Full wwPDB X-ray Structure Validation Report (i)

Jun 16, 2024 – 11:29 PM EDT

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 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 (i) 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 (i)) were used in the production of this report:

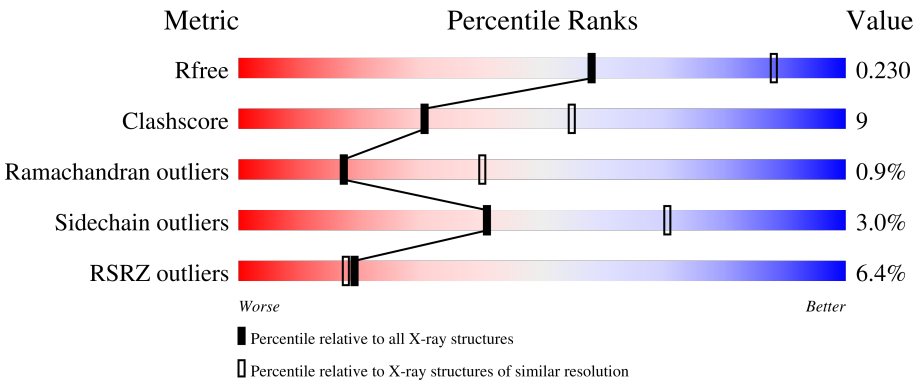
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

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}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (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 <=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	4% 65% 16% 18%
1	B	565	7% 65% 18% • • 14%
1	C	565	6% 68% 11% • 20%
1	D	565	4% 71% 11% 18%

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 (i)

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.

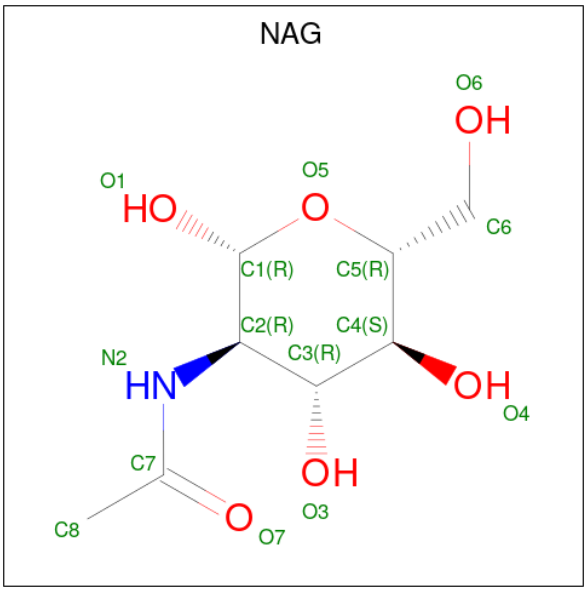
- Molecule 1 is a protein called HUMAN COMPLEMENT FACTOR I.

