



Full wwPDB X-ray Structure Validation 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 full wwPDB 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/ValidationPDFNotes.html>

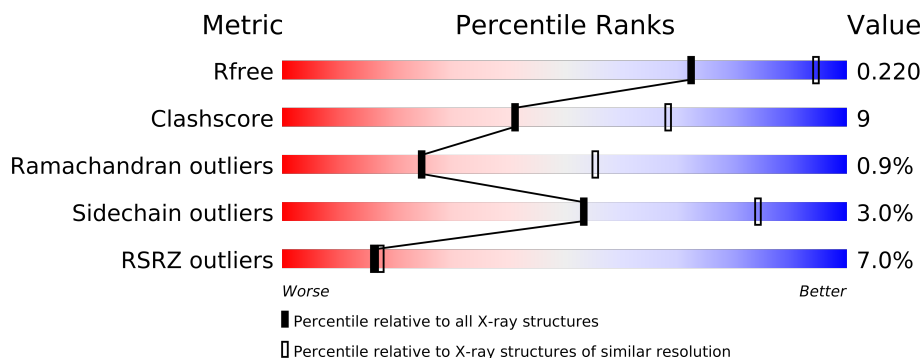
The following versions of software and data (see [references](#)) were used in the production of this report:

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		

Continued on next page...

Continued from previous page...

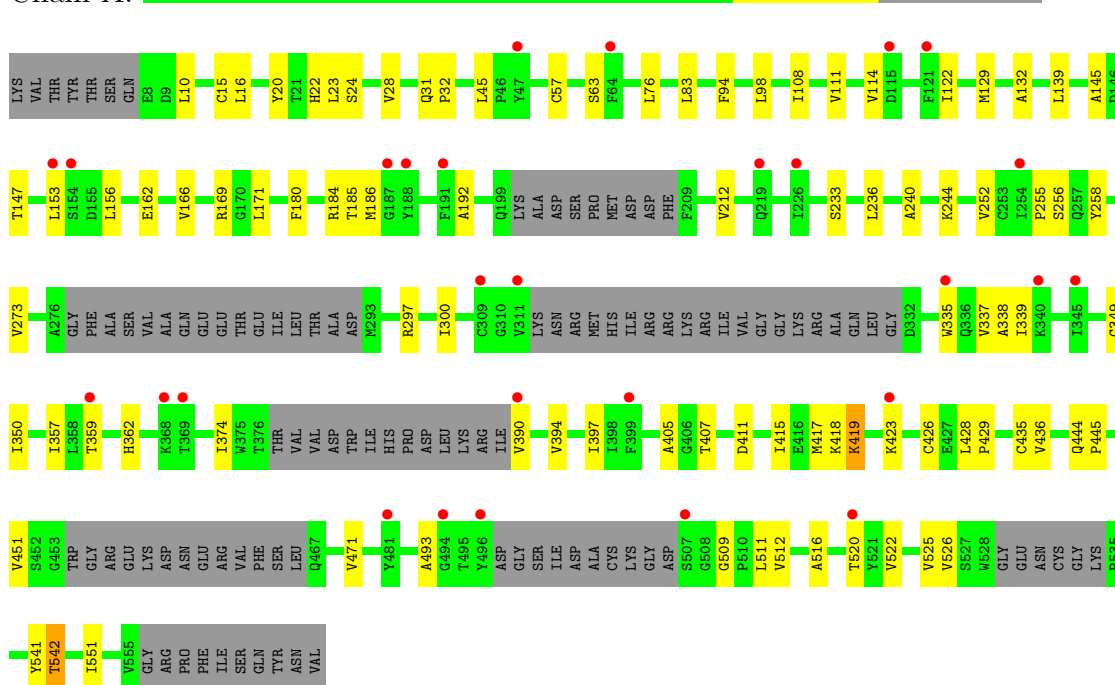
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	D	1	Total	C	N	O	0	0
			14	8	1	5		
3	D	1	Total	C	N	O	0	0
			14	8	1	5		
3	D	1	Total	C	N	O	0	0
			14	8	1	5		
3	D	1	Total	C	N	O	0	0
			14	8	1	5		

3 Residue-property plots

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.

