



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 12:49 PM UTC

PDB ID : 2XRC / pdb_00002xrc
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 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 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

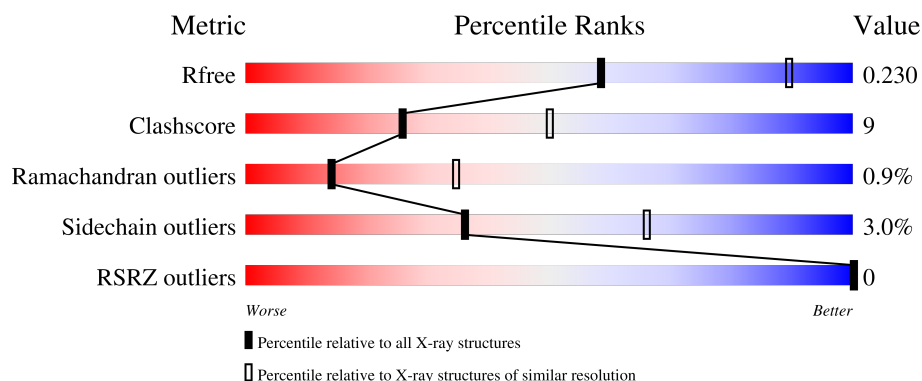
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.69 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}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (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 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	565	
1	B	565	
1	C	565	
1	D	565	

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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAG	A	646	X	-	-	-
3	NAG	A	659	X	-	-	-
3	NAG	A	676	X	-	-	-
3	NAG	B	646	X	-	-	-
3	NAG	D	646	X	-	-	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 14897 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.

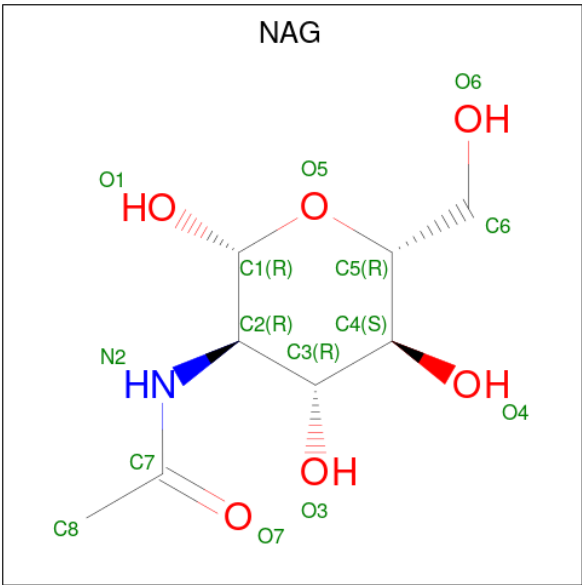
- Molecule 1 is a protein called HUMAN COMPLEMENT FACTOR I.

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 (CCD ID: CA) (formula: Ca).

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

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: 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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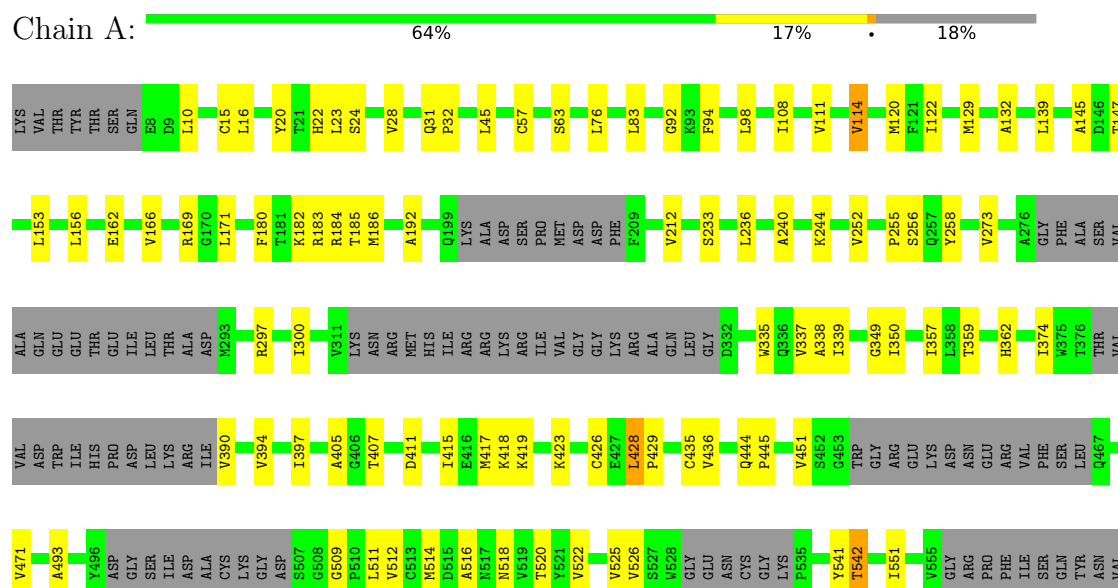
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	D	1	Total	C	N	O	0	0
			14	8	1	5		
3	D	1	Total	C	N	O	0	0
			14	8	1	5		
3	D	1	Total	C	N	O	0	0
			14	8	1	5		
3	D	1	Total	C	N	O	0	0
			14	8	1	5		

