



Full wwPDB X-ray Structure Validation Report ⓘ

May 18, 2020 – 10:00 pm BST

PDB ID : 5UU3
Title : Insulin with proline analog DfP at position B28 in the R6 state
Authors : Lieblich, S.A.; Fang, K.Y.; Tirrell, D.A.
Deposited on : 2017-02-16
Resolution : 2.25 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/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 : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
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) : 2.11

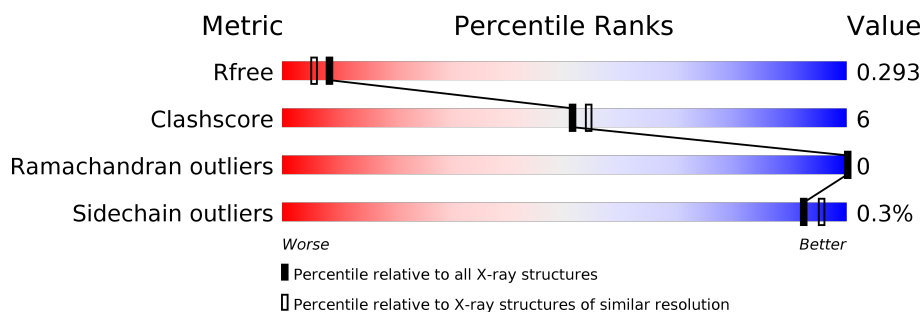
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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.

















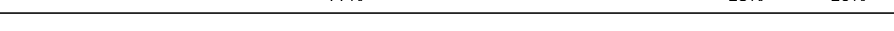


Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1377 (2.26-2.26)
Clashscore	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)

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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	21	90% 10%
1	C	21	86% 10% 5%
1	E	21	81% 14% 5%
1	G	21	81% 14% 5%
1	I	21	86% 14%
1	K	21	81% 19%
1	M	21	86% 14%

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Mol	Chain	Length	Quality of chain
1	O	21	 90% 10%
1	Q	21	 86% 14%
1	S	21	 81% 19%
1	U	21	 86% 14%
1	W	21	 81% 14% 5%
2	B	30	 77% 13% 10%
2	D	30	 70% 20% 10%
2	F	30	 77% 10% 13%
2	H	30	 93% 7%
2	J	30	 70% 23% 7%
2	L	30	 87% 7% 7%
2	N	30	 70% 20% 10%
2	P	30	 77% 13% 10%
2	R	30	 77% 13% 10%
2	T	30	 90% 7%
2	V	30	 77% 13% 10%
2	X	30	 80% 7% 13%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 4123 atoms, of which 6 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, chain B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	19	Total	C	N	O	S	0	0	0
			113	67	19	23	4			
1	C	20	Total	C	N	O	S	0	0	0
			147	90	23	30	4			
1	E	20	Total	C	N	O	S	0	0	0
			134	81	22	27	4			
1	G	20	Total	C	N	O	S	0	0	0
			143	89	21	29	4			
1	I	21	Total	C	N	O	S	0	0	0
			133	81	23	25	4			
1	K	21	Total	C	N	O	S	0	0	0
			150	91	24	31	4			
1	M	21	Total	C	N	O	S	0	0	0
			137	82	24	27	4			
1	O	21	Total	C	N	O	S	0	0	0
			151	93	24	30	4			
1	Q	21	Total	C	N	O	S	0	0	0
			139	84	23	28	4			
1	S	21	Total	C	N	O	S	0	0	0
			153	94	24	31	4			
1	U	21	Total	C	N	O	S	0	0	0
			137	83	24	26	4			
1	W	20	Total	C	N	O	S	0	0	0
			124	74	22	24	4			

- Molecule 2 is a protein called Insulin, chain A.