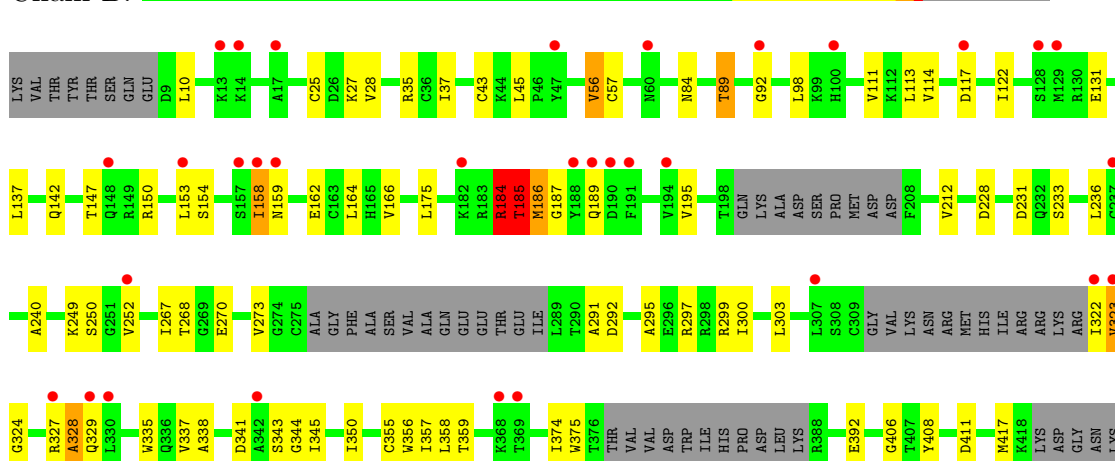
• Molecule 1: HUMAN COMPLEMENT FACTOR I

Chain A:



• Molecule 1: HUMAN COMPLEMENT FACTOR I

Chain B:



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.

