/1030 (0.1%)
1	B	0.92	0/757	0.74	0/1015
1	C	0.84	0/763	0.81	1/1022 (0.1%)
1	D	0.98	0/772	0.82	1/1033 (0.1%)
1	E	0.93	1/754 (0.1%)	0.78	0/1007
1	F	0.70	0/722	0.74	0/969
1	G	0.79	1/731 (0.1%)	0.72	0/977
1	H	0.66	0/766	0.69	0/1026
1	I	0.88	2/758 (0.3%)	0.82	1/1015 (0.1%)
1	J	0.80	0/776	0.85	1/1037 (0.1%)
1	K	0.90	0/752	0.80	0/1008
1	L	0.95	1/758 (0.1%)	0.86	1/1015 (0.1%)
1	M	0.72	0/744	0.74	0/996
1	N	0.81	0/759	0.78	0/1014
1	O	0.77	0/759	0.77	0/1016
1	P	0.79	1/746 (0.1%)	0.77	1/999 (0.1%)
1	Q	0.87	0/718	0.77	1/961 (0.1%)
1	R	0.73	0/762	0.70	0/1021
1	S	0.84	1/762 (0.1%)	0.80	0/1019
1	T	0.74	0/761	0.79	1/1019 (0.1%)
All	All	0.84	7/15091 (0.0%)	0.78	9/20199 (0.0%)

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	69	GLU	CD-OE2	-5.43	1.19	1.25
1	I	69	GLU	CG-CD	-5.39	1.43	1.51
1	E	33	GLU	CD-OE2	-5.31	1.19	1.25
1	G	86	CYS	CB-SG	-5.28	1.73	1.81
1	P	3	CYS	CB-SG	-5.22	1.73	1.81

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	93	PHE	C-N-CD	-8.77	101.30	120.60
1	I	12	MET	CG-SD-CE	7.88	112.81	100.20
1	L	12	MET	CG-SD-CE	5.59	109.15	100.20
1	J	67	ASP	CB-CG-OD1	5.33	123.09	118.30
1	Q	58	LEU	CA-CB-CG	5.26	127.40	115.30

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	754	0	742	13	0
1	B	740	0	710	17	0
1	C	746	0	718	20	0
1	D	752	0	732	20	0
1	E	741	0	722	18	0
1	F	709	0	662	18	0
1	G	718	0	693	20	0
1	H	752	0	722	11	0
1	I	744	0	718	5	0
1	J	756	0	743	11	0
1	K	738	0	707	11	0
1	L	744	0	718	12	0
1	M	731	0	700	30	0
1	N	743	0	722	15	0
1	O	745	0	720	14	0
1	P	733	0	700	12	0
1	Q	702	0	671	19	0
1	R	745	0	716	9	0
1	S	748	0	729	14	0
1	T	744	0	718	10	0
2	A	56	0	48	0	0
2	B	56	0	48	4	0
2	C	56	0	48	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	56	0	48	0	0
2	E	56	0	48	2	0
2	F	56	0	48	2	0
2	G	56	0	48	2	0
2	H	56	0	48	0	0
2	I	56	0	48	0	0
2	J	56	0	48	0	0
2	K	56	0	48	0	0
2	L	56	0	48	1	0
2	M	56	0	48	3	0
2	N	56	0	48	2	0
2	O	56	0	48	1	0
2	P	56	0	48	2	0
2	Q	56	0	48	1	0
2	R	56	0	48	1	0
2	S	56	0	48	2	0
2	T	56	0	48	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
3	E	2	0	0	0	0
3	F	2	0	0	0	0
3	G	2	0	0	0	0
3	H	2	0	0	0	0
3	I	2	0	0	0	0
3	J	2	0	0	0	0
3	K	2	0	0	0	0
3	L	2	0	0	0	0
3	M	2	0	0	0	0
3	N	2	0	0	0	0
3	O	2	0	0	0	0
3	P	2	0	0	0	0
3	Q	2	0	0	0	0
3	R	2	0	0	0	0
3	S	2	0	0	0	0
3	T	2	0	0	0	0
4	A	57	0	0	0	0
4	B	75	0	0	1	0
4	C	56	0	0	2	0
4	D	48	0	0	2	0
4	E	47	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	F	41	0	0	1	0
4	G	28	0	0	0	0
4	H	26	0	0	3	0
4	I	51	0	0	0	0
4	J	65	0	0	0	0
4	K	52	0	0	0	0
4	L	53	0	0	1	0
4	M	35	0	0	0	0
4	N	49	0	0	3	0
4	O	33	0	0	0	0
4	P	42	0	0	0	0
4	Q	28	0	0	0	0
4	R	32	0	0	4	0
4	S	60	0	0	1	0
4	T	32	0	0	1	0
All	All	16855	0	15223	256	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 8.

