



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 9, 2016 – 10:52 AM EST

PDB ID : 5IKC
Title : X-RAY STRUCTURE OF THE N-TERMINAL DOMAIN OF HUMAN DOUBLECORTIN in complex with FAB
Authors : Ruf, A.; Stihle, M.; Benz, J.; Thoma, R.; Rudolph, M.G.
Deposited on : 2016-03-03
Resolution : 2.06 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

<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	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20028442
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)	:	rb-20028442

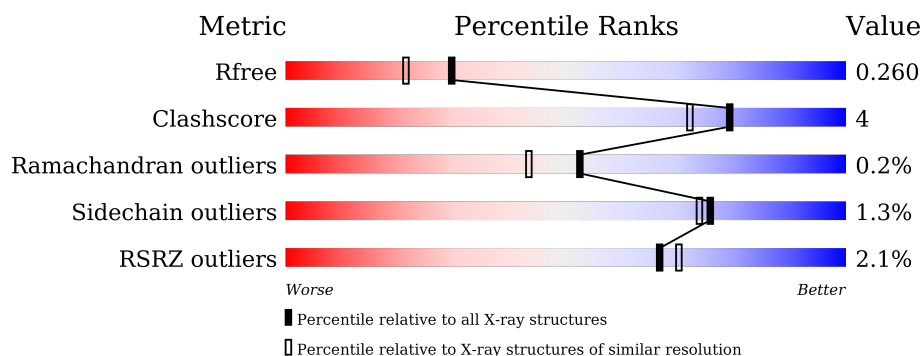
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.06 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	1799 (2.08-2.04)
Clashscore	102246	1910 (2.08-2.04)
Ramachandran outliers	100387	1893 (2.08-2.04)
Sidechain outliers	100360	1893 (2.08-2.04)
RSRZ outliers	91569	1802 (2.08-2.04)

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	213	<div> <div>2%</div> <div>89%</div> <div>11%</div> </div>
1	L	213	<div> <div>89%</div> <div>9%</div> <div>.</div> </div>
2	B	215	<div> <div>%</div> <div>86%</div> <div>11%</div> <div>..</div> </div>
2	H	215	<div> <div>5%</div> <div>89%</div> <div>11%</div> </div>
3	M	90	<div> <div>2%</div> <div>93%</div> <div>6%</div> <div>.</div> </div>
3	N	90	<div> <div>%</div> <div>90%</div> <div>10%</div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8308 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 MAb 6H10 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	213	Total	C	N	O	S	0	0	0
			1651	1029	279	336	7			
1	L	211	Total	C	N	O	S	0	0	0
			1635	1019	276	333	7			

There are 70 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	ASP	-	expression tag	UNP A0A0U5BC76
A	7	SER	THR	conflict	UNP A0A0U5BC76
A	8	GLN	PRO	conflict	UNP A0A0U5BC76
A	10	LEU	PHE	conflict	UNP A0A0U5BC76
A	11	MET	LEU	conflict	UNP A0A0U5BC76
A	12	SER	PHE	conflict	UNP A0A0U5BC76
A	13	THR	VAL	conflict	UNP A0A0U5BC76
A	15	VAL	ALA	conflict	UNP A0A0U5BC76
A	20	SER	THR	conflict	UNP A0A0U5BC76
A	22	THR	SER	conflict	UNP A0A0U5BC76
A	28	ILE	ARG	conflict	UNP A0A0U5BC76
A	30	ASP	LEU	conflict	UNP A0A0U5BC76
A	31	THR	ASN	conflict	UNP A0A0U5BC76
A	32	ALA	ASP	conflict	UNP A0A0U5BC76
A	38	GLN	GLU	conflict	UNP A0A0U5BC76
A	46	PRO	LEU	conflict	UNP A0A0U5BC76
A	50	LEU	TYR	conflict	UNP A0A0U5BC76
A	55	HIS	PHE	conflict	UNP A0A0U5BC76
A	63	THR	SER	conflict	UNP A0A0U5BC76
A	67	SER	TYR	conflict	UNP A0A0U5BC76
A	73	LEU	PHE	conflict	UNP A0A0U5BC76
A	76	ASN	SER	conflict	UNP A0A0U5BC76
A	77	ASN	THR	conflict	UNP A0A0U5BC76
A	80	SER	ALA	conflict	UNP A0A0U5BC76
A	81	ASP	GLU	conflict	UNP A0A0U5BC76