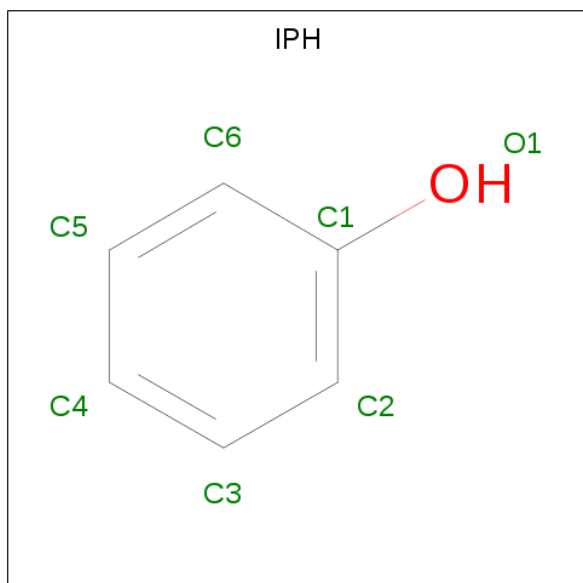
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	27	Total	C	F	N	O	S	0	0
			194	127	2	31	32	2		
2	D	27	Total	C	F	N	O	S	0	0
			195	129	2	31	31	2		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	26	Total	C	N	O	S	0	0	0
			195	128	33	32	2			
2	H	28	Total	C	F	N	O	S	0	0
			196	129	2	32	31	2		
2	J	28	Total	C	F	N	O	S	0	0
			210	137	2	35	34	2		
2	L	28	Total	C	F	N	O	S	0	0
			198	131	2	32	31	2		
2	N	27	Total	C	F	N	O	S	0	0
			203	133	2	34	32	2		
2	P	27	Total	C	F	N	O	S	0	0
			191	125	2	31	31	2		
2	R	27	Total	C	F	N	O	S	0	0
			200	130	2	34	32	2		
2	T	28	Total	C	F	N	O	S	0	0
			198	131	2	32	31	2		
2	V	27	Total	C	F	N	O	S	0	0
			201	131	2	34	32	2		
2	X	26	Total	C	F	N	O	S	0	0
			188	124	2	30	30	2		

- Molecule 3 is PHENOL (three-letter code: IPH) (formula: C₆H₆O).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			7	6	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	1	Total C H O 13 6 6 1	0	0
3	E	1	Total C O 7 6 1	0	0
3	G	1	Total C O 7 6 1	0	0
3	I	1	Total C O 7 6 1	0	0
3	K	1	Total C O 7 6 1	0	0
3	M	1	Total C O 7 6 1	0	0
3	Q	1	Total C O 7 6 1	0	0
3	S	1	Total C O 7 6 1	0	0
3	U	1	Total C O 7 6 1	0	0
3	W	1	Total C O 7 6 1	0	0

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	P	1	Total Zn 1 1	0	0
4	B	1	Total Zn 1 1	0	0
4	D	1	Total Zn 1 1	0	0
4	N	1	Total Zn 1 1	0	0

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	P	1	Total Cl 1 1	0	0
5	D	1	Total Cl 1 1	0	0
5	N	1	Total Cl 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	F	1	Total	Cl	0	0
			1	1		


- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	T	1	Total	O	0	0
			1	1		
6	X	1	Total	O	0	0
			1	1		

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 the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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 B