The worst 5 of 256 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:Q:12[A]:MET:HE1	4:R:1326:HOH:O	1.52	1.08
1:A:93:PHE:N	1:A:94:PRO:CD	2.16	1.04
1:A:92:GLY:O	1:A:93:PHE:HB2	1.59	1.00
1:M:12:MET:SD	1:N:12[A]:MET:SD	2.59	0.99
1:A:93:PHE:N	1:A:94:PRO:HD2	1.82	0.94

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	92/101 (91%)	91 (99%)	0	1 (1%)	17	18
1	B	92/101 (91%)	91 (99%)	1 (1%)	0	100	100
1	C	92/101 (91%)	90 (98%)	1 (1%)	1 (1%)	17	18
1	D	93/101 (92%)	92 (99%)	1 (1%)	0	100	100
1	E	90/101 (89%)	88 (98%)	2 (2%)	0	100	100
1	F	86/101 (85%)	83 (96%)	3 (4%)	0	100	100
1	G	86/101 (85%)	85 (99%)	1 (1%)	0	100	100
1	H	92/101 (91%)	87 (95%)	5 (5%)	0	100	100
1	I	91/101 (90%)	90 (99%)	1 (1%)	0	100	100
1	J	93/101 (92%)	92 (99%)	1 (1%)	0	100	100
1	K	91/101 (90%)	90 (99%)	0	1 (1%)	17	18
1	L	91/101 (90%)	88 (97%)	2 (2%)	1 (1%)	17	18
1	M	90/101 (89%)	90 (100%)	0	0	100	100
1	N	91/101 (90%)	91 (100%)	0	0	100	100
1	O	91/101 (90%)	87 (96%)	4 (4%)	0	100	100
1	P	90/101 (89%)	89 (99%)	1 (1%)	0	100	100
1	Q	85/101 (84%)	82 (96%)	2 (2%)	1 (1%)	16	16
1	R	92/101 (91%)	89 (97%)	2 (2%)	1 (1%)	17	18
1	S	91/101 (90%)	88 (97%)	3 (3%)	0	100	100
1	T	92/101 (91%)	87 (95%)	4 (4%)	1 (1%)	17	18
All	All	1811/2020 (90%)	1770 (98%)	34 (2%)	7 (0%)	39	48

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	93	PHE
1	C	93	PHE
1	T	47	GLY
1	R	93	PHE
1	Q	94	PRO

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	85/92 (92%)	77 (91%)	8 (9%)	11	12
1	B	82/92 (89%)	77 (94%)	5 (6%)	23	30
1	C	83/92 (90%)	76 (92%)	7 (8%)	14	16
1	D	85/92 (92%)	74 (87%)	11 (13%)	5	5
1	E	83/92 (90%)	73 (88%)	10 (12%)	6	6
1	F	78/92 (85%)	73 (94%)	5 (6%)	22	28
1	G	80/92 (87%)	72 (90%)	8 (10%)	9	11
1	H	84/92 (91%)	74 (88%)	10 (12%)	6	7
1	I	83/92 (90%)	76 (92%)	7 (8%)	14	16
1	J	86/92 (94%)	76 (88%)	10 (12%)	7	7
1	K	82/92 (89%)	78 (95%)	4 (5%)	31	41
1	L	83/92 (90%)	79 (95%)	4 (5%)	31	42
1	M	81/92 (88%)	73 (90%)	8 (10%)	10	11
1	N	83/92 (90%)	76 (92%)	7 (8%)	14	16
1	O	83/92 (90%)	78 (94%)	5 (6%)	24	31
1	P	81/92 (88%)	76 (94%)	5 (6%)	23	30
1	Q	79/92 (86%)	73 (92%)	6 (8%)	16	20
1	R	83/92 (90%)	76 (92%)	7 (8%)	14	16
1	S	84/92 (91%)	78 (93%)	6 (7%)	18	23
1	T	83/92 (90%)	78 (94%)	5 (6%)	24	31
All	All	1651/1840 (90%)	1513 (92%)	138 (8%)	14	16