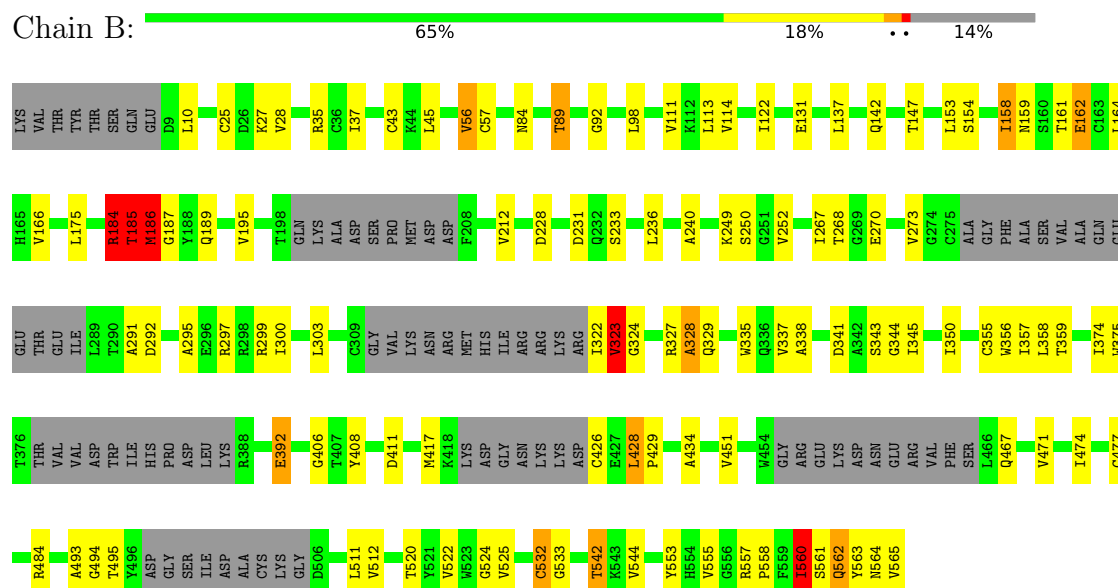
3 Residue-property plots

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.

