wwPDB X-ray Structure Validation Summary Report (i)

Jun 23, 2024 – 09:39 PM EDT

PDB ID	:	5MAM
Title	:	Human insulin in complex with serotonin
Authors	:	Brzozowski, A.M.; Turkenburg, J.P.; Jiracek, J.; Zakova, L.
Deposited on	:	2016-11-03
Resolution	:	2.20 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 (1)) were used in the production of this report:

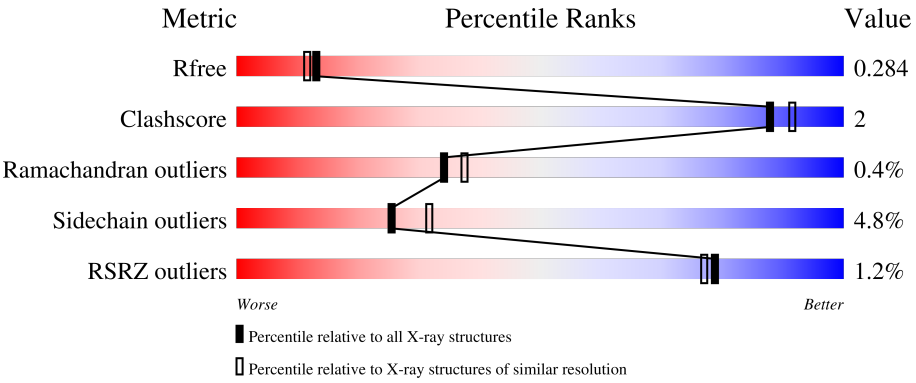
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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	0	21	5% 95% 5%
1	2	21	100%
1	4	21	95% 5%
1	A	21	81% 14% 5%
1	C	21	90% 10%

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Mol	Chain	Length	Quality of chain
1	E	21	90% 5% 5%
1	G	21	86% 14%
1	I	21	86% 14%
1	K	21	86% 14%
1	M	21	100%
1	O	21	90% 10%
1	Q	21	100%
1	S	21	5% 95% 5%
1	U	21	90% 10%
1	W	21	86% 14%
1	Y	21	95% 5%
2	1	30	77% 10% 10%
2	3	30	77% 20%
2	5	30	3% 90% 7%
2	B	30	3% 83% 13%
2	D	30	3% 87% 7% 7%
2	F	30	83% 17%
2	H	30	90% 7%
2	J	30	83% 10%
2	L	30	3% 80% 7% 13%
2	N	30	70% 13% 17%
2	P	30	77% 20%
2	R	30	97%
2	T	30	80% 17%
2	V	30	3% 80% 17%

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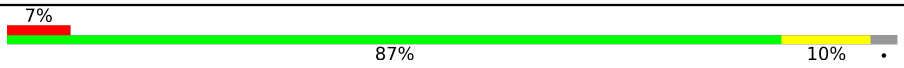
Mol	Chain	Length	Quality of chain
2	X	30	
2	Z	30	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	SRO	Y	101	-	-	-	X

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 6207 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 A chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	20	Total	C	N	O	S	0	0	0
			140	84	23	29	4			
1	C	21	Total	C	N	O	S	0	0	0
			159	97	25	33	4			
1	E	20	Total	C	N	O	S	0	0	0
			149	91	24	30	4			
1	G	21	Total	C	N	O	S	0	0	0
			163	99	25	35	4			
1	I	21	Total	C	N	O	S	0	0	0
			159	97	25	33	4			
1	K	21	Total	C	N	O	S	0	0	0
			150	91	25	30	4			
1	M	21	Total	C	N	O	S	0	0	0
			159	96	25	34	4			
1	O	21	Total	C	N	O	S	0	0	0
			159	97	25	33	4			
1	Q	21	Total	C	N	O	S	0	0	0
			159	97	25	33	4			
1	S	21	Total	C	N	O	S	0	0	0
			146	89	23	30	4			
1	U	21	Total	C	N	O	S	0	0	0
			142	85	23	30	4			
1	W	21	Total	C	N	O	S	0	0	0
			161	99	24	34	4			
1	Y	21	Total	C	N	O	S	0	0	0
			153	93	24	32	4			
1	0	21	Total	C	N	O	S	0	0	0
			158	97	25	32	4			
1	2	21	Total	C	N	O	S	0	0	0
			147	90	23	30	4			
1	4	21	Total	C	N	O	S	0	0	0
			162	99	24	35	4			