All (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
1:B:37:ILE:HG21	1:B:562:GLN:HA	1.57	0.86
1:B:337:VAL:HG11	1:B:357:ILE:HD13	1.57	0.84
1:A:525:VAL:HG23	1:A:542:THR:HG23	1.61	0.82
1:B:186:MET:HB3	1:B:187:GLY:HA3	1.64	0.80
1:A:98:LEU:HD11	1:A:139:LEU:HD13	1.62	0.79
1:D:350:ILE:HD13	1:D:522:VAL:HG22	1.63	0.79
1:C:311:VAL:HG12	1:C:432:ILE:HG21	1.65	0.79
1:A:108:ILE:HD11	1:A:153:LEU:HD11	1.63	0.78
1:A:390:VAL:HG11	1:A:428:LEU:HD21	1.64	0.78
1:D:357:ILE:HD12	1:D:374:ILE:HD13	1.67	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:337:VAL:HG11	1:A:357:ILE:HD13	1.66	0.75
1:C:122:ILE:HD12	1:C:166:VAL:CG2	2.16	0.75
1:A:525:VAL:CG2	1:A:542:THR:HG23	2.16	0.74
1:B:350:ILE:HD13	1:B:522:VAL:HG13	1.70	0.73
1:A:357:ILE:HD12	1:A:374:ILE:CD1	2.17	0.73
1:B:350:ILE:HD11	1:B:522:VAL:HG22	1.71	0.71
1:B:358:LEU:HD23	1:B:522:VAL:HG11	1.73	0.71
1:D:147:THR:HG21	1:D:217:ILE:HA	1.71	0.71
1:A:15:CYS:SG	1:A:16:LEU:N	2.63	0.71
1:A:512:VAL:CG1	1:A:520:THR:HG23	2.21	0.70
1:B:561:SER:HA	1:B:562:GLN:CB	2.21	0.70
1:C:430:ARG:HB3	1:C:431:SER:HA	1.73	0.70
1:C:92:GLY:HA3	1:C:114:VAL:HG13	1.76	0.68
1:B:524:GLY:HA2	1:B:544:VAL:HG23	1.74	0.68
1:D:512:VAL:CG1	1:D:520:THR:HG22	2.23	0.67
1:C:451:VAL:HG23	1:C:471:VAL:HG11	1.77	0.67
1:B:512:VAL:HG13	1:B:520:THR:HG23	1.77	0.66
1:A:337:VAL:CG1	1:A:374:ILE:HG23	2.26	0.66
1:B:158:ILE:HG22	1:B:159:ASN:H	1.61	0.66
1:A:273:VAL:HG11	1:A:516:ALA:HB3	1.79	0.65
1:C:151:PHE:CZ	1:C:153:LEU:HD11	2.33	0.64
1:B:565:VAL:O	1:B:565:VAL:HG12	1.98	0.64
1:A:273:VAL:HG11	1:A:516:ALA:CB	2.28	0.63
1:A:45:LEU:HD13	1:A:76:LEU:HD11	1.80	0.63
1:B:561:SER:HA	1:B:562:GLN:HB2	1.79	0.63
1:A:108:ILE:HD11	1:A:153:LEU:HD21	1.80	0.63
1:A:350:ILE:CD1	1:A:522:VAL:HG22	2.28	0.63
1:A:111:VAL:HG21	1:A:122:ILE:HD11	1.80	0.62
1:D:122:ILE:HD12	1:D:166:VAL:HG21	1.82	0.60
1:A:405:ALA:HB3	1:B:408:TYR:CD1	2.37	0.60
1:C:350:ILE:HD13	1:C:522:VAL:HG22	1.82	0.60
1:B:322:ILE:HG22	1:B:323:VAL:HG23	1.82	0.60
1:C:374:ILE:HD11	1:C:394:VAL:HG22	1.84	0.60
1:D:167:HIS:HB3	1:D:179:THR:HG22	1.83	0.59
1:C:411:ASP:O	1:C:542:THR:HG21	2.03	0.58
1:B:350:ILE:CD1	1:B:522:VAL:HG22	2.33	0.58
1:C:151:PHE:CE1	1:C:153:LEU:HD21	2.38	0.58
1:B:327:ARG:O	1:B:328:ALA:HB3	2.02	0.58
1:B:350:ILE:HG23	1:B:358:LEU:HB3	1.85	0.58
1:B:428:LEU:HD13	1:B:429:PRO:HD2	1.85	0.58
1:B:322:ILE:HD12	1:B:322:ILE:N	2.18	0.58
1:B:512:VAL:CG1	1:B:520:THR:HG23	2.34	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:512:VAL:HG12	1:D:520:THR:HG22	1.86	0.57
1:C:357:ILE:HD11	1:C:374:ILE:HG21	1.86	0.57
1:A:493:ALA:HB3	1:A:541:TYR:CE2	2.39	0.57
1:B:451:VAL:HG22	1:B:511:LEU:CD1	2.34	0.57
1:B:323:VAL:HG12	1:B:324:GLY:H	1.68	0.57
1:A:394:VAL:HG13	1:A:415:ILE:HG23	1.87	0.57
1:B:45:LEU:HD21	1:B:565:VAL:N	2.19	0.57
1:A:411:ASP:O	1:A:542:THR:HG21	2.05	0.56
1:A:122:ILE:HB	1:A:192:ALA:HB3	1.87	0.56
1:A:337:VAL:HG13	1:A:374:ILE:HG23	1.86	0.56
1:A:45:LEU:CD1	1:A:76:LEU:HD11	2.34	0.56
1:A:297:ARG:HA	1:A:300:ILE:HD12	1.87	0.56