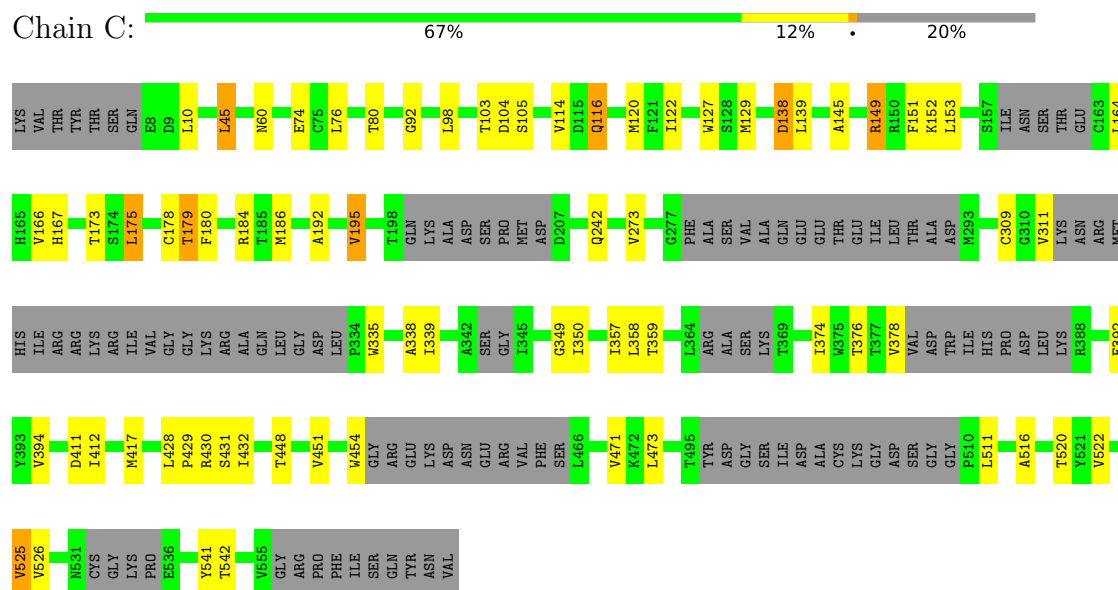
• Molecule 1: HUMAN COMPLEMENT FACTOR I



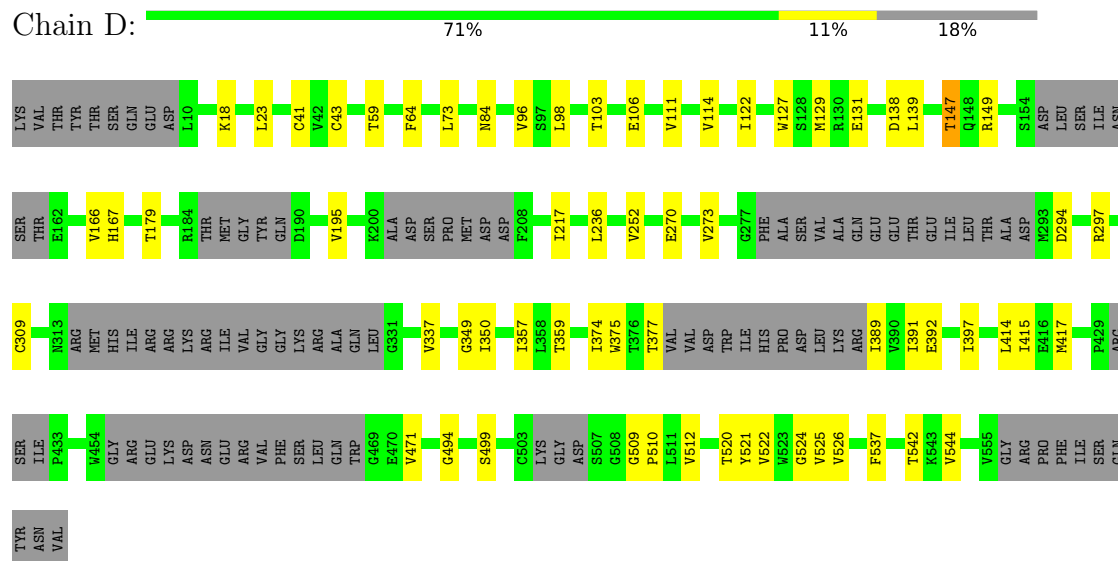
• Molecule 1: HUMAN COMPLEMENT FACTOR I



• Molecule 1: HUMAN COMPLEMENT FACTOR I



• Molecule 1: HUMAN COMPLEMENT FACTOR I



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 79.00 – 2.69	Depositor EDS
% Data completeness (in resolution range)	90.0 (79.00-2.69) 65.1 (79.00-2.69)	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 (Not available) , 0.230	Depositor DCC
R_{free} test set	2488 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	43.3	Xtriage
Anisotropy	0.479	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 6.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	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
Outliers	0 of 49895 reflections	Xtriage
F_o, F_c correlation	0.94	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.

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, CA

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	0.43	0/3681	0.66	0/4966
1	B	0.45	0/3879	0.68	0/5235
1	C	0.44	0/3641	0.65	0/4908
1	D	0.44	0/3682	0.65	0/4960
All	All	0.44	0/14883	0.66	0/20069

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.

There are no bond angle outliers.

