wwPDB X-ray Structure Validation Summary Report (i)

Jan 8, 2024 – 07:36 am GMT

PDB ID	:	5MT3
Title	:	Human insulin in complex with serotonin and arginine
Authors	:	Brzozowski, A.M.; Turkenburg, J.P.; Jiracek, J.; Zakova, L.
Deposited on	:	2017-01-06
Resolution	:	2.02 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

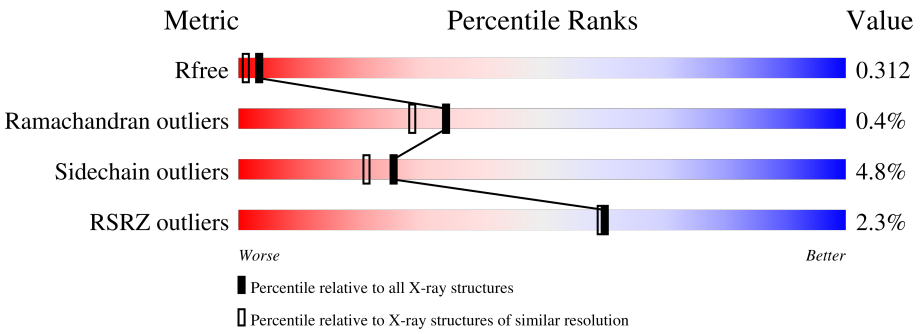
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.02 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	10434 (2.04-2.00)
Ramachandran outliers	138981	11493 (2.04-2.00)
Sidechain outliers	138945	11492 (2.04-2.00)
RSRZ outliers	127900	10220 (2.04-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	21	19%, 62%, 38%
1	C	21	5%, 100%
1	E	21	10%, 95%, 5%
1	G	21	100%
1	I	21	5%, 95%, 5%
1	K	21	90%, 5%, 5%

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Mol	Chain	Length	Quality of chain
1	M	21	5% 100%
1	O	21	95% 5%
1	Q	21	90% 10%
1	S	21	90% 10%
1	U	21	95% 5%
1	W	21	95% 5%
1	Y	21	5% 95% 5%
1	a	21	100%
1	c	21	100%
1	e	21	100%
2	B	30	77% 20%
2	D	30	87% 10%
2	F	30	87% 13%
2	H	30	83% 10% 7%
2	J	30	87% 7% 7%
2	L	30	7% 83% 7% 10%
2	N	30	3% 90% 10%
2	P	30	90% 7%
2	R	30	3% 80% 7% 13%
2	T	30	83% 10% 7%
2	V	30	3% 83% 13%
2	X	30	87% 7% 7%
2	Z	30	7% 77% 20%
2	b	30	93%
2	d	30	77% 20%

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Mol	Chain	Length	Quality of chain
2	f	30	87% 7% 7%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 6195 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 Insulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	13	101	61	15	21	4	0	0	0
			Total	C	N	O	S			
1	C	21	158	94	26	34	4	0	1	0
			Total	C	N	O	S			
1	E	20	146	87	24	31	4	0	0	0
			Total	C	N	O	S			
1	G	21	163	99	25	35	4	0	0	0
			Total	C	N	O	S			
1	I	21	157	96	25	32	4	0	0	0
			Total	C	N	O	S			
1	K	20	137	83	22	28	4	0	0	0
			Total	C	N	O	S			
1	M	21	154	93	25	32	4	0	0	0
			Total	C	N	O	S			
1	O	21	159	97	25	33	4	0	0	0
			Total	C	N	O	S			
1	Q	21	154	94	24	32	4	0	0	0
			Total	C	N	O	S			
1	S	21	157	96	25	32	4	0	0	0
			Total	C	N	O	S			
1	U	21	144	87	23	30	4	0	0	0
			Total	C	N	O	S			
1	W	21	158	97	25	32	4	0	0	0
			Total	C	N	O	S			
1	Y	21	144	89	22	29	4	0	0	0
			Total	C	N	O	S			
1	a	21	159	97	25	33	4	0	0	0
			Total	C	N	O	S			
1	c	21	147	90	23	30	4	0	0	0
			Total	C	N	O	S			
1	e	21	169	102	26	37	4	0	1	0