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Chain	Residue	Modelled	Actual	Comment	Reference
A	85	ASP	VAL	conflict	UNP A0A0U5BC76
A	89	LEU	GLN	conflict	UNP A0A0U5BC76
A	91	HIS	ASP	conflict	UNP A0A0U5BC76
A	92	TRP	TYR	conflict	UNP A0A0U5BC76
A	93	ASN	ARG	conflict	UNP A0A0U5BC76
A	94	TYR	SER	conflict	UNP A0A0U5BC76
A	96	LEU	TRP	conflict	UNP A0A0U5BC76
A	100	ALA	GLY	conflict	UNP A0A0U5BC76
A	106	LEU	ILE	conflict	UNP A0A0U5BC76
A	108	GLY	ARG	conflict	UNP A0A0U5BC76
L	1	ASP	-	expression tag	UNP A0A0U5BC76
L	7	SER	THR	conflict	UNP A0A0U5BC76
L	8	GLN	PRO	conflict	UNP A0A0U5BC76
L	10	LEU	PHE	conflict	UNP A0A0U5BC76
L	11	MET	LEU	conflict	UNP A0A0U5BC76
L	12	SER	PHE	conflict	UNP A0A0U5BC76
L	13	THR	VAL	conflict	UNP A0A0U5BC76
L	15	VAL	ALA	conflict	UNP A0A0U5BC76
L	20	SER	THR	conflict	UNP A0A0U5BC76
L	22	THR	SER	conflict	UNP A0A0U5BC76
L	28	ILE	ARG	conflict	UNP A0A0U5BC76
L	30	ASP	LEU	conflict	UNP A0A0U5BC76
L	31	THR	ASN	conflict	UNP A0A0U5BC76
L	32	ALA	ASP	conflict	UNP A0A0U5BC76
L	38	GLN	GLU	conflict	UNP A0A0U5BC76
L	46	PRO	LEU	conflict	UNP A0A0U5BC76
L	50	LEU	TYR	conflict	UNP A0A0U5BC76
L	55	HIS	PHE	conflict	UNP A0A0U5BC76
L	63	THR	SER	conflict	UNP A0A0U5BC76
L	67	SER	TYR	conflict	UNP A0A0U5BC76
L	73	LEU	PHE	conflict	UNP A0A0U5BC76
L	76	ASN	SER	conflict	UNP A0A0U5BC76
L	77	ASN	THR	conflict	UNP A0A0U5BC76
L	80	SER	ALA	conflict	UNP A0A0U5BC76
L	81	ASP	GLU	conflict	UNP A0A0U5BC76
L	85	ASP	VAL	conflict	UNP A0A0U5BC76
L	89	LEU	GLN	conflict	UNP A0A0U5BC76
L	91	HIS	ASP	conflict	UNP A0A0U5BC76
L	92	TRP	TYR	conflict	UNP A0A0U5BC76
L	93	ASN	ARG	conflict	UNP A0A0U5BC76
L	94	TYR	SER	conflict	UNP A0A0U5BC76
L	96	LEU	TRP	conflict	UNP A0A0U5BC76

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Chain	Residue	Modelled	Actual	Comment	Reference
L	100	ALA	GLY	conflict	UNP A0A0U5BC76
L	106	LEU	ILE	conflict	UNP A0A0U5BC76
L	108	GLY	ARG	conflict	UNP A0A0U5BC76

- Molecule 2 is a protein called Ighg protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	211	Total	C	N	O	S	0	0	0
			1578	991	258	323	6			
2	H	215	Total	C	N	O	S	0	0	0
			1602	1005	262	329	6			