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 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	3606	0	3439	83	0
1	B	3798	0	3631	90	0
1	C	3568	0	3401	59	0
1	D	3609	0	3442	47	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	276	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 9.

All (276) 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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:B:565:VAL:HG12	1:B:565:VAL:O	1.98	0.62
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:B:474:ILE:HD12	1:B:474:ILE:C	2.26	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: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:N	1:B:322:ILE:HD12	2.18	0.58
1:B:327:ARG:O	1:B:328:ALA:HB3	2.02	0.58
1:B:512:VAL:CG1	1:B:520:THR:HG23	2.34	0.57
1:C:357:ILE:HD11	1:C:374:ILE:HG21	1.86	0.57
1:D:512:VAL:HG12	1:D:520:THR:HG22	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:122:ILE:HB	1:A:192:ALA:HB3	1.87	0.56
1:A:411:ASP:O	1:A:542:THR:HG21	2.05	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:HH11	1:B:184:ARG:CG	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: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: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:335:TRP:NE1	1:A:512:VAL:HG21	2.22	0.55
1:A:374:ILE:HD11	1:A:415:ILE:HG21	1.89	0.55
1:C:120:MET:HE3	1:C:164:LEU:HD11	1.88	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:A:120:MET:HE1	1:A:182:LYS:HE2	1.90	0.54
1:B:137:LEU:HD13	1:B:142:GLN:HA	1.89	0.54
1:C:392:GLU:HG2	1:C:417:MET:HE3	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:B:27:LYS:HB3	1:B:236:LEU:HD22	1.89	0.54
1:D:167:HIS:HB3	1:D:179:THR:CG2	2.37	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:A:185:THR:HG22	1:A:186:MET:O	2.08	0.54
1:D:64:PHE:CZ	1:D:73:LEU:HD13	2.42	0.54
1:B:147:THR:HG21	1:B:228:ASP:HB3	1.89	0.54
1:B:553:TYR:HA	1:B:560:ILE:HD11	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:356:TRP:NE1	1:B:555:VAL:HG13	2.23	0.53
1:D:375:TRP:CH2	1:D:391:ILE:HD11	2.44	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:C:116:GLN:HG2	1:C:120:MET:HE2	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:428:LEU:HD22	1:A:429:PRO:HD2	1.92	0.51
1:A:525:VAL:HG23	1:A:542:THR:CG2	2.35	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:A:236:LEU:HD23	1:A:252:VAL:HG13	1.93	0.51
1:C:122:ILE:HG21	1:C:127:TRP:CZ3	2.45	0.51
1:B:212:VAL:HG23	1:B:233:SER:HB3	1.93	0.51
1:B:563:TYR:HD1	1:B:565:VAL:HG13	1.75	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:A:255:PRO:O	1:A:258:TYR:HB2	2.12	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: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:D:397:ILE:HG23	1:D:415:ILE:HD13	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:111:VAL:CG2	1:A:122:ILE:HD11	2.43	0.49
1:A:394:VAL:CG1	1:A:415:ILE:HG23	2.42	0.49
1:C:339:ILE:HD12	1:C:339:ILE:N	2.28	0.49
1:D:392:GLU:HG3	1:D:417:MET:HE3	1.95	0.49
1:B:231:ASP:OD1	1:B:233:SER:OG	2.28	0.49
1:C:335:TRP:CD1	1:C:350:ILE:HD11	2.48	0.49
1:C:129:MET:HE2	1:C:129:MET:HA	1.95	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:B:471:VAL:HG23	1:B:494:GLY:C	2.38	0.48
1:A:397:ILE:HD12	1:A:397:ILE:N	2.29	0.48
1:B:184:ARG:HH11	1:B:184:ARG:HG2	1.76	0.48
1:C:166:VAL:HG11	1:C:175:LEU:HD21	1.96	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:C:60:ASN:ND2	1:C:80:THR:HG21	2.28	0.47
1:D:397:ILE:HG23	1:D:415:ILE:CD1	2.44	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:C:138:ASP:OD2	1:C:138:ASP:C	2.58	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:C:473:LEU:HD21	1:C:511:LEU:HD21	1.97	0.46
