



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 02:33 PM GMT

PDB ID : 3ZS2
Title : TYRB25,NMEPHEB26,LYSB28,PROB29-INSULIN ANALOGUE CRYSTAL STRUCTURE
Authors : Antolikova, E.; Zakova, L.; Turkenburg, J.P.; Watson, C.J.; Hanclova, I.; Sanda, M.; Cooper, A.; Kraus, T.; Brzozowski, A.M.; Jiracek, J.A.
Deposited on : 2011-06-21
Resolution : 1.97 Å(reported)

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

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

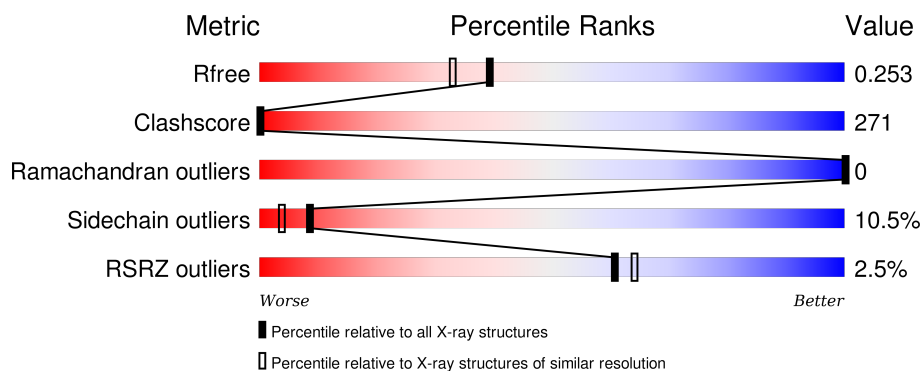
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.97 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	8664 (2.00-1.96)
Clashscore	102246	9905 (2.00-1.96)
Ramachandran outliers	100387	9792 (2.00-1.96)
Sidechain outliers	100360	9791 (2.00-1.96)
RSRZ outliers	91569	8679 (2.00-1.96)

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

Mol	Chain	Length	Quality of chain
1	A	21	<div> <div>19%</div> <div>86%</div> <div>10%</div> <div>5%</div> </div>
1	C	21	<div> <div>5%</div> <div>90%</div> <div>5%</div> </div>
1	E	21	<div> <div>81%</div> <div>19%</div> </div>
1	G	21	<div> <div>14%</div> <div>67%</div> <div>14%</div> <div>5%</div> </div>
1	I	21	<div> <div>5%</div> <div>90%</div> <div>5%</div> </div>

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Mol	Chain	Length	Quality of chain
1	K	21	
2	B	30	
2	D	30	
2	F	30	
2	H	30	
2	J	30	
2	L	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
2	MEA	D	26	-	X	-	-
2	MEA	F	26	-	X	X	-
2	MEA	H	26	-	X	-	-
2	MEA	J	26	-	X	-	-
2	MEA	L	26	-	X	-	-
3	IPH	A	1022	-	X	-	-
3	IPH	C	1022	-	X	-	-
3	IPH	E	1022	-	X	-	-
3	IPH	G	1022	-	X	-	-
3	IPH	I	1022	-	X	-	-
3	IPH	K	1022	-	X	-	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 2440 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
			159	97	24	34	4			
1	C	21	Total	C	N	O	S	0	0	0
			163	99	25	35	4			
1	E	21	Total	C	N	O	S	0	0	0
			163	99	25	35	4			
1	G	20	Total	C	N	O	S	0	0	0
			159	97	24	34	4			
1	I	21	Total	C	N	O	S	0	0	0
			163	99	25	35	4			
1	K	21	Total	C	N	O	S	0	0	0
			163	99	25	35	4			

- Molecule 2 is a protein called INSULIN B CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	27	Total	C	N	O	S	0	0	0
			219	144	36	37	2			
2	D	25	Total	C	N	O	S	0	0	0
			194	125	34	33	2			
2	F	25	Total	C	N	O	S	0	0	0
			194	125	34	33	2			
2	H	28	Total	C	N	O	S	0	0	1
			220	144	37	37	2			
2	J	29	Total	C	N	O	S	0	0	0
			235	155	39	39	2			
2	L	26	Total	C	N	O	S	0	0	0
			212	140	35	35	2			