1:C:45:LEU:HD12	1:C:76:LEU:HD11	1.87	0.56
1:B:474:ILE:HD11	1:B:477:CYS:HB2	1.88	0.56
1:A:436:VAL:HG11	1:A:551:ILE:HD13	1.87	0.56
1:B:184:ARG:CG	1:B:184:ARG:HH11	2.19	0.56
1:C:349:GLY:HA2	1:C:359:THR:HG22	1.87	0.56
1:B:357:ILE:CD1	1:B:374:ILE:HD13	2.32	0.56
1:B:474:ILE:C	1:B:474:ILE:HD12	2.26	0.56
1:A:129:MET:SD	1:A:147:THR:HG22	2.46	0.56
1:C:149:ARG:HB3	1:C:195:VAL:HG11	1.88	0.56
1:C:120:MET:HE3	1:C:164:LEU:HD11	1.88	0.55
1:D:525:VAL:HG22	1:D:542:THR:CG2	2.37	0.55
1:C:103:THR:HG22	1:C:105:SER:H	1.71	0.55
1:D:122:ILE:HD12	1:D:166:VAL:CG2	2.35	0.55
1:B:471:VAL:HG23	1:B:495:THR:HA	1.88	0.55
1:A:512:VAL:HG13	1:A:520:THR:HG23	1.89	0.55
1:A:374:ILE:HD11	1:A:415:ILE:HG21	1.89	0.55
1:A:335:TRP:NE1	1:A:512:VAL:HG21	2.22	0.55
1:C:376:THR:HG23	1:C:378:VAL:HG23	1.88	0.55
1:D:294:ASP:OD1	1:D:297:ARG:NH1	2.40	0.55
1:B:137:LEU:HD13	1:B:142:GLN:HA	1.89	0.54
1:A:98:LEU:HD11	1:A:139:LEU:CD1	2.35	0.54
1:A:350:ILE:HD11	1:A:522:VAL:HG22	1.88	0.54
1:D:122:ILE:HG21	1:D:127:TRP:CZ3	2.41	0.54
1:D:471:VAL:HG23	1:D:494:GLY:O	2.08	0.54
1:A:122:ILE:HD12	1:A:166:VAL:CG2	2.38	0.54
1:D:167:HIS:HB3	1:D:179:THR:CG2	2.37	0.54
1:B:27:LYS:HB3	1:B:236:LEU:HD22	1.89	0.54
1:C:526:VAL:HG22	1:C:541:TYR:CE1	2.43	0.54
1:D:98:LEU:CD1	1:D:139:LEU:HD11	2.38	0.54
1:D:64:PHE:CZ	1:D:73:LEU:HD13	2.42	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:185:THR:HG22	1:A:186:MET:O	2.08	0.54
1:B:553:TYR:HA	1:B:560:ILE:HD11	1.90	0.54
1:B:147:THR:HG21	1:B:228:ASP:HB3	1.89	0.54
1:A:24:SER:O	1:A:28:VAL:HG12	2.07	0.54
1:B:327:ARG:O	1:B:328:ALA:CB	2.57	0.53
1:A:512:VAL:HG11	1:A:520:THR:HG23	1.89	0.53
1:B:297:ARG:HA	1:B:300:ILE:HD12	1.90	0.53
1:C:74:GLU:OE2	1:C:173:THR:OG1	2.20	0.53
1:D:375:TRP:CH2	1:D:391:ILE:HD11	2.44	0.53
1:B:356:TRP:NE1	1:B:555:VAL:HG13	2.23	0.53
1:D:98:LEU:HD11	1:D:139:LEU:HD11	1.91	0.53
1:C:10:LEU:HD11	1:C:242:GLN:HB3	1.91	0.52
1:A:22:HIS:CD2	1:A:23:LEU:HD23	2.45	0.52
1:D:111:VAL:HG21	1:D:122:ILE:HD11	1.90	0.52
1:A:349:GLY:HA2	1:A:359:THR:HG22	1.92	0.52
1:B:563:TYR:CD1	1:B:565:VAL:HG13	2.44	0.52
1:B:299:ARG:NH1	1:B:303:LEU:HD11	2.25	0.52
1:D:524:GLY:HA2	1:D:544:VAL:HG23	1.91	0.52
1:C:525:VAL:O	1:C:542:THR:HG22	2.08	0.52
1:B:343:SER:O	1:B:345:ILE:N	2.38	0.52
1:A:525:VAL:HG23	1:A:542:THR:CG2	2.35	0.51
1:A:428:LEU:HD22	1:A:429:PRO:HD2	1.92	0.51
1:B:270:GLU:O	1:B:273:VAL:HG12	2.10	0.51
1:C:273:VAL:HG11	1:C:516:ALA:HB1	1.92	0.51
1:A:20:TYR:O	1:A:236:LEU:HD12	2.11	0.51
1:C:311:VAL:CG1	1:C:432:ILE:HD13	2.40	0.51
1:C:122:ILE:HG21	1:C:127:TRP:CZ3	2.45	0.51
1:A:236:LEU:HD23	1:A:252:VAL:HG13	1.93	0.51
1:B:563:TYR:HD1	1:B:565:VAL:HG13	1.75	0.51
1:B:212:VAL:HG23	1:B:233:SER:HB3	1.93	0.51
1:D:357:ILE:CD1	1:D:374:ILE:HD13	2.38	0.50
1:A:108:ILE:CD1	1:A:153:LEU:HD21	2.41	0.50
1:C:357:ILE:HG22	1:C:359:THR:HG23	1.93	0.50
1:B:338:ALA:HB3	1:B:375:TRP:HB2	1.93	0.50
1:B:249:LYS:HB2	1:B:268:THR:HG21	1.94	0.50
1:B:292:ASP:OD1	1:B:295:ALA:N	2.40	0.50
1:B:532:CYS:HB3	1:B:533:GLY:HA2	1.93	0.49