5 of 138 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	61	ASN
1	J	62	LEU
1	S	7	LYS
1	I	31	LYS
1	I	60	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
1	H	17	HIS
1	H	73	GLN
1	P	17	HIS
1	F	17	HIS
1	F	68	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 80 ligands modelled in this entry, 40 are monoatomic - leaving 40 for Mogul analysis.

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	TFP	A	201	-	31,31,31	2.09	4 (12%)	45,45,45	2.12	13 (28%)
2	TFP	A	202	-	31,31,31	1.69	5 (16%)	45,45,45	1.60	10 (22%)
2	TFP	B	201	-	31,31,31	2.17	5 (16%)	45,45,45	1.78	8 (17%)
2	TFP	B	202	-	31,31,31	1.77	4 (12%)	45,45,45	1.59	11 (24%)
2	TFP	C	201	-	31,31,31	2.31	5 (16%)	45,45,45	1.88	12 (26%)
2	TFP	C	202	-	31,31,31	1.62	4 (12%)	45,45,45	1.36	8 (17%)
2	TFP	D	201	-	31,31,31	2.19	5 (16%)	45,45,45	1.70	14 (31%)
2	TFP	D	202	-	31,31,31	1.94	4 (12%)	45,45,45	1.40	5 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	TFP	E	201	-	31,31,31	2.26	4 (12%)	45,45,45	1.82	10 (22%)
2	TFP	E	202	-	31,31,31	1.72	3 (9%)	45,45,45	1.39	5 (11%)
2	TFP	F	201	-	31,31,31	2.17	4 (12%)	45,45,45	1.34	7 (15%)
2	TFP	F	202	-	31,31,31	1.58	3 (9%)	45,45,45	1.39	7 (15%)
2	TFP	G	201	-	31,31,31	2.20	4 (12%)	45,45,45	1.44	10 (22%)
2	TFP	G	202	-	31,31,31	1.88	5 (16%)	45,45,45	1.66	11 (24%)
2	TFP	H	201	-	31,31,31	2.28	5 (16%)	45,45,45	1.46	6 (13%)
2	TFP	H	202	-	31,31,31	1.85	4 (12%)	45,45,45	1.26	4 (8%)
2	TFP	I	201	-	31,31,31	1.96	4 (12%)	45,45,45	1.74	7 (15%)
2	TFP	I	202	-	31,31,31	1.63	4 (12%)	45,45,45	1.63	9 (20%)
2	TFP	J	201	-	31,31,31	2.11	5 (16%)	45,45,45	2.08	13 (28%)
2	TFP	J	202	-	31,31,31	1.91	4 (12%)	45,45,45	1.36	4 (8%)
2	TFP	K	201	-	31,31,31	2.05	4 (12%)	45,45,45	1.84	14 (31%)
2	TFP	K	202	-	31,31,31	1.68	4 (12%)	45,45,45	1.60	12 (26%)
2	TFP	L	201	-	31,31,31	2.06	4 (12%)	45,45,45	1.97	12 (26%)
2	TFP	L	202	-	31,31,31	1.84	4 (12%)	45,45,45	1.63	9 (20%)
2	TFP	M	201	-	31,31,31	2.19	4 (12%)	45,45,45	1.51	9 (20%)
2	TFP	M	202	-	31,31,31	2.03	3 (9%)	45,45,45	1.41	8 (17%)
2	TFP	N	201	-	31,31,31	2.17	6 (19%)	45,45,45	1.35	7 (15%)
2	TFP	N	202	-	31,31,31	1.80	4 (12%)	45,45,45	1.53	10 (22%)
2	TFP	O	201	-	31,31,31	2.19	4 (12%)	45,45,45	2.05	13 (28%)
2	TFP	O	202	-	31,31,31	1.70	4 (12%)	45,45,45	1.31	6 (13%)
2	TFP	P	201	-	31,31,31	2.15	4 (12%)	45,45,45	1.77	13 (28%)
2	TFP	P	202	-	31,31,31	1.67	4 (12%)	45,45,45	1.55	9 (20%)
2	TFP	Q	201	-	31,31,31	2.18	4 (12%)	45,45,45	1.35	5 (11%)
2	TFP	Q	202	-	31,31,31	1.95	5 (16%)	45,45,45	1.53	9 (20%)
2	TFP	R	201	-	31,31,31	1.92	4 (12%)	45,45,45	1.67	9 (20%)
2	TFP	R	202	-	31,31,31	1.99	4 (12%)	45,45,45	1.61	6 (13%)
2	TFP	S	201	-	31,31,31	2.13	4 (12%)	45,45,45	1.73	12 (26%)
2	TFP	S	202	-	31,31,31	1.76	4 (12%)	45,45,45	1.50	9 (20%)
2	TFP	T	201	-	31,31,31	2.15	5 (16%)	45,45,45	1.64	8 (17%)
2	TFP	T	202	-	31,31,31	1.93	4 (12%)	45,45,45	1.92	12 (26%)