- Molecule 2 is a protein called Insulin B chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	26	Total	C	N	O	S	0	0	0
			180	120	28	30	2			
2	D	28	Total	C	N	O	S	0	1	0
			225	145	41	37	2			
2	F	25	Total	C	N	O	S	0	0	0
			186	123	30	31	2			
2	H	29	Total	C	N	O	S	0	1	0
			239	157	40	40	2			
2	J	29	Total	C	N	O	S	0	1	0
			230	148	42	38	2			
2	L	26	Total	C	N	O	S	0	0	0
			195	129	32	32	2			
2	N	25	Total	C	N	O	S	0	0	0
			196	129	32	33	2			
2	P	30	Total	C	N	O	S	0	1	0
			235	151	40	42	2			
2	R	29	Total	C	N	O	S	0	0	0
			221	147	37	35	2			
2	T	25	Total	C	N	O	S	0	0	0
			185	120	32	31	2			
2	V	25	Total	C	N	O	S	0	0	0
			189	124	32	31	2			
2	X	29	Total	C	N	O	S	0	0	0
			210	136	37	35	2			
2	Z	26	Total	C	N	O	S	0	0	0
			191	126	31	32	2			
2	1	27	Total	C	N	O	S	0	0	0
			210	137	36	35	2			
2	3	24	Total	C	N	O	S	0	1	0
			187	120	32	33	2			
2	5	28	Total	C	N	O	S	0	0	0
			206	135	36	33	2			

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

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

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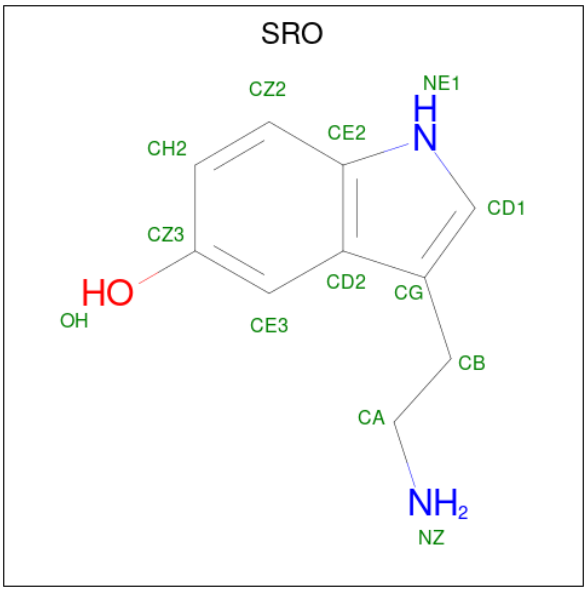
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	H	1	Total Zn 1 1	0	0
3	R	1	Total Zn 1 1	0	0
3	T	1	Total Zn 1 1	0	0
3	3	1	Total Zn 1 1	0	0
3	5	1	Total Zn 1 1	0	0

- 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	P	1	Total Cl 1 1	0	0
4	T	1	Total Cl 1 1	0	0
4	X	1	Total Cl 1 1	0	0
4	3	1	Total Cl 1 1	0	0
4	5	1	Total Cl 1 1	0	0

- Molecule 5 is SEROTONIN (three-letter code: SRO) (formula: $C_{10}H_{12}N_2O$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	1	Total C N O 13 10 2 1	0	0
5	E	1	Total C N O 13 10 2 1	0	0
5	G	1	Total C N O 13 10 2 1	0	0
5	I	1	Total C N O 13 10 2 1	0	0
5	K	1	Total C N O 13 10 2 1	0	0
5	M	1	Total C N O 13 10 2 1	0	0
5	O	1	Total C N O 13 10 2 1	0	0
5	Q	1	Total C N O 13 10 2 1	0	0
5	W	1	Total C N O 13 10 2 1	0	0
5	Y	1	Total C N O 13 10 2 1	0	0
5	Y	1	Total C N O 13 10 2 1	0	0
5	0	1	Total C N O 13 10 2 1	0	0
5	2	1	Total C N O 13 10 2 1	0	0
5	3	1	Total C N O 13 10 2 1	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	10	Total O 10 10	0	0
6	B	6	Total O 6 6	0	0
6	C	3	Total O 3 3	0	0
6	D	12	Total O 12 12	0	0
6	E	7	Total O 7 7	0	0
6	F	9	Total O 9 9	0	0
6	G	11	Total O 11 11	0	0
6	H	9	Total O 9 9	0	0
6	I	9	Total O 9 9	0	0
6	J	8	Total O 8 8	0	0
6	K	4	Total O 4 4	0	0
6	L	9	Total O 9 9	0	0
6	M	7	Total O 7 7	0	0
6	N	8	Total O 8 8	0	0
6	O	12	Total O 12 12	0	0
6	P	12	Total O 12 12	0	0
6	Q	11	Total O 11 11	0	0
6	R	11	Total O 11 11	0	0
6	S	9	Total O 9 9	0	0
6	T	8	Total O 8 8	0	0
6	U	8	Total O 8 8	0	0