- Molecule 2 is a protein called Insulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	24	181	120	27	32	2	0	1	0
2	D	27	210	137	36	35	2	0	0	0
2	F	26	194	129	31	32	2	0	0	0
2	H	28	221	146	37	36	2	0	0	0
2	J	28	219	142	38	37	2	0	1	0
2	L	27	204	135	32	35	2	0	0	0
2	N	27	201	131	32	36	2	0	0	0
2	P	28	220	144	38	36	2	0	0	0
2	R	26	200	131	33	34	2	0	1	0
2	T	28	223	145	38	38	2	0	0	0
2	V	26	190	125	31	32	2	0	0	0
2	X	28	207	134	36	35	2	0	0	0
2	Z	24	184	119	31	32	2	0	0	0
2	b	29	225	149	37	37	2	0	0	0
2	d	24	187	120	32	33	2	0	1	0
2	f	28	212	137	37	36	2	0	0	0

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
3	B	1	1	1	0	0
3	D	1	1	1	0	0
3	E	1	1	1	0	0

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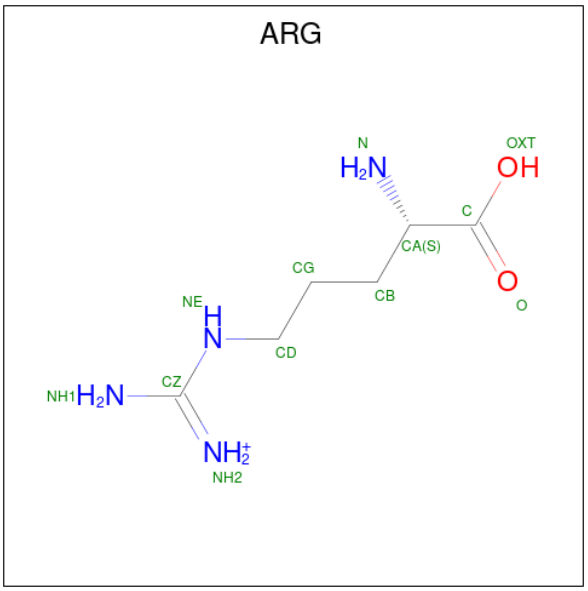
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	F	1	Total Zn 1 1	0	0
3	H	1	Total Zn 1 1	0	0
3	T	1	Total Zn 1 1	0	0
3	d	1	Total Zn 1 1	0	0
3	f	1	Total Zn 1 1	0	0

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

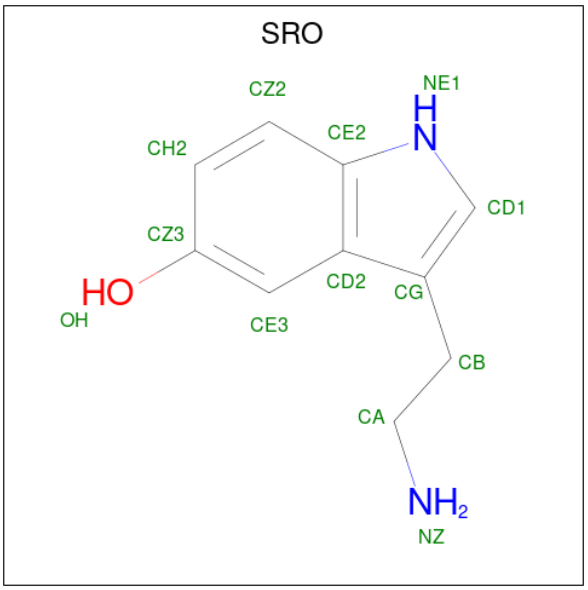
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total Cl 1 1	0	0
4	D	1	Total Cl 1 1	0	0
4	F	1	Total Cl 1 1	0	0
4	H	1	Total Cl 1 1	0	0
4	T	1	Total Cl 1 1	0	0
4	f	1	Total Cl 1 1	0	0

- Molecule 5 is ARGININE (three-letter code: ARG) (formula: $C_6H_{15}N_4O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
5	B	1	12	6	4	2	0	0
			Total	C	N	O		
5	F	1	12	6	4	2	0	0
			Total	C	N	O		
5	L	1	12	6	4	2	0	0
			Total	C	N	O		
5	N	1	12	6	4	2	0	0

