



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 06:31 PM UTC

PDB ID : 5BPB / pdb_00005bpb
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 wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

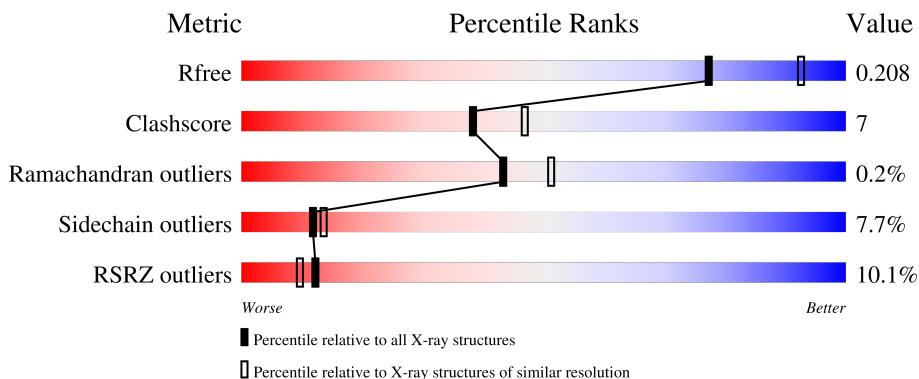
1 Overall quality at a glance

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}	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	 7% 66% 13% • 20%
1	B	149	 7% 70% 13% • 15%
1	C	149	 9% 64% 13% • 21%
1	D	149	 11% 70% 12% • • 13%

2 Entry composition i

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

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 (CCD ID: 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		

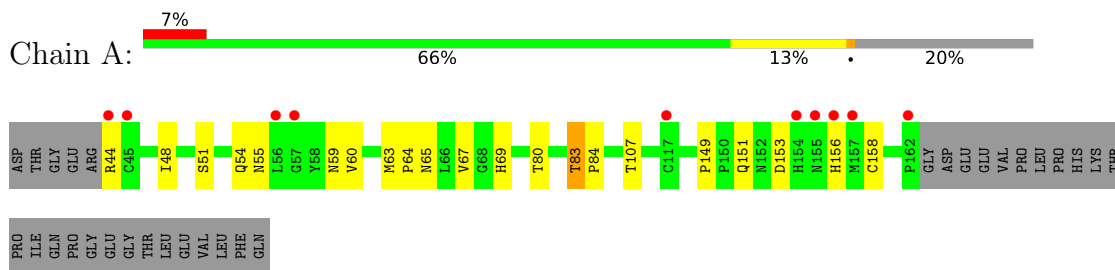
- Molecule 3 is water.

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		

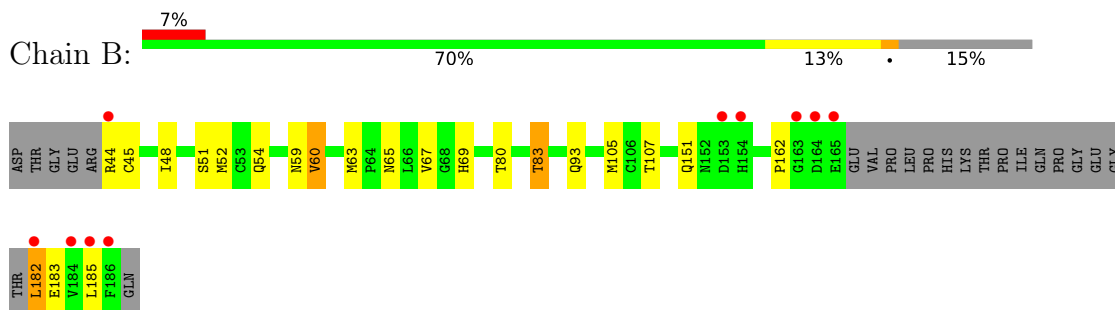
3 Residue-property plots [i](#)

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.