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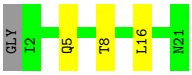
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	V	4	Total O 4 4	0	0
6	W	3	Total O 3 3	0	0
6	X	4	Total O 4 4	0	0
6	Y	7	Total O 7 7	0	0
6	Z	8	Total O 8 8	0	0
6	0	4	Total O 4 4	0	0
6	1	8	Total O 8 8	0	0
6	2	8	Total O 8 8	0	0
6	3	11	Total O 11 11	0	0
6	4	8	Total O 8 8	0	0
6	5	10	Total O 10 10	0	0

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 A chain

Chain A:

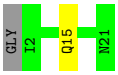


- Molecule 1: Insulin A chain

Chain C:

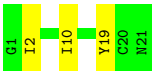
- Molecule 1: Insulin A chain

Chain E:



- Molecule 1: Insulin A chain

Chain G:



- Molecule 1: Insulin A chain

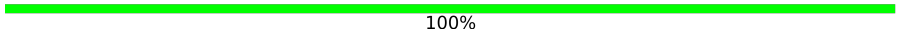
Chain I:

- Molecule 1: Insulin A chain

Chain K:

• Molecule 1: Insulin A chain

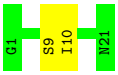
Chain M:



There are no outlier residues recorded for this chain.

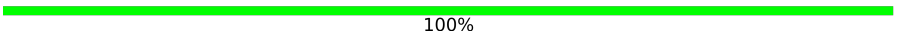
• Molecule 1: Insulin A chain

Chain O:



• Molecule 1: Insulin A chain

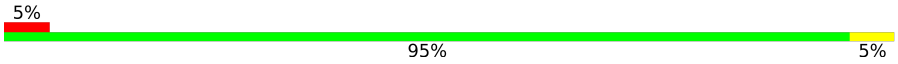
Chain Q:

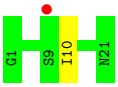


There are no outlier residues recorded for this chain.

• Molecule 1: Insulin A chain

Chain S:



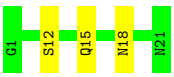


• Molecule 1: Insulin A chain

Chain U:

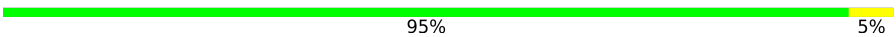
• Molecule 1: Insulin A chain

Chain W:



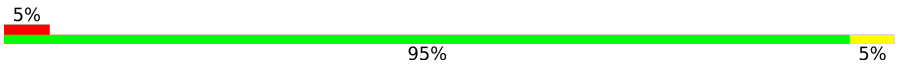
• Molecule 1: Insulin A chain

Chain Y:



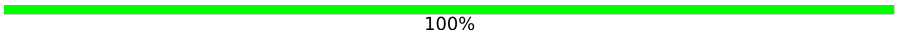
• Molecule 1: Insulin A chain

Chain 0:



• Molecule 1: Insulin A chain

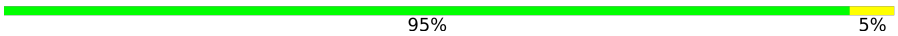
Chain 2:



There are no outlier residues recorded for this chain.

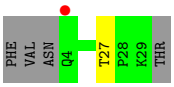
• Molecule 1: Insulin A chain

Chain 4:



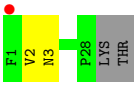
• Molecule 2: Insulin B chain

Chain B:



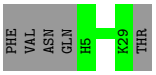
• Molecule 2: Insulin B chain

Chain D:



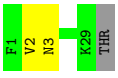
• Molecule 2: Insulin B chain

Chain F:



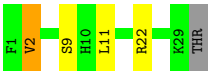
• Molecule 2: Insulin B chain

Chain H:



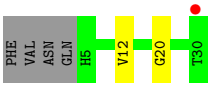
• Molecule 2: Insulin B chain

Chain J:



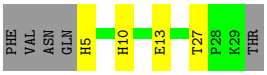
• Molecule 2: Insulin B chain

Chain L:



• Molecule 2: Insulin B chain

Chain N:

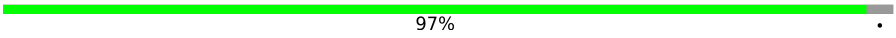


• Molecule 2: Insulin B chain

Chain P:

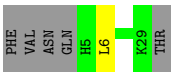
• Molecule 2: Insulin B chain

Chain R:



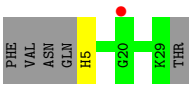
• Molecule 2: Insulin B chain

Chain T:



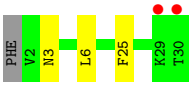
• Molecule 2: Insulin B chain

Chain V:



• Molecule 2: Insulin B chain

Chain X:



• Molecule 2: Insulin B chain

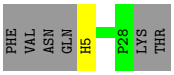
Chain Z:

• Molecule 2: Insulin B chain

Chain 1:

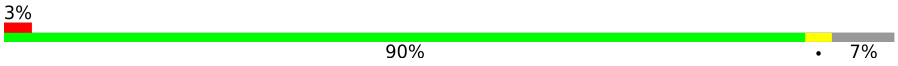
• Molecule 2: Insulin B chain

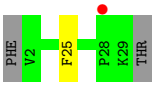
Chain 3:



• Molecule 2: Insulin B chain

Chain 5:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α, β, γ	158.96Å 158.96Å 76.53Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	51.18 – 2.20 51.18 – 2.20	Depositor EDS
% Data completeness (in resolution range)	98.4 (51.18-2.20) 98.4 (51.18-2.20)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.82 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.8.0155	Depositor
R, R_{free}	0.202 , 0.280 0.208 , 0.284	Depositor DCC
R_{free} test set	1786 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å^2)	36.5	Xtriage
Anisotropy	0.289	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 45.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.52$, $< L^2 > = 0.36$	Xtriage
Estimated twinning fraction	0.030 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	6207	wwPDB-VP
Average B, all atoms (Å^2)	46.0	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 68.82 % 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 4.0983e-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: SRO, ZN, CL

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	0	0.65	0/159	0.67	0/214
1	2	0.63	0/148	0.75	0/198
1	4	0.72	0/163	0.76	0/218
1	A	0.63	0/141	0.66	0/189
1	C	0.61	0/160	0.66	0/215
1	E	0.70	0/150	0.76	0/201
1	G	0.83	0/164	0.78	0/220
1	I	0.76	0/160	0.79	0/215
1	K	0.66	0/151	0.70	0/203
1	M	0.71	0/160	0.73	0/214
1	O	0.82	0/160	0.78	0/215
1	Q	0.69	0/160	0.77	0/215
1	S	0.68	0/147	0.76	0/197
1	U	0.58	0/142	0.69	0/190
1	W	0.67	0/162	0.72	0/216
1	Y	0.62	0/154	0.74	0/207
2	1	0.73	0/216	0.78	0/293
2	3	0.74	0/192	0.74	0/259
2	5	0.72	0/212	0.71	0/287
2	B	0.66	0/185	0.74	0/251
2	D	0.61	0/231	0.71	0/312
2	F	0.70	0/191	0.81	0/259
2	H	0.83	0/246	0.78	0/332
2	J	0.82	1/236 (0.4%)	0.80	0/319
2	L	0.74	0/200	0.82	0/270
2	N	0.81	0/202	0.91	0/273
2	P	0.83	1/241 (0.4%)	0.85	0/325
2	R	0.72	0/228	0.73	0/309
2	T	0.73	0/190	0.84	0/257
2	V	0.77	0/195	0.73	0/263
2	X	0.72	0/216	0.73	0/291
2	Z	0.76	0/196	0.75	0/266

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
All	All	0.72	2/5858 (0.0%)	0.76	0/7893

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	9	SER	CB-OG	-5.19	1.35	1.42
2	P	9	SER	CB-OG	-5.03	1.35	1.42