- Molecule 6 is SEROTONIN (three-letter code: SRO) (formula: $C_{10}H_{12}N_2O$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
6	C	1	13	10	2	1	0	0
6	E	1	13	10	2	1	0	0
6	G	1	13	10	2	1	0	0
6	I	1	13	10	2	1	0	0
6	K	1	13	10	2	1	0	0
6	O	1	13	10	2	1	0	0
6	Q	1	13	10	2	1	0	0
6	S	1	13	10	2	1	0	0
6	W	1	13	10	2	1	0	0
6	a	1	13	10	2	1	0	0
6	c	1	13	10	2	1	0	0
6	d	1	13	10	2	1	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
7	A	6	6	6	0	0
7	B	6	6	6	0	0
7	C	7	7	7	0	0
7	D	3	3	3	0	0
7	E	6	6	6	0	0
7	F	8	8	8	0	0
7	G	9	9	9	0	0
7	H	16	16	16	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	I	9	Total O 9 9	0	0
7	J	12	Total O 12 12	0	0
7	K	5	Total O 5 5	0	0
7	L	8	Total O 8 8	0	0
7	M	9	Total O 9 9	0	0
7	N	6	Total O 6 6	0	0
7	O	12	Total O 12 12	0	0
7	P	11	Total O 11 11	0	0
7	Q	7	Total O 7 7	0	0
7	R	13	Total O 13 13	0	0
7	S	4	Total O 4 4	0	0
7	T	14	Total O 14 14	0	0
7	U	4	Total O 4 4	0	0
7	V	5	Total O 5 5	0	0
7	W	9	Total O 9 9	0	0
7	X	14	Total O 14 14	0	0
7	Y	3	Total O 3 3	0	0
7	Z	15	Total O 15 15	0	0
7	a	9	Total O 9 9	0	0
7	b	16	Total O 16 16	0	0
7	c	8	Total O 8 8	0	0

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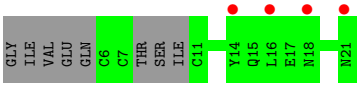
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
7	d	18	18	18	0	0
			Total	O		
7	e	10	10	10	0	0
			Total	O		
7	f	10	10	10	0	0

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.

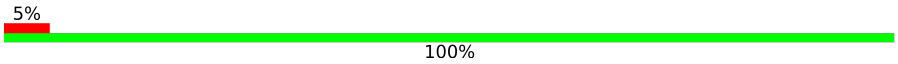
- Molecule 1: Insulin

Chain A:



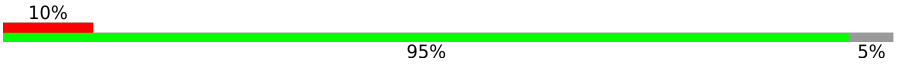
- Molecule 1: Insulin

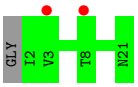
Chain C:



- Molecule 1: Insulin

Chain E:





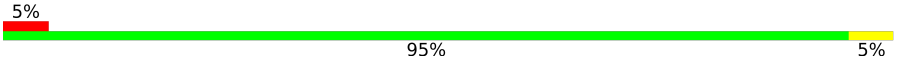
- Molecule 1: Insulin

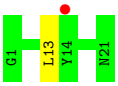
Chain G:

There are no outlier residues recorded for this chain.

- Molecule 1: Insulin

Chain I:

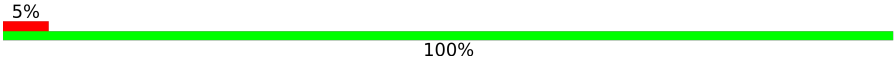




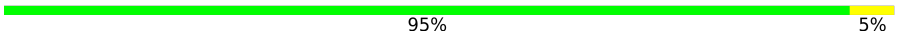
- Molecule 1: Insulin

Chain K:

• Molecule 1: Insulin

Chain M: 

• Molecule 1: Insulin

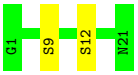
Chain O: 

• Molecule 1: Insulin

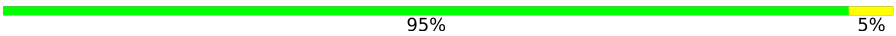
Chain Q:

• Molecule 1: Insulin

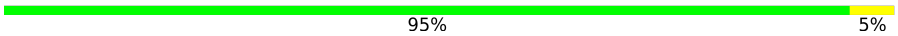
Chain S:



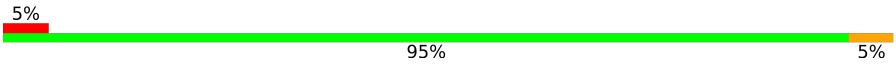
• Molecule 1: Insulin

Chain U: 

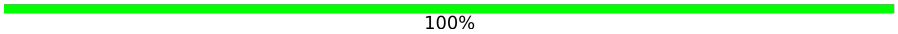
• Molecule 1: Insulin

Chain W: 

• Molecule 1: Insulin

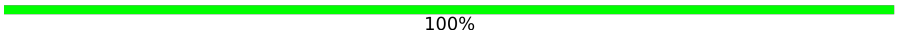
Chain Y: 

• Molecule 1: Insulin

Chain a: 

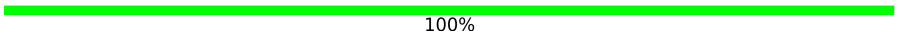
There are no outlier residues recorded for this chain.

• Molecule 1: Insulin

Chain c: 

There are no outlier residues recorded for this chain.

• Molecule 1: Insulin

Chain e: 

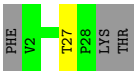
There are no outlier residues recorded for this chain.

• Molecule 2: Insulin

Chain B:

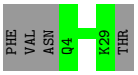
• Molecule 2: Insulin

Chain D:



• Molecule 2: Insulin

Chain F:

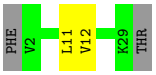


• Molecule 2: Insulin

Chain H:

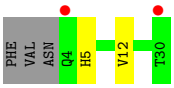
• Molecule 2: Insulin

Chain J:

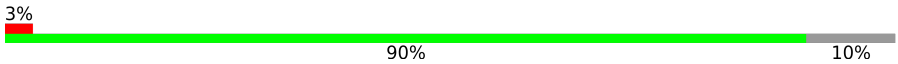


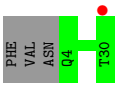
• Molecule 2: Insulin

Chain L:



• Molecule 2: Insulin

Chain N: 

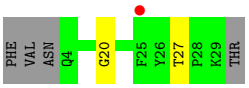


• Molecule 2: Insulin

Chain P:

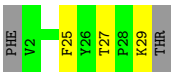
• Molecule 2: Insulin

Chain R:



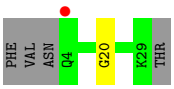
• Molecule 2: Insulin

Chain T:



• Molecule 2: Insulin

Chain V:

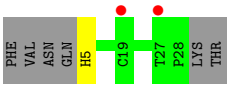


• Molecule 2: Insulin

Chain X:

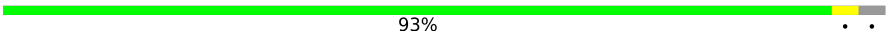
• Molecule 2: Insulin

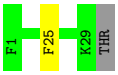
Chain Z:



• Molecule 2: Insulin

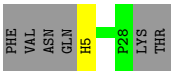
Chain b:





• Molecule 2: Insulin

Chain d:



• Molecule 2: Insulin

Chain f:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α, β, γ	158.64Å 158.64Å 76.10Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	42.89 – 2.02 42.89 – 2.02	Depositor EDS
% Data completeness (in resolution range)	98.3 (42.89-2.02) 98.3 (42.89-2.02)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.75 (at 2.01Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.236 , 0.310 0.244 , 0.312	Depositor DCC
R_{free} test set	2266 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å^2)	31.9	Xtriage
Anisotropy	0.319	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 57.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.53$, $< L^2 > = 0.37$	Xtriage
Estimated twinning fraction	0.035 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	6195	wwPDB-VP
Average B, all atoms (Å^2)	42.0	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 75.15 % 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 1.3348e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: CL, SRO, ZN