Chain A:  90% 10%




- Molecule 1: Insulin, chain B

Chain C:  86% 10% 5%




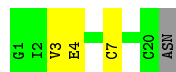
- Molecule 1: Insulin, chain B

Chain E:  81% 14% 5%




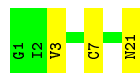
- Molecule 1: Insulin, chain B

Chain G:  81% 14% 5%




- Molecule 1: Insulin, chain B

Chain I:  86% 14%

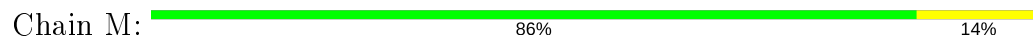


- Molecule 1: Insulin, chain B

Chain K:  81% 19%



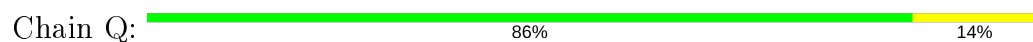
- Molecule 1: Insulin, chain B



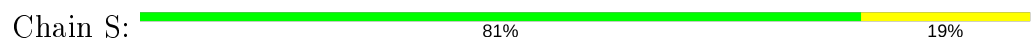
- Molecule 1: Insulin, chain B



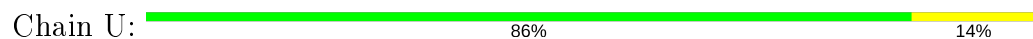
- Molecule 1: Insulin, chain B



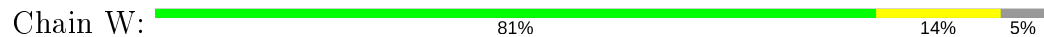
- Molecule 1: Insulin, chain B



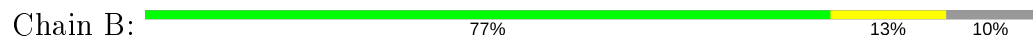
- Molecule 1: Insulin, chain B



- Molecule 1: Insulin, chain B



- Molecule 2: Insulin, chain A





- Molecule 2: Insulin, chain A

Chain D: 70% 20% 10%



- Molecule 2: Insulin, chain A

Chain F: 77% 10% 13%



- Molecule 2: Insulin, chain A

Chain H: 93% 7%



- Molecule 2: Insulin, chain A

Chain J: 70% 23% 7%



- Molecule 2: Insulin, chain A

Chain L: 87% 7% 7%



- Molecule 2: Insulin, chain A

Chain N: 70% 20% 10%



- Molecule 2: Insulin, chain A

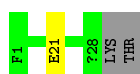
Chain P: 77% 13% 10%



- Molecule 2: Insulin, chain A



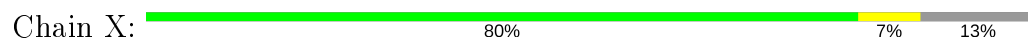
- Molecule 2: Insulin, chain A



- Molecule 2: Insulin, chain A



- Molecule 2: Insulin, chain A



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	40.60 Å 47.42 Å 78.70 Å 89.96° 89.93° 73.41°	Depositor
Resolution (Å)	34.90 – 2.25 39.35 – 1.72	Depositor EDS
% Data completeness (in resolution range)	87.2 (34.90-2.25) 83.4 (39.35-1.72)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.39 (at 1.72 Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.243 , 0.292 0.247 , 0.293	Depositor DCC
R_{free} test set	2412 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å ²)	26.3	Xtriage
Anisotropy	0.107	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 84.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.049 for -h,-k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4123	wwPDB-VP
Average B, all atoms (Å ²)	79.0	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 89.32 % 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 3.5603e-08. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PDF, ZN, IPH, 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	A	0.21	0/113	0.38	0/154
1	C	0.21	0/148	0.37	0/200
1	E	0.21	0/134	0.38	0/181
1	G	0.21	0/144	0.38	0/195
1	I	0.21	0/133	0.37	0/181
1	K	0.20	0/151	0.38	0/204
1	M	0.24	0/137	0.43	0/186
1	O	0.22	0/152	0.37	0/206
1	Q	0.22	0/139	0.36	0/188
1	S	0.21	0/154	0.36	0/208
1	U	0.21	0/137	0.39	0/186
1	W	0.21	0/124	0.37	0/169
2	B	0.24	0/190	0.36	0/258
2	D	0.25	0/191	0.35	0/260
2	F	0.24	0/200	0.36	0/270
2	H	0.23	0/192	0.35	0/261
2	J	0.25	0/205	0.39	0/276
2	L	0.26	0/194	0.35	0/264
2	N	0.26	0/199	0.37	0/269
2	P	0.26	0/187	0.39	0/254
2	R	0.26	0/196	0.39	0/265
2	T	0.26	0/194	0.36	0/264
2	V	0.24	0/197	0.36	0/266
2	X	0.23	0/184	0.35	0/250
All	All	0.23	0/3995	0.37	0/5415