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	0	158	0	142	1	0
1	2	147	0	126	0	0
1	4	162	0	147	0	0
1	A	140	0	101	0	0
1	C	159	0	142	1	0
1	E	149	0	124	2	0
1	G	163	0	149	3	0
1	I	159	0	145	2	0
1	K	150	0	120	1	0
1	M	159	0	136	0	0
1	O	159	0	145	3	0
1	Q	159	0	145	0	0
1	S	146	0	121	0	0
1	U	142	0	118	1	0
1	W	161	0	147	1	0
1	Y	153	0	133	1	0
2	1	210	0	196	2	0
2	3	187	0	169	0	0
2	5	206	0	184	0	0
2	B	180	0	157	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	225	0	209	0	0
2	F	186	0	170	0	0
2	H	239	0	226	3	0
2	J	230	0	214	3	0
2	L	195	0	183	1	0
2	N	196	0	181	1	0
2	P	235	0	212	5	0
2	R	221	0	204	0	0
2	T	185	0	169	0	0
2	V	189	0	173	0	0
2	X	210	0	184	1	0
2	Z	191	0	172	3	0
3	3	1	0	0	0	0
3	5	1	0	0	0	0
3	B	1	0	0	0	0
3	D	1	0	0	0	0
3	F	1	0	0	0	0
3	H	1	0	0	0	0
3	R	1	0	0	0	0
3	T	1	0	0	0	0
4	3	1	0	0	0	1
4	5	1	0	0	0	0
4	B	1	0	0	0	0
4	D	1	0	0	0	0
4	F	1	0	0	0	0
4	P	1	0	0	0	0
4	T	1	0	0	0	0
4	X	1	0	0	0	0
5	0	13	0	11	0	0
5	2	13	0	11	0	0
5	3	13	0	11	0	0
5	C	13	0	11	1	0
5	E	13	0	12	0	0
5	G	13	0	11	0	0
5	I	13	0	11	0	0
5	K	13	0	11	1	0
5	M	13	0	11	0	0
5	O	13	0	11	0	0
5	Q	13	0	12	0	0
5	W	13	0	11	0	0
5	Y	26	0	23	0	0
6	0	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	1	8	0	0	0	0
6	2	8	0	0	0	0
6	3	11	0	0	0	0
6	4	8	0	0	0	0
6	5	10	0	0	0	0
6	A	10	0	0	0	0
6	B	6	0	0	0	0
6	C	3	0	0	0	0
6	D	12	0	0	0	0
6	E	7	0	0	0	0
6	F	9	0	0	0	0
6	G	11	0	0	0	0
6	H	9	0	0	0	0
6	I	9	0	0	0	0
6	J	8	0	0	0	0
6	K	4	0	0	0	0
6	L	9	0	0	1	0
6	M	7	0	0	0	0
6	N	8	0	0	0	0
6	O	12	0	0	0	0
6	P	12	0	0	0	0
6	Q	11	0	0	0	0
6	R	11	0	0	0	0
6	S	9	0	0	0	0
6	T	8	0	0	0	0
6	U	8	0	0	0	0
6	V	4	0	0	0	0
6	W	3	0	0	0	0
6	X	4	0	0	0	0
6	Y	7	0	0	0	0
6	Z	8	0	0	0	0
All	All	6207	0	5301	23	1

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.

The worst 5 of 23 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)
2:P:13[B]:GLU:HA	2:P:13[B]:GLU:OE1	1.83	0.78
1:G:10:ILE:HD13	2:J:2:VAL:HG12	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:28:PRO:HB2	2:P:29:LYS:CA	2.33	0.58
1:E:15:GLN:HG2	2:Z:25:PHE:CE1	2.41	0.56
2:P:13[B]:GLU:OE1	2:P:13[B]:GLU:CA	2.54	0.55

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:3:102:CL:CL	4:3:102:CL:CL[3_675]	1.91	0.29

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	0	19/21 (90%)	18 (95%)	1 (5%)	0	100	100
1	2	19/21 (90%)	19 (100%)	0	0	100	100
1	4	19/21 (90%)	19 (100%)	0	0	100	100
1	A	18/21 (86%)	16 (89%)	1 (6%)	1 (6%)	2	0
1	C	19/21 (90%)	16 (84%)	3 (16%)	0	100	100
1	E	18/21 (86%)	18 (100%)	0	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	19/21 (90%)	19 (100%)	0	0	100	100
1	M	19/21 (90%)	18 (95%)	1 (5%)	0	100	100
1	O	19/21 (90%)	19 (100%)	0	0	100	100
1	Q	19/21 (90%)	19 (100%)	0	0	100	100
1	S	19/21 (90%)	18 (95%)	1 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	U	19/21 (90%)	17 (90%)	2 (10%)	0	100	100
1	W	19/21 (90%)	18 (95%)	1 (5%)	0	100	100
1	Y	19/21 (90%)	18 (95%)	1 (5%)	0	100	100
2	1	25/30 (83%)	25 (100%)	0	0	100	100
2	3	23/30 (77%)	23 (100%)	0	0	100	100
2	5	26/30 (87%)	26 (100%)	0	0	100	100
2	B	24/30 (80%)	23 (96%)	1 (4%)	0	100	100
2	D	27/30 (90%)	26 (96%)	1 (4%)	0	100	100
2	F	23/30 (77%)	23 (100%)	0	0	100	100
2	H	28/30 (93%)	28 (100%)	0	0	100	100
2	J	28/30 (93%)	27 (96%)	0	1 (4%)	3	1
2	L	24/30 (80%)	24 (100%)	0	0	100	100
2	N	23/30 (77%)	23 (100%)	0	0	100	100
2	P	29/30 (97%)	27 (93%)	2 (7%)	0	100	100
2	R	27/30 (90%)	27 (100%)	0	0	100	100
2	T	23/30 (77%)	22 (96%)	0	1 (4%)	2	1
2	V	23/30 (77%)	23 (100%)	0	0	100	100
2	X	27/30 (90%)	25 (93%)	2 (7%)	0	100	100
2	Z	24/30 (80%)	23 (96%)	1 (4%)	0	100	100
All	All	706/816 (86%)	685 (97%)	18 (2%)	3 (0%)	34	37