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	TFP	A	201	-	-	0/12/34/34	0/4/4/4
2	TFP	A	202	-	-	0/12/34/34	0/4/4/4
2	TFP	B	201	-	-	0/12/34/34	0/4/4/4
2	TFP	B	202	-	-	0/12/34/34	0/4/4/4
2	TFP	C	201	-	-	0/12/34/34	0/4/4/4
2	TFP	C	202	-	-	0/12/34/34	0/4/4/4
2	TFP	D	201	-	-	0/12/34/34	0/4/4/4
2	TFP	D	202	-	-	0/12/34/34	0/4/4/4
2	TFP	E	201	-	-	0/12/34/34	0/3/4/4
2	TFP	E	202	-	-	0/12/34/34	0/3/4/4
2	TFP	F	201	-	-	0/12/34/34	0/3/4/4
2	TFP	F	202	-	-	0/12/34/34	0/4/4/4
2	TFP	G	201	-	-	0/12/34/34	0/3/4/4
2	TFP	G	202	-	-	0/12/34/34	0/4/4/4
2	TFP	H	201	-	-	0/12/34/34	0/4/4/4
2	TFP	H	202	-	-	0/12/34/34	0/4/4/4
2	TFP	I	201	-	-	0/12/34/34	0/4/4/4
2	TFP	I	202	-	-	0/12/34/34	0/3/4/4
2	TFP	J	201	-	-	0/12/34/34	0/3/4/4
2	TFP	J	202	-	-	0/12/34/34	0/3/4/4
2	TFP	K	201	-	-	0/12/34/34	0/4/4/4
2	TFP	K	202	-	-	0/12/34/34	0/4/4/4
2	TFP	L	201	-	-	0/12/34/34	0/4/4/4
2	TFP	L	202	-	-	0/12/34/34	0/3/4/4
2	TFP	M	201	-	-	0/12/34/34	0/3/4/4
2	TFP	M	202	-	-	0/12/34/34	0/4/4/4
2	TFP	N	201	-	-	0/12/34/34	0/4/4/4
2	TFP	N	202	-	-	0/12/34/34	0/3/4/4
2	TFP	O	201	-	-	0/12/34/34	0/4/4/4
2	TFP	O	202	-	-	0/12/34/34	0/4/4/4
2	TFP	P	201	-	-	0/12/34/34	0/3/4/4
2	TFP	P	202	-	-	0/12/34/34	0/3/4/4
2	TFP	Q	201	-	-	0/12/34/34	0/4/4/4
2	TFP	Q	202	-	-	0/12/34/34	0/3/4/4
2	TFP	R	201	-	-	0/12/34/34	0/4/4/4
2	TFP	R	202	-	-	0/12/34/34	0/4/4/4
2	TFP	S	201	-	-	0/12/34/34	0/4/4/4
2	TFP	S	202	-	-	0/12/34/34	0/3/4/4
2	TFP	T	201	-	-	0/12/34/34	0/4/4/4
2	TFP	T	202	-	-	0/12/34/34	0/4/4/4

