



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2020 – 03:14 PM BST

PDB ID : 5BPB
Title : Crystal structure of the cysteine-rich domain of human Frizzled 4 - Crystal Form I
Authors : Chang, T.-H.; Hsieh, F.-L.; Harlos, K.; Jones, E.Y.
Deposited on : 2015-05-27
Resolution : 2.20 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 : 2.13.1
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) : 2.13.1

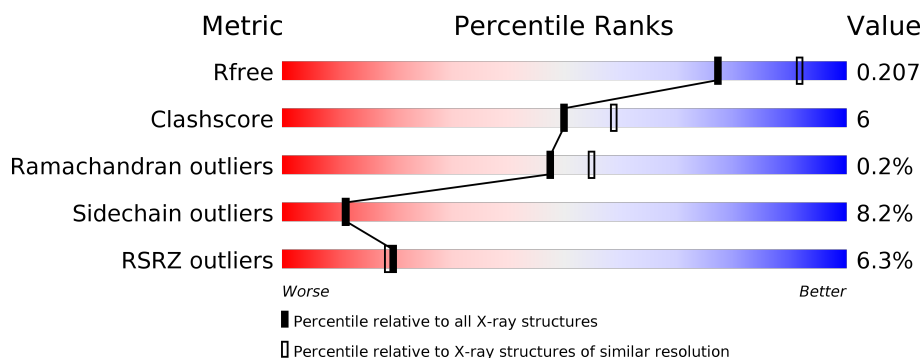
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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 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 $\leq 5\%$. 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	149	<div> <div>3%</div> <div> <div></div> <div>67%</div> <div>12%</div> <div>•</div> <div>20%</div> </div> </div>
1	B	149	<div> <div>3%</div> <div> <div></div> <div>71%</div> <div>13%</div> <div>•</div> <div>15%</div> </div> </div>
1	C	149	<div> <div>8%</div> <div> <div></div> <div>64%</div> <div>12%</div> <div>•</div> <div>21%</div> </div> </div>
1	D	149	<div> <div>7%</div> <div> <div></div> <div>71%</div> <div>13%</div> <div>••</div> <div>13%</div> </div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	B	202	-	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4070 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 Frizzled-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	119	Total	C	N	O	S	0	0	0
			930	588	157	169	16			
1	B	127	Total	C	N	O	S	0	0	0
			994	630	165	183	16			
1	D	130	Total	C	N	O	S	0	0	0
			1019	643	174	186	16			
1	C	118	Total	C	N	O	S	0	0	0
			923	583	156	168	16			

There are 44 discrepancies between the modelled and reference sequences:

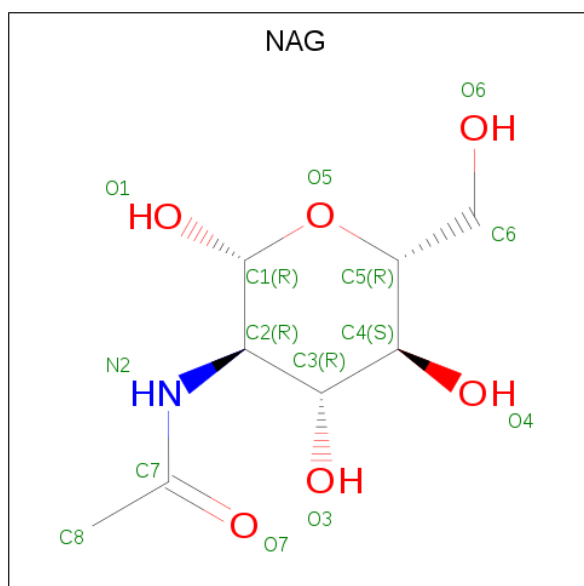
Chain	Residue	Modelled	Actual	Comment	Reference
A	39	ASP	-	expression tag	UNP Q9ULV1
A	40	THR	-	expression tag	UNP Q9ULV1
A	41	GLY	-	expression tag	UNP Q9ULV1
A	180	GLY	-	expression tag	UNP Q9ULV1
A	181	THR	-	expression tag	UNP Q9ULV1
A	182	LEU	-	expression tag	UNP Q9ULV1
A	183	GLU	-	expression tag	UNP Q9ULV1
A	184	VAL	-	expression tag	UNP Q9ULV1
A	185	LEU	-	expression tag	UNP Q9ULV1
A	186	PHE	-	expression tag	UNP Q9ULV1
A	187	GLN	-	expression tag	UNP Q9ULV1
B	39	ASP	-	expression tag	UNP Q9ULV1
B	40	THR	-	expression tag	UNP Q9ULV1
B	41	GLY	-	expression tag	UNP Q9ULV1
B	180	GLY	-	expression tag	UNP Q9ULV1
B	181	THR	-	expression tag	UNP Q9ULV1
B	182	LEU	-	expression tag	UNP Q9ULV1
B	183	GLU	-	expression tag	UNP Q9ULV1
B	184	VAL	-	expression tag	UNP Q9ULV1
B	185	LEU	-	expression tag	UNP Q9ULV1
B	186	PHE	-	expression tag	UNP Q9ULV1