1:B:186:MET:CB	1:B:187:GLY:HA3	2.38	0.49
1:B:451:VAL:HG22	1:B:511:LEU:HD13	1.95	0.49
1:A:339:ILE:HD13	1:A:359:THR:HG21	1.94	0.49
1:B:84:ASN:HB3	1:B:114:VAL:HG11	1.93	0.49
1:A:255:PRO:O	1:A:258:TYR:HB2	2.12	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:397:ILE:HG23	1:D:415:ILE:HD13	1.94	0.49
1:A:394:VAL:CG1	1:A:415:ILE:HG23	2.42	0.49
1:A:111:VAL:CG2	1:A:122:ILE:HD11	2.43	0.49
1:C:339:ILE:N	1:C:339:ILE:HD12	2.28	0.49
1:C:335:TRP:CD1	1:C:350:ILE:HD11	2.48	0.49
1:B:291:ALA:HA	3:B:685:NAG:H83	1.94	0.49
1:C:357:ILE:CD1	1:C:374:ILE:HD13	2.43	0.48
1:D:96:VAL:HG21	1:D:138:ASP:OD1	2.13	0.48
1:C:116:GLN:HG2	1:C:120:MET:HE2	1.95	0.48
1:C:166:VAL:HG11	1:C:175:LEU:HD21	1.96	0.48
1:B:184:ARG:HH11	1:B:184:ARG:HG2	1.76	0.48
1:A:397:ILE:N	1:A:397:ILE:HD12	2.29	0.48
1:A:509:GLY:O	1:A:526:VAL:HG23	2.14	0.48
1:A:212:VAL:HG23	1:A:233:SER:OG	2.14	0.48
1:D:397:ILE:HG23	1:D:415:ILE:CD1	2.44	0.47
1:C:60:ASN:ND2	1:C:80:THR:HG21	2.28	0.47
1:B:111:VAL:HG12	1:B:113:LEU:HD12	1.97	0.47
1:A:357:ILE:CD1	1:A:374:ILE:HD13	2.28	0.47
1:B:27:LYS:O	1:B:267:ILE:HD13	2.14	0.47
1:B:122:ILE:HD12	1:B:166:VAL:HG23	1.95	0.47
1:A:428:LEU:HD13	1:A:429:PRO:HD2	1.96	0.47
1:A:526:VAL:HG22	1:A:541:TYR:CE1	2.50	0.47
1:D:510:PRO:HA	1:D:525:VAL:HA	1.97	0.46
1:C:473:LEU:HD21	1:C:511:LEU:HD21	1.97	0.46
1:C:129:MET:HE1	1:C:132:ALA:HB3	1.97	0.46
1:D:374:ILE:HD12	1:D:417:MET:HG2	1.97	0.46
1:D:375:TRP:CZ2	1:D:391:ILE:HD11	2.50	0.46
1:B:185:THR:HG22	1:B:186:MET:N	2.31	0.46
1:C:357:ILE:HD11	1:C:374:ILE:HD13	1.97	0.46
1:B:392:GLU:HB3	1:B:417:MET:HE2	1.98	0.46
1:D:23:LEU:HD22	1:D:41:CYS:O	2.16	0.46
1:C:122:ILE:HD13	1:C:164:LEU:HB2	1.98	0.46
1:B:561:SER:CA	1:B:562:GLN:CB	2.93	0.45
1:C:335:TRP:CZ2	1:C:520:THR:HG21	2.52	0.45
1:B:355:CYS:SG	1:B:426:CYS:N	2.89	0.45
1:B:341:ASP:HB3	1:B:343:SER:O	2.16	0.45
1:C:122:ILE:HG21	1:C:127:TRP:CE3	2.52	0.45
1:D:414:LEU:O	1:D:415:ILE:HD13	2.16	0.45
1:A:419:LYS:HB2	1:A:426:CYS:SG	2.57	0.45
1:D:512:VAL:HG12	1:D:520:THR:CG2	2.47	0.45
1:B:231:ASP:OD1	1:B:233:SER:OG	2.28	0.45
1:A:83:LEU:HD11	1:A:94:PHE:H	1.81	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:362:HIS:HB2	1:B:484:ARG:NH2	2.32	0.45
1:B:35:ARG:NH1	1:B:43:CYS:O	2.50	0.45
1:D:84:ASN:OD1	1:D:114:VAL:HG11	2.17	0.45
1:C:122:ILE:HB	1:C:192:ALA:HB3	1.99	0.44
1:D:106:GLU:HG2	1:D:195:VAL:HG22	1.99	0.44
1:B:411:ASP:O	1:B:542:THR:HG21	2.17	0.44
1:C:45:LEU:CD1	1:C:45:LEU:N	2.79	0.44
1:B:356:TRP:CD2	1:B:555:VAL:HG22	2.52	0.44
1:D:349:GLY:HA2	1:D:359:THR:HG22	1.99	0.44
1:B:335:TRP:CH2	1:B:520:THR:HG21	2.52	0.44
1:C:122:ILE:HG23	1:C:166:VAL:HG23	2.00	0.44
1:B:356:TRP:CE3	1:B:555:VAL:HG22	2.53	0.44
1:B:122:ILE:HD13	1:B:164:LEU:HB2	1.99	0.44
1:A:10:LEU:HD22	1:A:240:ALA:O	2.18	0.44
1:A:525:VAL:HG22	1:A:542:THR:HG23	2.00	0.44
1:B:471:VAL:HG23	1:B:494:GLY:C	2.38	0.44
1:B:350:ILE:HD13	1:B:522:VAL:CG1	2.44	0.43
1:C:349:GLY:CA	1:C:359:THR:HG22	2.48	0.43
1:A:335:TRP:CZ3	1:A:520:THR:HG21	2.53	0.43