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	8	THR
2	T	6	LEU
2	J	2	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	0	18/20 (90%)	18 (100%)	0	100	100
1	2	16/20 (80%)	16 (100%)	0	100	100
1	4	20/20 (100%)	19 (95%)	1 (5%)	24	30
1	A	14/20 (70%)	12 (86%)	2 (14%)	3	2
1	C	18/20 (90%)	17 (94%)	1 (6%)	21	25
1	E	16/20 (80%)	16 (100%)	0	100	100
1	G	20/20 (100%)	20 (100%)	0	100	100
1	I	19/20 (95%)	18 (95%)	1 (5%)	22	27
1	K	15/20 (75%)	13 (87%)	2 (13%)	4	3
1	M	18/20 (90%)	18 (100%)	0	100	100
1	O	19/20 (95%)	18 (95%)	1 (5%)	22	27
1	Q	19/20 (95%)	19 (100%)	0	100	100
1	S	15/20 (75%)	14 (93%)	1 (7%)	16	18
1	U	16/20 (80%)	16 (100%)	0	100	100
1	W	19/20 (95%)	18 (95%)	1 (5%)	22	27
1	Y	17/20 (85%)	17 (100%)	0	100	100
2	1	22/26 (85%)	19 (86%)	3 (14%)	3	3
2	3	20/26 (77%)	19 (95%)	1 (5%)	24	30
2	5	19/26 (73%)	18 (95%)	1 (5%)	22	27
2	B	16/26 (62%)	15 (94%)	1 (6%)	18	20
2	D	23/26 (88%)	21 (91%)	2 (9%)	10	10
2	F	18/26 (69%)	18 (100%)	0	100	100
2	H	25/26 (96%)	24 (96%)	1 (4%)	31	40
2	J	23/26 (88%)	22 (96%)	1 (4%)	29	36
2	L	19/26 (73%)	18 (95%)	1 (5%)	22	27
2	N	20/26 (77%)	18 (90%)	2 (10%)	7	7
2	P	23/26 (88%)	21 (91%)	2 (9%)	10	10
2	R	22/26 (85%)	22 (100%)	0	100	100
2	T	18/26 (69%)	18 (100%)	0	100	100
2	V	19/26 (73%)	18 (95%)	1 (5%)	22	27
2	X	20/26 (77%)	18 (90%)	2 (10%)	7	7
2	Z	18/26 (69%)	17 (94%)	1 (6%)	21	25

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	604/736 (82%)	575 (95%)	29 (5%)	25 32

5 of 29 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	O	9	SER
1	4	18	ASN
1	S	10	ILE
2	1	25	PHE
2	P	27	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
1	I	18	ASN
1	Y	18	ASN
1	Q	21	ASN
1	4	18	ASN
2	V	5	HIS