There are 58 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1	PCA	-	expression tag	UNP Q569X1
B	5	GLN	LEU	conflict	UNP Q569X1
B	9	ALA	THR	conflict	UNP Q569X1
B	10	ASP	GLU	conflict	UNP Q569X1
B	28	ASP	SER	conflict	UNP Q569X1
B	32	ASP	SER	conflict	UNP Q569X1
B	33	TYR	LEU	conflict	UNP Q569X1
B	34	VAL	LEU	conflict	UNP Q569X1
B	38	LYS	MET	conflict	UNP Q569X1
B	50	ARG	TRP	conflict	UNP Q569X1
B	54	ALA	GLU	conflict	UNP Q569X1
B	55	ASN	ASP	conflict	UNP Q569X1
B	57	ALA	GLU	conflict	UNP Q569X1
B	61	ALA	VAL	conflict	UNP Q569X1
B	73	ASP	ALA	conflict	UNP Q569X1
B	89	GLU	GLY	conflict	UNP Q569X1
B	93	VAL	THR	conflict	UNP Q569X1
B	?	-	LEU	deletion	UNP Q569X1
B	?	-	PHE	deletion	UNP Q569X1
B	?	-	TYR	deletion	UNP Q569X1
B	?	-	GLY	deletion	UNP Q569X1
B	?	-	TYR	deletion	UNP Q569X1
B	?	-	ASP	deletion	UNP Q569X1
B	97	GLY	ASP	conflict	UNP Q569X1
B	98	ARG	GLY	conflict	UNP Q569X1
B	99	SER	ARG	conflict	UNP Q569X1
B	100	LYS	ASP	conflict	UNP Q569X1

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Chain	Residue	Modelled	Actual	Comment	Reference
B	104	SER	TYR	conflict	UNP Q569X1
B	111	LEU	ILE	conflict	UNP Q569X1
H	1	PCA	-	expression tag	UNP Q569X1
H	5	GLN	LEU	conflict	UNP Q569X1
H	9	ALA	THR	conflict	UNP Q569X1
H	10	ASP	GLU	conflict	UNP Q569X1
H	28	ASP	SER	conflict	UNP Q569X1
H	32	ASP	SER	conflict	UNP Q569X1
H	33	TYR	LEU	conflict	UNP Q569X1
H	34	VAL	LEU	conflict	UNP Q569X1
H	38	LYS	MET	conflict	UNP Q569X1
H	50	ARG	TRP	conflict	UNP Q569X1
H	54	ALA	GLU	conflict	UNP Q569X1
H	55	ASN	ASP	conflict	UNP Q569X1
H	57	ALA	GLU	conflict	UNP Q569X1
H	61	ALA	VAL	conflict	UNP Q569X1
H	73	ASP	ALA	conflict	UNP Q569X1
H	89	GLU	GLY	conflict	UNP Q569X1
H	93	VAL	THR	conflict	UNP Q569X1
H	?	-	LEU	deletion	UNP Q569X1
H	?	-	PHE	deletion	UNP Q569X1
H	?	-	TYR	deletion	UNP Q569X1
H	?	-	GLY	deletion	UNP Q569X1
H	?	-	TYR	deletion	UNP Q569X1
H	?	-	ASP	deletion	UNP Q569X1
H	97	GLY	ASP	conflict	UNP Q569X1
H	98	ARG	GLY	conflict	UNP Q569X1
H	99	SER	ARG	conflict	UNP Q569X1
H	100	LYS	ASP	conflict	UNP Q569X1
H	104	SER	TYR	conflict	UNP Q569X1
H	111	LEU	ILE	conflict	UNP Q569X1

- Molecule 3 is a protein called Neuronal migration protein doublecortin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	M	89	Total	C	N	O	S	0	0	0
			723	457	124	140	2			
3	N	90	Total	C	N	O	S	0	0	0
			732	463	126	141	2			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	51	ALA	-	expression tag	UNP O43602
N	51	ALA	-	expression tag	UNP O43602

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	H	1	Total Cl 1 1	0	0
4	B	1	Total Cl 1 1	0	0

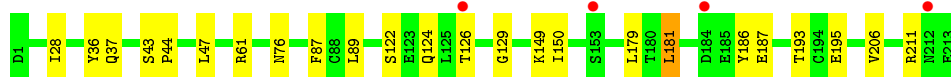
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	85	Total O 85 85	0	0
5	B	62	Total O 62 62	0	0
5	H	88	Total O 88 88	0	0
5	L	75	Total O 75 75	0	0
5	M	27	Total O 27 27	0	0
5	N	48	Total O 48 48	0	0

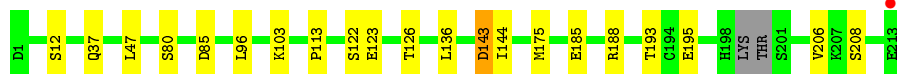
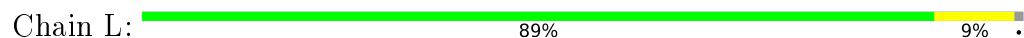
3 Residue-property plots [i](#)

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.

