



wwPDB X-ray Structure Validation Summary Report

Mar 1, 2014 – 02:50 AM GMT

PDB ID : 2XRC
Title : HUMAN COMPLEMENT FACTOR I
Authors : Roversi, P.; Johnson, S.; Lea, S.M.
Deposited on : 2010-09-13
Resolution : 2.69 Å(reported)

This is a wwPDB 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/ValidationPDFNotes.html>

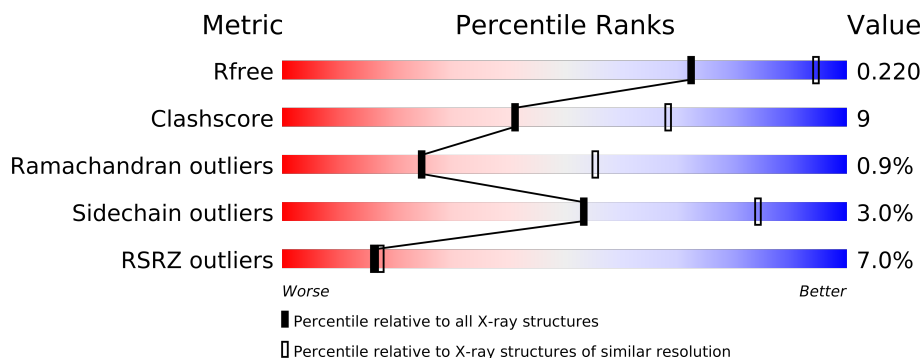
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.69 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}	66092	1557 (2.70-2.70)
Clashscore	79885	1939 (2.70-2.70)
Ramachandran outliers	78287	1905 (2.70-2.70)
Sidechain outliers	78261	1905 (2.70-2.70)
RSRZ outliers	66119	1559 (2.70-2.70)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	565	
1	B	565	
1	C	565	
1	D	565	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	NAG	A	646	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 14897 atoms, of which 0 are hydrogen and 0 are deuterium.

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 HUMAN COMPLEMENT FACTOR I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	461	Total	C	N	O	S	0	0	0
			3606	2262	617	681	46			
1	B	485	Total	C	N	O	S	0	0	0
			3798	2388	652	711	47			
1	C	454	Total	C	N	O	S	0	0	0
			3568	2245	609	668	46			
1	D	464	Total	C	N	O	S	0	0	0
			3609	2264	619	679	47			

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total	Ca	0	0
			2	2		
2	A	2	Total	Ca	0	0
			2	2		
2	D	2	Total	Ca	0	0
			2	2		
2	C	2	Total	Ca	0	0
			2	2		

- Molecule 3 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: C₈H₁₅NO₆).

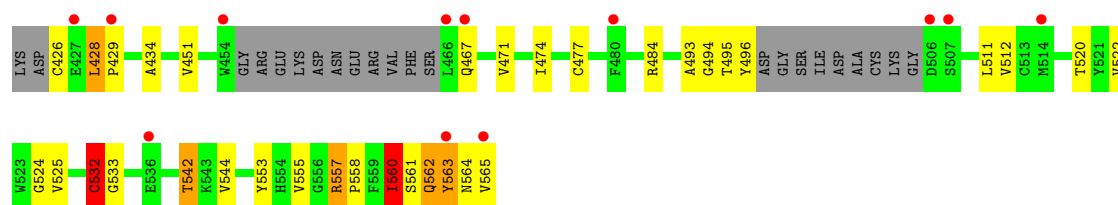


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1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