There are 24 discrepancies between the modelled and reference sequences:

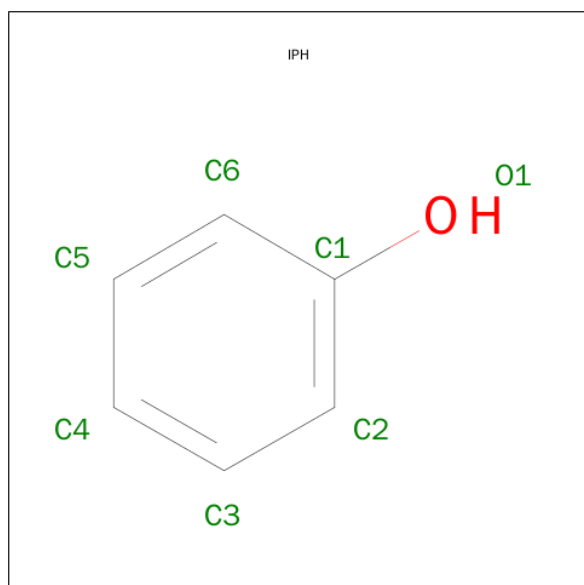
Chain	Residue	Modelled	Actual	Comment	Reference
B	25	TYR	PHE	ENGINEERED MUTATION	UNP P01308

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Chain	Residue	Modelled	Actual	Comment	Reference
B	26	MEA	TYR	ENGINEERED MUTATION	UNP P01308
B	28	LYS	PRO	ENGINEERED MUTATION	UNP P01308
B	29	PRO	LYS	ENGINEERED MUTATION	UNP P01308
D	25	TYR	PHE	ENGINEERED MUTATION	UNP P01308
D	26	MEA	TYR	ENGINEERED MUTATION	UNP P01308
D	28	LYS	PRO	ENGINEERED MUTATION	UNP P01308
D	29	PRO	LYS	ENGINEERED MUTATION	UNP P01308
F	25	TYR	PHE	ENGINEERED MUTATION	UNP P01308
F	26	MEA	TYR	ENGINEERED MUTATION	UNP P01308
F	28	LYS	PRO	ENGINEERED MUTATION	UNP P01308
F	29	PRO	LYS	ENGINEERED MUTATION	UNP P01308
H	25	TYR	PHE	ENGINEERED MUTATION	UNP P01308
H	26	MEA	TYR	ENGINEERED MUTATION	UNP P01308
H	28	LYS	PRO	ENGINEERED MUTATION	UNP P01308
H	29	PRO	LYS	ENGINEERED MUTATION	UNP P01308
J	25	TYR	PHE	ENGINEERED MUTATION	UNP P01308
J	26	MEA	TYR	ENGINEERED MUTATION	UNP P01308
J	28	LYS	PRO	ENGINEERED MUTATION	UNP P01308
J	29	PRO	LYS	ENGINEERED MUTATION	UNP P01308
L	25	TYR	PHE	ENGINEERED MUTATION	UNP P01308
L	26	MEA	TYR	ENGINEERED MUTATION	UNP P01308
L	28	LYS	PRO	ENGINEERED MUTATION	UNP P01308
L	29	PRO	LYS	ENGINEERED MUTATION	UNP P01308

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



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

- 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	C	1	Total Cl 1 1	0	0

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	2	Total O 2 2	0	0
6	B	17	Total O 17 17	0	0
6	C	17	Total O 17 17	0	0
6	D	10	Total O 10 10	0	0
6	E	7	Total O 7 7	0	0

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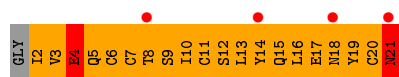
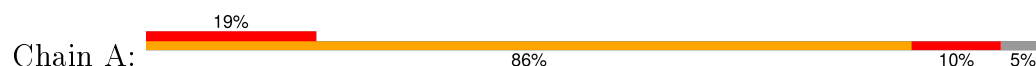
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	F	15	Total 15	O 15	0	0
6	G	17	Total 17	O 17	0	0
6	H	17	Total 17	O 17	0	0
6	I	19	Total 19	O 19	0	0
6	J	16	Total 16	O 16	0	0
6	K	9	Total 9	O 9	0	0
6	L	4	Total 4	O 4	0	0

