



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2020 – 11:58 PM BST

PDB ID : 5W21
Title : Crystal Structure of a 1:1:1 FGF23-FGFR1c-aKlotho Ternary Complex
Authors : Mohammadi, M.
Deposited on : 2017-06-05
Resolution : 3.00 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
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) : 2.13.1

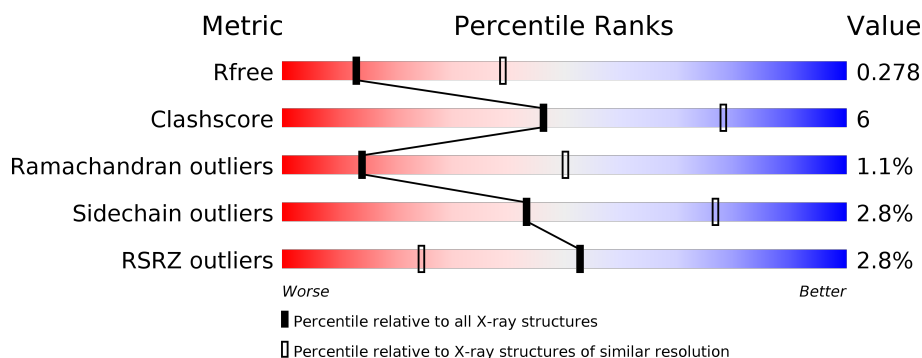
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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 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	981	<div> <div>2%</div> <div> <div></div> <div>77%</div> <div>15%</div> <div>• 6%</div> </div> </div>
2	B	226	<div> <div>5%</div> <div> <div></div> <div>65%</div> <div>14%</div> <div>• 19%</div> </div> </div>
3	C	226	<div> <div>5%</div> <div> <div></div> <div>76%</div> <div>18%</div> <div>6%</div> </div> </div>

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 10701 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 Klotho.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	922	Total	C	N	O	S	0	0	0
			7511	4874	1273	1335	29			

- Molecule 2 is a protein called Fibroblast growth factor 23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	182	Total	C	N	O	S	0	0	0
			1434	908	259	259	8			

There are 50 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-21	MET	-	expression tag	UNP Q9GZV9
B	-20	HIS	-	expression tag	UNP Q9GZV9
B	-19	HIS	-	expression tag	UNP Q9GZV9
B	-18	HIS	-	expression tag	UNP Q9GZV9
B	-17	HIS	-	expression tag	UNP Q9GZV9
B	-16	HIS	-	expression tag	UNP Q9GZV9
B	-15	HIS	-	expression tag	UNP Q9GZV9
B	-14	SER	-	expression tag	UNP Q9GZV9
B	-13	SER	-	expression tag	UNP Q9GZV9
B	-12	GLY	-	expression tag	UNP Q9GZV9
B	-11	LEU	-	expression tag	UNP Q9GZV9
B	-10	VAL	-	expression tag	UNP Q9GZV9
B	-9	PRO	-	expression tag	UNP Q9GZV9
B	-8	ARG	-	expression tag	UNP Q9GZV9
B	-7	GLY	-	expression tag	UNP Q9GZV9
B	-6	SER	-	expression tag	UNP Q9GZV9
B	-5	GLY	-	expression tag	UNP Q9GZV9
B	-4	MET	-	expression tag	UNP Q9GZV9
B	-3	LYS	-	expression tag	UNP Q9GZV9
B	-2	GLU	-	expression tag	UNP Q9GZV9

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-1	THR	-	expression tag	UNP Q9GZV9
B	0	ALA	-	expression tag	UNP Q9GZV9
B	1	ALA	-	expression tag	UNP Q9GZV9
B	2	ALA	-	expression tag	UNP Q9GZV9
B	3	LYS	-	expression tag	UNP Q9GZV9
B	4	PHE	-	expression tag	UNP Q9GZV9
B	5	GLU	-	expression tag	UNP Q9GZV9
B	6	ARG	-	expression tag	UNP Q9GZV9
B	7	GLN	-	expression tag	UNP Q9GZV9
B	8	HIS	-	expression tag	UNP Q9GZV9
B	9	MET	-	expression tag	UNP Q9GZV9
B	10	ASP	-	expression tag	UNP Q9GZV9
B	11	SER	-	expression tag	UNP Q9GZV9
B	12	PRO	-	expression tag	UNP Q9GZV9
B	13	ASP	-	expression tag	UNP Q9GZV9
B	14	LEU	-	expression tag	UNP Q9GZV9
B	15	GLY	-	expression tag	UNP Q9GZV9
B	16	THR	-	expression tag	UNP Q9GZV9
B	17	ASP	-	expression tag	UNP Q9GZV9
B	18	ASP	-	expression tag	UNP Q9GZV9
B	19	ASP	-	expression tag	UNP Q9GZV9
B	20	ASP	-	expression tag	UNP Q9GZV9
B	21	LYS	-	expression tag	UNP Q9GZV9
B	22	ALA	-	expression tag	UNP Q9GZV9
B	23	MET	-	expression tag	UNP Q9GZV9
B	24	GLY	-	expression tag	UNP Q9GZV9
B	140	ALA	ARG	conflict	UNP Q9GZV9
B	143	ALA	ARG	conflict	UNP Q9GZV9
B	176	GLN	ARG	conflict	UNP Q9GZV9
B	179	GLN	ARG	conflict	UNP Q9GZV9

