



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:23 PM GMT

PDB ID : 4RRY
Title : Crystal Structure of Apo Murine H90W Cyclooxygenase-2
Authors : Xu, S.; Blobaum, A.L.; Banerjee, S.; Marnett, L.J.
Deposited on : 2014-11-06
Resolution : 2.43 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
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

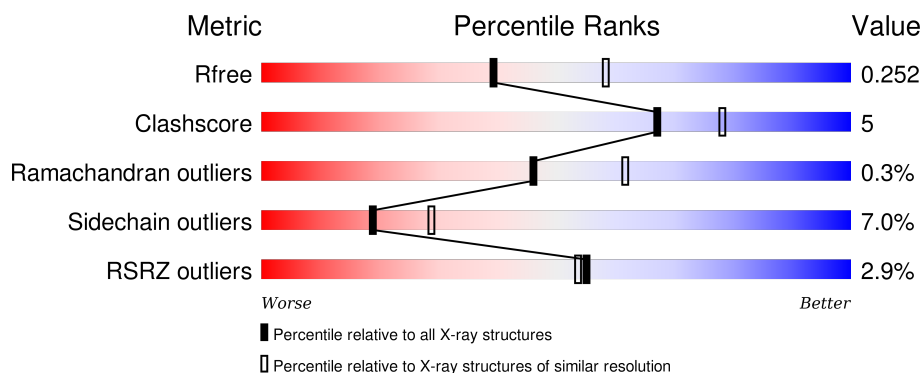
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.43 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}	91344	3386 (2.44-2.40)
Clashscore	102246	3897 (2.44-2.40)
Ramachandran outliers	100387	3837 (2.44-2.40)
Sidechain outliers	100360	3838 (2.44-2.40)
RSRZ outliers	91569	3396 (2.44-2.40)

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. 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	587	<div> <div>3%</div> <div>79%</div> <div>13%</div> <div>6%</div> </div>
1	B	587	<div> <div>2%</div> <div>80%</div> <div>12%</div> <div>6%</div> </div>
1	C	587	<div> <div>4%</div> <div>78%</div> <div>14%</div> <div>6%</div> </div>
1	D	587	<div> <div>2%</div> <div>80%</div> <div>12%</div> <div>6%</div> </div>

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
2	NAG	B	701	-	-	-	X
4	BOG	A	705	-	-	-	X
4	BOG	A	706	-	-	-	X
4	BOG	B	705	-	-	-	X
4	BOG	C	705	-	-	-	X
4	BOG	C	706	-	-	-	X
4	BOG	D	705	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 18993 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 Prostaglandin G/H synthase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	552	Total	C	N	O	S	0	0	0
			4478	2890	749	814	25			
1	B	552	Total	C	N	O	S	0	0	0
			4478	2890	749	814	25			
1	C	552	Total	C	N	O	S	0	0	0
			4478	2890	749	814	25			
1	D	552	Total	C	N	O	S	0	0	0
			4478	2890	749	814	25			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	90	TRP	HIS	ENGINEERED MUTATION	UNP Q05769
B	90	TRP	HIS	ENGINEERED MUTATION	UNP Q05769
C	90	TRP	HIS	ENGINEERED MUTATION	UNP Q05769
D	90	TRP	HIS	ENGINEERED MUTATION	UNP Q05769

- Molecule 2 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: C₈H₁₅NO₆).

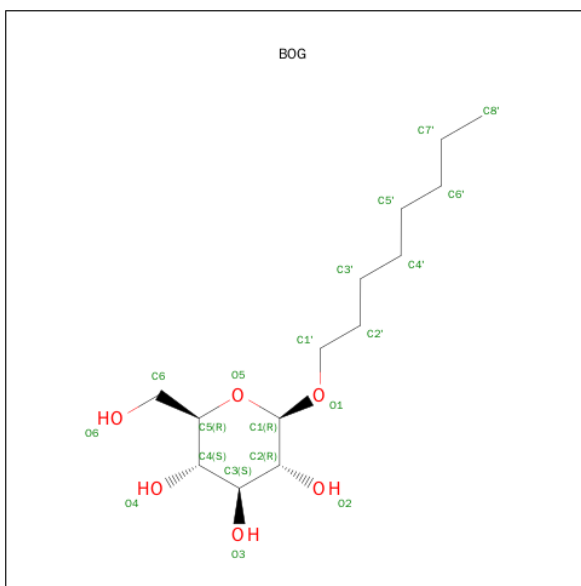


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	D	1	Total	C	N	O	0	0
			14	8	1	5		
2	D	1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