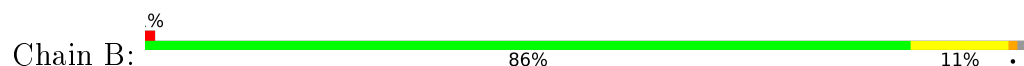
- Molecule 1: MAb 6H10 light chain



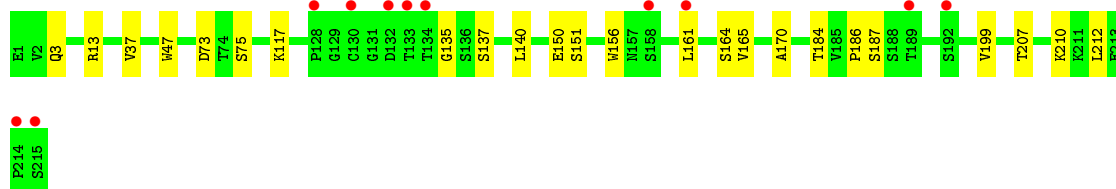
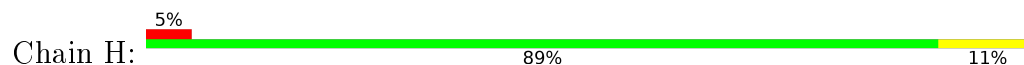
- Molecule 1: MAb 6H10 light chain



- Molecule 2: IgH protein



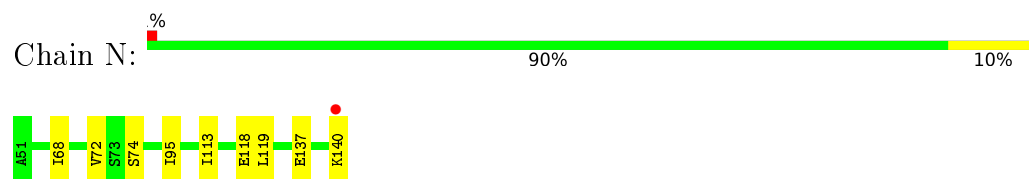
- Molecule 2: IgH protein



- Molecule 3: Neuronal migration protein doublecortin



- Molecule 3: Neuronal migration protein doublecortin



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	66.86 Å 110.40 Å 75.09 Å 90.00° 106.54° 90.00°	Depositor
Resolution (Å)	41.83 – 2.06 41.83 – 2.06	Depositor EDS
% Data completeness (in resolution range)	98.9 (41.83-2.06) 87.0 (41.83-2.06)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.52 (at 2.06 Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.198 , 0.265 0.192 , 0.260	Depositor DCC
R_{free} test set	2807 reflections (5.00%)	DCC
Wilson B-factor (Å ²)	26.3	Xtriage
Anisotropy	0.318	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 43.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8308	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.17% 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, 0.333 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: PCA, 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	0.41	0/1688	0.57	0/2296
1	L	0.41	0/1671	0.58	0/2272
2	B	0.41	0/1610	0.60	0/2205
2	H	0.43	0/1635	0.61	0/2240
3	M	0.42	0/736	0.54	0/987
3	N	0.44	0/745	0.60	0/998
All	All	0.42	0/8085	0.59	0/10998

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 [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1651	0	1584	14	0
1	L	1635	0	1563	11	0
2	B	1578	0	1525	14	0
2	H	1602	0	1550	11	1
3	M	723	0	702	3	0
3	N	732	0	715	6	1
4	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	H	1	0	0	0	0
5	A	85	0	0	1	0
5	B	62	0	0	0	0
5	H	88	0	0	0	0
5	L	75	0	0	0	0
5	M	27	0	0	0	0
5	N	48	0	0	0	0
All	All	8308	0	7639	55	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 4.