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	113	0	66	0	0
1	C	147	0	130	1	0
1	E	134	0	112	2	0
1	G	143	0	121	2	0
1	I	133	0	105	2	0
1	K	150	0	125	3	0
1	M	137	0	109	2	0
1	O	151	0	129	1	0
1	Q	139	0	114	2	0
1	S	153	0	128	3	0
1	U	137	0	111	2	0
1	W	124	0	83	2	0
2	B	194	0	159	4	0
2	D	195	0	169	6	0
2	F	195	0	174	3	0
2	H	196	0	162	0	0
2	J	210	0	186	6	0
2	L	198	0	169	2	0
2	N	203	0	179	6	0
2	P	191	0	155	4	0
2	R	200	0	170	4	0
2	T	198	0	169	1	0
2	V	201	0	172	4	0
2	X	188	0	160	2	0
3	A	7	0	5	0	0
3	C	7	6	6	0	0
3	E	7	0	6	0	0
3	G	7	0	5	0	0
3	I	7	0	5	0	0
3	K	7	0	5	1	0
3	M	7	0	5	0	0
3	Q	7	0	5	0	0
3	S	7	0	5	1	0
3	U	7	0	5	0	0
3	W	7	0	5	1	0
4	B	1	0	0	0	0
4	D	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	N	1	0	0	0	0
4	P	1	0	0	0	0
5	D	1	0	0	0	0
5	F	1	0	0	0	0
5	N	1	0	0	0	0
5	P	1	0	0	0	0
6	T	1	0	0	0	0
6	X	1	0	0	0	0
All	All	4117	6	3414	42	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 6.

All (42) 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:B:23:GLY:HA3	2:D:27:THR:HG22	1.63	0.80
2:N:23:GLY:HA3	2:P:27:THR:HG22	1.66	0.77
1:S:4:GLU:N	1:S:4:GLU:OE1	2.26	0.66
2:J:2:VAL:HG12	2:J:4:GLN:H	1.60	0.65
1:G:4:GLU:OE1	1:G:4:GLU:N	2.29	0.63
2:D:14:ALA:O	2:D:18:VAL:HG12	2.00	0.61
2:N:25:PHE:HB3	2:P:25:PHE:CE2	2.35	0.61
1:I:3:VAL:O	1:I:7:CYS:HB2	2.03	0.59
1:K:6:CYS:O	3:K:101:IPH:O1	2.22	0.57
1:G:3:VAL:O	1:G:7:CYS:HB2	2.05	0.57
1:O:3:VAL:O	1:O:7:CYS:HB2	2.06	0.56
1:C:3:VAL:O	1:C:7:CYS:HB2	2.06	0.55
2:N:10:HIS:CD2	2:R:6:LEU:HD22	2.44	0.53
1:E:17:GLU:CG	2:F:22:ARG:HH22	2.21	0.52
1:Q:3:VAL:O	1:Q:7:CYS:HB2	2.10	0.52
1:K:3:VAL:O	1:K:7:CYS:HB2	2.10	0.52
2:R:28:PDF:F2	2:T:21:GLU:HA	1.98	0.52
1:U:21:ASN:HB2	2:V:22:ARG:O	2.11	0.50
2:J:25:PHE:HB3	2:L:25:PHE:CE1	2.47	0.49
2:R:10:HIS:CD2	2:V:6:LEU:HD22	2.47	0.49
1:W:6:CYS:O	3:W:101:IPH:O1	2.31	0.49
2:N:21:GLU:HA	2:P:28:PDF:F1	2.03	0.49
2:N:28:PDF:F1	2:P:21:GLU:HA	2.02	0.49
1:S:3:VAL:O	1:S:7:CYS:HB2	2.13	0.48
2:D:15:LEU:HA	2:D:18:VAL:CG1	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:17:GLU:CG	2:R:22:ARG:HH22	2.27	0.48
2:F:17:LEU:O	1:K:13:LEU:HD11	2.14	0.48
2:V:28:PDF:F1	2:X:21:GLU:HA	2.04	0.47
2:F:10:HIS:CD2	2:J:6:LEU:HD22	2.50	0.47
1:S:6:CYS:O	3:S:101:IPH:O1	2.33	0.47
1:M:3:VAL:O	1:M:7:CYS:HB2	2.15	0.47
1:E:3:VAL:O	1:E:7:CYS:HB2	2.15	0.46
2:B:6:LEU:HD22	2:J:10:HIS:CD2	2.50	0.46
2:D:15:LEU:HA	2:D:18:VAL:HG12	1.98	0.45
1:I:21:ASN:ND2	2:J:25:PHE:HD2	2.14	0.45
1:M:21:ASN:HB2	2:N:22:ARG:O	2.17	0.45
2:V:23:GLY:HA3	2:X:27:THR:HG22	1.98	0.44
1:U:3:VAL:O	1:U:7:CYS:HB2	2.17	0.44
1:W:3:VAL:O	1:W:7:CYS:HB2	2.17	0.44
2:B:28:PDF:F1	2:D:21:GLU:HA	2.07	0.44
2:J:21:GLU:HA	2:L:28:PDF:F1	2.09	0.42
2:B:25:PHE:HB2	2:D:25:PHE:CE1	2.56	0.41