- Molecule 3 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	2	Total	C	N	O	0	0
			28	16	2	10		
3	B	2	Total	C	N	O	0	0
			28	16	2	10		
3	C	2	Total	C	N	O	0	0
			28	16	2	10		
3	D	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 4 is SUGAR (B-OCTYLGLUCOSIDE) (three-letter code: BOG) (formula: C₁₄H₂₈O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			20	14	6		
4	A	1	Total	C	O	0	0
			20	14	6		
4	B	1	Total	C	O	0	0
			20	14	6		
4	C	1	Total	C	O	0	0
			20	14	6		
4	C	1	Total	C	O	0	0
			20	14	6		
4	D	1	Total	C	O	0	0
			20	14	6		

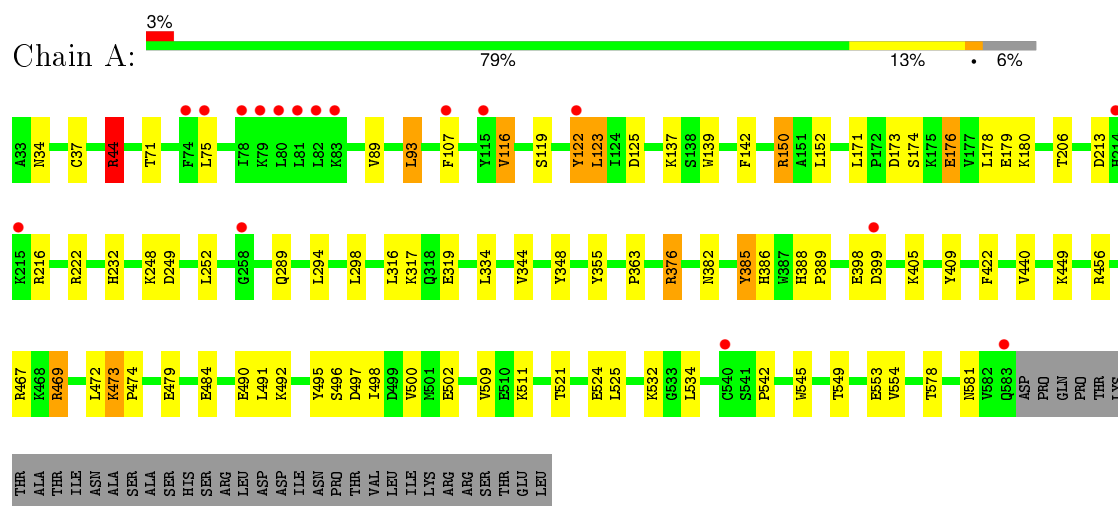
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	214	Total	O	0	0
			214	214		
5	B	212	Total	O	0	0
			212	212		
5	C	145	Total	O	0	0
			145	145		
5	D	166	Total	O	0	0
			166	166		

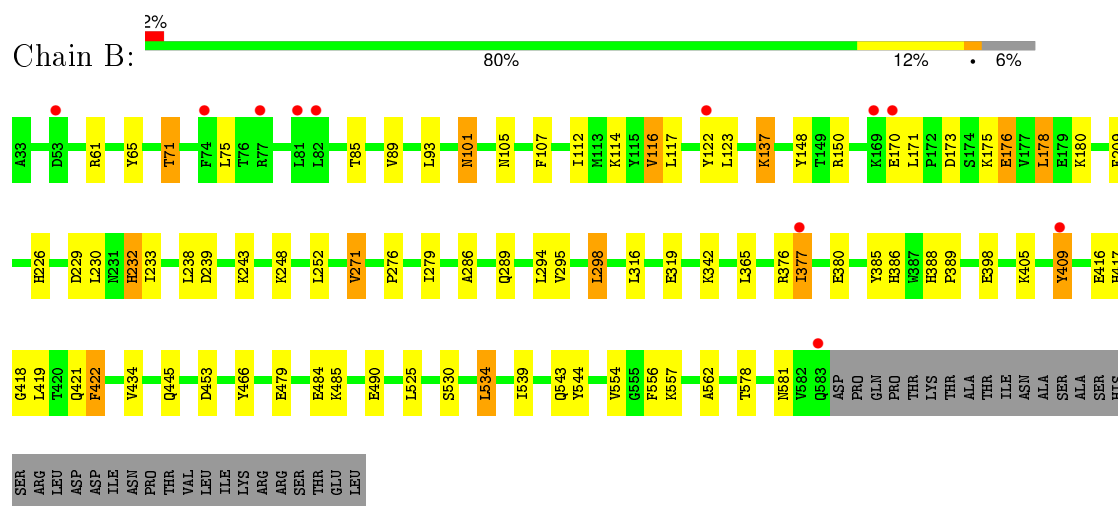
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