All (55) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:195:GLU:HG2	1:L:206:VAL:HG22	1.67	0.74
2:H:140:LEU:HB3	2:H:212:LEU:HD22	1.75	0.69
2:B:30:LYS:HD3	2:B:74:THR:HG21	1.75	0.69
2:B:38:LYS:HE2	2:B:40:ARG:HD2	1.76	0.66
3:N:137:GLU:HB3	3:N:140:LYS:HB2	1.76	0.66
2:B:103:ASP:OD2	3:M:63:ARG:NH1	2.31	0.62
1:L:193:THR:HG1	1:L:208:SER:HG	1.47	0.62
1:A:150:ILE:HD11	1:A:179:LEU:HD21	1.82	0.61
1:L:37:GLN:HB2	1:L:47:LEU:HD11	1.84	0.60
2:B:121:PRO:HB3	2:B:147:TYR:HB3	1.84	0.59
1:L:143:ASP:OD1	1:L:143:ASP:N	2.28	0.59
1:A:37:GLN:HB2	1:A:47:LEU:HD11	1.88	0.56
3:N:72:VAL:HG11	3:N:119:LEU:HD12	1.88	0.54
2:B:43:GLN:N	2:B:43:GLN:OE1	2.41	0.54
3:N:113:ILE:HG23	3:N:118:GLU:HB2	1.90	0.53
1:L:113:PRO:HG3	1:L:144:ILE:HD11	1.92	0.51
2:H:156:TRP:HZ3	2:H:212:LEU:HD13	1.76	0.51
1:L:122:SER:O	1:L:126:THR:HG23	2.10	0.51
1:L:85:ASP:OD1	1:L:103:LYS:HD3	2.10	0.51
2:B:165:VAL:HG22	2:B:183:VAL:HG23	1.93	0.50
3:M:101:VAL:HG13	3:M:127:CYS:HB3	1.94	0.50
2:B:67:LYS:NZ	2:B:90:ASP:OD2	2.40	0.49
2:H:150:GLU:OE2	2:H:170:ALA:HB3	2.14	0.48
1:A:195:GLU:HG2	1:A:206:VAL:HG22	1.96	0.47
2:H:37:VAL:HG12	2:H:47:TRP:HA	1.95	0.47
2:B:1:PCA:HB2	2:B:2:VAL:H	1.56	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:150:GLU:O	2:B:151:SER:HB3	2.15	0.47
1:A:61:ARG:HB2	1:A:76:ASN:O	2.15	0.46
2:H:73:ASP:OD1	2:H:75:SER:OG	2.31	0.46
1:A:44:PRO:HD2	2:B:105:TRP:CE3	2.51	0.46
2:H:199:VAL:O	2:H:207:THR:HA	2.16	0.46
1:A:187:GLU:HA	1:A:211:ARG:NH2	2.31	0.45
1:A:122:SER:O	1:A:126:THR:HG23	2.17	0.44
1:A:124:GLN:HG2	1:A:129:GLY:O	2.17	0.44
1:A:28:ILE:HD12	5:A:372:HOH:O	2.16	0.43
1:L:185:GLU:HG3	1:L:188:ARG:HH21	1.82	0.43
1:L:136:LEU:HB2	1:L:175:MET:HG2	1.99	0.43
2:H:161:LEU:O	2:H:165:VAL:HG23	2.18	0.43
1:A:36:TYR:HB2	1:A:87:PHE:CE1	2.54	0.42
3:N:72:VAL:HG11	3:N:119:LEU:CD1	2.48	0.42
2:H:137:SER:HA	2:H:186:PRO:HA	2.01	0.42
1:A:181:LEU:CD1	1:A:186:TYR:HB2	2.49	0.42
2:H:135:GLY:O	2:H:187:SER:OG	2.23	0.42
2:H:210:LYS:HD3	2:H:210:LYS:HA	1.90	0.41
1:L:123:GLU:HG3	1:L:123:GLU:H	1.52	0.41
2:B:67:LYS:HB2	2:B:67:LYS:HE3	1.98	0.41
2:H:164:SER:OG	2:H:184:THR:HB	2.21	0.41
1:L:96:LEU:HD11	3:N:95:ILE:HD11	2.03	0.41
3:M:54:LYS:HE3	3:M:69:VAL:HG11	2.03	0.41
1:A:181:LEU:HD13	1:A:186:TYR:HB2	2.03	0.41
1:A:149:LYS:HB2	1:A:193:THR:HB	2.03	0.41
1:A:43:SER:HB3	2:B:95:TYR:CE1	2.56	0.40
2:B:163:SER:HB2	2:B:184:THR:O	2.21	0.40
2:B:60:TYR:CE2	2:B:70:LEU:HD13	2.56	0.40
3:N:68:ILE:HG21	3:N:68:ILE:HD13	1.77	0.40

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)
2:H:13:ARG:NH1	3:N:74:SER:O[1_455]	2.13	0.07