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	17/21 (81%)	17 (100%)	0	0	100	100
1	C	18/21 (86%)	18 (100%)	0	0	100	100
1	E	18/21 (86%)	18 (100%)	0	0	100	100
1	G	18/21 (86%)	18 (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%)	19 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	19 (100%)	0	0	100	100
1	U	19/21 (90%)	19 (100%)	0	0	100	100
1	W	18/21 (86%)	18 (100%)	0	0	100	100
2	B	25/30 (83%)	25 (100%)	0	0	100	100
2	D	25/30 (83%)	25 (100%)	0	0	100	100
2	F	24/30 (80%)	24 (100%)	0	0	100	100
2	H	26/30 (87%)	26 (100%)	0	0	100	100
2	J	25/30 (83%)	25 (100%)	0	0	100	100
2	L	26/30 (87%)	26 (100%)	0	0	100	100
2	N	25/30 (83%)	25 (100%)	0	0	100	100
2	P	25/30 (83%)	25 (100%)	0	0	100	100
2	R	25/30 (83%)	25 (100%)	0	0	100	100
2	T	26/30 (87%)	26 (100%)	0	0	100	100
2	V	25/30 (83%)	25 (100%)	0	0	100	100
2	X	24/30 (80%)	24 (100%)	0	0	100	100
All	All	523/612 (86%)	523 (100%)	0	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	8/20 (40%)	8 (100%)	0	100	100
1	C	17/20 (85%)	17 (100%)	0	100	100
1	E	14/20 (70%)	14 (100%)	0	100	100
1	G	15/20 (75%)	15 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	I	12/20 (60%)	12 (100%)	0	100	100
1	K	16/20 (80%)	16 (100%)	0	100	100
1	M	13/20 (65%)	13 (100%)	0	100	100
1	O	16/20 (80%)	16 (100%)	0	100	100
1	Q	14/20 (70%)	14 (100%)	0	100	100
1	S	16/20 (80%)	16 (100%)	0	100	100
1	U	13/20 (65%)	13 (100%)	0	100	100
1	W	10/20 (50%)	10 (100%)	0	100	100
2	B	16/25 (64%)	16 (100%)	0	100	100
2	D	17/25 (68%)	17 (100%)	0	100	100
2	F	18/25 (72%)	18 (100%)	0	100	100
2	H	15/25 (60%)	15 (100%)	0	100	100
2	J	19/25 (76%)	18 (95%)	1 (5%)	22	23
2	L	16/25 (64%)	16 (100%)	0	100	100
2	N	18/25 (72%)	18 (100%)	0	100	100
2	P	15/25 (60%)	15 (100%)	0	100	100
2	R	17/25 (68%)	17 (100%)	0	100	100
2	T	16/25 (64%)	16 (100%)	0	100	100
2	V	17/25 (68%)	17 (100%)	0	100	100
2	X	16/25 (64%)	16 (100%)	0	100	100
All	All	364/540 (67%)	363 (100%)	1 (0%)	92	95

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	J	17	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

11 non-standard protein/DNA/RNA residues are modelled in this entry.