1:D:510:PRO:HA	1:D:525:VAL:HA	1.97	0.46
1:B:392:GLU:CB	1:B:417:MET:HE2	2.45	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: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:129:MET:HE1	1:C:145:ALA:CB	2.47	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:B:392:GLU:HG2	1:B:417:MET:HE2	1.99	0.45
1:A:419:LYS:HB2	1:A:426:CYS:SG	2.57	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:83:LEU:HD11	1:A:94:PHE:H	1.81	0.45
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:512:VAL:HG12	1:D:520:THR:CG2	2.47	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:73:LEU:HD23	1:D:73:LEU:C	2.42	0.44
1:D:106:GLU:HG2	1:D:195:VAL:HG22	1.99	0.44
1:A:514:MET:HE3	1:A:520:THR:OG1	2.17	0.44
1:B:411:ASP:O	1:B:542:THR:HG21	2.17	0.44
1:B:356:TRP:CD2	1:B:555:VAL:HG22	2.52	0.44
1:C:45:LEU:CD1	1:C:45:LEU:N	2.79	0.44
1:D:349:GLY:HA2	1:D:359:THR:HG22	1.99	0.44
1:A:10:LEU:HD22	1:A:240:ALA:O	2.18	0.44
1:B:122:ILE:HD13	1:B:164:LEU:HB2	1.99	0.44
1:B:161:THR:O	1:B:162:GLU:C	2.61	0.44
1:B:335:TRP:CH2	1:B:520:THR:HG21	2.52	0.44
1:B:356:TRP:CE3	1:B:555:VAL:HG22	2.53	0.44
1:C:122:ILE:HG23	1:C:166:VAL:HG23	2.00	0.44
1:D:129:MET:HE2	1:D:129:MET:HA	1.99	0.44
1:A:525:VAL:HG22	1:A:542:THR:HG23	2.00	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:169:ARG:CZ	1:A:171:LEU:HD12	2.47	0.43
1:A:335:TRP:CZ3	1:A:520:THR:HG21	2.53	0.43
1:B:122:ILE:HD12	1:B:166:VAL:CG2	2.47	0.43
1:D:64:PHE:CE1	1:D:73:LEU:HD13	2.53	0.43
1:A:418:LYS:O	1:A:419:LYS:HB3	2.18	0.43
1:B:565:VAL:O	1:B:565:VAL:CG1	2.65	0.43
1:D:512:VAL:HG13	1:D:521:TYR:O	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:A:244:LYS:O	1:A:256:SER:OG	2.37	0.43
1:C:149:ARG:HB3	1:C:195:VAL:HG21	2.00	0.43
1:D:509:GLY:O	1:D:526:VAL:HG23	2.19	0.43
1:A:444:GLN:HB3	1:A:445:PRO:HD2	2.00	0.43
1:B:525:VAL:HG22	1:B:542:THR:HG23	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:356:TRP:CE2	1:B:555:VAL:HG13	2.55	0.42
1:C:151:PHE:CE1	1:C:153:LEU:HD11	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:B:557:ARG:N	1:B:558:PRO:HD3	2.34	0.42
1:C:167:HIS:HB3	1:C:179:THR:HG23	2.01	0.42
1:C:152:LYS:O	1:C:153:LEU:HD13	2.20	0.42
1:C:175:LEU:HD22	1:C:180:PHE:HZ	1.84	0.42
1:B:89:THR:HG21	1:B:92:GLY:HA3	2.02	0.42
1:C:451:VAL:HG23	1:C:471:VAL:CG1	2.47	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:A:514:MET:HE2	1:A:518:ASN:C	2.46	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:B:56:VAL:HG13	1:B:57:CYS:N	2.35	0.41
1:D:64:PHE:HZ	1:D:73:LEU:HD13	1.84	0.41
1:B:236:LEU:HD23	1:B:252:VAL:HG13	2.03	0.41
1:A:98:LEU:HD12	1:A:98:LEU:N	2.36	0.41
1:B:175:LEU:HD23	1:B:175:LEU:HA	1.97	0.41
1:C:60:ASN:HD21	1:C:80:THR:HG21	1.86	0.41
1:D:350:ILE:HD13	1:D:522:VAL:CG2	2.44	0.41
1:B:212:VAL:HG23	1:B:233:SER:CB	2.50	0.41
1:B:471:VAL:HG22	1:B:493:ALA:HB1	2.02	0.41
1:C:120:MET:CE	1:C:164:LEU:HD21	2.51	0.41
1:D:149:ARG:HD2	1:D:195:VAL:HG11	2.03	0.41
1:A:132:ALA:HB1	1:A:145:ALA:HB2	2.04	0.40
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:525:VAL:CG2	1:D:542:THR:CG2	2.99	0.40
1:A:390:VAL:HG11	1:A:428:LEU:CD2	2.43	0.40
1:B:335:TRP:O	1:B:337:VAL:HG23	2.21	0.40
1:A:92:GLY:C	1:A:114:VAL:HG23	2.47	0.40
1:A:132:ALA:HB1	1:A:145:ALA:CB	2.51	0.40
1:B:250:SER:HB2	1:B:267:ILE:HD11	2.04	0.40
1:B:350:ILE:HD11	1:B:434: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%)	30	54
1	B	469/565 (83%)	404 (86%)	52 (11%)	13 (3%)	4	9
1	C	432/565 (76%)	398 (92%)	34 (8%)	0	100	100
1	D	444/565 (79%)	412 (93%)	31 (7%)	1 (0%)	43	68
All	All	1790/2260 (79%)	1618 (90%)	156 (9%)	16 (1%)	14	35