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	0.61	0/101	0.57	0/133
1	C	0.56	0/158	0.68	0/212
1	E	0.67	0/147	0.65	0/196
1	G	0.81	0/164	0.79	0/220
1	I	0.75	0/158	0.74	0/212
1	K	0.68	0/138	0.74	0/184
1	M	0.66	0/155	0.73	0/207
1	O	0.87	0/160	0.85	0/215
1	Q	0.53	0/155	0.69	0/208
1	S	0.66	0/158	0.76	0/212
1	U	0.61	0/145	0.73	0/194
1	W	0.75	0/159	0.73	0/215
1	Y	0.59	0/145	0.78	1/195 (0.5%)
1	a	0.74	0/160	0.80	0/215
1	c	0.71	0/148	0.70	0/198
1	e	0.78	0/170	0.83	0/228
2	B	0.73	0/186	0.71	0/252
2	D	0.69	0/216	0.75	0/293
2	F	0.77	0/200	0.87	0/271
2	H	0.85	1/228 (0.4%)	0.76	0/309
2	J	0.88	0/225	0.87	0/304
2	L	0.73	0/210	0.79	0/283
2	N	0.71	0/206	0.80	0/277
2	P	0.77	0/226	0.78	0/305
2	R	0.76	0/206	0.78	0/279
2	T	0.80	0/229	0.85	0/309
2	V	0.73	0/195	0.83	0/264
2	X	0.73	0/213	0.75	0/288
2	Z	0.80	0/189	0.86	0/256
2	b	0.85	0/232	0.81	0/314
2	d	0.85	0/192	0.77	0/259
2	f	0.87	1/218 (0.5%)	0.75	0/295

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
All	All	0.75	2/5792 (0.0%)	0.78	1/7802 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	f	9	SER	CB-OG	-6.65	1.33	1.42
2	H	9	SER	CB-OG	-5.11	1.35	1.42

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	Y	11	CYS	CA-CB-SG	5.22	123.40	114.00

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	9/21 (43%)	8 (89%)	1 (11%)	0	100	100
1	C	20/21 (95%)	17 (85%)	3 (15%)	0	100	100
1	E	18/21 (86%)	17 (94%)	1 (6%)	0	100	100
1	G	19/21 (90%)	19 (100%)	0	0	100	100
1	I	19/21 (90%)	19 (100%)	0	0	100	100
1	K	18/21 (86%)	14 (78%)	3 (17%)	1 (6%)	2	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	M	19/21 (90%)	17 (90%)	2 (10%)	0	100	100
1	O	19/21 (90%)	19 (100%)	0	0	100	100
1	Q	19/21 (90%)	18 (95%)	1 (5%)	0	100	100
1	S	19/21 (90%)	18 (95%)	1 (5%)	0	100	100
1	U	19/21 (90%)	13 (68%)	6 (32%)	0	100	100
1	W	19/21 (90%)	19 (100%)	0	0	100	100
1	Y	19/21 (90%)	17 (90%)	2 (10%)	0	100	100
1	a	19/21 (90%)	19 (100%)	0	0	100	100
1	c	19/21 (90%)	18 (95%)	1 (5%)	0	100	100
1	e	20/21 (95%)	20 (100%)	0	0	100	100
2	B	23/30 (77%)	22 (96%)	1 (4%)	0	100	100
2	D	25/30 (83%)	24 (96%)	1 (4%)	0	100	100
2	F	24/30 (80%)	23 (96%)	1 (4%)	0	100	100
2	H	26/30 (87%)	26 (100%)	0	0	100	100
2	J	27/30 (90%)	27 (100%)	0	0	100	100
2	L	25/30 (83%)	24 (96%)	1 (4%)	0	100	100
2	N	25/30 (83%)	23 (92%)	2 (8%)	0	100	100
2	P	26/30 (87%)	26 (100%)	0	0	100	100
2	R	24/30 (80%)	22 (92%)	1 (4%)	1 (4%)	3	0
2	T	26/30 (87%)	25 (96%)	1 (4%)	0	100	100
2	V	24/30 (80%)	22 (92%)	1 (4%)	1 (4%)	3	0
2	X	26/30 (87%)	26 (100%)	0	0	100	100
2	Z	22/30 (73%)	22 (100%)	0	0	100	100
2	b	27/30 (90%)	26 (96%)	1 (4%)	0	100	100
2	d	23/30 (77%)	23 (100%)	0	0	100	100
2	f	26/30 (87%)	25 (96%)	1 (4%)	0	100	100
All	All	693/816 (85%)	658 (95%)	32 (5%)	3 (0%)	34	28