- Molecule 3 is a protein called Fibroblast growth factor receptor 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	213	Total	C	N	O	S	0	0	0
			1656	1056	282	309	9			

There are 3 discrepancies between the modelled and reference sequences:

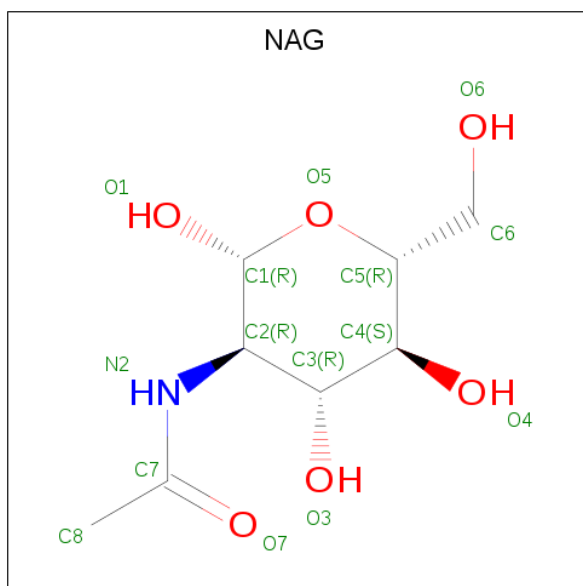
Chain	Residue	Modelled	Actual	Comment	Reference
C	140	MET	-	expression tag	UNP P11362
C	141	ALA	-	expression tag	UNP P11362

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Chain	Residue	Modelled	Actual	Comment	Reference
C	185	GLN	ASN	conflict	UNP P11362

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

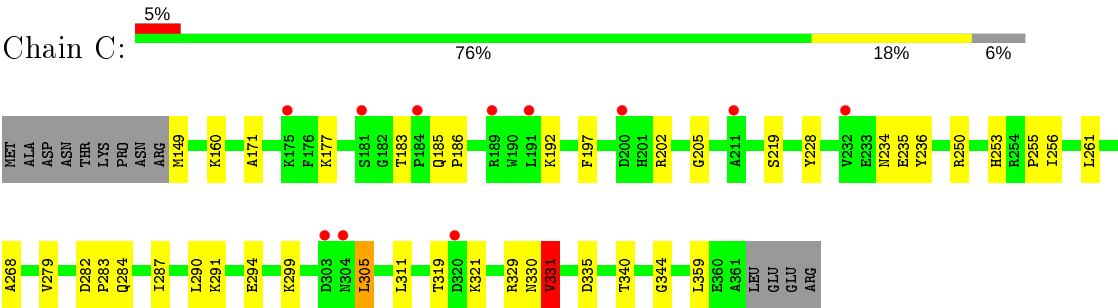
- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Zn	0	0
			1	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	O	0	0
			1	1		

● Molecule 3: Fibroblast growth factor receptor 1



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	283.30Å 72.59Å 95.33Å 90.00° 91.98° 90.00°	Depositor
Resolution (Å)	48.80 – 3.00 48.80 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.5 (48.80-3.00) 99.8 (48.80-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.72 (at 3.01Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, R_{free}	0.230 , 0.278 0.230 , 0.278	Depositor DCC
R_{free} test set	1954 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	66.0	Xtriage
Anisotropy	1.168	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 72.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.023 for -h,-k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	10701	wwPDB-VP
Average B, all atoms (Å ²)	115.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.11% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, 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	0.24	0/7754	0.41	0/10552
2	B	0.25	0/1479	0.43	0/2013
3	C	0.24	0/1703	0.42	0/2324
All	All	0.24	0/10936	0.41	0/14889

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-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 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	7511	0	7217	96	0
2	B	1434	0	1349	21	0
3	C	1656	0	1613	24	0
4	A	98	0	91	1	0
5	A	1	0	0	0	0
6	A	1	0	0	0	0
All	All	10701	0	10270	132	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 6.