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Chain	Residue	Modelled	Actual	Comment	Reference
B	187	GLN	-	expression tag	UNP Q9ULV1
D	39	ASP	-	expression tag	UNP Q9ULV1
D	40	THR	-	expression tag	UNP Q9ULV1
D	41	GLY	-	expression tag	UNP Q9ULV1
D	180	GLY	-	expression tag	UNP Q9ULV1
D	181	THR	-	expression tag	UNP Q9ULV1
D	182	LEU	-	expression tag	UNP Q9ULV1
D	183	GLU	-	expression tag	UNP Q9ULV1
D	184	VAL	-	expression tag	UNP Q9ULV1
D	185	LEU	-	expression tag	UNP Q9ULV1
D	186	PHE	-	expression tag	UNP Q9ULV1
D	187	GLN	-	expression tag	UNP Q9ULV1
C	39	ASP	-	expression tag	UNP Q9ULV1
C	40	THR	-	expression tag	UNP Q9ULV1
C	41	GLY	-	expression tag	UNP Q9ULV1
C	180	GLY	-	expression tag	UNP Q9ULV1
C	181	THR	-	expression tag	UNP Q9ULV1
C	182	LEU	-	expression tag	UNP Q9ULV1
C	183	GLU	-	expression tag	UNP Q9ULV1
C	184	VAL	-	expression tag	UNP Q9ULV1
C	185	LEU	-	expression tag	UNP Q9ULV1
C	186	PHE	-	expression tag	UNP Q9ULV1
C	187	GLN	-	expression tag	UNP Q9ULV1

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	D	1	Total	C	N	O	0	0
			14	8	1	5		

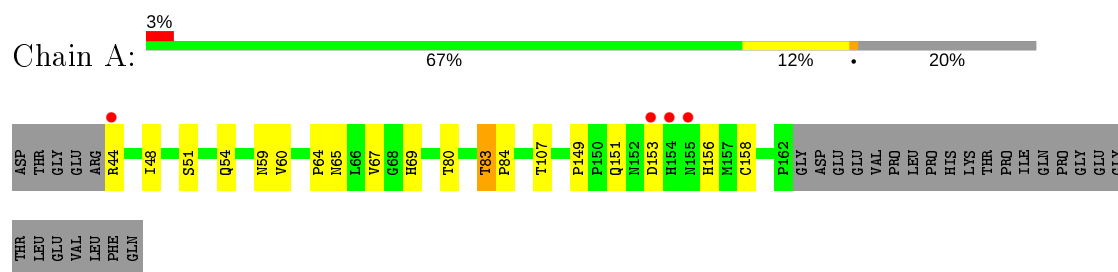
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	48	Total	O	0	0
			48	48		
3	B	52	Total	O	0	0
			52	52		
3	D	30	Total	O	0	0
			30	30		
3	C	18	Total	O	0	0
			18	18		