1:D:64:PHE:CE1	1:D:73:LEU:HD13	2.53	0.43
1:B:122:ILE:HD12	1:B:166:VAL:CG2	2.47	0.43
1:A:169:ARG:CZ	1:A:171:LEU:HD12	2.47	0.43
1:D:512:VAL:HG13	1:D:521:TYR:O	2.18	0.43
1:B:565:VAL:O	1:B:565:VAL:CG1	2.65	0.43
1:A:418:LYS:O	1:A:419:LYS:HB3	2.18	0.43
1:A:339:ILE:CD1	1:A:359:THR:HG21	2.47	0.43
1:A:451:VAL:HG22	1:A:511:LEU:HD13	2.01	0.43
1:A:166:VAL:HG22	1:A:180:PHE:CD1	2.54	0.43
1:C:429:PRO:HA	1:C:430:ARG:HA	1.82	0.43
1:C:149:ARG:HB3	1:C:195:VAL:HG21	2.00	0.43
1:A:244:LYS:O	1:A:256:SER:OG	2.37	0.43
1:D:509:GLY:O	1:D:526:VAL:HG23	2.19	0.43
1:B:525:VAL:HG22	1:B:542:THR:HG23	2.01	0.43
1:A:444:GLN:HB3	1:A:445:PRO:HD2	2.00	0.43
1:D:270:GLU:HA	1:D:273:VAL:HG22	2.01	0.42
1:A:451:VAL:HG23	1:A:471:VAL:CG1	2.49	0.42
1:A:337:VAL:HG12	1:A:338:ALA:N	2.33	0.42
1:C:151:PHE:CE1	1:C:153:LEU:HD11	2.55	0.42
1:B:356:TRP:CE2	1:B:555:VAL:HG13	2.55	0.42
1:C:473:LEU:CD2	1:C:511:LEU:HD21	2.49	0.42
1:D:349:GLY:CA	1:D:359:THR:HG22	2.49	0.42
1:C:138:ASP:C	1:C:138:ASP:OD2	2.58	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:167:HIS:HB3	1:C:179:THR:HG23	2.01	0.42
1:B:557:ARG:N	1:B:558:PRO:HD3	2.34	0.42
1:B:56:VAL:CG1	1:B:57:CYS:N	2.82	0.42
1:C:175:LEU:HD22	1:C:180:PHE:HZ	1.84	0.42
1:C:152:LYS:O	1:C:153:LEU:HD13	2.20	0.42
1:C:451:VAL:HG23	1:C:471:VAL:CG1	2.47	0.42
1:B:89:THR:HG21	1:B:92:GLY:HA3	2.02	0.42
1:A:32:PRO:HB2	1:A:300:ILE:HG22	2.01	0.42
1:A:57:CYS:SG	1:A:83:LEU:HD23	2.60	0.42
1:D:103:THR:HG22	1:D:106:GLU:HB2	2.02	0.42
1:A:350:ILE:HD13	1:A:522:VAL:HG13	2.02	0.42
1:C:358:LEU:HD11	1:C:412:ILE:HD11	2.01	0.42
1:B:350:ILE:HD11	1:B:434:ALA:HB3	2.02	0.41
1:C:338:ALA:HB2	1:C:454:TRP:CZ3	2.55	0.41
1:A:108:ILE:HD11	1:A:153:LEU:CD1	2.41	0.41
1:A:405:ALA:HB2	1:B:406:GLY:O	2.20	0.41
1:C:103:THR:HG22	1:C:104:ASP:N	2.35	0.41
1:D:236:LEU:HD23	1:D:252:VAL:HG13	2.02	0.41
1:A:493:ALA:HB3	1:A:541:TYR:HE2	1.86	0.41
1:D:64:PHE:HZ	1:D:73:LEU:HD13	1.84	0.41
1:B:392:GLU:CB	1:B:417:MET:HE2	2.50	0.41
1:B:56:VAL:HG13	1:B:57:CYS:N	2.35	0.41
1:B:236:LEU:HD23	1:B:252:VAL:HG13	2.03	0.41
1:A:98:LEU:N	1:A:98:LEU:HD12	2.36	0.41
1:D:350:ILE:HD13	1:D:522:VAL:CG2	2.44	0.41
1:C:60:ASN:HD21	1:C:80:THR:HG21	1.86	0.41
1:B:175:LEU:HD23	1:B:175:LEU:HA	1.97	0.41
1:C:120:MET:CE	1:C:164:LEU:HD21	2.51	0.41
1:B:471:VAL:HG22	1:B:493:ALA:HB1	2.02	0.41
1:B:212:VAL:HG23	1:B:233:SER:CB	2.50	0.41
1:D:149:ARG:HD2	1:D:195:VAL:HG11	2.03	0.41
1:A:374:ILE:HD12	1:A:417:MET:HG2	2.03	0.40
1:B:335:TRP:CZ2	1:B:512:VAL:HG21	2.56	0.40
1:C:175:LEU:HD23	1:C:178:CYS:SG	2.61	0.40
1:D:525:VAL:CG2	1:D:542:THR:CG2	2.99	0.40
1:A:132:ALA:HB1	1:A:145:ALA:HB2	2.04	0.40
1:B:335:TRP:O	1:B:337:VAL:HG23	2.21	0.40
1:A:390:VAL:HG11	1:A:428:LEU:CD2	2.43	0.40
1:B:350:ILE:HD11	1:B:434:ALA:CB	2.51	0.40
1:B:250:SER:HB2	1:B:267:ILE:HD11	2.04	0.40
1:A:132:ALA:HB1	1:A:145:ALA:CB	2.51	0.40
1:B:195:VAL:HG13	1:B:195:VAL:O	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	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