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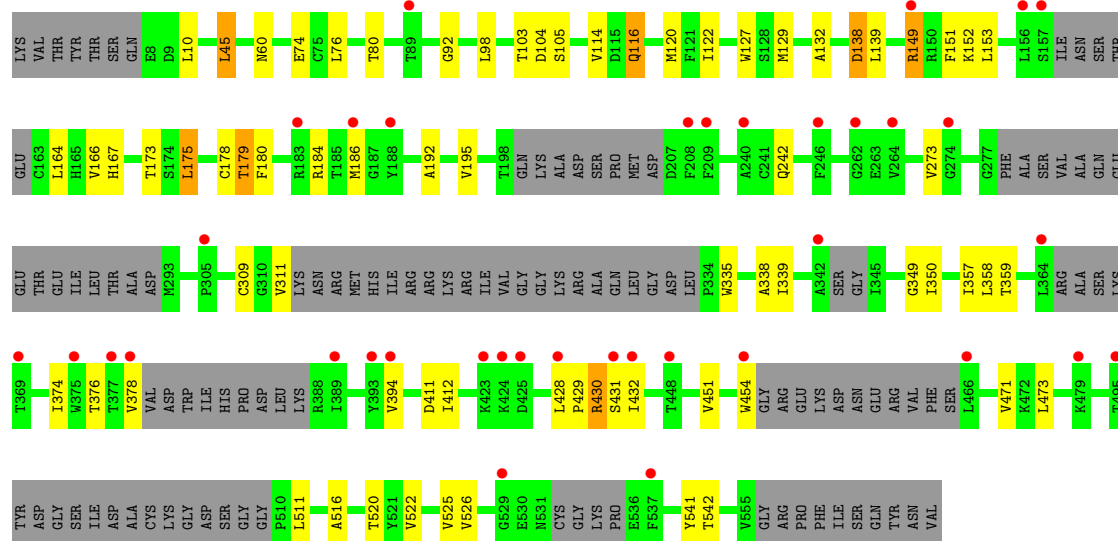
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	D	1	Total	C	N	O	0	0
			14	8	1	5		
3	D	1	Total	C	N	O	0	0
			14	8	1	5		
3	D	1	Total	C	N	O	0	0
	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



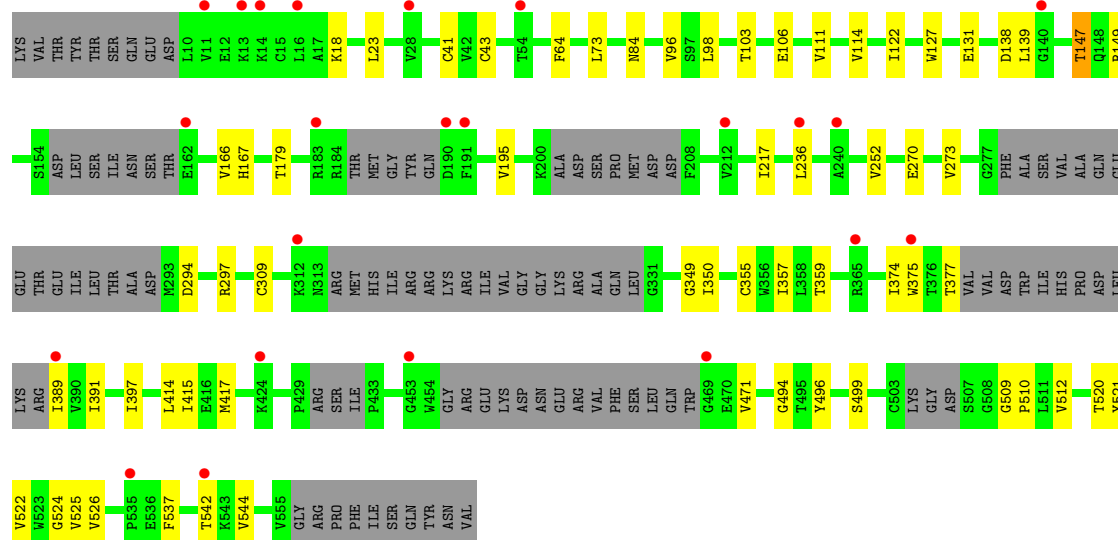
• Molecule 1: HUMAN COMPLEMENT FACTOR I

Chain C:



• Molecule 1: HUMAN COMPLEMENT FACTOR I

Chain D:



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	71.32Å 234.72Å 40.30Å 89.98° 90.18° 90.03°	Depositor
Resolution (Å)	79.00 – 2.69 78.24 – 2.65	Depositor EDS
% Data completeness (in resolution range)	90.0 (79.00-2.69) 65.1 (78.24-2.65)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.15 (at 2.65Å)	Xtriage
Refinement program	REFMAC 5.6.0079	Depositor
R, R_{free}	0.200 , 0.238 0.205 , 0.220	Depositor DCC
R_{free} test set	2488 reflections (5.23%)	DCC
Wilson B-factor (Å ²)	43.3	Xtriage
Anisotropy	0.479	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 3.5	EDS
Estimated twinning fraction	0.334 for H, K, L 0.359 for -H, K, -L 0.187 for -H, -K, L 0.119 for H, -K, -L 0.339 for -h,-k,l 0.317 for h,-k,-l 0.409 for -h,k,-l	Xtriage
Reported twinning fraction	0.334 for H, K, L 0.359 for -H, K, -L 0.187 for -H, -K, L 0.119 for H, -K, -L	Depositor
L-test for twinning	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.24$	Xtriage
Outliers	0 of 49895 reflections	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	14897	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.17% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, 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	0.32	0/3681	0.47	0/4966
1	B	0.32	0/3879	0.51	1/5235 (0.0%)
1	C	0.33	0/3641	0.47	0/4908
1	D	0.32	0/3682	0.47	0/4960
All	All	0.32	0/14883	0.48	1/20069 (0.0%)

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	B	0	2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	184	ARG	NE-CZ-NH1	6.65	123.62	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	184	ARG	Peptide
1	B	185	THR	Peptide

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3606	0	3439	79	0
1	B	3798	0	3631	90	0
1	C	3568	0	3401	57	0
1	D	3609	0	3442	44	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
3	A	84	0	78	0	0
3	B	84	0	78	1	0
3	C	70	0	65	0	0
3	D	70	0	65	0	0
All	All	14897	0	14199	267	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 9.

The worst 5 of 267 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:357:ILE:HD12	1:A:374:ILE:HD13	1.40	1.03
1:D:377:THR:HG22	1:D:389:ILE:HG22	1.52	0.92
1:B:357:ILE:HD12	1:B:374:ILE:HD13	1.53	0.91
1:B:10:LEU:HD22	1:B:240:ALA:HB3	1.53	0.90
1:C:98:LEU:HD11	1:C:139:LEU:HD13	1.55	0.88

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	445/565 (79%)	404 (91%)	39 (9%)	2 (0%)	43	76
1	B	469/565 (83%)	404 (86%)	52 (11%)	13 (3%)	8	18
1	C	432/565 (76%)	398 (92%)	34 (8%)	0	100	100
1	D	444/565 (79%)	412 (93%)	31 (7%)	1 (0%)	56	86
All	All	1790/2260 (79%)	1618 (90%)	156 (9%)	16 (1%)	25	55

5 of 16 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	158	ILE
1	B	185	THR
1	B	186	MET
1	B	323	VAL
1	B	560	ILE

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	401/489 (82%)	392 (98%)	9 (2%)	64	90
1	B	420/489 (86%)	400 (95%)	20 (5%)	35	68
1	C	396/489 (81%)	385 (97%)	11 (3%)	56	86
1	D	399/489 (82%)	391 (98%)	8 (2%)	68	92
All	All	1616/1956 (83%)	1568 (97%)	48 (3%)	53	84