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	211/213 (99%)	206 (98%)	5 (2%)	0	100	100
1	L	207/213 (97%)	201 (97%)	6 (3%)	0	100	100
2	B	207/215 (96%)	201 (97%)	5 (2%)	1 (0%)	34	22
2	H	213/215 (99%)	205 (96%)	7 (3%)	1 (0%)	34	22
3	M	87/90 (97%)	85 (98%)	2 (2%)	0	100	100
3	N	88/90 (98%)	87 (99%)	1 (1%)	0	100	100
All	All	1013/1036 (98%)	985 (97%)	26 (3%)	2 (0%)	52	43

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	151	SER
2	B	151	SER

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	189/189 (100%)	187 (99%)	2 (1%)	80	79
1	L	187/189 (99%)	184 (98%)	3 (2%)	70	67
2	B	180/183 (98%)	175 (97%)	5 (3%)	51	45
2	H	183/183 (100%)	181 (99%)	2 (1%)	80	79
3	M	78/79 (99%)	78 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	N	79/79 (100%)	79 (100%)	0	100	100
All	All	896/902 (99%)	884 (99%)	12 (1%)	76	74

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	89	LEU
1	A	181	LEU
2	B	3	GLN
2	B	50	ARG
2	B	150	GLU
2	B	182	SER
2	B	209	ASP
2	H	3	GLN
2	H	117	LYS
1	L	12	SER
1	L	80	SER
1	L	143	ASP

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 ⓘ

2 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	PCA	B	1	2	7,8,9	1.76	1 (14%)	9,10,12	2.06	4 (44%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	PCA	H	1	2	7,8,9	1.67	1 (14%)	9,10,12	2.00	5 (55%)

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	PCA	B	1	2	-	0/0/11/13	0/1/1/1
2	PCA	H	1	2	-	0/0/11/13	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	1	PCA	CD-N	4.33	1.46	1.33
2	B	1	PCA	CD-N	4.55	1.47	1.33

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	PCA	CB-CA-C	-3.21	108.04	112.80
2	H	1	PCA	O-C-CA	-3.06	117.32	125.69
2	B	1	PCA	OE-CD-CG	-2.87	121.17	126.85
2	H	1	PCA	CA-N-CD	-2.74	103.78	113.53
2	B	1	PCA	CA-N-CD	-2.62	104.19	113.53
2	H	1	PCA	OE-CD-CG	-2.56	121.79	126.85
2	H	1	PCA	CG-CD-N	2.02	114.40	108.28
2	B	1	PCA	CB-CA-N	2.08	109.64	103.34
2	H	1	PCA	CB-CA-N	2.80	111.85	103.34

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1	PCA	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

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.

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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	213/213 (100%)	-0.06	4 (1%) 70 73	20, 37, 73, 100	0
1	L	211/213 (99%)	-0.16	1 (0%) 91 93	21, 38, 65, 101	0
2	B	210/215 (97%)	-0.04	3 (1%) 78 80	21, 40, 74, 108	0
2	H	214/215 (99%)	0.13	11 (5%) 32 34	21, 35, 94, 128	0
3	M	89/90 (98%)	0.19	2 (2%) 65 69	24, 43, 69, 76	0
3	N	90/90 (100%)	-0.38	1 (1%) 82 85	19, 31, 53, 106	0
All	All	1027/1036 (99%)	-0.04	22 (2%) 67 70	19, 38, 75, 128	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	130	CYS	8.1
2	H	134	THR	4.1
2	H	161	LEU	4.0
2	H	192	SER	4.0
2	B	130	CYS	3.5
2	B	163	SER	3.5
3	N	140	LYS	3.4
2	H	189	THR	2.8
2	B	131	GLY	2.6
1	A	184	ASP	2.5
1	A	212	ASN	2.4
1	L	213	GLU	2.4
2	H	132	ASP	2.3
2	H	215	SER	2.3
3	M	95	ILE	2.3
1	A	153	SER	2.2
2	H	128	PRO	2.2
2	H	158	SER	2.1
2	H	214	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	126	THR	2.1
2	H	133	THR	2.1
3	M	89	ARG	2.0

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	PCA	B	1	8/9	0.82	0.19	-	60,88,92,92	0
2	PCA	H	1	8/9	0.85	0.25	-	53,78,89,90	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
4	CL	B	301	1/1	0.99	0.13	-0.27	34,34,34,34	0
4	CL	H	301	1/1	1.00	0.06	-5.48	21,21,21,21	0

6.5 Other polymers [i](#)

There are no such residues in this entry.