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	PDF	H	28	2	5,9,10	2.16	2 (40%)	7,13,15	1.55	2 (28%)
2	PDF	N	28	2	5,9,10	2.20	2 (40%)	7,13,15	1.52	2 (28%)
2	PDF	L	28	2	5,9,10	2.20	2 (40%)	7,13,15	1.61	2 (28%)
2	PDF	R	28	2	5,9,10	2.27	2 (40%)	7,13,15	1.57	2 (28%)
2	PDF	P	28	2	5,9,10	2.24	2 (40%)	7,13,15	1.40	1 (14%)
2	PDF	V	28	2	5,9,10	2.25	2 (40%)	7,13,15	1.47	2 (28%)
2	PDF	T	28	2	5,9,10	2.21	2 (40%)	7,13,15	1.54	2 (28%)
2	PDF	X	28	2	5,9,10	2.20	2 (40%)	7,13,15	1.51	2 (28%)
2	PDF	B	28	2	5,9,10	2.21	2 (40%)	7,13,15	1.48	2 (28%)
2	PDF	D	28	2	5,9,10	2.21	2 (40%)	7,13,15	1.66	2 (28%)
2	PDF	J	28	2	5,9,10	2.20	2 (40%)	7,13,15	1.48	2 (28%)

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	PDF	H	28	2	-	0/0/13/15	0/1/1/1
2	PDF	N	28	2	-	0/0/13/15	0/1/1/1
2	PDF	L	28	2	-	0/0/13/15	0/1/1/1
2	PDF	R	28	2	-	0/0/13/15	0/1/1/1
2	PDF	P	28	2	-	0/0/13/15	0/1/1/1
2	PDF	V	28	2	-	0/0/13/15	0/1/1/1
2	PDF	T	28	2	-	0/0/13/15	0/1/1/1
2	PDF	X	28	2	-	0/0/13/15	0/1/1/1
2	PDF	B	28	2	-	0/0/13/15	0/1/1/1
2	PDF	D	28	2	-	0/0/13/15	0/1/1/1
2	PDF	J	28	2	-	0/0/13/15	0/1/1/1

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	R	28	PDF	F2-CG	-3.49	1.32	1.38
2	P	28	PDF	F1-CG	-3.46	1.32	1.38
2	V	28	PDF	F1-CG	-3.45	1.32	1.38
2	T	28	PDF	F1-CG	-3.43	1.32	1.38
2	N	28	PDF	F1-CG	-3.41	1.32	1.38
2	J	28	PDF	F1-CG	-3.40	1.32	1.38
2	D	28	PDF	F1-CG	-3.40	1.32	1.38
2	X	28	PDF	F1-CG	-3.40	1.32	1.38
2	R	28	PDF	F1-CG	-3.38	1.32	1.38
2	B	28	PDF	F1-CG	-3.38	1.32	1.38
2	L	28	PDF	F1-CG	-3.32	1.32	1.38
2	V	28	PDF	F2-CG	-3.32	1.32	1.38
2	P	28	PDF	F2-CG	-3.30	1.32	1.38
2	L	28	PDF	F2-CG	-3.29	1.32	1.38
2	H	28	PDF	F1-CG	-3.29	1.32	1.38
2	B	28	PDF	F2-CG	-3.27	1.32	1.38
2	D	28	PDF	F2-CG	-3.27	1.32	1.38
2	J	28	PDF	F2-CG	-3.26	1.32	1.38
2	T	28	PDF	F2-CG	-3.23	1.32	1.38
2	N	28	PDF	F2-CG	-3.23	1.32	1.38
2	X	28	PDF	F2-CG	-3.22	1.32	1.38
2	H	28	PDF	F2-CG	-3.22	1.32	1.38