5 of 48 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	467	GLN
1	B	560	ILE
1	D	309	CYS
1	B	496	TYR
1	B	542	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	564	ASN
1	C	148	GLN
1	D	410	ASN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 30 ligands modelled in this entry, 8 are monoatomic - leaving 22 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	NAG	A	618	1	12,14,15	0.40	0	15,19,21	1.00	2 (13%)
3	NAG	A	646	1	12,14,15	0.43	0	15,19,21	0.70	0
3	NAG	A	652	1	12,14,15	0.46	0	15,19,21	0.59	0
3	NAG	A	659	1	12,14,15	0.41	0	15,19,21	0.99	1 (6%)
3	NAG	A	676	1	12,14,15	0.41	0	15,19,21	1.15	2 (13%)
3	NAG	A	685	1	12,14,15	0.37	0	15,19,21	0.93	1 (6%)
3	NAG	B	618	1	12,14,15	0.34	0	15,19,21	0.69	0
3	NAG	B	646	1	12,14,15	0.58	0	15,19,21	0.88	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	B	652	1	12,14,15	0.36	0	15,19,21	0.92	1 (6%)
3	NAG	B	659	1	12,14,15	0.36	0	15,19,21	0.73	1 (6%)
3	NAG	B	676	1	12,14,15	0.40	0	15,19,21	0.81	0
3	NAG	B	685	1	12,14,15	0.32	0	15,19,21	0.79	0
3	NAG	C	618	1	12,14,15	0.47	0	15,19,21	1.14	3 (20%)
3	NAG	C	646	1	12,14,15	0.34	0	15,19,21	0.80	1 (6%)
3	NAG	C	652	1	12,14,15	0.36	0	15,19,21	0.69	1 (6%)
3	NAG	C	676	1	12,14,15	0.37	0	15,19,21	1.06	1 (6%)
3	NAG	C	685	1	12,14,15	0.30	0	15,19,21	0.77	0
3	NAG	D	618	1	12,14,15	0.34	0	15,19,21	1.18	1 (6%)
3	NAG	D	646	1	12,14,15	0.65	0	15,19,21	1.16	2 (13%)
3	NAG	D	652	1	12,14,15	0.43	0	15,19,21	0.83	1 (6%)
3	NAG	D	676	1	12,14,15	0.37	0	15,19,21	0.94	1 (6%)
3	NAG	D	685	1	12,14,15	0.43	0	15,19,21	1.25	2 (13%)

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	NAG	A	618	1	-	0/6/23/26	0/1/1/1
3	NAG	A	646	1	1/1/5/7	0/6/23/26	1/1/1/1
3	NAG	A	652	1	-	0/6/23/26	0/1/1/1
3	NAG	A	659	1	1/1/5/7	0/6/23/26	0/1/1/1
3	NAG	A	676	1	1/1/5/7	0/6/23/26	0/1/1/1
3	NAG	A	685	1	-	0/6/23/26	0/1/1/1
3	NAG	B	618	1	-	0/6/23/26	0/1/1/1
3	NAG	B	646	1	1/1/5/7	0/6/23/26	0/1/1/1
3	NAG	B	652	1	-	0/6/23/26	0/1/1/1
3	NAG	B	659	1	-	0/6/23/26	0/1/1/1
3	NAG	B	676	1	-	0/6/23/26	0/1/1/1
3	NAG	B	685	1	-	0/6/23/26	0/1/1/1
3	NAG	C	618	1	-	0/6/23/26	0/1/1/1
3	NAG	C	646	1	-	0/6/23/26	0/1/1/1
3	NAG	C	652	1	-	0/6/23/26	0/1/1/1
3	NAG	C	676	1	-	0/6/23/26	0/1/1/1
3	NAG	C	685	1	-	0/6/23/26	0/1/1/1
3	NAG	D	618	1	-	0/6/23/26	0/1/1/1
3	NAG	D	646	1	1/1/5/7	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	D	652	1	-	0/6/23/26	0/1/1/1
3	NAG	D	676	1	-	0/6/23/26	0/1/1/1
3	NAG	D	685	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	618	NAG	O5-C5-C6	3.46	110.61	106.98
3	A	659	NAG	O5-C5-C6	3.12	110.26	106.98
3	D	685	NAG	O5-C5-C6	3.10	110.23	106.98
3	C	676	NAG	O5-C5-C6	3.04	110.17	106.98
3	D	685	NAG	O5-C5-C4	-2.90	106.97	110.65

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	659	NAG	C1
3	A	646	NAG	C1
3	B	646	NAG	C1
3	D	646	NAG	C1
3	A	676	NAG	C1

There are no torsion outliers.