All (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
1	B	562	GLN
1	A	114	VAL
1	B	154	SER
1	D	499	SER
1	B	162	GLU
1	B	328	ALA
1	A	156	LEU
1	B	329	GLN
1	B	532	CYS
1	B	189	GLN
1	B	344	GLY

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

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	GLN
1	A	63	SER
1	A	162	GLU
1	A	184	ARG
1	A	407	THR
1	A	419	LYS
1	A	423	LYS
1	A	435	CYS
1	A	542	THR
1	B	25	CYS
1	B	28	VAL
1	B	56	VAL
1	B	89	THR
1	B	98	LEU
1	B	117	ASP
1	B	131	GLU
1	B	150	ARG
1	B	153	LEU
1	B	184	ARG
1	B	359	THR
1	B	428	LEU
1	B	467	GLN
1	B	496	TYR
1	B	532	CYS
1	B	542	THR
1	B	557	ARG
1	B	560	ILE
1	B	563	TYR
1	B	564	ASN
1	C	45	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	116	GLN
1	C	138	ASP
1	C	149	ARG
1	C	175	LEU
1	C	179	THR
1	C	184	ARG
1	C	186	MET
1	C	309	CYS
1	C	428	LEU
1	C	430	ARG
1	D	18	LYS
1	D	43	CYS
1	D	131	GLU
1	D	147	THR
1	D	309	CYS
1	D	355	CYS
1	D	496	TYR
1	D	537	PHE

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%)
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
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.

All (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
3	D	676	NAG	O5-C5-C6	2.85	109.97	106.98
3	B	652	NAG	O5-C5-C6	2.76	109.88	106.98
3	A	676	NAG	O5-C5-C6	2.75	109.87	106.98
3	C	646	NAG	O5-C5-C6	2.60	109.71	106.98
3	C	618	NAG	O5-C5-C4	-2.54	107.43	110.65
3	A	676	NAG	C3-C2-N2	-2.52	107.92	111.76
3	C	618	NAG	O5-C5-C6	2.35	109.44	106.98
3	D	646	NAG	C4-C3-C2	2.31	116.98	111.32
3	A	618	NAG	O5-C5-C6	2.26	109.35	106.98
3	C	652	NAG	O5-C5-C6	2.23	109.32	106.98
3	A	685	NAG	O5-C5-C6	2.20	109.29	106.98

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	618	NAG	C3-C2-N2	-2.20	108.41	111.76
3	D	652	NAG	O5-C5-C6	2.14	109.23	106.98
3	B	646	NAG	C3-C4-C5	2.09	113.93	110.20
3	A	618	NAG	O5-C5-C4	-2.08	108.01	110.65
3	D	646	NAG	C3-C4-C5	2.05	113.87	110.20
3	B	659	NAG	O5-C5-C6	2.01	109.09	106.98