All (132) 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:594:ARG:NH2	1:A:688:ASN:OD1	2.18	0.77
2:B:173:ILE:H	2:B:174:PRO:HD2	1.51	0.76
1:A:731:GLN:HA	1:A:807:SER:HB3	1.75	0.69
1:A:564:VAL:HG13	1:A:565:THR:HG23	1.76	0.68
1:A:684:TRP:HB2	1:A:726:ILE:HG12	1.76	0.68
1:A:884:ASP:OD2	1:A:940:SER:N	2.28	0.67
2:B:128:HIS:HB3	2:B:135:LEU:HD23	1.79	0.65
3:C:291:LYS:HB2	3:C:311:LEU:HD11	1.79	0.65
2:B:173:ILE:H	2:B:174:PRO:CD	2.10	0.65
1:A:620:ARG:NH2	1:A:676:GLU:OE1	2.29	0.64
1:A:238:ASP:HA	1:A:297:ALA:HB3	1.79	0.64
1:A:781:ARG:O	1:A:782:ASN:ND2	2.30	0.64
2:B:29:SER:HB3	2:B:30:PRO:HD2	1.81	0.62
1:A:303:ILE:HD11	1:A:320:LEU:HG	1.82	0.62
1:A:568:ARG:NH2	3:C:335:ASP:OD1	2.32	0.62
1:A:776:ASP:OD1	1:A:780:GLN:NE2	2.34	0.61
1:A:134:ARG:NH1	1:A:486:LYS:O	2.33	0.61
1:A:246:HIS:NE2	1:A:379:LEU:O	2.29	0.61
1:A:136:THR:HG21	1:A:179:ARG:HG2	1.83	0.60
1:A:756:ASP:OD1	2:B:198:ARG:NH2	2.30	0.60
1:A:752:VAL:HG22	1:A:828:LEU:HD23	1.83	0.60
1:A:91:ASP:O	1:A:95:HIS:ND1	2.35	0.59
3:C:319:THR:HG22	3:C:321:LYS:H	1.68	0.59
1:A:639:GLN:HG2	1:A:688:ASN:HB3	1.84	0.58
1:A:786:LEU:HD12	1:A:787:PRO:HD2	1.85	0.58
1:A:303:ILE:HD13	1:A:316:CYS:HB3	1.86	0.58
1:A:217:ARG:HG3	1:A:281:LEU:HD22	1.85	0.58
2:B:77:SER:HA	2:B:83:VAL:HA	1.85	0.58
3:C:192:LYS:HB2	3:C:197:PHE:HD1	1.70	0.57
1:A:594:ARG:NH1	1:A:872:SER:OG	2.34	0.56
3:C:160:LYS:HB3	3:C:177:LYS:HE3	1.88	0.55
1:A:923:PRO:HB2	1:A:924:ARG:HD3	1.88	0.55
1:A:414:GLU:HG3	1:A:458:TRP:HB2	1.88	0.55
1:A:811:THR:HG21	1:A:851:GLY:HA3	1.90	0.54
3:C:192:LYS:HG3	3:C:228:TYR:HE2	1.72	0.53
3:C:202:ARG:NH1	3:C:205:GLY:O	2.41	0.53
2:B:54:GLN:HE21	2:B:70:TYR:HB2	1.74	0.53
1:A:804:LEU:HD21	1:A:859:LEU:HD13	1.92	0.52
1:A:392:PRO:HG3	2:B:189:PRO:HB2	1.92	0.52
1:A:395:ARG:HB2	1:A:440:GLU:HB3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:629:VAL:HA	4:A:1006:NAG:H82	1.92	0.52
1:A:530:ASN:HB3	1:A:639:GLN:HE22	1.76	0.51
2:B:46:THR:O	2:B:48:ARG:N	2.38	0.51
1:A:901:ALA:HB1	1:A:907:ILE:HG13	1.93	0.51
1:A:526:GLY:HA3	1:A:592:HIS:O	2.10	0.50