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	646	NAG	C1-C2-C3-C4-C5-O5

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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	461/565 (81%)	0.64	28 (6%)	21 22	18, 46, 74, 100	0
1	B	485/565 (85%)	0.73	44 (9%)	9 9	26, 50, 82, 108	0
1	C	454/565 (80%)	0.75	37 (8%)	12 12	24, 46, 75, 95	0
1	D	464/565 (82%)	0.61	23 (4%)	28 30	25, 46, 67, 95	0
All	All	1864/2260 (82%)	0.68	132 (7%)	16 17	18, 47, 77, 108	0

The worst 5 of 132 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	156	LEU	7.8
1	B	188	TYR	5.7
1	C	425	ASP	5.2
1	C	157	SER	5.0
1	A	191	PHE	4.6

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	NAG	A	646	14/15	0.34	2.23	66,73,79,79	0
3	NAG	D	646	14/15	0.22	1.75	63,65,68,69	0
3	NAG	B	659	14/15	0.33	1.04	90,93,95,96	0
3	NAG	C	618	14/15	0.20	0.97	64,66,70,73	0
3	NAG	C	646	14/15	0.22	0.47	62,64,67,68	0
3	NAG	B	676	14/15	0.25	0.47	64,67,74,75	0
3	NAG	A	618	14/15	0.21	0.14	64,67,68,69	0
3	NAG	C	685	14/15	0.20	-0.17	55,57,62,64	0
3	NAG	B	618	14/15	0.20	-0.19	49,51,51,51	0
3	NAG	B	685	14/15	0.17	-0.21	50,52,56,57	0
3	NAG	A	652	14/15	0.19	-0.38	60,62,63,64	0
3	NAG	C	676	14/15	0.22	-0.39	61,63,65,65	0
3	NAG	A	676	14/15	0.19	-0.44	65,69,74,75	0
3	NAG	D	676	14/15	0.24	-0.46	65,67,67,68	0
2	CA	A	601	1/1	0.18	-0.50	43,43,43,43	0
3	NAG	D	685	14/15	0.19	-0.54	50,53,56,57	0
3	NAG	B	652	14/15	0.24	-0.64	73,77,81,83	0
3	NAG	D	652	14/15	0.20	-0.64	79,85,87,88	0
3	NAG	D	618	14/15	0.19	-0.65	53,55,56,57	0
3	NAG	A	659	14/15	0.20	-0.65	73,75,77,77	0
3	NAG	A	685	14/15	0.18	-0.78	49,52,56,56	0
2	CA	B	601	1/1	0.16	-1.00	60,60,60,60	0
3	NAG	C	652	14/15	0.20	-1.04	65,67,67,67	0
2	CA	C	601	1/1	0.17	-1.09	37,37,37,37	0
2	CA	D	601	1/1	0.15	-1.16	61,61,61,61	0
2	CA	B	600	1/1	0.14	-1.78	58,58,58,58	0
2	CA	C	600	1/1	0.14	-1.88	41,41,41,41	0
2	CA	A	600	1/1	0.14	-2.39	33,33,33,33	0
2	CA	D	600	1/1	0.09	-2.62	45,45,45,45	0
3	NAG	B	646	14/15	0.27	-	59,63,70,71	0

6.5 Other polymers ⓘ

There are no such residues in this entry.