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, 16 are monoatomic - leaving 14 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	$\#\|Z\| > 2$
5	SRO	M	101	-	12,14,14	1.17	1 (8%)	12,19,19	1.41	1 (8%)
5	SRO	I	101	-	12,14,14	1.15	1 (8%)	12,19,19	1.38	2 (16%)
5	SRO	Y	101	-	12,14,14	1.16	1 (8%)	12,19,19	1.23	1 (8%)
5	SRO	O	101	-	12,14,14	1.14	1 (8%)	12,19,19	1.51	1 (8%)
5	SRO	K	101	-	12,14,14	1.20	1 (8%)	12,19,19	1.49	2 (16%)
5	SRO	2	101	-	12,14,14	1.17	1 (8%)	12,19,19	1.58	5 (41%)
5	SRO	Q	101	-	12,14,14	1.19	1 (8%)	12,19,19	1.53	1 (8%)
5	SRO	C	101	-	12,14,14	1.16	1 (8%)	12,19,19	1.41	1 (8%)
5	SRO	G	101	-	12,14,14	1.16	1 (8%)	12,19,19	1.76	2 (16%)
5	SRO	3	103	-	12,14,14	1.16	1 (8%)	12,19,19	1.52	2 (16%)
5	SRO	E	101	-	12,14,14	1.16	1 (8%)	12,19,19	1.83	3 (25%)
5	SRO	Y	102	-	12,14,14	1.17	1 (8%)	12,19,19	1.57	2 (16%)
5	SRO	0	101	-	12,14,14	1.16	1 (8%)	12,19,19	1.45	1 (8%)
5	SRO	W	101	-	12,14,14	1.15	1 (8%)	12,19,19	1.65	3 (25%)

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
5	SRO	M	101	-	-	1/3/3/3	0/2/2/2
5	SRO	I	101	-	-	1/3/3/3	0/2/2/2
5	SRO	Y	101	-	-	2/3/3/3	0/2/2/2
5	SRO	O	101	-	-	1/3/3/3	0/2/2/2
5	SRO	K	101	-	-	1/3/3/3	0/2/2/2
5	SRO	2	101	-	-	0/3/3/3	0/2/2/2
5	SRO	Q	101	-	-	1/3/3/3	0/2/2/2
5	SRO	C	101	-	-	1/3/3/3	0/2/2/2
5	SRO	G	101	-	-	0/3/3/3	0/2/2/2
5	SRO	3	103	-	-	1/3/3/3	0/2/2/2
5	SRO	E	101	-	-	0/3/3/3	0/2/2/2
5	SRO	Y	102	-	-	0/3/3/3	0/2/2/2
5	SRO	0	101	-	-	1/3/3/3	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	SRO	W	101	-	-	1/3/3/3	0/2/2/2

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	K	101	SRO	CD2-CE2	2.51	1.49	1.42
5	Y	102	SRO	CD2-CE2	2.49	1.49	1.42
5	Y	101	SRO	CD2-CE2	2.43	1.49	1.42
5	M	101	SRO	CD2-CE2	2.41	1.49	1.42
5	Q	101	SRO	CD2-CE2	2.39	1.49	1.42

The worst 5 of 27 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	G	101	SRO	CZ3-CE3-CD2	-4.28	117.65	120.64
5	M	101	SRO	CZ3-CE3-CD2	-3.50	118.19	120.64
5	E	101	SRO	CZ3-CE3-CD2	-3.46	118.22	120.64
5	3	103	SRO	CZ3-CE3-CD2	-3.46	118.22	120.64
5	C	101	SRO	CZ3-CE3-CD2	-3.40	118.26	120.64

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	101	SRO	NZ-CA-CB-CG
5	I	101	SRO	NZ-CA-CB-CG
5	K	101	SRO	NZ-CA-CB-CG
5	O	101	SRO	NZ-CA-CB-CG
5	Q	101	SRO	NZ-CA-CB-CG