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	V	20	GLY
2	R	20	GLY

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Mol	Chain	Res	Type
1	K	3	VAL

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	12/20 (60%)	12 (100%)	0	100	100
1	C	19/20 (95%)	19 (100%)	0	100	100
1	E	16/20 (80%)	16 (100%)	0	100	100
1	G	20/20 (100%)	20 (100%)	0	100	100
1	I	18/20 (90%)	17 (94%)	1 (6%)	21	16
1	K	13/20 (65%)	13 (100%)	0	100	100
1	M	17/20 (85%)	17 (100%)	0	100	100
1	O	19/20 (95%)	18 (95%)	1 (5%)	22	17
1	Q	18/20 (90%)	16 (89%)	2 (11%)	6	3
1	S	19/20 (95%)	17 (90%)	2 (10%)	7	3
1	U	15/20 (75%)	14 (93%)	1 (7%)	16	11
1	W	19/20 (95%)	18 (95%)	1 (5%)	22	17
1	Y	14/20 (70%)	13 (93%)	1 (7%)	14	9
1	a	19/20 (95%)	19 (100%)	0	100	100
1	c	16/20 (80%)	16 (100%)	0	100	100
1	e	21/20 (105%)	21 (100%)	0	100	100
2	B	18/26 (69%)	17 (94%)	1 (6%)	21	16
2	D	22/26 (85%)	21 (96%)	1 (4%)	27	23
2	F	19/26 (73%)	19 (100%)	0	100	100
2	H	23/26 (88%)	21 (91%)	2 (9%)	10	6
2	J	22/26 (85%)	20 (91%)	2 (9%)	9	5
2	L	19/26 (73%)	17 (90%)	2 (10%)	7	3
2	N	19/26 (73%)	19 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	P	23/26 (88%)	22 (96%)	1 (4%)	29	25
2	R	20/26 (77%)	19 (95%)	1 (5%)	24	19
2	T	24/26 (92%)	21 (88%)	3 (12%)	4	2
2	V	18/26 (69%)	18 (100%)	0	100	100
2	X	20/26 (77%)	18 (90%)	2 (10%)	7	4
2	Z	19/26 (73%)	18 (95%)	1 (5%)	22	17
2	b	23/26 (88%)	22 (96%)	1 (4%)	29	25
2	d	20/26 (77%)	19 (95%)	1 (5%)	24	19
2	f	21/26 (81%)	20 (95%)	1 (5%)	25	21
All	All	605/736 (82%)	577 (95%)	28 (5%)	25	22

5 of 28 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	S	9	SER
2	f	25	PHE
2	T	27	THR
2	Z	5	HIS
2	T	25	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
1	Y	18	ASN
2	b	5	HIS
2	b	4	GLN
1	M	5	GLN
1	W	15	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)

Of 30 ligands modelled in this entry, 14 are monoatomic - leaving 16 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	$\#\|Z\| > 2$
6	SRO	I	101	-	12,14,14	1.09	0	12,19,19	1.23	1 (8%)
6	SRO	Q	101	-	12,14,14	1.23	1 (8%)	12,19,19	1.50	1 (8%)
6	SRO	W	101	-	12,14,14	1.37	1 (8%)	12,19,19	1.68	2 (16%)
6	SRO	a	101	-	12,14,14	1.53	3 (25%)	12,19,19	1.14	0
6	SRO	C	101	-	12,14,14	1.15	2 (16%)	12,19,19	1.29	2 (16%)
5	ARG	L	101	-	10,11,11	0.56	0	11,13,13	1.50	2 (18%)
5	ARG	B	103	-	10,11,11	0.93	1 (10%)	11,13,13	1.77	2 (18%)
6	SRO	G	101	-	12,14,14	1.30	1 (8%)	12,19,19	1.52	2 (16%)
6	SRO	O	101	-	12,14,14	1.10	1 (8%)	12,19,19	0.80	0
5	ARG	N	101	-	10,11,11	0.91	0	11,13,13	2.19	2 (18%)
6	SRO	K	101	-	12,14,14	1.09	0	12,19,19	1.24	1 (8%)
6	SRO	c	101	-	12,14,14	1.35	0	12,19,19	2.40	4 (33%)
6	SRO	d	102	-	12,14,14	1.39	2 (16%)	12,19,19	1.65	5 (41%)
6	SRO	S	101	-	12,14,14	1.30	2 (16%)	12,19,19	1.93	2 (16%)
6	SRO	E	102	-	12,14,14	1.24	1 (8%)	12,19,19	1.56	2 (16%)
5	ARG	F	103	-	10,11,11	0.67	0	11,13,13	1.65	2 (18%)