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

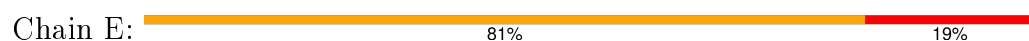
- Molecule 1: INSULIN A CHAIN



- Molecule 1: INSULIN A CHAIN



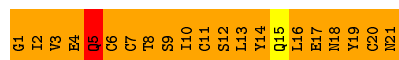
- Molecule 1: INSULIN A CHAIN



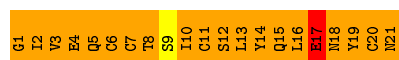
- Molecule 1: INSULIN A CHAIN



- Molecule 1: INSULIN A CHAIN



- Molecule 1: INSULIN A CHAIN



F1	V2	N3	Q4	H5	L6	C7	G8	S9	H10	L11	V12	E13	A14	L15	Y16	L17	V18	C19	G20	E21	R22	G23	F24	Y25	F26	T27	LVS	PRO	THR
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PHE	V2	N3	Q4	H5	L6	C7	G8	S9	H10	L11	V12	E13	A14	L15	Y16	L17	V18	C19	G20	E21	R22	G23	F24	Y25	F26	THR	LVS	PRO	THR
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PHE	V2	N3	H4	L6	C7	S8	G9	H10	L11	V12	E13	A14	L15	Y16	L17	V18	C19	G20	E21	R22	G23	F24	Y25	F26	THR	LYS	PRO	THR
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F1	V2	N3	Q4	H5	L6	C7	S8	H10	L11	V12	E13	A14	L15	Y16	L17	V18	C19	G20	E21	R22	G23	F24	Y25	F26	T27	K28	THR
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F1	V2	N3	Q4	H5	L6	C7	G8	S9	H10	L11	V12	E13	A14	L15	Y16	L17	V18	C19	G20	E21	R22	G23	F24	Y25	F26	T27	K28	P29	THR
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F1	V2	N3	Q4	H5	L6	C7	G8	S9	H10	L11	V12	E13	A14	L15	Y16	L17	V18	C19	G20	E21	R22	G23	F24	Y25	F26	THR	LYS	PRO	THR
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4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	46.68 Å 62.17 Å 57.66 Å 90.00° 111.32° 90.00°	Depositor
Resolution (Å)	53.68 – 1.97 29.03 – 1.97	Depositor EDS
% Data completeness (in resolution range)	89.9 (53.68-1.97) 56.7 (29.03-1.97)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.97 (at 1.96 Å)	Xtriage
Refinement program	REFMAC 5.6.0116	Depositor
R, R_{free}	0.193 , 0.252 0.196 , 0.253	Depositor DCC
R_{free} test set	617 reflections (5.25%)	DCC
Wilson B-factor (Å ²)	30.8	Xtriage
Anisotropy	0.551	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 48.1	EDS
Estimated twinning fraction	0.051 for h,-k,-h-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 12370 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	2440	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.26% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MEA, 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	8.64	89/160 (55.6%)	6.45	74/215 (34.4%)
1	C	9.23	114/164 (69.5%)	5.50	68/220 (30.9%)
1	E	8.84	92/164 (56.1%)	5.86	98/220 (44.5%)
1	G	8.32	76/160 (47.5%)	5.40	68/215 (31.6%)
1	I	9.44	104/164 (63.4%)	5.56	77/220 (35.0%)
1	K	9.06	106/164 (64.6%)	5.30	78/220 (35.5%)
2	B	9.26	128/211 (60.7%)	6.53	115/283 (40.6%)
2	D	8.05	104/185 (56.2%)	5.47	87/249 (34.9%)
2	F	7.48	89/185 (48.1%)	5.67	111/249 (44.6%)
2	H	8.79	116/212 (54.7%)	5.73	103/285 (36.1%)
2	J	8.32	130/228 (57.0%)	5.93	102/306 (33.3%)
2	L	8.93	133/205 (64.9%)	6.40	100/276 (36.2%)
All	All	8.70	1281/2202 (58.2%)	5.85	1081/2958 (36.5%)