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

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Mol	Chain	Res	Type
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%)	391 (98%)	10 (2%)	42	71
1	B	420/489 (86%)	403 (96%)	17 (4%)	28	56
1	C	396/489 (81%)	383 (97%)	13 (3%)	33	63
1	D	399/489 (82%)	391 (98%)	8 (2%)	48	76
All	All	1616/1956 (83%)	1568 (97%)	48 (3%)	36	66

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	183	ARG
1	A	184	ARG
1	A	407	THR
1	A	423	LYS
1	A	428	LEU
1	A	435	CYS
1	A	542	THR
1	B	25	CYS
1	B	28	VAL

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Mol	Chain	Res	Type
1	B	56	VAL
1	B	89	THR
1	B	98	LEU
1	B	131	GLU
1	B	153	LEU
1	B	184	ARG
1	B	186	MET
1	B	323	VAL
1	B	359	THR
1	B	392	GLU
1	B	428	LEU
1	B	467	GLN
1	B	542	THR
1	B	560	ILE
1	B	564	ASN
1	C	45	LEU
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	195	VAL
1	C	309	CYS
1	C	428	LEU
1	C	448	THR
1	C	525	VAL
1	D	18	LYS
1	D	43	CYS
1	D	59	THR
1	D	131	GLU
1	D	147	THR
1	D	309	CYS
1	D	337	VAL
1	D	537	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	31	GLN
1	A	70	GLN

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Mol	Chain	Res	Type
1	A	116	GLN
1	A	189	GLN
1	A	336	GLN
1	A	404	ASN
1	B	77	HIS
1	B	84	ASN
1	B	210	GLN
1	B	564	ASN
1	C	70	GLN
1	C	148	GLN
1	C	483	ASN
1	D	70	GLN
1	D	143	GLN
1	D	232	GLN
1	D	373	GLN
1	D	410	ASN
1	D	554	HIS

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](#)

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	B	659	1	14,14,15	0.30	0	17,19,21	0.99	1 (5%)
3	NAG	B	646	1	14,14,15	0.48	0	17,19,21	1.14	3 (17%)
3	NAG	C	676	1	14,14,15	0.31	0	17,19,21	0.53	0
3	NAG	A	652	1	14,14,15	0.32	0	17,19,21	0.67	0
3	NAG	B	652	1	14,14,15	0.28	0	17,19,21	0.61	0
3	NAG	C	646	1	14,14,15	0.28	0	17,19,21	0.46	0
3	NAG	A	676	1	14,14,15	0.43	0	17,19,21	1.31	1 (5%)
3	NAG	A	646	1	14,14,15	0.39	0	17,19,21	0.77	1 (5%)
3	NAG	A	659	1	14,14,15	0.35	0	17,19,21	0.60	0
3	NAG	C	618	1	14,14,15	0.47	0	17,19,21	0.85	0
3	NAG	C	685	1	14,14,15	0.37	0	17,19,21	1.47	2 (11%)
3	NAG	D	652	1	14,14,15	0.30	0	17,19,21	0.81	0
3	NAG	A	618	1	14,14,15	0.40	0	17,19,21	0.83	1 (5%)
3	NAG	A	685	1	14,14,15	0.43	0	17,19,21	1.36	1 (5%)
3	NAG	B	685	1	14,14,15	0.34	0	17,19,21	1.35	2 (11%)
3	NAG	D	676	1	14,14,15	0.34	0	17,19,21	0.71	0
3	NAG	D	646	1	14,14,15	0.62	0	17,19,21	1.43	3 (17%)
3	NAG	B	676	1	14,14,15	0.30	0	17,19,21	0.66	0
3	NAG	D	618	1	14,14,15	0.31	0	17,19,21	0.89	0
3	NAG	D	685	1	14,14,15	0.49	0	17,19,21	0.95	0
3	NAG	B	618	1	14,14,15	0.33	0	17,19,21	0.93	1 (5%)
3	NAG	C	652	1	14,14,15	0.43	0	17,19,21	1.06	1 (5%)