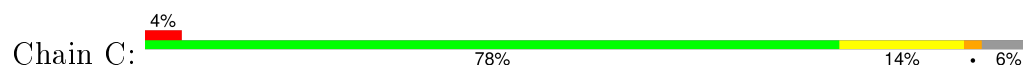
• Molecule 1: Prostaglandin G/H synthase 2

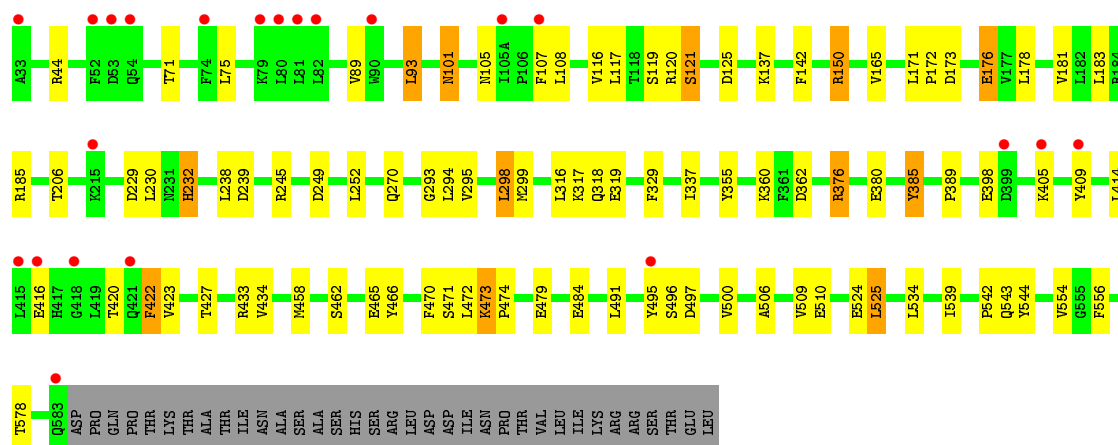


• Molecule 1: Prostaglandin G/H synthase 2

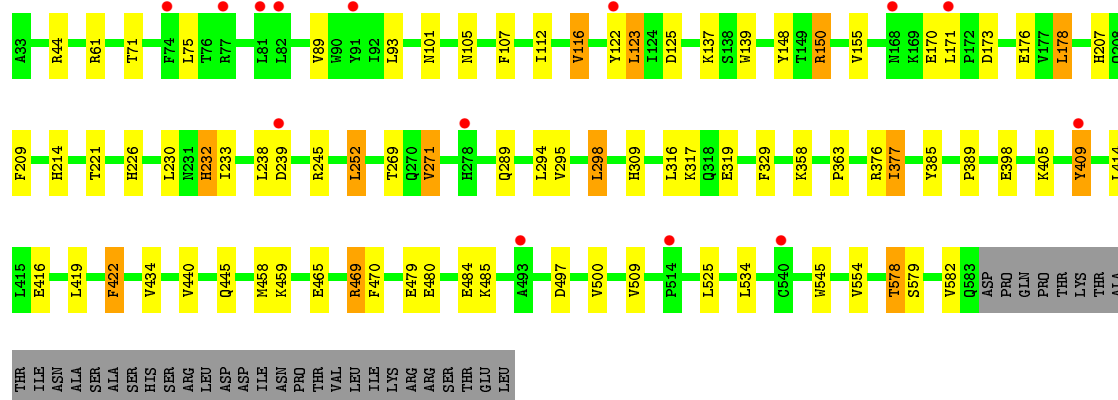
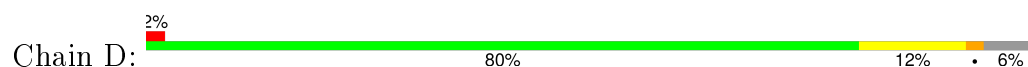


• Molecule 1: Prostaglandin G/H synthase 2





• Molecule 1: Prostaglandin G/H synthase 2



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	181.19Å 134.47Å 121.89Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.36 – 2.43 49.36 – 2.43	Depositor EDS
% Data completeness (in resolution range)	99.6 (49.36-2.43) 87.3 (49.36-2.43)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.73 (at 2.42Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, R_{free}	0.209 , 0.259 0.213 , 0.252	Depositor DCC
R_{free} test set	3370 reflections (3.53%)	DCC
Wilson B-factor (Å ²)	36.0	Xtriage
Anisotropy	0.655	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 41.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	6 of 112349 reflections (0.005%)	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	18993	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 48.89 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 8.0641e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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, BOG

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	0.31	0/4606	0.46	1/6247 (0.0%)
1	B	0.30	0/4606	0.45	0/6247
1	C	0.33	0/4606	0.46	0/6247
1	D	0.30	0/4606	0.46	0/6247
All	All	0.31	0/18424	0.46	1/24988 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	44	ARG	NE-CZ-NH1	5.69	123.14	120.30

There are no chirality outliers.