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	28	PDF	CB-CA-C	-2.95	108.96	113.36
2	P	28	PDF	O-C-CA	-2.57	118.03	124.78
2	R	28	PDF	CB-CA-C	-2.57	109.52	113.36
2	L	28	PDF	CB-CA-C	-2.54	109.57	113.36
2	L	28	PDF	O-C-CA	-2.52	118.17	124.78
2	H	28	PDF	O-C-CA	-2.50	118.23	124.78
2	T	28	PDF	O-C-CA	-2.46	118.32	124.78
2	X	28	PDF	CB-CA-C	-2.42	109.74	113.36
2	V	28	PDF	O-C-CA	-2.39	118.50	124.78
2	N	28	PDF	O-C-CA	-2.37	118.56	124.78
2	H	28	PDF	CB-CA-C	-2.36	109.83	113.36
2	N	28	PDF	CB-CA-C	-2.36	109.84	113.36
2	R	28	PDF	O-C-CA	-2.34	118.64	124.78
2	D	28	PDF	O-C-CA	-2.33	118.67	124.78
2	X	28	PDF	O-C-CA	-2.32	118.71	124.78
2	B	28	PDF	O-C-CA	-2.29	118.79	124.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	28	PDF	CB-CA-C	-2.26	109.99	113.36
2	T	28	PDF	CB-CA-C	-2.24	110.01	113.36
2	V	28	PDF	CB-CA-C	-2.22	110.04	113.36
2	B	28	PDF	CB-CA-C	-2.19	110.09	113.36
2	J	28	PDF	O-C-CA	-2.15	119.16	124.78

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	N	28	PDF	1	0
2	L	28	PDF	1	0
2	R	28	PDF	1	0
2	P	28	PDF	1	0
2	V	28	PDF	1	0
2	B	28	PDF	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 19 ligands modelled in this entry, 8 are monoatomic - leaving 11 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	$\# Z > 2$
3	IPH	M	101	-	7,7,7	0.34	0	8,8,8	0.28	0
3	IPH	K	101	-	7,7,7	0.38	0	8,8,8	0.21	0
3	IPH	I	101	-	7,7,7	0.36	0	8,8,8	0.29	0
3	IPH	W	101	-	7,7,7	0.42	0	8,8,8	0.27	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	IPH	U	101	-	7,7,7	0.40	0	8,8,8	0.30	0
3	IPH	S	101	-	7,7,7	0.37	0	8,8,8	0.26	0
3	IPH	Q	101	-	7,7,7	0.37	0	8,8,8	0.28	0
3	IPH	G	101	-	7,7,7	0.40	0	8,8,8	0.25	0
3	IPH	E	101	-	7,7,7	0.38	0	8,8,8	0.30	0
3	IPH	C	101	-	7,7,7	0.59	0	8,8,8	0.26	0
3	IPH	A	101	-	7,7,7	0.36	0	8,8,8	0.26	0

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
3	IPH	M	101	-	-	-	0/1/1/1
3	IPH	K	101	-	-	-	0/1/1/1
3	IPH	I	101	-	-	-	0/1/1/1
3	IPH	W	101	-	-	-	0/1/1/1
3	IPH	U	101	-	-	-	0/1/1/1
3	IPH	S	101	-	-	-	0/1/1/1
3	IPH	Q	101	-	-	-	0/1/1/1
3	IPH	G	101	-	-	-	0/1/1/1
3	IPH	E	101	-	-	-	0/1/1/1
3	IPH	C	101	-	-	-	0/1/1/1
3	IPH	A	101	-	-	-	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	K	101	IPH	1	0
3	W	101	IPH	1	0
3	S	101	IPH	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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers

Unable to reproduce the depositors R factor - this section is therefore empty.