1:A:377:PHE:N	1:A:390:GLU:OE1	2.45	0.50
1:A:771:PRO:HG2	1:A:774:MET:HE3	1.92	0.50
3:C:268:ALA:HA	3:C:359:LEU:H	1.77	0.49
1:A:131:ASN:HB3	1:A:134:ARG:HB3	1.95	0.49
1:A:589:HIS:ND1	1:A:949:ASP:OD1	2.41	0.48
1:A:345:LEU:HB3	1:A:349:LEU:HB2	1.94	0.48
1:A:748:VAL:HG12	1:A:751:ARG:HH21	1.77	0.48
1:A:759:TRP:HB2	1:A:774:MET:HE1	1.95	0.48
2:B:166:LEU:HA	2:B:169:PHE:HD1	1.78	0.48
1:A:729:ALA:HA	1:A:805:ALA:HB3	1.94	0.48
1:A:251:GLY:HA2	1:A:256:GLY:HA3	1.95	0.48
1:A:345:LEU:HD12	1:A:348:ILE:HD11	1.95	0.48
1:A:237:ILE:HD13	1:A:271:LEU:HD12	1.96	0.48
2:B:138:LEU:HB2	2:B:154:TYR:HB3	1.96	0.48
1:A:564:VAL:HG22	1:A:565:THR:H	1.79	0.48
3:C:255:PRO:HG2	3:C:344:GLY:HA2	1.96	0.47
1:A:842:PRO:HG2	1:A:878:GLY:HA2	1.97	0.47
1:A:728:ILE:HD11	1:A:765:PHE:HE1	1.81	0.46
1:A:324:LEU:HD23	1:A:400:TRP:HZ3	1.80	0.46
1:A:884:ASP:HB3	1:A:888:VAL:HG23	1.97	0.46
3:C:234:ASN:OD1	3:C:235:GLU:N	2.44	0.46
2:B:92:ARG:NH1	2:B:104:GLY:O	2.49	0.46
1:A:548:LEU:HB3	3:C:305:LEU:HD13	1.98	0.46
1:A:570:SER:O	1:A:617:GLN:NE2	2.50	0.45
1:A:76:THR:HA	1:A:126:SER:HB3	1.98	0.45
1:A:965:GLU:OE1	1:A:965:GLU:N	2.49	0.45
3:C:282:ASP:HB3	3:C:283:PRO:HD3	1.98	0.45
1:A:272:LEU:HD21	1:A:330:PRO:HB2	1.99	0.45
1:A:234:TRP:HB2	1:A:294:VAL:HG22	1.98	0.45
1:A:869:TYR:OH	1:A:973:CYS:O	2.19	0.45
1:A:734:TRP:HB3	1:A:811:THR:HG22	1.98	0.44
1:A:79:GLY:N	1:A:123:ASP:O	2.43	0.44
1:A:882:GLU:HB3	1:A:885:GLN:HG3	1.99	0.44
1:A:356:GLU:O	1:A:360:ILE:HG13	2.18	0.44
1:A:696:THR:HG23	1:A:699:ALA:H	1.83	0.44
1:A:707:HIS:CE1	1:A:728:ILE:HG23	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:428:ALA:HA	1:A:431:MET:HG2	1.99	0.44
1:A:436:LYS:NZ	1:A:440:GLU:OE2	2.38	0.44
1:A:592:HIS:CD2	1:A:632:THR:HB	2.52	0.44
1:A:594:ARG:NH1	1:A:871:ILE:O	2.50	0.44
2:B:135:LEU:HD21	2:B:145:PHE:HB2	2.00	0.44
2:B:69:ILE:HB	2:B:89:MET:HG3	2.00	0.44
2:B:29:SER:HB3	2:B:30:PRO:CD	2.48	0.43
1:A:588:MET:HE2	1:A:928:TYR:HE1	1.83	0.43
3:C:329:ARG:O	3:C:331:VAL:N	2.46	0.43
1:A:85:LYS:HD2	1:A:155:ARG:HE	1.83	0.43
1:A:524:ALA:HB3	1:A:911:GLY:HA3	2.01	0.43