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
6	SRO	I	101	-	-	0/3/3/3	0/2/2/2
6	SRO	Q	101	-	-	2/3/3/3	0/2/2/2
6	SRO	W	101	-	-	0/3/3/3	0/2/2/2
6	SRO	a	101	-	-	0/3/3/3	0/2/2/2
6	SRO	C	101	-	-	0/3/3/3	0/2/2/2
5	ARG	L	101	-	-	2/11/11/11	-
5	ARG	B	103	-	-	5/11/11/11	-
6	SRO	G	101	-	-	0/3/3/3	0/2/2/2
6	SRO	O	101	-	-	1/3/3/3	0/2/2/2
5	ARG	N	101	-	-	6/11/11/11	-
6	SRO	K	101	-	-	1/3/3/3	0/2/2/2
6	SRO	c	101	-	-	2/3/3/3	0/2/2/2
6	SRO	d	102	-	-	0/3/3/3	0/2/2/2
6	SRO	S	101	-	-	1/3/3/3	0/2/2/2
6	SRO	E	102	-	-	1/3/3/3	0/2/2/2
5	ARG	F	103	-	-	5/11/11/11	-

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	W	101	SRO	CE3-CD2	-3.22	1.35	1.42
6	d	102	SRO	CE3-CD2	-2.73	1.36	1.42
6	a	101	SRO	CZ2-CH2	2.52	1.41	1.36
6	a	101	SRO	CE3-CD2	-2.51	1.37	1.42
6	a	101	SRO	CD2-CE2	2.32	1.48	1.42

The worst 5 of 30 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	c	101	SRO	CZ3-CE3-CD2	-5.45	116.83	120.64
5	N	101	ARG	OXT-C-O	-4.84	113.11	124.09
5	N	101	ARG	OXT-C-CA	4.45	128.56	113.38
6	S	101	SRO	CZ3-CE3-CD2	-4.43	117.54	120.64
5	B	103	ARG	OXT-C-O	-4.06	114.87	124.09

There are no chirality outliers.

5 of 26 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	103	ARG	C-CA-CB-CG
5	F	103	ARG	O-C-CA-N

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Mol	Chain	Res	Type	Atoms
5	F	103	ARG	N-CA-CB-CG
5	F	103	ARG	C-CA-CB-CG
5	N	101	ARG	C-CA-CB-CG

There are no ring outliers.

No monomer is involved in short contacts.