There are no planarity outliers.

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	4478	0	4376	46	0
1	B	4478	0	4376	42	0
1	C	4478	0	4376	52	0
1	D	4478	0	4376	41	0
2	A	28	0	26	0	0
2	B	28	0	26	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	28	0	26	0	0
2	D	28	0	26	0	0
3	A	28	0	25	1	0
3	B	28	0	25	0	0
3	C	28	0	25	0	0
3	D	28	0	25	0	0
4	A	40	0	56	3	0
4	B	20	0	28	2	0
4	C	40	0	56	5	0
4	D	20	0	28	1	0
5	A	214	0	0	5	0
5	B	212	0	0	5	0
5	C	145	0	0	0	0
5	D	166	0	0	6	0
All	All	18993	0	17876	173	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 5.

All (173) 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:C:120:ARG:HD3	4:C:706:BOG:O2	1.73	0.88
1:A:44:ARG:HH11	1:A:44:ARG:HG2	1.46	0.80
1:B:150:ARG:HD3	5:B:939:HOH:O	1.82	0.79
1:B:294:LEU:HD22	1:B:409:TYR:HD1	1.49	0.76
1:A:123:LEU:O	1:A:469:ARG:NH2	2.20	0.74
1:C:319:GLU:HG3	1:C:554:VAL:HG11	1.70	0.72
1:C:543:GLN:NE2	1:D:125:ASP:OD1	2.22	0.71
1:C:172:PRO:HG2	1:C:495:TYR:CZ	2.26	0.71
1:D:150:ARG:NH2	1:D:458:MET:O	2.25	0.69
1:B:319:GLU:HG3	1:B:554:VAL:HG11	1.75	0.69
1:B:479:GLU:OE2	1:B:485:LYS:HG2	1.94	0.68
1:C:116:VAL:O	1:C:120:ARG:HG2	1.94	0.66
1:A:319:GLU:HG3	1:A:554:VAL:HG11	1.77	0.65
1:D:479:GLU:CD	5:D:879:HOH:O	2.36	0.63
1:A:142:PHE:O	1:A:376:ARG:NH2	2.21	0.63
1:C:173:ASP:HB3	1:C:176:GLU:HB2	1.80	0.62
1:D:319:GLU:HG3	1:D:554:VAL:HG11	1.81	0.62
1:D:389:PRO:HG2	1:D:434:VAL:HA	1.81	0.61
1:D:485:LYS:NZ	5:D:879:HOH:O	2.32	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:150:ARG:NH2	1:C:458:MET:O	2.33	0.61
1:A:125:ASP:OD1	1:B:543:GLN:NE2	2.30	0.60
1:D:123:LEU:O	1:D:469:ARG:NH2	2.28	0.60
1:B:226:HIS:HA	1:B:377:ILE:HD13	1.83	0.60
1:D:245:ARG:HD3	1:D:329:PHE:CD1	2.36	0.60
1:C:116:VAL:HB	4:C:706:BOG:H2'2	1.83	0.60
1:B:294:LEU:HD22	1:B:409:TYR:CD1	2.34	0.59
1:C:44:ARG:HH11	1:C:44:ARG:HG2	1.68	0.59
1:B:175:LYS:NZ	5:B:822:HOH:O	2.34	0.59
1:A:294:LEU:HD22	1:A:409:TYR:HD1	1.67	0.58
1:C:294:LEU:HD22	1:C:409:TYR:HD1	1.67	0.58
1:D:294:LEU:HD22	1:D:409:TYR:HD1	1.67	0.58
1:D:209:PHE:HB2	1:D:377:ILE:HD12	1.85	0.58
1:C:172:PRO:CG	1:C:495:TYR:CE1	2.86	0.58
1:C:542:PRO:O	1:D:61:ARG:NH1	2.37	0.57
1:C:470:PHE:O	1:C:471:SER:HB2	2.04	0.57
1:A:495:TYR:O	1:A:496:SER:HB3	2.04	0.56
1:B:389:PRO:HG2	1:B:434:VAL:HA	1.89	0.55
1:B:85:THR:O	1:B:89:VAL:HG23	2.06	0.55