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	B	659	1	-	2/6/23/26	0/1/1/1
3	NAG	B	646	1	1/1/5/7	0/6/23/26	0/1/1/1
3	NAG	C	676	1	-	0/6/23/26	0/1/1/1
3	NAG	A	652	1	-	0/6/23/26	0/1/1/1
3	NAG	B	652	1	-	0/6/23/26	0/1/1/1
3	NAG	C	646	1	-	1/6/23/26	0/1/1/1
3	NAG	A	676	1	1/1/5/7	0/6/23/26	0/1/1/1
3	NAG	A	646	1	1/1/5/7	1/6/23/26	0/1/1/1
3	NAG	A	659	1	1/1/5/7	2/6/23/26	0/1/1/1
3	NAG	C	618	1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	C	685	1	-	2/6/23/26	0/1/1/1
3	NAG	D	652	1	-	0/6/23/26	0/1/1/1
3	NAG	A	618	1	-	3/6/23/26	0/1/1/1
3	NAG	A	685	1	-	2/6/23/26	0/1/1/1
3	NAG	B	685	1	-	4/6/23/26	0/1/1/1
3	NAG	D	676	1	-	0/6/23/26	0/1/1/1
3	NAG	D	646	1	1/1/5/7	4/6/23/26	0/1/1/1
3	NAG	B	676	1	-	0/6/23/26	0/1/1/1
3	NAG	D	618	1	-	1/6/23/26	0/1/1/1
3	NAG	D	685	1	-	4/6/23/26	0/1/1/1
3	NAG	B	618	1	-	1/6/23/26	0/1/1/1
3	NAG	C	652	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	685	NAG	C1-O5-C5	4.68	118.46	112.19
3	A	685	NAG	C1-O5-C5	4.50	118.22	112.19
3	A	676	NAG	O5-C1-C2	-4.14	104.89	111.29
3	D	646	NAG	C4-C3-C2	4.07	116.98	111.02
3	C	652	NAG	C1-O5-C5	3.90	117.41	112.19
3	B	659	NAG	C1-O5-C5	3.43	116.78	112.19
3	B	618	NAG	C1-O5-C5	3.31	116.63	112.19
3	B	685	NAG	C1-O5-C5	3.17	116.43	112.19
3	B	685	NAG	O5-C1-C2	-3.11	106.48	111.29
3	B	646	NAG	C4-C3-C2	2.93	115.31	111.02
3	B	646	NAG	O5-C1-C2	-2.58	107.29	111.29
3	D	646	NAG	O5-C1-C2	-2.48	107.46	111.29
3	C	685	NAG	C4-C3-C2	-2.24	107.74	111.02
3	A	646	NAG	C1-O5-C5	2.22	115.16	112.19
3	B	646	NAG	C3-C4-C5	2.04	113.93	110.23
3	A	618	NAG	C1-O5-C5	2.03	114.91	112.19
3	D	646	NAG	C3-C4-C5	2.01	113.87	110.23