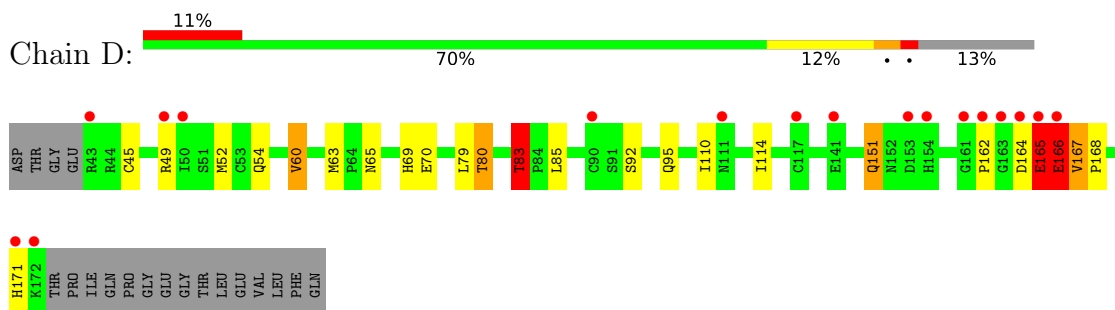
- Molecule 1: Frizzled-4



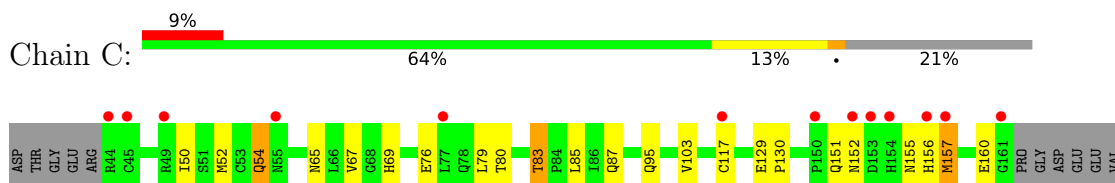
- Molecule 1: Frizzled-4



- Molecule 1: Frizzled-4



- Molecule 1: Frizzled-4



PRO
LEU
PRO
HIS
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 40.00 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.0 (40.00-2.20) 99.0 (40.00-2.20)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.26 (at 2.20Å)	Xtrriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.177 , 0.223 0.209 , 0.208	Depositor DCC
R_{free} test set	2190 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	33.9	Xtrriage
Anisotropy	0.425	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 43.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
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

Xtrriage'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.*

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: 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	0.60	0/954	0.78	0/1293
1	B	0.64	0/1018	0.75	0/1378
1	C	0.54	0/946	0.72	0/1281
1	D	0.95	6/1046 (0.6%)	0.96	4/1418 (0.3%)
All	All	0.71	6/3964 (0.2%)	0.81	4/5370 (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

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	166	GLU	CA-C	-8.88	1.43	1.52
1	D	80	THR	C-O	-6.08	1.16	1.24
1	D	167	VAL	N-CA	-6.04	1.41	1.46
1	D	83	THR	C-O	-5.88	1.19	1.24
1	D	168	PRO	N-CD	5.41	1.55	1.47

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	167	VAL	N-CA-C	8.72	116.57	107.76
1	D	167	VAL	CA-C-O	7.47	123.56	119.15
1	D	167	VAL	CA-C-N	-6.29	113.50	119.85
1	D	167	VAL	C-N-CA	-6.29	113.50	119.85

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 [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	930	0	902	13	0
1	B	994	0	959	10	0
1	C	923	0	896	15	0
1	D	1019	0	988	16	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	53	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 7.

The worst 5 of 53 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:52:MET:HE3	1:D:95:GLN:HE22	1.24	1.00
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

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	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%)	16	16
All	All	484/596 (81%)	480 (99%)	3 (1%)	1 (0%)	43	51

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	162	PRO

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	109/135 (81%)	102 (94%)	7 (6%)	16	19
1	B	116/135 (86%)	105 (90%)	11 (10%)	8	8
1	C	108/135 (80%)	101 (94%)	7 (6%)	15	18
1	D	119/135 (88%)	109 (92%)	10 (8%)	10	11
All	All	452/540 (84%)	417 (92%)	35 (8%)	12	13

5 of 35 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	54	GLN
1	C	83	THR
1	C	151	GLN
1	B	83	THR
1	B	67	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

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

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 oligosaccharides 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	B	202	1	14,14,15	0.46	0	17,19,21	0.85	0
2	NAG	A	201	1	14,14,15	0.48	0	17,19,21	2.00	6 (35%)
2	NAG	B	201	1	14,14,15	0.49	0	17,19,21	1.93	5 (29%)
2	NAG	D	201	1	14,14,15	0.50	0	17,19,21	1.86	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	B	202	1	-	0/6/23/26	0/1/1/1
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	D	201	1	-	5/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	201	NAG	C1-O5-C5	4.57	118.31	112.19
2	D	201	NAG	C2-N2-C7	4.18	128.50	122.90
2	D	201	NAG	C8-C7-N2	3.55	122.00	116.12
2	A	201	NAG	C1-O5-C5	3.51	116.88	112.19
2	A	201	NAG	C8-C7-N2	3.44	121.83	116.12

There are no chirality outliers.

5 of 13 torsion outliers are listed below:

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

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 [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	119/149 (79%)	0.45	10 (8%) 17 14	23, 37, 74, 100	0
1	B	127/149 (85%)	0.41	10 (7%) 18 16	23, 35, 68, 88	0
1	C	118/149 (79%)	0.93	13 (11%) 10 8	28, 56, 91, 135	0
1	D	130/149 (87%)	0.69	17 (13%) 7 5	24, 43, 67, 89	0
All	All	494/596 (82%)	0.62	50 (10%) 12 10	23, 41, 77, 135	0

The worst 5 of 50 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	165	GLU	7.3
1	B	186	PHE	6.4
1	D	162	PRO	5.6
1	C	154	HIS	5.4
1	D	166	GLU	5.1

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 oligosaccharides 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(\AA^2)	Q<0.9
2	NAG	B	202	14/15	0.51	0.20	35,37,44,49	0
2	NAG	D	201	14/15	0.64	0.17	30,33,41,42	0
2	NAG	A	201	14/15	0.74	0.15	29,32,37,38	0
2	NAG	B	201	14/15	0.86	0.12	23,24,31,33	0

6.5 Other polymers [i](#)

There are no such residues in this entry.