3:C:171:ALA:HA	3:C:219:SER:HA	2.00	0.43
1:A:254:ALA:HB3	1:A:255:PRO:HD3	2.00	0.43
1:A:330:PRO:O	1:A:335:GLY:HA2	2.19	0.43
1:A:557:LEU:HD21	3:C:290:LEU:HD21	2.00	0.43
1:A:755:PHE:CZ	1:A:774:MET:HG3	2.53	0.43
1:A:194:TRP:CD1	1:A:194:TRP:N	2.86	0.43
2:B:173:ILE:O	2:B:175:ARG:N	2.50	0.43
1:A:728:ILE:HD11	1:A:765:PHE:CE1	2.54	0.43
3:C:330:ASN:O	3:C:331:VAL:HG22	2.18	0.43
1:A:860:LYS:HD2	1:A:907:ILE:HD13	2.01	0.42
1:A:140:ARG:HG3	1:A:183:LEU:HD13	2.01	0.42
1:A:585:LEU:HD23	1:A:588:MET:HE3	2.00	0.42
3:C:253:HIS:CD2	3:C:256:ILE:HD11	2.54	0.42
3:C:279:VAL:HG21	3:C:287:ILE:HD12	2.02	0.42
1:A:588:MET:HG3	1:A:941:MET:HG2	2.01	0.42
1:A:806:LEU:HD23	1:A:807:SER:N	2.35	0.42
1:A:871:ILE:HD12	1:A:871:ILE:HA	1.93	0.42
1:A:90:TRP:CE2	1:A:254:ALA:HB2	2.55	0.42
1:A:532:ILE:HD11	1:A:593:PHE:HE2	1.85	0.42
3:C:149:MET:O	3:C:183:THR:OG1	2.38	0.42
1:A:436:LYS:HA	1:A:439:MET:HB2	2.02	0.41
1:A:748:VAL:HG12	1:A:751:ARG:NH2	2.35	0.41
1:A:701:HIS:HD2	1:A:705:LYS:HE3	1.84	0.41
3:C:185:GLN:HA	3:C:186:PRO:HD3	1.95	0.41
1:A:44:ARG:HA	1:A:44:ARG:NH2	2.36	0.41
1:A:549:TRP:CH2	3:C:340:THR:HG21	2.55	0.41
1:A:888:VAL:HG13	1:A:943:HIS:CD2	2.54	0.41
2:B:143:ALA:HB3	2:B:152:PRO:HG3	2.02	0.41
1:A:179:ARG:O	1:A:183:LEU:HG	2.20	0.41
1:A:702:ASN:HA	1:A:705:LYS:HD2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:182:GLU:O	2:B:184:ASP:N	2.48	0.41
1:A:78:GLY:O	1:A:155:ARG:NH2	2.54	0.40
2:B:25:TYR:CE2	3:C:261:LEU:HD21	2.56	0.40
1:A:836:ILE:HD13	2:B:192:VAL:HG22	2.02	0.40
1:A:453:ILE:HA	1:A:453:ILE:HD12	1.96	0.40
3:C:261:LEU:HA	3:C:261:LEU:HD23	1.92	0.40
1:A:526:GLY:HA2	1:A:590:VAL:HG13	2.02	0.40
1:A:68:ALA:HB2	1:A:146:HIS:HB2	2.03	0.40
3:C:294:GLU:HB3	3:C:299:LYS:HB3	2.03	0.40
1:A:436:LYS:HD3	2:B:190:LEU:HD13	2.04	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	916/981 (93%)	827 (90%)	81 (9%)	8 (1%)	17	55
2	B	180/226 (80%)	150 (83%)	25 (14%)	5 (3%)	5	25
3	C	211/226 (93%)	186 (88%)	23 (11%)	2 (1%)	17	55
All	All	1307/1433 (91%)	1163 (89%)	129 (10%)	15 (1%)	14	50