The worst 5 of 1281 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	7	CYS	CB-SG	29.76	2.32	1.82
1	I	12	SER	CB-OG	28.65	1.79	1.42
1	K	20	CYS	CB-SG	28.63	2.31	1.82
2	H	25	TYR	CG-CD2	25.70	1.72	1.39
1	G	6	CYS	CB-SG	25.51	2.25	1.82

The worst 5 of 1081 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	22	ARG	NE-CZ-NH1	-39.15	100.72	120.30
1	A	14	TYR	CB-CG-CD1	-33.41	100.95	121.00
2	J	16	TYR	CB-CG-CD1	-29.25	103.45	121.00
2	J	22	ARG	NE-CZ-NH1	29.24	134.92	120.30
2	B	24	PHE	CB-CG-CD2	26.18	139.13	120.80

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	159	0	142	88	0
1	C	163	0	149	108	0
1	E	163	0	148	131	0
1	G	159	0	143	73	0
1	I	163	0	149	112	0
1	K	163	0	146	122	0
2	B	219	0	205	146	0
2	D	194	0	178	94	0
2	F	194	0	180	63	0
2	H	220	0	206	96	0
2	J	235	0	219	132	0
2	L	212	0	195	117	0
3	A	7	0	5	2	0
3	C	7	0	6	0	0
3	E	7	0	5	0	0
3	G	7	0	6	2	0
3	I	7	0	5	1	0
3	K	7	0	5	2	0
4	B	1	0	0	0	0
4	C	1	0	0	1	0
5	B	1	0	0	0	0
5	D	1	0	0	0	0
6	A	2	0	0	0	0
6	B	17	0	0	5	0
6	C	17	0	0	3	0
6	D	10	0	0	6	0
6	E	7	0	0	1	0
6	F	15	0	0	5	0
6	G	17	0	0	6	0
6	H	17	0	0	3	0
6	I	19	0	0	6	0
6	J	16	0	0	1	0
6	K	9	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	L	4	0	0	0	0
All	All	2440	0	2092	1179	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 271.

The worst 5 of 1179 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:H:10:HIS:CB	2:H:10:HIS:CG	1.75	1.70
1:I:14:TYR:CE1	1:I:14:TYR:CD1	1.75	1.70
1:I:14:TYR:CD2	1:I:14:TYR:CE2	1.75	1.68
2:B:24:PHE:CB	2:B:24:PHE:CG	1.77	1.68
2:H:24:PHE:CD1	2:H:24:PHE:CE1	1.75	1.65

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	18/21 (86%)	17 (94%)	1 (6%)	0	100	100
1	C	19/21 (90%)	17 (90%)	2 (10%)	0	100	100
1	E	19/21 (90%)	17 (90%)	2 (10%)	0	100	100
1	G	18/21 (86%)	17 (94%)	1 (6%)	0	100	100
1	I	19/21 (90%)	19 (100%)	0	0	100	100
1	K	19/21 (90%)	18 (95%)	1 (5%)	0	100	100
2	B	24/30 (80%)	24 (100%)	0	0	100	100
2	D	23/30 (77%)	22 (96%)	1 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	F	23/30 (77%)	22 (96%)	1 (4%)	0	100	100
2	H	25/30 (83%)	24 (96%)	1 (4%)	0	100	100
2	J	26/30 (87%)	24 (92%)	2 (8%)	0	100	100
2	L	24/30 (80%)	23 (96%)	1 (4%)	0	100	100
All	All	257/306 (84%)	244 (95%)	13 (5%)	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	20/20 (100%)	18 (90%)	2 (10%)	9	4
1	C	20/20 (100%)	19 (95%)	1 (5%)	30	22
1	E	20/20 (100%)	16 (80%)	4 (20%)	1	0
1	G	20/20 (100%)	17 (85%)	3 (15%)	3	1
1	I	20/20 (100%)	19 (95%)	1 (5%)	30	22
1	K	20/20 (100%)	19 (95%)	1 (5%)	30	22
2	B	22/25 (88%)	20 (91%)	2 (9%)	12	6
2	D	19/25 (76%)	15 (79%)	4 (21%)	1	0
2	F	19/25 (76%)	18 (95%)	1 (5%)	28	20
2	H	22/25 (88%)	20 (91%)	2 (9%)	12	6
2	J	24/25 (96%)	22 (92%)	2 (8%)	14	7
2	L	21/25 (84%)	18 (86%)	3 (14%)	4	1
All	All	247/270 (92%)	221 (90%)	26 (10%)	8	4