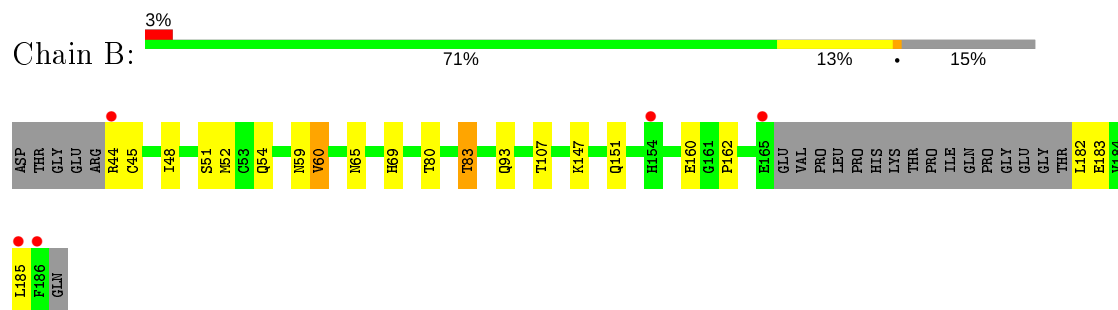
3 Residue-property plots [i](#)

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.

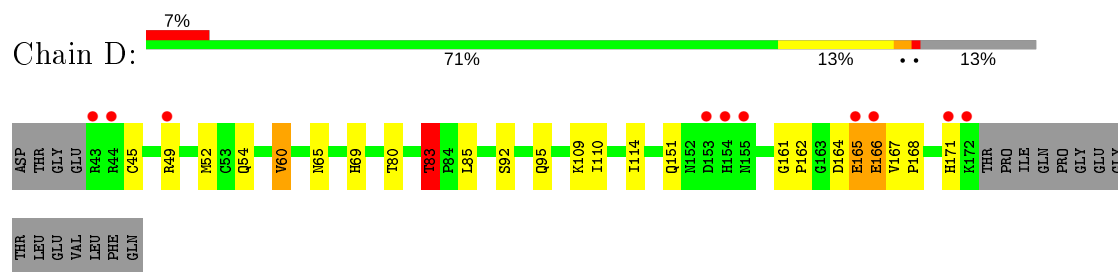
• Molecule 1: Frizzled-4



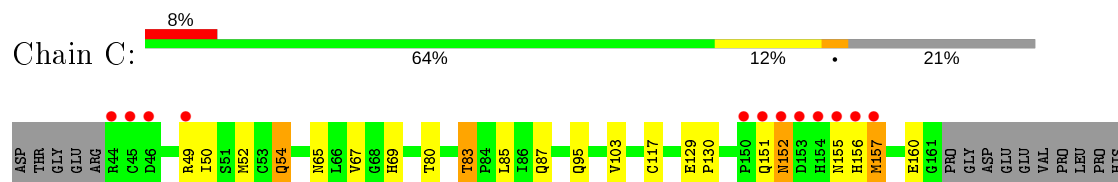
• Molecule 1: Frizzled-4



• Molecule 1: Frizzled-4



• Molecule 1: Frizzled-4



LYS
THR
PRO
ILE
GLN
PRO
GLY
GLY
THR
LEU
GLU
VAL
LEU
PHE
GLN

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	72.61Å 102.14Å 116.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.20 41.77 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.0 (40.00-2.20) 99.0 (41.77-2.20)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.26 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.177 , 0.223 0.208 , 0.207	Depositor DCC
R_{free} test set	2190 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	33.9	Xtriage
Anisotropy	0.425	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 40.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4070	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 38.99 % 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 3.3941e-04. 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:
NAG