The worst 5 of 168 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	M	201	TFP	C4-S	-5.02	1.67	1.76
2	Q	201	TFP	C7-S	-4.52	1.67	1.76
2	D	201	TFP	C4-S	-4.31	1.68	1.76
2	S	202	TFP	C7-S	-4.31	1.68	1.76
2	G	201	TFP	C4-S	-4.24	1.68	1.76

The worst 5 of 366 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	201	TFP	C16-C17-N3	-6.30	104.13	110.79
2	R	202	TFP	C16-C17-N3	-6.08	104.37	110.79
2	J	201	TFP	C13-N1-C12	-5.95	111.03	119.01
2	O	201	TFP	C6-C5-N1	-5.94	114.33	121.75
2	P	201	TFP	C13-N1-C5	-5.82	111.21	119.01

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

16 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	201	TFP	4	0
2	E	201	TFP	2	0
2	F	201	TFP	2	0
2	G	201	TFP	2	0
2	L	201	TFP	1	0
2	M	201	TFP	2	0
2	M	202	TFP	1	0
2	N	201	TFP	1	0
2	N	202	TFP	1	0
2	O	202	TFP	1	0
2	P	201	TFP	1	0
2	P	202	TFP	1	0
2	Q	201	TFP	1	0
2	R	202	TFP	1	0
2	S	201	TFP	1	0
2	S	202	TFP	1	0

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, 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	93/101 (92%)	0.40	5 (5%) 29 38	13, 20, 47, 57	0
1	B	93/101 (92%)	0.28	7 (7%) 17 24	14, 22, 48, 66	0
1	C	93/101 (92%)	0.18	3 (3%) 51 60	11, 21, 37, 48	0
1	D	93/101 (92%)	0.62	10 (10%) 8 11	17, 25, 70, 77	0
1	E	92/101 (91%)	0.20	5 (5%) 29 38	14, 24, 45, 51	0
1	F	90/101 (89%)	0.53	10 (11%) 7 11	15, 27, 51, 69	1 (1%)
1	G	90/101 (89%)	0.64	13 (14%) 3 5	7, 27, 49, 56	3 (3%)
1	H	94/101 (93%)	1.20	27 (28%) 1 1	20, 33, 63, 67	1 (1%)
1	I	93/101 (92%)	0.37	5 (5%) 29 38	15, 27, 42, 49	1 (1%)
1	J	93/101 (92%)	0.20	3 (3%) 51 60	13, 22, 39, 49	0
1	K	93/101 (92%)	0.33	6 (6%) 22 30	13, 23, 48, 54	0
1	L	93/101 (92%)	0.23	4 (4%) 39 48	15, 23, 46, 60	0
1	M	92/101 (91%)	0.43	7 (7%) 17 24	17, 28, 53, 60	2 (2%)
1	N	92/101 (91%)	0.22	4 (4%) 39 48	12, 21, 45, 52	1 (1%)
1	O	93/101 (92%)	0.43	8 (8%) 13 18	11, 29, 43, 49	2 (2%)
1	P	92/101 (91%)	0.27	5 (5%) 29 38	15, 26, 44, 50	0
1	Q	88/101 (87%)	0.70	11 (12%) 5 8	22, 33, 56, 58	2 (2%)
1	R	93/101 (92%)	0.38	7 (7%) 17 24	21, 30, 49, 56	0
1	S	93/101 (92%)	0.20	7 (7%) 17 24	5, 21, 39, 45	2 (2%)
1	T	93/101 (92%)	0.66	11 (11%) 6 10	12, 27, 58, 64	1 (1%)
All	All	1846/2020 (91%)	0.42	158 (8%) 13 18	5, 26, 49, 77	16 (0%)