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	968	THR
2	B	173	ILE
3	C	331	VAL
1	A	916	SER
3	C	284	GLN
1	A	255	PRO
1	A	257	ILE

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Mol	Chain	Res	Type
2	B	35	SER
2	B	197	ALA
1	A	962	PHE
1	A	971	THR
2	B	29	SER
2	B	172	PRO
1	A	163	GLY
1	A	49	PRO

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	789/842 (94%)	766 (97%)	23 (3%)	42	76
2	B	151/191 (79%)	147 (97%)	4 (3%)	46	78
3	C	182/198 (92%)	178 (98%)	4 (2%)	52	81
All	All	1122/1231 (91%)	1091 (97%)	31 (3%)	43	77

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	144	VAL
1	A	179	ARG
1	A	195	ASP
1	A	263	LEU
1	A	303	ILE
1	A	467	HIS
1	A	497	TYR
1	A	500	LEU
1	A	515	LEU
1	A	687	MET
1	A	720	HIS
1	A	756	ASP
1	A	780	GLN
1	A	782	ASN

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Mol	Chain	Res	Type
1	A	828	LEU
1	A	839	LEU
1	A	875	ILE
1	A	917	PHE
1	A	919	ASP
1	A	924	ARG
1	A	965	GLU
1	A	971	THR
1	A	973	CYS
2	B	39	LEU
2	B	89	MET
2	B	149	MET
2	B	198	ARG
3	C	236	TYR
3	C	250	ARG
3	C	305	LEU
3	C	331	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	54	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 1 is monoatomic - leaving 7 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	$\# Z > 2$
4	NAG	A	1004	1	14,14,15	0.34	0	17,19,21	0.41	0
4	NAG	A	1007	1	14,14,15	0.32	0	17,19,21	0.55	0
4	NAG	A	1003	1	14,14,15	0.25	0	17,19,21	0.40	0
4	NAG	A	1002	1	14,14,15	0.24	0	17,19,21	0.45	0
4	NAG	A	1005	1	14,14,15	0.20	0	17,19,21	0.42	0
4	NAG	A	1001	1	14,14,15	0.22	0	17,19,21	0.42	0
4	NAG	A	1006	1	14,14,15	0.22	0	17,19,21	0.42	0

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
4	NAG	A	1004	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1007	1	-	3/6/23/26	0/1/1/1
4	NAG	A	1003	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1002	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1005	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1001	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1006	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1001	NAG	O5-C5-C6-O6
4	A	1003	NAG	O5-C5-C6-O6
4	A	1001	NAG	C4-C5-C6-O6
4	A	1003	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
4	A	1006	NAG	O5-C5-C6-O6
4	A	1007	NAG	O5-C5-C6-O6
4	A	1007	NAG	C4-C5-C6-O6
4	A	1006	NAG	C4-C5-C6-O6
4	A	1002	NAG	C4-C5-C6-O6
4	A	1007	NAG	C3-C2-N2-C7
4	A	1002	NAG	O5-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1006	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

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	922/981 (93%)	-0.08	15 (1%)	72 44	54, 97, 169, 294	0
2	B	182/226 (80%)	0.28	11 (6%)	21 7	75, 121, 214, 332	0
3	C	213/226 (94%)	0.21	11 (5%)	27 10	88, 136, 201, 225	0
All	All	1317/1433 (91%)	0.02	37 (2%)	53 25	54, 106, 197, 332	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	177	HIS	13.7
2	B	178	THR	8.1
1	A	254	ALA	7.4
2	B	179	GLN	5.3
2	B	180	SER	4.2
1	A	160	GLY	3.8
1	A	977	HIS	3.8
3	C	232	VAL	3.5
1	A	116	PRO	3.5
1	A	963	CYS	3.2
3	C	211	ALA	3.2
3	C	304	ASN	3.2
1	A	969	VAL	3.2
1	A	883	ASP	3.2
1	A	881	ALA	2.9
1	A	59	GLY	2.9
1	A	257	ILE	2.8
3	C	184	PRO	2.6
3	C	320	ASP	2.6
3	C	191	LEU	2.6
2	B	149	MET	2.5
2	B	145	PHE	2.4
3	C	200	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	970	CYS	2.4
1	A	975	PHE	2.3
3	C	189	ARG	2.3
2	B	35	SER	2.3
1	A	973	CYS	2.2
3	C	181	SER	2.2
2	B	200	THR	2.2
2	B	176	GLN	2.2
2	B	19	ASP	2.2
1	A	877	ASP	2.1
3	C	303	ASP	2.1
3	C	175	LYS	2.0
1	A	259	GLY	2.0
2	B	34	SER	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 monosaccharides 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. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	NAG	A	1003	14/15	0.63	0.32	217,234,247,249	0
4	NAG	A	1004	14/15	0.70	0.31	175,182,188,191	0
4	NAG	A	1001	14/15	0.71	0.39	145,183,197,197	0
4	NAG	A	1002	14/15	0.74	0.31	157,180,210,218	0
4	NAG	A	1007	14/15	0.79	0.23	139,158,165,168	0
4	NAG	A	1005	14/15	0.81	0.34	134,164,171,183	0
4	NAG	A	1006	14/15	0.84	0.25	148,163,171,176	0
5	ZN	A	1008	1/1	0.97	0.21	116,116,116,116	0

6.5 Other polymers ⓘ

There are no such residues in this entry.