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

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

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

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

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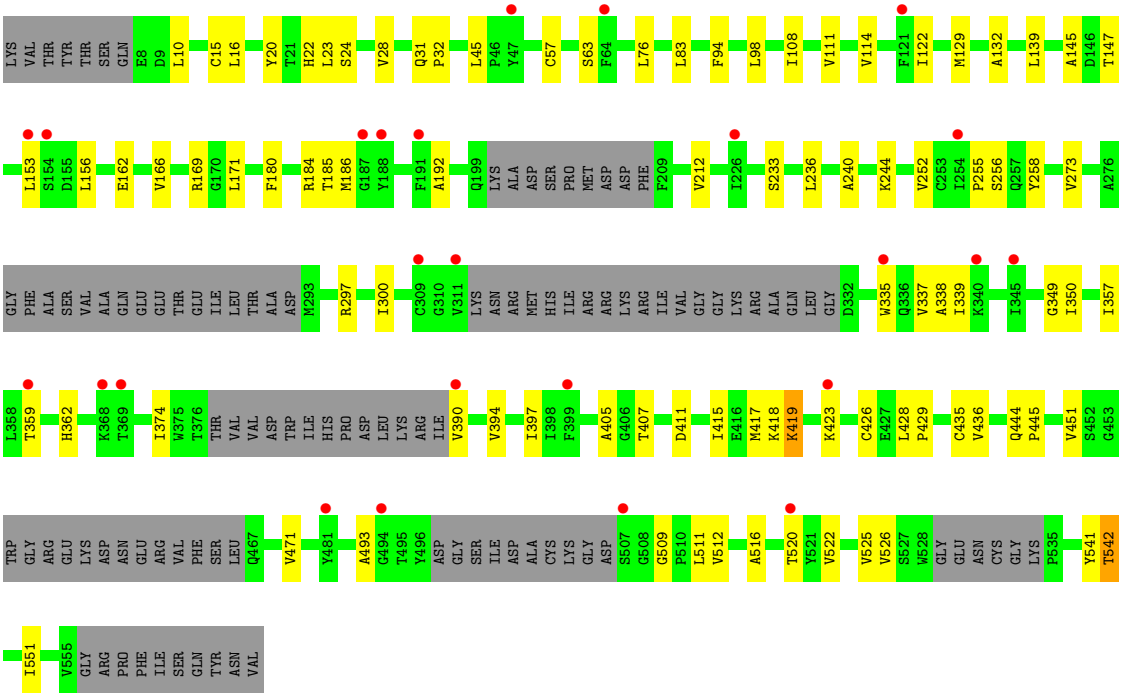
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	C	1	14	8	1	5	0	0
			Total	C	N	O		
3	C	1	14	8	1	5	0	0
			Total	C	N	O		
3	C	1	14	8	1	5	0	0
			Total	C	N	O		
3	D	1	14	8	1	5	0	0
			Total	C	N	O		
3	D	1	14	8	1	5	0	0
			Total	C	N	O		
3	D	1	14	8	1	5	0	0
			Total	C	N	O		
3	D	1	14	8	1	5	0	0
			Total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

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.

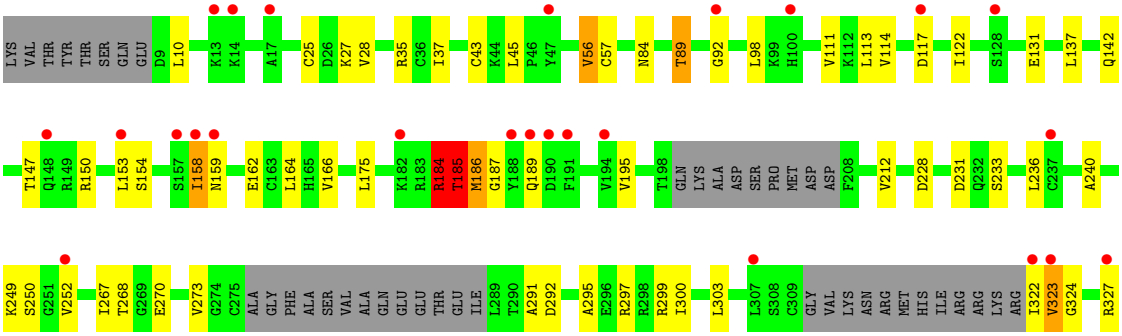
• Molecule 1: HUMAN COMPLEMENT FACTOR I

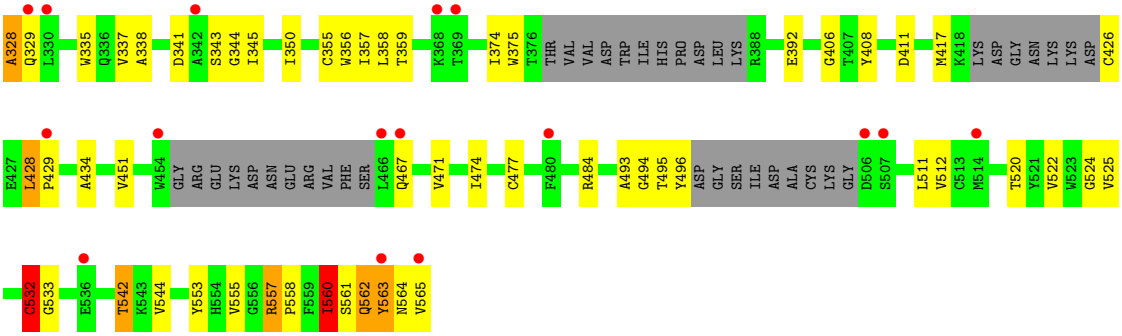
Chain A:



• Molecule 1: HUMAN COMPLEMENT FACTOR I

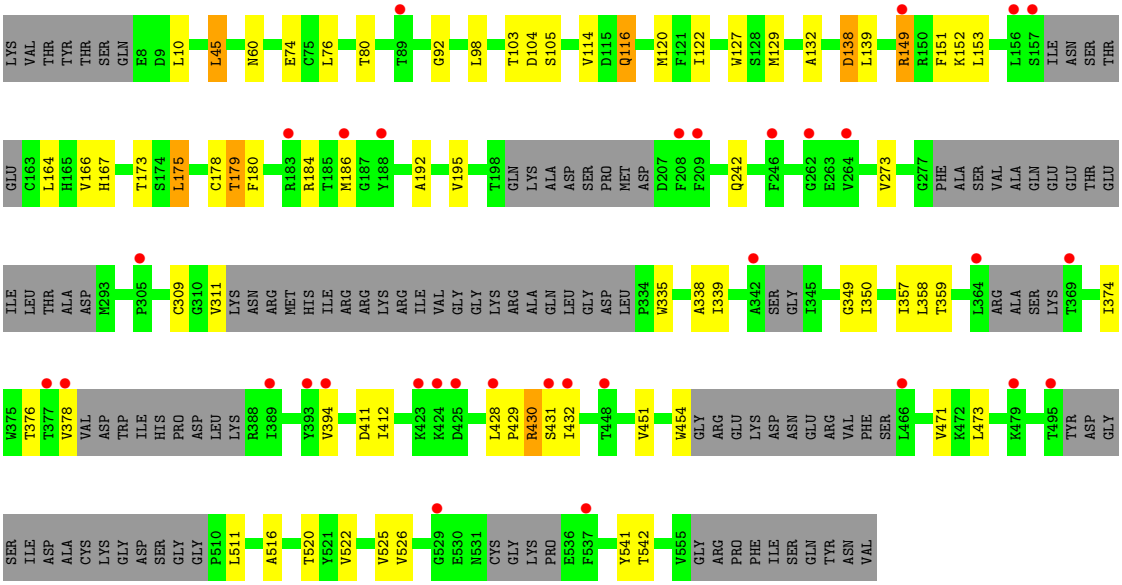
Chain B:





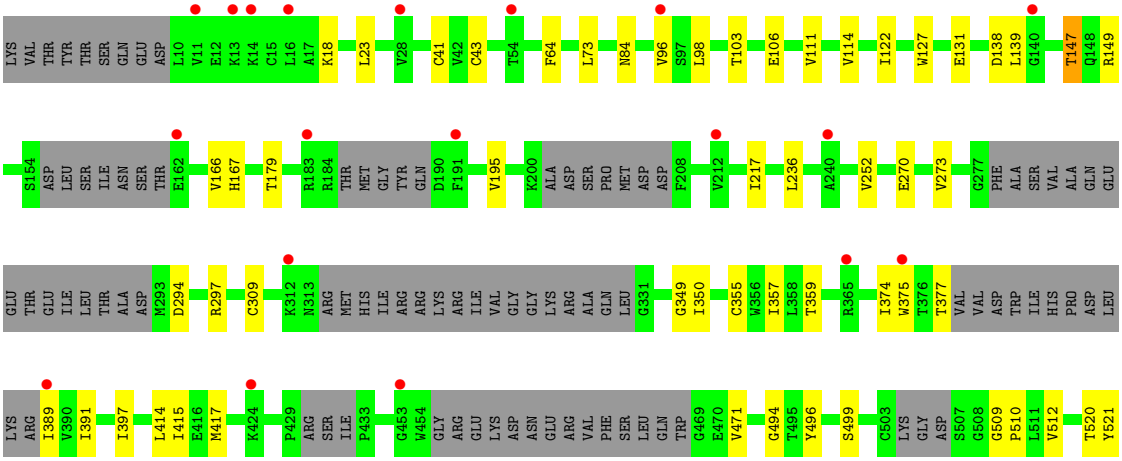
- Molecule 1: HUMAN COMPLEMENT FACTOR I

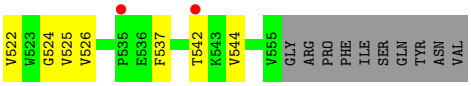
Chain C:



- Molecule 1: HUMAN COMPLEMENT FACTOR I

Chain D:




V522
W523
G524
V525
V526
P535
E536
F537
T542
K543
V544
V555
GLY
ARG
PRO
PHE
ILE
SER
GLN
TYR
ASN
VAL

4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [1]	2.15 (at 2.65Å)	Xtriage
Refinement program	REFMAC 5.6.0079	Depositor
R, R_{free}	0.200 , 0.238 0.202 , 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)	0.31 , 4.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.42$, $< L^2 > = 0.24$	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	0.91	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.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: 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(^{o})	Ideal(^{o})
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 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	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

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 (267) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (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:HG12	1:B:565:VAL:O	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:N	1:B:322:ILE:HD12	2.18	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:B:474:ILE:HD12	1:B:474:ILE:C	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: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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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: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: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: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:A:419:LYS:HB2	1:A:426:CYS:SG	2.57	0.45
1:C:122:ILE:HG21	1:C:127:TRP:CE3	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:231:ASP:OD1	1:B:233:SER:OG	2.28	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: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: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: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: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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:356:TRP:CE2	1:B:555:VAL:HG13	2.55	0.42
1:C:138:ASP:C	1:C:138:ASP:OD2	2.58	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:B:56:VAL:CG1	1:B:57:CYS:N	2.82	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: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:B:392:GLU:CB	1:B:417:MET:HE2	2.50	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
1:D:525:VAL:CG2	1:D:542:THR:CG2	2.99	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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 (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	445/565 (79%)	404 (91%)	39 (9%)	2 (0%)	34 60
1	B	469/565 (83%)	404 (86%)	52 (11%)	13 (3%)	5 11
1	C	432/565 (76%)	398 (92%)	34 (8%)	0	100 100
1	D	444/565 (79%)	412 (93%)	31 (7%)	1 (0%)	47 73
All	All	1790/2260 (79%)	1618 (90%)	156 (9%)	16 (1%)	17 40

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

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Mol	Chain	Res	Type
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 (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	401/489 (82%)	392 (98%)	9 (2%)	52	79
1	B	420/489 (86%)	400 (95%)	20 (5%)	25	53
1	C	396/489 (81%)	385 (97%)	11 (3%)	43	73
1	D	399/489 (82%)	391 (98%)	8 (2%)	55	81
All	All	1616/1956 (83%)	1568 (97%)	48 (3%)	41	70

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

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Mol	Chain	Res	Type
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
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

Sometimes 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 (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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	C	652	1	14,14,15	0.43	0	17,19,21	1.06	1 (5%)
3	NAG	C	676	1	14,14,15	0.31	0	17,19,21	0.53	0
3	NAG	B	618	1	14,14,15	0.33	0	17,19,21	0.93	1 (5%)
3	NAG	B	676	1	14,14,15	0.30	0	17,19,21	0.66	0
3	NAG	B	652	1	14,14,15	0.28	0	17,19,21	0.61	0
3	NAG	B	659	1	14,14,15	0.30	0	17,19,21	0.99	1 (5%)
3	NAG	D	618	1	14,14,15	0.31	0	17,19,21	0.89	0
3	NAG	A	659	1	14,14,15	0.35	0	17,19,21	0.60	0
3	NAG	D	652	1	14,14,15	0.30	0	17,19,21	0.81	0
3	NAG	D	676	1	14,14,15	0.34	0	17,19,21	0.71	0
3	NAG	C	646	1	14,14,15	0.28	0	17,19,21	0.46	0
3	NAG	A	618	1	14,14,15	0.40	0	17,19,21	0.83	1 (5%)
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	B	646	1	14,14,15	0.48	0	17,19,21	1.14	3 (17%)
3	NAG	C	685	1	14,14,15	0.37	0	17,19,21	1.47	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	NAG	D	646	1	14,14,15	0.62	0	17,19,21	1.43	3 (17%)
3	NAG	C	618	1	14,14,15	0.47	0	17,19,21	0.85	0
3	NAG	B	685	1	14,14,15	0.34	0	17,19,21	1.35	2 (11%)
3	NAG	D	685	1	14,14,15	0.49	0	17,19,21	0.95	0
3	NAG	A	652	1	14,14,15	0.32	0	17,19,21	0.67	0
3	NAG	A	685	1	14,14,15	0.43	0	17,19,21	1.36	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	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	B	618	1	-	1/6/23/26	0/1/1/1
3	NAG	B	676	1	-	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	-	2/6/23/26	0/1/1/1
3	NAG	D	618	1	-	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	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	C	646	1	-	1/6/23/26	0/1/1/1
3	NAG	A	618	1	-	3/6/23/26	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	B	646	1	1/1/5/7	0/6/23/26	0/1/1/1
3	NAG	C	685	1	-	2/6/23/26	0/1/1/1
3	NAG	D	646	1	1/1/5/7	4/6/23/26	0/1/1/1
3	NAG	C	618	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	685	1	-	4/6/23/26	0/1/1/1
3	NAG	A	652	1	-	0/6/23/26	0/1/1/1
3	NAG	A	685	1	-	2/6/23/26	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(^{o})	Ideal(^{o})
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
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