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

All (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
1	B	329	GLN	4.4
1	B	191	PHE	4.4
1	C	466	LEU	4.4
1	B	454	TRP	4.4
1	C	389	ILE	4.4
1	C	424	LYS	4.3
1	C	208	PHE	4.1
1	B	330	LEU	4.0
1	D	16	LEU	3.9
1	D	162	GLU	3.8
1	B	153	LEU	3.8
1	D	535	PRO	3.7
1	B	189	GLN	3.7
1	B	368	LYS	3.6
1	D	389	ILE	3.5
1	C	89	THR	3.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	378	VAL	3.4
1	C	369	THR	3.4
1	A	494	GLY	3.4
1	B	506	ASP	3.3
1	B	369	THR	3.3
1	D	13	LYS	3.2
1	B	190	ASP	3.2
1	A	309	CYS	3.2
1	B	158	ILE	3.2
1	A	121	PHE	3.2
1	C	432	ILE	3.2
1	C	448	THR	3.1
1	A	345	ILE	3.1
1	D	453	GLY	3.1
1	A	507	SER	3.1
1	C	393	TYR	3.0
1	B	157	SER	3.0
1	C	537	PHE	2.9
1	D	312	LYS	2.9
1	B	148	GLN	2.9
1	B	100	HIS	2.9
1	C	431	SER	2.9
1	B	194	VAL	2.9
1	B	323	VAL	2.9
1	B	514	MET	2.9
1	B	507	SER	2.9
1	C	209	PHE	2.8
1	D	140	GLY	2.8
1	B	322	ILE	2.8
1	D	424	LYS	2.8
1	D	375	TRP	2.7
1	B	47	TYR	2.7
1	C	495	THR	2.7
1	C	149	ARG	2.7
1	D	54	THR	2.7
1	C	188	TYR	2.7
1	C	364	LEU	2.7
1	B	536	GLU	2.6
1	C	246	PHE	2.6
1	B	307	LEU	2.6
1	C	529	GLY	2.6
1	D	191	PHE	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	377	THR	2.6
1	C	264	VAL	2.6
1	C	423	LYS	2.6
1	A	311	VAL	2.6
1	B	565	VAL	2.6
1	B	237	CYS	2.5
1	C	183	ARG	2.5
1	C	428	LEU	2.5
1	A	64	PHE	2.5
1	A	369	THR	2.5
1	C	394	VAL	2.5
1	A	187	GLY	2.4
1	B	13	LYS	2.4
1	B	14	LYS	2.4
1	B	342	ALA	2.4
1	D	212	VAL	2.4
1	A	340	LYS	2.4
1	D	14	LYS	2.4
1	A	423	LYS	2.4
1	A	153	LEU	2.4
1	D	183	ARG	2.4
1	A	188	TYR	2.3
1	B	128	SER	2.3
1	B	429	PRO	2.3
1	B	117	ASP	2.3
1	D	365	ARG	2.3
1	A	47	TYR	2.3
1	C	342	ALA	2.3
1	B	92	GLY	2.3
1	B	563	TYR	2.3
1	A	368	LYS	2.2
1	A	335	TRP	2.2
1	D	240	ALA	2.2
1	A	154	SER	2.2
1	B	327	ARG	2.2
1	C	305	PRO	2.2
1	B	182	LYS	2.2
1	A	481	TYR	2.2
1	C	186	MET	2.2
1	B	466	LEU	2.2
1	C	479	LYS	2.2
1	B	159	ASN	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	252	VAL	2.1
1	A	226	ILE	2.1
1	A	399	PHE	2.1
1	B	480	PHE	2.1
1	B	467	GLN	2.1
1	A	390	VAL	2.1
1	D	28	VAL	2.1
1	A	254	ILE	2.1
1	C	262	GLY	2.1
1	D	542	THR	2.1
1	C	454	TRP	2.1
1	D	11	VAL	2.1
1	B	17	ALA	2.1
1	C	240	ALA	2.1
1	A	359	THR	2.0
1	A	520	THR	2.0
1	A	219	GLN	2.0
1	B	129	MET	2.0
1	A	496	TYR	2.0
1	C	274	GLY	2.0
1	D	469	GLY	2.0
1	C	375	TRP	2.0
1	B	427	GLU	2.0
1	A	115	ASP	2.0
1	B	60	ASN	2.0
1	D	236	LEU	2.0
1	D	190	ASP	2.0

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(Å 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.