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	646	NAG	C1
3	A	659	NAG	C1

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

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	646	NAG	O5-C5-C6-O6
3	A	618	NAG	O5-C5-C6-O6
3	B	659	NAG	O5-C5-C6-O6
3	C	618	NAG	O5-C5-C6-O6
3	C	618	NAG	C4-C5-C6-O6
3	D	685	NAG	O5-C5-C6-O6
3	B	659	NAG	C4-C5-C6-O6
3	D	646	NAG	C4-C5-C6-O6
3	D	685	NAG	C4-C5-C6-O6
3	A	618	NAG	C4-C5-C6-O6
3	A	659	NAG	C4-C5-C6-O6
3	A	659	NAG	O5-C5-C6-O6
3	A	646	NAG	O5-C5-C6-O6
3	D	618	NAG	O5-C5-C6-O6
3	B	685	NAG	C4-C5-C6-O6
3	B	618	NAG	O5-C5-C6-O6
3	A	685	NAG	C1-C2-N2-C7
3	C	685	NAG	C1-C2-N2-C7
3	D	685	NAG	C1-C2-N2-C7
3	B	685	NAG	O5-C5-C6-O6
3	B	685	NAG	C3-C2-N2-C7
3	D	646	NAG	C3-C2-N2-C7
3	D	685	NAG	C3-C2-N2-C7
3	C	646	NAG	C4-C5-C6-O6
3	B	685	NAG	C1-C2-N2-C7
3	D	646	NAG	C1-C2-N2-C7
3	A	618	NAG	C3-C2-N2-C7
3	A	685	NAG	C3-C2-N2-C7
3	C	685	NAG	C3-C2-N2-C7

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	685	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	461/565 (81%)	-0.82	0 100 100	18, 46, 74, 100	0
1	B	485/565 (85%)	-0.81	0 100 100	26, 50, 82, 108	0
1	C	454/565 (80%)	-0.82	0 100 100	24, 46, 75, 95	0
1	D	464/565 (82%)	-0.82	0 100 100	25, 46, 67, 95	0
All	All	1864/2260 (82%)	-0.82	0 100 100	18, 47, 77, 108	0

There are no RSRZ outliers to report.

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(Å ²)	Q<0.9
3	NAG	A	646	14/15	0.94	0.09	66,73,79,79	0
3	NAG	D	652	14/15	0.95	0.07	79,85,87,88	0
3	NAG	A	676	14/15	0.96	0.06	65,69,74,75	0
3	NAG	B	646	14/15	0.96	0.06	59,63,70,71	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	NAG	B	676	14/15	0.96	0.07	64,67,74,75	0
3	NAG	D	646	14/15	0.96	0.06	63,65,68,69	0
3	NAG	A	659	14/15	0.96	0.06	73,75,77,77	0
3	NAG	D	676	14/15	0.96	0.09	65,67,67,68	0
3	NAG	C	652	14/15	0.97	0.06	65,67,67,67	0
3	NAG	B	652	14/15	0.97	0.07	73,77,81,83	0
3	NAG	B	659	14/15	0.97	0.08	90,93,95,96	0
3	NAG	B	618	14/15	0.97	0.06	49,51,51,51	0
3	NAG	C	618	14/15	0.98	0.06	64,66,70,73	0
3	NAG	C	646	14/15	0.98	0.04	62,64,67,68	0
3	NAG	A	685	14/15	0.98	0.05	49,52,56,56	0
3	NAG	C	676	14/15	0.98	0.06	61,63,65,65	0
3	NAG	D	618	14/15	0.98	0.05	53,55,56,57	0
3	NAG	A	618	14/15	0.98	0.06	64,67,68,69	0
3	NAG	A	652	14/15	0.98	0.06	60,62,63,64	0
3	NAG	B	685	14/15	0.98	0.05	50,52,56,57	0
3	NAG	D	685	14/15	0.98	0.06	50,53,56,57	0
2	CA	D	601	1/1	0.99	0.03	61,61,61,61	0
2	CA	B	600	1/1	0.99	0.03	58,58,58,58	0
3	NAG	C	685	14/15	0.99	0.05	55,57,62,64	0
2	CA	D	600	1/1	0.99	0.04	45,45,45,45	0
2	CA	C	601	1/1	1.00	0.02	37,37,37,37	0
2	CA	A	601	1/1	1.00	0.01	43,43,43,43	0
2	CA	A	600	1/1	1.00	0.01	33,33,33,33	0
2	CA	B	601	1/1	1.00	0.02	60,60,60,60	0
2	CA	C	600	1/1	1.00	0.01	41,41,41,41	0

6.5 Other polymers [i](#)

There are no such residues in this entry.