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Mol	Chain	Res	Type	Atoms
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%)	0.57	25 (5%)	25	24	18, 46, 74, 100	0
1	B	485/565 (85%)	0.67	41 (8%)	10	9	26, 50, 82, 108	0
1	C	454/565 (80%)	0.68	33 (7%)	15	13	24, 46, 75, 95	0
1	D	464/565 (82%)	0.55	21 (4%)	33	31	25, 46, 67, 95	0
All	All	1864/2260 (82%)	0.62	120 (6%)	19	18	18, 47, 77, 108	0

All (120) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	156	LEU	7.6
1	B	188	TYR	5.5
1	C	425	ASP	5.0
1	C	157	SER	4.9
1	A	191	PHE	4.5
1	C	389	ILE	4.3
1	B	191	PHE	4.3
1	B	329	GLN	4.3
1	C	466	LEU	4.3
1	B	454	TRP	4.2
1	C	424	LYS	4.2
1	C	208	PHE	4.0
1	B	330	LEU	3.9
1	D	16	LEU	3.8
1	D	162	GLU	3.8
1	B	153	LEU	3.7
1	D	535	PRO	3.6
1	B	368	LYS	3.6
1	D	389	ILE	3.6
1	B	189	GLN	3.6
1	C	89	THR	3.5