5 of 26 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	8	THR

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Mol	Chain	Res	Type
1	G	3	VAL
2	L	17	LEU
1	E	9	SER
2	F	3	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	5	GLN
1	E	21	ASN
1	I	5	GLN
2	D	4	GLN
1	I	21	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

6 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	MEA	B	26	2	10,12,13	6.33	6 (60%)	10,14,16	3.84	7 (70%)
2	MEA	D	26	2	10,12,13	9.90	7 (70%)	10,14,16	8.88	10 (100%)
2	MEA	F	26	2	10,12,13	9.23	7 (70%)	10,14,16	7.87	8 (80%)
2	MEA	H	26	2	10,12,13	6.13	6 (60%)	10,14,16	2.94	8 (80%)
2	MEA	J	26	2	10,12,13	25.75	6 (60%)	10,14,16	41.74	10 (100%)
2	MEA	L	26	2	10,12,13	4.99	9 (90%)	10,14,16	5.33	8 (80%)

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	MEA	B	26	2	-	0/4/8/10	0/1/1/1
2	MEA	D	26	2	-	0/4/8/10	0/1/1/1
2	MEA	F	26	2	-	0/4/8/10	0/1/1/1
2	MEA	H	26	2	-	0/4/8/10	0/1/1/1
2	MEA	J	26	2	-	0/4/8/10	1/1/1/1
2	MEA	L	26	2	-	0/4/8/10	0/1/1/1

The worst 5 of 41 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	26	MEA	CA-N	-16.73	1.16	1.47
2	D	26	MEA	CA-N	-15.90	1.18	1.47
2	F	26	MEA	CB-CG	-9.06	1.29	1.51
2	F	26	MEA	CE2-CD2	-8.61	1.21	1.38
2	D	26	MEA	CE1-CD1	-8.51	1.21	1.38

The worst 5 of 51 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	26	MEA	CZ-CE1-CD1	-63.73	26.90	120.19
2	J	26	MEA	CZ-CE2-CD2	-60.21	32.04	120.19
2	J	26	MEA	CE2-CD2-CG	-59.28	26.44	120.65
2	J	26	MEA	CE1-CD1-CG	-56.06	31.55	120.65
2	J	26	MEA	CD2-CG-CD1	-37.48	58.13	118.13

There are no chirality outliers.

There are no torsion outliers.

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	J	26	MEA	CD1-CD2-CE1-CE2-CG-CZ

6 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	26	MEA	3	0
2	D	26	MEA	4	0
2	F	26	MEA	7	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	26	MEA	2	0
2	J	26	MEA	5	0
2	L	26	MEA	3	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 4 are monoatomic - leaving 6 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	A	1022	-	7,7,7	8.26	5 (71%)	8,8,8	7.51	8 (100%)
3	IPH	C	1022	-	7,7,7	4.58	4 (57%)	8,8,8	3.65	6 (75%)
3	IPH	E	1022	-	7,7,7	2.20	2 (28%)	8,8,8	2.53	6 (75%)
3	IPH	G	1022	-	7,7,7	7.72	7 (100%)	8,8,8	7.77	7 (87%)
3	IPH	I	1022	-	7,7,7	2.36	4 (57%)	8,8,8	3.00	5 (62%)
3	IPH	K	1022	-	7,7,7	6.59	5 (71%)	8,8,8	4.83	7 (87%)