The worst 5 of 158 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	53	ALA	7.0
1	H	54	ALA	6.4
1	K	2	ALA	6.0
1	P	2	ALA	5.9
1	C	94	PRO	5.8

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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	LLDF	B-factors(Å ²)	Q<0.9
2	TFP	O	202	28/28	0.94	0.16	1.80	14,27,31,33	0
2	TFP	Q	202	28/28	0.94	0.16	1.40	24,31,35,36	0
2	TFP	A	202	28/28	0.96	0.17	1.16	6,14,24,26	0
2	TFP	S	202	28/28	0.97	0.18	1.15	10,14,21,22	0
2	TFP	B	202	28/28	0.97	0.19	1.14	13,16,27,27	0
2	TFP	E	202	28/28	0.95	0.14	0.98	13,21,26,27	0
2	TFP	J	202	28/28	0.97	0.18	0.94	10,13,24,25	0
2	TFP	K	202	28/28	0.96	0.18	0.93	9,18,27,27	0
2	TFP	G	202	28/28	0.96	0.15	0.80	14,24,32,33	0
2	TFP	L	202	28/28	0.97	0.16	0.64	14,17,26,27	0
2	TFP	F	202	28/28	0.94	0.14	0.59	19,26,29,30	0
2	TFP	I	202	28/28	0.95	0.19	0.40	16,22,32,32	0
2	TFP	J	201	28/28	0.90	0.16	0.33	31,34,40,40	0
2	TFP	C	202	28/28	0.95	0.17	0.26	12,16,24,25	0
2	TFP	R	202	28/28	0.97	0.17	0.24	17,28,33,34	0
2	TFP	M	202	28/28	0.94	0.16	0.21	15,24,28,29	0
2	TFP	E	201	28/28	0.91	0.17	0.20	37,38,40,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	TFP	P	202	28/28	0.94	0.15	0.17	11,20,27,29	0
2	TFP	D	201	28/28	0.91	0.15	0.04	37,40,45,46	0
2	TFP	H	202	28/28	0.95	0.15	0.03	14,21,29,30	0
2	TFP	P	201	28/28	0.90	0.17	0.03	36,40,44,44	0
2	TFP	O	201	28/28	0.89	0.17	-0.00	31,37,39,39	0
3	CA	K	302	1/1	0.98	0.13	-0.03	20,20,20,20	0
2	TFP	R	201	28/28	0.93	0.15	-0.13	30,32,36,37	0
2	TFP	F	201	28/28	0.85	0.18	-0.15	40,42,49,49	0
2	TFP	K	201	28/28	0.93	0.14	-0.15	32,34,38,39	0
2	TFP	H	201	28/28	0.86	0.16	-0.22	27,30,31,31	0
2	TFP	N	202	28/28	0.97	0.13	-0.22	12,14,22,24	0
2	TFP	B	201	28/28	0.90	0.15	-0.24	37,39,40,41	0
2	TFP	T	202	28/28	0.96	0.14	-0.25	12,18,26,27	0
2	TFP	G	201	28/28	0.88	0.17	-0.30	44,45,47,47	0
2	TFP	S	201	28/28	0.94	0.13	-0.33	22,26,32,33	0
2	TFP	I	201	28/28	0.92	0.15	-0.37	25,29,33,34	0
2	TFP	M	201	28/28	0.92	0.15	-0.40	41,45,49,50	0
3	CA	C	302	1/1	0.95	0.11	-0.42	17,17,17,17	0
2	TFP	Q	201	28/28	0.89	0.14	-0.44	44,47,50,50	0
2	TFP	L	201	28/28	0.94	0.13	-0.53	28,31,34,34	0