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	K	101	SRO	1	0
5	C	101	SRO	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, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	0	21/21 (100%)	-0.23	1 (4%) 30 29	41, 54, 67, 82	0
1	2	21/21 (100%)	-0.41	0 100 100	38, 49, 68, 76	0
1	4	21/21 (100%)	-0.45	0 100 100	29, 42, 56, 70	0
1	A	20/21 (95%)	0.16	0 100 100	60, 74, 85, 87	0
1	C	21/21 (100%)	-0.20	0 100 100	46, 57, 69, 78	0
1	E	20/21 (95%)	-0.12	0 100 100	40, 58, 71, 78	0
1	G	21/21 (100%)	-0.45	0 100 100	30, 34, 45, 56	0
1	I	21/21 (100%)	-0.39	0 100 100	32, 40, 52, 62	0
1	K	21/21 (100%)	-0.15	0 100 100	43, 61, 79, 82	0
1	M	21/21 (100%)	-0.19	0 100 100	39, 52, 69, 81	0
1	O	21/21 (100%)	-0.54	0 100 100	29, 37, 50, 59	0
1	Q	21/21 (100%)	-0.35	0 100 100	32, 40, 56, 64	0
1	S	21/21 (100%)	-0.19	1 (4%) 30 29	46, 59, 75, 80	0
1	U	21/21 (100%)	-0.25	0 100 100	46, 54, 67, 73	0
1	W	21/21 (100%)	-0.54	0 100 100	29, 42, 60, 66	0
1	Y	21/21 (100%)	-0.19	0 100 100	41, 56, 61, 72	0
2	1	27/30 (90%)	-0.20	0 100 100	25, 39, 66, 76	0
2	3	24/30 (80%)	-0.07	0 100 100	27, 37, 52, 70	0
2	5	28/30 (93%)	-0.24	1 (3%) 42 41	26, 36, 65, 80	0
2	B	26/30 (86%)	-0.21	1 (3%) 40 38	36, 43, 66, 74	0
2	D	28/30 (93%)	-0.06	1 (3%) 42 41	33, 46, 74, 101	0
2	F	25/30 (83%)	-0.41	0 100 100	25, 32, 51, 68	0
2	H	29/30 (96%)	-0.51	0 100 100	21, 30, 44, 75	0
2	J	29/30 (96%)	-0.45	0 100 100	23, 32, 49, 56	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
2	L	26/30 (86%)	-0.14	1 (3%) 40 38	25, 35, 63, 98	0
2	N	25/30 (83%)	-0.29	0 100 100	25, 35, 56, 68	0
2	P	30/30 (100%)	-0.36	0 100 100	23, 32, 60, 84	0
2	R	29/30 (96%)	-0.37	0 100 100	25, 35, 66, 92	0
2	T	25/30 (83%)	-0.12	0 100 100	28, 40, 61, 75	0
2	V	25/30 (83%)	-0.20	1 (4%) 38 36	31, 41, 70, 71	0
2	X	29/30 (96%)	0.06	2 (6%) 16 15	26, 37, 90, 134	0
2	Z	26/30 (86%)	-0.21	0 100 100	31, 45, 64, 71	0
All	All	765/816 (93%)	-0.26	9 (1%) 79 77	21, 44, 74, 134	0

The worst 5 of 9 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	X	30	THR	6.9
2	D	1	PHE	6.2
2	L	30	THR	5.5
2	X	29	LYS	2.9
1	0	21	ASN	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
5	SRO	Y	101	13/13	0.27	0.47	105,120,132,132	0
5	SRO	Y	102	13/13	0.78	0.23	53,62,67,69	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	SRO	K	101	13/13	0.83	0.20	42,48,63,65	0
4	CL	5	102	1/1	0.86	0.16	29,29,29,29	1
5	SRO	E	101	13/13	0.87	0.25	38,49,75,78	0
4	CL	P	101	1/1	0.88	0.12	24,24,24,24	0
5	SRO	M	101	13/13	0.90	0.20	59,64,74,77	0
4	CL	F	102	1/1	0.91	0.20	64,64,64,64	0
5	SRO	2	101	13/13	0.91	0.14	42,48,51,51	0
4	CL	X	101	1/1	0.92	0.12	27,27,27,27	0
4	CL	B	102	1/1	0.92	0.29	120,120,120,120	1
5	SRO	0	101	13/13	0.93	0.10	48,55,57,59	0
5	SRO	Q	101	13/13	0.94	0.13	36,43,46,47	0
5	SRO	I	101	13/13	0.95	0.12	33,35,40,41	0
5	SRO	C	101	13/13	0.95	0.15	41,44,54,55	0
5	SRO	G	101	13/13	0.96	0.10	29,32,34,35	0
5	SRO	W	101	13/13	0.96	0.13	30,33,37,38	0
5	SRO	O	101	13/13	0.96	0.10	30,31,34,34	0
5	SRO	3	103	13/13	0.96	0.12	34,39,41,42	0
4	CL	3	102	1/1	0.97	0.30	72,72,72,72	0
4	CL	D	102	1/1	0.97	0.17	36,36,36,36	1
4	CL	T	102	1/1	0.98	0.07	60,60,60,60	0
3	ZN	R	101	1/1	0.98	0.10	24,24,24,24	0
3	ZN	5	101	1/1	0.98	0.14	26,26,26,26	1
3	ZN	T	101	1/1	0.99	0.11	36,36,36,36	0
3	ZN	H	101	1/1	0.99	0.14	21,21,21,21	0
3	ZN	D	101	1/1	0.99	0.09	33,33,33,33	1
3	ZN	3	101	1/1	1.00	0.10	32,32,32,32	1
3	ZN	F	101	1/1	1.00	0.11	36,36,36,36	0
3	ZN	B	101	1/1	1.00	0.12	45,45,45,45	1

6.5 Other polymers (i)

There are no such residues in this entry.