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	0.42	0/954	0.58	0/1293
1	B	0.45	0/1018	0.57	0/1378
1	C	0.37	0/946	0.52	0/1281
1	D	0.63	1/1046 (0.1%)	0.70	3/1418 (0.2%)
All	All	0.48	1/3964 (0.0%)	0.60	3/5370 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	168	PRO	N-CD	5.34	1.55	1.47

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	161	GLY	C-N-CD	-5.99	107.43	120.60
1	D	83	THR	C-N-CD	5.49	139.93	128.40
1	D	167	VAL	C-N-CD	5.15	139.21	128.40

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	164	ASP	Peptide
1	D	166	GLU	Peptide

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	930	0	902	11	0
1	B	994	0	959	8	0
1	C	923	0	896	13	0
1	D	1019	0	988	13	0
2	A	14	0	13	1	0
2	B	28	0	26	0	0
2	D	14	0	13	1	0
3	A	48	0	0	0	0
3	B	52	0	0	0	0
3	C	18	0	0	0	0
3	D	30	0	0	0	0
All	All	4070	0	3797	45	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 (45) 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:D:92:SER:OG	1:D:165:GLU:N	2.13	0.80
1:D:80:THR:O	1:D:83:THR:HG23	1.87	0.75
1:C:117:CYS:SG	1:C:160:GLU:HG2	2.36	0.66
1:C:65:ASN:HD21	1:C:69:HIS:HD2	1.45	0.65
1:C:80:THR:O	1:C:83:THR:HG23	1.98	0.64
1:D:52:MET:HE3	1:D:95:GLN:HE22	1.64	0.62
1:D:92:SER:CB	1:D:165:GLU:HB3	2.30	0.62
1:B:65:ASN:HD21	1:B:69:HIS:HD2	1.47	0.61
1:D:65:ASN:HD21	1:D:69:HIS:HD2	1.48	0.61
2:A:201:NAG:H3	2:A:201:NAG:H83	1.84	0.60
1:D:52:MET:CE	1:D:95:GLN:HE22	2.17	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:80:THR:HA	1:A:83:THR:CG2	2.36	0.55
1:A:51:SER:OG	1:C:83:THR:HG21	2.07	0.55
1:A:48:ILE:HD12	1:A:59:ASN:HA	1.89	0.54
1:A:65:ASN:HD21	1:A:69:HIS:HD2	1.54	0.54
1:D:65:ASN:HD21	1:D:69:HIS:CD2	2.26	0.53
1:C:52:MET:O	1:C:95:GLN:NE2	2.42	0.52
1:D:92:SER:HG	1:D:165:GLU:H	1.48	0.51
1:C:50:ILE:HD12	1:C:103:VAL:HG11	1.94	0.50
1:D:92:SER:HB2	1:D:165:GLU:HB3	1.93	0.50
2:D:201:NAG:H83	2:D:201:NAG:H3	1.93	0.49
1:A:80:THR:HA	1:A:83:THR:HG23	1.95	0.49
1:B:80:THR:HA	1:B:83:THR:CG2	2.44	0.47
1:C:67:VAL:O	1:C:67:VAL:HG12	2.15	0.47
1:B:65:ASN:HD21	1:B:69:HIS:CD2	2.29	0.47
1:C:65:ASN:HD21	1:C:69:HIS:CD2	2.29	0.45
1:C:152:ASN:ND2	1:C:157:MET:HA	2.31	0.45
1:A:65:ASN:HD21	1:A:69:HIS:CD2	2.34	0.44
1:B:80:THR:HA	1:B:83:THR:HG23	2.00	0.44
1:B:93:GLN:OE1	1:B:162:PRO:O	2.36	0.44
1:B:45:CYS:HB3	1:B:60:VAL:HG13	1.99	0.44
1:C:129:GLU:N	1:C:130:PRO:CD	2.81	0.43
1:A:64:PRO:HA	1:A:69:HIS:O	2.19	0.43
1:A:153:ASP:N	1:A:156:HIS:O	2.35	0.42
1:D:110:ILE:HG21	1:D:114:ILE:HD11	2.02	0.42
1:D:45:CYS:HB3	1:D:60:VAL:HG13	2.01	0.42
1:D:165:GLU:OE1	1:D:166:GLU:HB2	2.20	0.42
1:A:153:ASP:HB2	1:A:156:HIS:H	1.85	0.41
1:B:48:ILE:HD12	1:B:59:ASN:HA	2.02	0.41
1:C:152:ASN:HD22	1:C:152:ASN:C	2.24	0.41
1:C:54:GLN:HE21	1:C:54:GLN:CA	2.34	0.41
1:A:149:PRO:HG2	1:A:158:CYS:HB3	2.03	0.41
1:A:83:THR:N	1:A:84:PRO:CD	2.84	0.41
1:C:152:ASN:ND2	1:C:156:HIS:O	2.53	0.40
1:B:51:SER:O	1:D:80:THR:HG21	2.21	0.40