2	TFP	T	201	28/28	0.91	0.13	-0.62	27,30,33,33	0
2	TFP	C	201	28/28	0.95	0.11	-0.70	24,26,31,32	0
3	CA	S	302	1/1	0.95	0.11	-0.71	13,13,13,13	0
2	TFP	A	201	28/28	0.96	0.10	-0.71	20,24,25,26	0
2	TFP	D	202	28/28	0.97	0.11	-0.77	10,21,29,30	0
3	CA	L	301	1/1	0.96	0.11	-0.79	17,17,17,17	0
3	CA	K	301	1/1	0.99	0.10	-0.82	17,17,17,17	0
3	CA	A	302	1/1	0.96	0.09	-0.95	12,12,12,12	0
2	TFP	N	201	28/28	0.95	0.11	-0.98	26,27,32,33	0
3	CA	B	302	1/1	0.98	0.10	-1.05	18,18,18,18	0
3	CA	E	302	1/1	0.99	0.09	-1.07	23,23,23,23	0
3	CA	L	302	1/1	0.99	0.08	-1.29	18,18,18,18	0
3	CA	B	301	1/1	0.96	0.09	-1.31	14,14,14,14	0
3	CA	S	301	1/1	0.99	0.09	-1.36	14,14,14,14	0
3	CA	J	302	1/1	0.99	0.09	-1.41	14,14,14,14	0
3	CA	A	301	1/1	0.98	0.09	-1.53	15,15,15,15	0
3	CA	C	301	1/1	0.98	0.06	-1.55	17,17,17,17	0
3	CA	J	301	1/1	0.99	0.07	-1.64	13,13,13,13	0
3	CA	R	301	1/1	0.99	0.06	-1.69	27,27,27,27	0
3	CA	D	301	1/1	0.96	0.07	-1.71	23,23,23,23	0
3	CA	P	302	1/1	0.95	0.05	-1.72	20,20,20,20	0
3	CA	M	301	1/1	0.96	0.09	-1.73	32,32,32,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	CA	G	302	1/1	0.90	0.05	-2.01	26,26,26,26	0
3	CA	N	301	1/1	0.97	0.06	-2.20	18,18,18,18	0
3	CA	D	302	1/1	0.97	0.04	-2.22	19,19,19,19	0
3	CA	R	302	1/1	0.96	0.03	-2.24	37,37,37,37	0
3	CA	T	301	1/1	0.93	0.04	-2.27	21,21,21,21	0
3	CA	T	302	1/1	0.94	0.04	-2.36	33,33,33,33	0
3	CA	P	301	1/1	1.00	0.03	-2.40	16,16,16,16	0
3	CA	I	301	1/1	0.97	0.07	-2.42	24,24,24,24	0
3	CA	F	302	1/1	0.95	0.03	-2.46	28,28,28,28	0
3	CA	N	302	1/1	0.97	0.05	-2.48	14,14,14,14	0
3	CA	H	302	1/1	0.89	0.05	-2.55	32,32,32,32	0
3	CA	I	302	1/1	0.99	0.02	-2.55	27,27,27,27	0
3	CA	Q	301	1/1	0.96	0.04	-2.57	30,30,30,30	0
3	CA	O	301	1/1	0.96	0.03	-2.67	31,31,31,31	0
3	CA	O	302	1/1	0.99	0.04	-2.70	25,25,25,25	0
3	CA	F	301	1/1	0.97	0.04	-2.73	23,23,23,23	0
3	CA	E	301	1/1	0.98	0.02	-3.07	19,19,19,19	0
3	CA	H	301	1/1	0.96	0.04	-3.27	38,38,38,38	0
3	CA	Q	302	1/1	0.94	0.04	-3.50	48,48,48,48	0
3	CA	G	301	1/1	0.97	0.03	-3.86	24,24,24,24	0
3	CA	M	302	1/1	0.89	0.04	-4.30	28,28,28,28	0

6.5 Other polymers [i](#)

There are no such residues in this entry.