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Mol	Chain	Res	Type	RSRZ
1	C	378	VAL	3.4
1	C	369	THR	3.4
1	A	494	GLY	3.3
1	B	369	THR	3.3
1	B	190	ASP	3.2
1	B	158	ILE	3.2
1	B	506	ASP	3.2
1	D	13	LYS	3.2
1	A	121	PHE	3.1
1	C	432	ILE	3.1
1	A	345	ILE	3.1
1	A	309	CYS	3.1
1	C	448	THR	3.0
1	A	507	SER	3.0
1	B	157	SER	3.0
1	D	453	GLY	3.0
1	B	148	GLN	2.9
1	D	312	LYS	2.9
1	C	393	TYR	2.9
1	C	537	PHE	2.9
1	B	194	VAL	2.9
1	B	100	HIS	2.9
1	B	507	SER	2.8
1	B	323	VAL	2.8
1	B	322	ILE	2.8
1	D	140	GLY	2.8
1	C	209	PHE	2.8
1	B	514	MET	2.7
1	B	47	TYR	2.7
1	D	375	TRP	2.7
1	D	424	LYS	2.7
1	C	149	ARG	2.6
1	C	495	THR	2.6
1	C	364	LEU	2.6
1	D	54	THR	2.6
1	C	188	TYR	2.6
1	B	307	LEU	2.6
1	C	246	PHE	2.6
1	C	377	THR	2.5
1	D	191	PHE	2.5
1	C	423	LYS	2.5
1	B	536	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	311	VAL	2.5
1	B	565	VAL	2.5
1	C	264	VAL	2.5
1	C	529	GLY	2.5
1	C	183	ARG	2.5
1	C	394	VAL	2.5
1	C	428	LEU	2.4
1	A	64	PHE	2.4
1	B	13	LYS	2.4
1	A	369	THR	2.4
1	B	237	CYS	2.4
1	A	340	LYS	2.4
1	B	14	LYS	2.4
1	C	431	SER	2.4
1	A	187	GLY	2.4
1	A	423	LYS	2.4
1	D	212	VAL	2.3
1	B	342	ALA	2.3
1	D	183	ARG	2.3
1	A	188	TYR	2.3
1	D	14	LYS	2.3
1	B	429	PRO	2.3
1	A	153	LEU	2.3
1	B	128	SER	2.3
1	D	365	ARG	2.3
1	C	342	ALA	2.2
1	B	92	GLY	2.2
1	B	563	TYR	2.2
1	D	96	VAL	2.2
1	B	117	ASP	2.2
1	D	240	ALA	2.2
1	A	368	LYS	2.2
1	C	305	PRO	2.2
1	B	327	ARG	2.2
1	A	47	TYR	2.2
1	A	335	TRP	2.2
1	A	481	TYR	2.1
1	B	182	LYS	2.1
1	B	159	ASN	2.1
1	A	154	SER	2.1
1	A	226	ILE	2.1
1	B	466	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	254	ILE	2.1
1	C	479	LYS	2.1
1	B	252	VAL	2.1
1	D	11	VAL	2.1
1	D	28	VAL	2.1
1	B	467	GLN	2.1
1	A	399	PHE	2.1
1	B	480	PHE	2.1
1	A	390	VAL	2.1
1	D	542	THR	2.1
1	C	186	MET	2.0
1	C	262	GLY	2.0
1	A	359	THR	2.0
1	A	520	THR	2.0
1	B	17	ALA	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	NAG	A	646	14/15	0.71	0.35	66,73,79,79	0
3	NAG	B	652	14/15	0.80	0.24	73,77,81,83	0
3	NAG	D	652	14/15	0.82	0.20	79,85,87,88	0
3	NAG	C	646	14/15	0.84	0.22	62,64,67,68	0
3	NAG	D	676	14/15	0.84	0.24	65,67,67,68	0
3	NAG	B	659	14/15	0.85	0.33	90,93,95,96	0
3	NAG	A	652	14/15	0.85	0.20	60,62,63,64	0
3	NAG	C	676	14/15	0.86	0.22	61,63,65,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	NAG	C	685	14/15	0.86	0.20	55,57,62,64	0
3	NAG	D	646	14/15	0.86	0.22	63,65,68,69	0
3	NAG	B	676	14/15	0.86	0.25	64,67,74,75	0
3	NAG	A	618	14/15	0.86	0.21	64,67,68,69	0
3	NAG	D	618	14/15	0.87	0.19	53,55,56,57	0
3	NAG	C	652	14/15	0.87	0.20	65,67,67,67	0
3	NAG	A	676	14/15	0.88	0.19	65,69,74,75	0
2	CA	D	601	1/1	0.88	0.15	61,61,61,61	0
3	NAG	C	618	14/15	0.89	0.20	64,66,70,73	0
3	NAG	A	659	14/15	0.89	0.21	73,75,77,77	0
3	NAG	B	685	14/15	0.89	0.17	50,52,56,57	0
3	NAG	D	685	14/15	0.89	0.19	50,53,56,57	0
3	NAG	B	646	14/15	0.90	0.27	59,63,70,71	0
2	CA	B	601	1/1	0.91	0.16	60,60,60,60	0
3	NAG	A	685	14/15	0.91	0.18	49,52,56,56	0
3	NAG	B	618	14/15	0.91	0.20	49,51,51,51	0
2	CA	B	600	1/1	0.92	0.14	58,58,58,58	0
2	CA	A	600	1/1	0.95	0.14	33,33,33,33	0
2	CA	C	601	1/1	0.97	0.17	37,37,37,37	0
2	CA	A	601	1/1	0.97	0.18	43,43,43,43	0
2	CA	C	600	1/1	0.97	0.13	41,41,41,41	0
2	CA	D	600	1/1	0.98	0.09	45,45,45,45	0

6.5 Other polymers (i)

There are no such residues in this entry.