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	117/149 (78%)	116 (99%)	1 (1%)	0	100	100
1	B	123/149 (83%)	122 (99%)	1 (1%)	0	100	100
1	C	116/149 (78%)	116 (100%)	0	0	100	100
1	D	128/149 (86%)	126 (98%)	1 (1%)	1 (1%)	19	19
All	All	484/596 (81%)	480 (99%)	3 (1%)	1 (0%)	47	55

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	162	PRO

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	109/135 (81%)	102 (94%)	7 (6%)	17	20
1	B	116/135 (86%)	104 (90%)	12 (10%)	7	6
1	C	108/135 (80%)	99 (92%)	9 (8%)	11	11
1	D	119/135 (88%)	110 (92%)	9 (8%)	13	14
All	All	452/540 (84%)	415 (92%)	37 (8%)	11	11

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	ARG
1	A	54	GLN
1	A	60	VAL
1	A	67	VAL
1	A	83	THR
1	A	107	THR
1	A	151	GLN
1	B	44	ARG
1	B	52	MET
1	B	54	GLN
1	B	60	VAL
1	B	83	THR
1	B	107	THR
1	B	147	LYS
1	B	151	GLN
1	B	160	GLU
1	B	182	LEU
1	B	183	GLU
1	B	185	LEU
1	D	49	ARG
1	D	54	GLN
1	D	60	VAL
1	D	83	THR
1	D	85	LEU
1	D	109	LYS
1	D	151	GLN
1	D	165	GLU
1	D	171	HIS
1	C	49	ARG
1	C	54	GLN
1	C	83	THR
1	C	85	LEU
1	C	87	GLN
1	C	151	GLN
1	C	152	ASN
1	C	155	ASN
1	C	157	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	69	HIS
1	A	78	GLN

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Mol	Chain	Res	Type
1	A	151	GLN
1	B	69	HIS
1	B	93	GLN
1	B	151	GLN
1	D	54	GLN
1	D	69	HIS
1	D	95	GLN
1	D	151	GLN
1	C	54	GLN
1	C	69	HIS
1	C	152	ASN

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](#)

4 ligands 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	NAG	A	201	1	14,14,15	0.48	0	17,19,21	1.95	6 (35%)
2	NAG	B	201	1	14,14,15	0.49	0	17,19,21	1.88	4 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	B	202	1	14,14,15	0.46	0	17,19,21	0.92	1 (5%)
2	NAG	D	201	1	14,14,15	0.51	0	17,19,21	1.81	5 (29%)

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	NAG	A	201	1	-	4/6/23/26	0/1/1/1
2	NAG	B	201	1	-	4/6/23/26	0/1/1/1
2	NAG	B	202	1	-	0/6/23/26	0/1/1/1
2	NAG	D	201	1	-	5/6/23/26	0/1/1/1