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	13/21 (61%)	1.40	4 (30%)	0	0	57, 70, 79, 84	0
1	C	21/21 (100%)	0.49	1 (4%)	30	30	47, 58, 72, 80	0
1	E	20/21 (95%)	0.82	2 (10%)	7	6	39, 52, 67, 75	0
1	G	21/21 (100%)	0.05	0	100	100	26, 33, 41, 59	0
1	I	21/21 (100%)	0.22	1 (4%)	30	30	32, 39, 56, 60	0
1	K	20/21 (95%)	0.51	0	100	100	44, 54, 74, 75	0
1	M	21/21 (100%)	0.89	1 (4%)	30	30	39, 48, 60, 67	0
1	O	21/21 (100%)	-0.13	0	100	100	30, 36, 44, 50	0
1	Q	21/21 (100%)	0.36	0	100	100	44, 55, 65, 77	0
1	S	21/21 (100%)	0.47	0	100	100	39, 52, 58, 60	0
1	U	21/21 (100%)	0.35	0	100	100	44, 57, 66, 77	0
1	W	21/21 (100%)	0.01	0	100	100	29, 40, 46, 54	0
1	Y	21/21 (100%)	0.36	1 (4%)	30	30	44, 56, 66, 76	0
1	a	21/21 (100%)	-0.03	0	100	100	29, 35, 45, 55	0
1	c	21/21 (100%)	0.12	0	100	100	38, 47, 58, 62	0
1	e	21/21 (100%)	0.11	0	100	100	25, 36, 47, 52	0
2	B	24/30 (80%)	0.40	0	100	100	32, 42, 59, 63	0
2	D	27/30 (90%)	0.28	0	100	100	31, 41, 67, 76	0
2	F	26/30 (86%)	0.06	0	100	100	23, 32, 53, 65	0
2	H	28/30 (93%)	-0.07	0	100	100	19, 28, 40, 43	0
2	J	28/30 (93%)	-0.00	0	100	100	19, 29, 43, 59	0
2	L	27/30 (90%)	0.17	2 (7%)	14	14	24, 36, 74, 87	0
2	N	27/30 (90%)	0.06	1 (3%)	41	41	25, 35, 60, 78	1 (3%)
2	P	28/30 (93%)	-0.03	0	100	100	19, 29, 47, 64	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
2	R	26/30 (86%)	0.26	1 (3%) 40 40	28, 41, 57, 64	0
2	T	28/30 (93%)	0.26	0 100 100	23, 37, 65, 90	0
2	V	26/30 (86%)	0.30	1 (3%) 40 40	30, 41, 60, 68	0
2	X	28/30 (93%)	0.04	0 100 100	24, 37, 57, 87	0
2	Z	24/30 (80%)	0.31	2 (8%) 11 10	25, 35, 53, 56	0
2	b	29/30 (96%)	0.01	0 100 100	21, 34, 56, 74	0
2	d	24/30 (80%)	0.29	0 100 100	26, 36, 49, 65	0
2	f	28/30 (93%)	0.08	0 100 100	22, 32, 57, 78	0
All	All	754/816 (92%)	0.23	17 (2%) 60 59	19, 41, 67, 90	1 (0%)

The worst 5 of 17 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	16	LEU	3.8
2	L	30	THR	3.4
2	N	30	THR	2.8
2	V	4	GLN	2.7
1	E	8	THR	2.6

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)

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
6	SRO	Q	101	13/13	0.57	0.38	29,30,33,33	13
5	ARG	B	103	12/12	0.64	0.35	52,78,85,86	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	SRO	K	101	13/13	0.69	0.37	34,35,37,37	13
5	ARG	L	101	12/12	0.69	0.34	47,72,78,80	0
5	ARG	F	103	12/12	0.70	0.32	48,74,79,80	0
5	ARG	N	101	12/12	0.78	0.28	41,56,73,74	0
6	SRO	c	101	13/13	0.80	0.32	27,29,33,35	13
6	SRO	C	101	13/13	0.90	0.15	40,45,49,49	0
6	SRO	S	101	13/13	0.91	0.15	39,48,53,54	0
6	SRO	E	102	13/13	0.91	0.26	19,21,22,24	13
6	SRO	a	101	13/13	0.92	0.11	30,33,35,35	0
4	CL	F	102	1/1	0.93	0.05	69,69,69,69	0
6	SRO	G	101	13/13	0.94	0.11	30,31,34,36	0
6	SRO	O	101	13/13	0.94	0.14	26,28,31,31	0
6	SRO	I	101	13/13	0.95	0.10	32,35,36,36	0
6	SRO	W	101	13/13	0.95	0.13	26,29,33,35	0
6	SRO	d	102	13/13	0.95	0.12	27,31,33,34	0
3	ZN	d	101	1/1	0.96	0.14	32,32,32,32	1
4	CL	D	102	1/1	0.97	0.18	27,27,27,27	1
4	CL	B	102	1/1	0.97	0.02	61,61,61,61	1
3	ZN	F	101	1/1	0.99	0.10	28,28,28,28	0
4	CL	H	102	1/1	0.99	0.10	18,18,18,18	0
3	ZN	f	101	1/1	0.99	0.13	25,25,25,25	1
3	ZN	H	101	1/1	1.00	0.11	19,19,19,19	0
3	ZN	T	101	1/1	1.00	0.11	22,22,22,22	0
3	ZN	D	101	1/1	1.00	0.07	33,33,33,33	1
4	CL	T	102	1/1	1.00	0.14	17,17,17,17	0
4	CL	f	102	1/1	1.00	0.16	14,14,14,14	1
3	ZN	E	101	1/1	1.00	0.13	32,32,32,32	0
3	ZN	B	101	1/1	1.00	0.06	39,39,39,39	1

6.5 Other polymers (i)

There are no such residues in this entry.