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	A	1022	-	-	0/0/0/0	0/1/1/1
3	IPH	C	1022	-	-	0/0/0/0	0/1/1/1
3	IPH	E	1022	-	-	0/0/0/0	0/1/1/1
3	IPH	G	1022	-	-	0/0/0/0	0/1/1/1
3	IPH	I	1022	-	-	0/0/0/0	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	IPH	K	1022	-	-	0/0/0/0	0/1/1/1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	K	1022	IPH	C3-C2	-9.77	1.18	1.38
3	K	1022	IPH	C5-C6	-9.49	1.19	1.38
3	K	1022	IPH	O1-C1	-7.66	1.18	1.37
3	G	1022	IPH	C2-C1	-6.44	1.25	1.38
3	K	1022	IPH	C6-C1	-5.64	1.27	1.38

The worst 5 of 39 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1022	IPH	C4-C5-C6	-11.69	103.07	120.19
3	A	1022	IPH	C3-C2-C1	-11.27	102.45	119.37
3	G	1022	IPH	C4-C5-C6	-11.14	103.88	120.19
3	G	1022	IPH	C3-C2-C1	-11.11	102.69	119.37
3	K	1022	IPH	C5-C6-C1	-7.99	107.37	119.37

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1022	IPH	2	0
3	G	1022	IPH	2	0
3	I	1022	IPH	1	0
3	K	1022	IPH	2	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 [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	20/21 (95%)	0.81	4 (20%) 1 1	39, 54, 68, 70	0
1	C	21/21 (100%)	-0.47	0 100 100	27, 36, 48, 55	0
1	E	21/21 (100%)	-0.39	0 100 100	28, 39, 57, 73	0
1	G	20/21 (95%)	-0.30	0 100 100	31, 36, 57, 66	0
1	I	21/21 (100%)	-0.55	0 100 100	27, 32, 44, 59	0
1	K	21/21 (100%)	-0.50	0 100 100	27, 37, 53, 59	0
2	B	26/30 (86%)	0.17	1 (3%) 44 48	24, 30, 69, 94	0
2	D	24/30 (80%)	0.10	0 100 100	21, 30, 59, 64	0
2	F	24/30 (80%)	0.08	0 100 100	24, 30, 52, 66	0
2	H	27/30 (90%)	0.12	1 (3%) 45 49	23, 30, 62, 76	0
2	J	28/30 (93%)	0.09	0 100 100	24, 29, 55, 73	0
2	L	25/30 (83%)	0.37	1 (4%) 42 46	23, 32, 55, 67	0
All	All	278/306 (90%)	-0.02	7 (2%) 61 64	21, 35, 65, 94	0

The worst 5 of 7 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	18	ASN	3.4
2	L	1	PHE	3.1
1	A	21	ASN	3.0
1	A	14	TYR	2.9
1	A	8	THR	2.7

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron

density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	MEA	D	26	12/13	0.89	0.10	-	53,65,71,73	0
2	MEA	B	26	12/13	0.84	0.17	-	83,90,94,95	0
2	MEA	L	26	12/13	0.76	0.19	-	58,69,80,82	0
2	MEA	J	26	12/13	0.97	0.11	-	28,31,37,39	0
2	MEA	H	26	12/13	0.95	0.07	-	36,41,45,46	0
2	MEA	F	26	12/13	0.95	0.11	-	44,49,53,53	0

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	IPH	C	1022	7/7	0.97	0.14	1.45	27,32,33,34	0
3	IPH	G	1022	7/7	0.99	0.14	0.90	25,27,29,32	0
3	IPH	K	1022	7/7	0.96	0.13	0.88	28,28,31,32	0
4	CL	B	1028	1/1	1.00	0.12	0.43	27,27,27,27	0
3	IPH	A	1022	7/7	0.96	0.09	-0.06	29,31,36,36	0
3	IPH	I	1022	7/7	0.98	0.09	-0.22	25,26,28,30	0
5	ZN	B	1030	1/1	1.00	0.10	-0.33	25,25,25,25	0
3	IPH	E	1022	7/7	0.96	0.09	-0.39	32,33,35,35	0
4	CL	C	1028	1/1	0.99	0.12	-1.24	25,25,25,25	0
5	ZN	D	1030	1/1	1.00	0.07	-4.75	23,23,23,23	0

6.5 Other polymers [i](#)

There are no such residues in this entry.