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	201	NAG	C1-O5-C5	4.51	118.31	112.19
2	D	201	NAG	C2-N2-C7	3.93	128.50	122.90
2	D	201	NAG	C8-C7-N2	3.49	122.00	116.10
2	A	201	NAG	C1-O5-C5	3.46	116.88	112.19
2	A	201	NAG	C8-C7-N2	3.38	121.83	116.10
2	A	201	NAG	C2-N2-C7	3.14	127.37	122.90
2	B	201	NAG	C2-N2-C7	3.10	127.32	122.90
2	A	201	NAG	C1-C2-N2	3.00	115.62	110.49
2	D	201	NAG	O5-C1-C2	-2.74	106.96	111.29
2	B	201	NAG	C8-C7-N2	2.72	120.70	116.10
2	B	201	NAG	C1-C2-N2	2.70	115.09	110.49
2	A	201	NAG	O5-C1-C2	-2.59	107.20	111.29
2	B	202	NAG	O5-C5-C6	2.39	110.96	107.20
2	A	201	NAG	O7-C7-C8	-2.29	117.80	122.06
2	D	201	NAG	O7-C7-C8	-2.14	118.09	122.06
2	D	201	NAG	C1-C2-N2	2.07	114.02	110.49

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	201	NAG	C8-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
2	A	201	NAG	O7-C7-N2-C2
2	B	201	NAG	C8-C7-N2-C2
2	B	201	NAG	O7-C7-N2-C2
2	D	201	NAG	C8-C7-N2-C2
2	D	201	NAG	O7-C7-N2-C2
2	D	201	NAG	C3-C2-N2-C7
2	A	201	NAG	O5-C5-C6-O6
2	D	201	NAG	C4-C5-C6-O6
2	A	201	NAG	C3-C2-N2-C7
2	B	201	NAG	C3-C2-N2-C7
2	D	201	NAG	O5-C5-C6-O6
2	B	201	NAG	C1-C2-N2-C7

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	201	NAG	1	0
2	D	201	NAG	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, 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	119/149 (79%)	0.06	4 (3%) 45 43	23, 37, 74, 100	0
1	B	127/149 (85%)	0.06	5 (3%) 39 37	23, 35, 68, 88	0
1	C	118/149 (79%)	0.49	12 (10%) 6 6	28, 56, 91, 135	0
1	D	130/149 (87%)	0.12	10 (7%) 13 12	24, 43, 67, 89	0
All	All	494/596 (82%)	0.18	31 (6%) 20 19	23, 41, 77, 135	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	154	HIS	7.8
1	D	154	HIS	6.1
1	A	154	HIS	6.0
1	C	153	ASP	5.7
1	D	165	GLU	5.3
1	B	186	PHE	5.1
1	C	150	PRO	4.0
1	C	155	ASN	3.8
1	D	43	ARG	3.4
1	B	185	LEU	3.3
1	C	152	ASN	3.3
1	D	172	LYS	3.3
1	C	156	HIS	3.0
1	C	49	ARG	3.0
1	D	166	GLU	2.9
1	C	157	MET	2.9
1	D	171	HIS	2.8
1	D	49	ARG	2.8
1	A	155	ASN	2.6
1	D	153	ASP	2.5
1	B	165	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	155	ASN	2.5
1	B	44	ARG	2.4
1	A	44	ARG	2.4
1	B	154	HIS	2.4
1	C	45	CYS	2.4
1	C	44	ARG	2.3
1	D	44	ARG	2.2
1	C	151	GLN	2.2
1	C	46	ASP	2.1
1	A	153	ASP	2.0

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
2	NAG	B	202	14/15	0.76	0.46	35,37,44,49	0
2	NAG	D	201	14/15	0.81	0.35	30,33,41,42	0
2	NAG	A	201	14/15	0.83	0.24	29,32,37,38	0
2	NAG	B	201	14/15	0.90	0.22	23,24,31,33	0

6.5 Other polymers [i](#)

There are no such residues in this entry.