1:D:214:HIS:ND1	5:D:946:HOH:O	2.33	0.55
1:C:500:VAL:O	1:C:500:VAL:HG12	2.07	0.55
1:C:543:GLN:HE22	1:D:44:ARG:HH22	1.54	0.55
1:D:479:GLU:HG2	1:D:480:GLU:N	2.22	0.55
1:D:178:LEU:HD11	1:D:445:GLN:HB2	1.89	0.54
1:C:472:LEU:HD21	1:C:524:GLU:HG3	1.87	0.54
1:A:150:ARG:NH1	1:A:152:LEU:O	2.40	0.54
1:C:495:TYR:O	1:C:497:ASP:N	2.41	0.54
1:B:557:LYS:NZ	5:B:965:HOH:O	2.29	0.54
1:A:472:LEU:HD21	1:A:524:GLU:HG3	1.90	0.54
1:A:93:LEU:HD21	4:A:706:BOG:H4'1	1.89	0.54
1:C:142:PHE:O	1:C:376:ARG:NH2	2.25	0.53
1:A:216:ARG:NH1	3:A:703:NAG:O7	2.42	0.53
1:C:294:LEU:HD22	1:C:409:TYR:CD1	2.44	0.52
1:B:116:VAL:HG12	4:B:705:BOG:H4'2	1.91	0.52
1:B:230:LEU:HD13	1:B:233:ILE:HD12	1.90	0.52
1:A:456:ARG:NH2	1:A:502:GLU:OE1	2.39	0.52
1:A:213:ASP:HB2	1:A:222:ARG:HG3	1.91	0.52
1:C:389:PRO:HG2	1:C:434:VAL:HA	1.92	0.51
1:D:44:ARG:N	5:D:887:HOH:O	2.35	0.51
1:A:389:PRO:HD3	1:A:440:VAL:HG22	1.92	0.51
1:B:150:ARG:NH2	5:B:811:HOH:O	2.29	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:423:VAL:O	1:C:427:THR:OG1	2.25	0.51
1:D:101:ASN:O	1:D:105:ASN:ND2	2.39	0.51
1:B:209:PHE:O	1:B:377:ILE:HD12	2.11	0.51
1:C:380:GLU:HG2	1:C:466:TYR:CE1	2.46	0.50
1:C:206:THR:HG21	1:C:385:TYR:CE1	2.47	0.50
1:C:44:ARG:NH2	1:C:125:ASP:OD1	2.44	0.50
1:A:497:ASP:HB3	1:A:500:VAL:HG23	1.93	0.50
1:A:44:ARG:CG	1:A:44:ARG:HH11	2.21	0.49
1:B:230:LEU:HA	1:B:232:HIS:CE1	2.47	0.49
1:A:549:THR:OG1	1:B:137:LYS:NZ	2.44	0.49
1:A:553:GLU:HG3	5:A:930:HOH:O	2.13	0.49
1:A:294:LEU:HD22	1:A:409:TYR:CD1	2.47	0.49
1:C:172:PRO:HG2	1:C:495:TYR:CE1	2.48	0.49
1:C:172:PRO:CG	1:C:495:TYR:CZ	2.95	0.49
1:A:116:VAL:HB	4:A:706:BOG:H2'2	1.95	0.48
1:D:230:LEU:HD13	1:D:233:ILE:HD12	1.94	0.48
1:D:497:ASP:HB3	1:D:500:VAL:HG23	1.96	0.48
1:B:226:HIS:ND1	1:B:377:ILE:HG12	2.29	0.48
1:D:294:LEU:HD22	1:D:409:TYR:CD1	2.47	0.48
1:C:360:LYS:HE2	1:C:362:ASP:HB2	1.96	0.48
1:B:380:GLU:HG2	1:B:466:TYR:CE1	2.49	0.48
1:D:207:HIS:NE2	5:D:962:HOH:O	2.35	0.47
1:B:342:LYS:HG2	1:B:562:ALA:HB3	1.95	0.47
1:D:269:THR:OG1	1:D:271:VAL:HG13	2.14	0.47
1:B:417:HIS:O	1:B:421:GLN:HB2	2.15	0.47
1:B:89:VAL:HG11	4:B:705:BOG:H3'2	1.97	0.47
1:A:249:ASP:OD1	1:A:317:LYS:HE3	2.15	0.47
1:B:180:LYS:HB3	1:B:490:GLU:HG2	1.96	0.47
1:B:243:LYS:HB3	1:B:271:VAL:HG12	1.96	0.47
1:D:173:ASP:HB3	1:D:176:GLU:HB2	1.97	0.46
1:B:112:ILE:O	1:B:116:VAL:HG13	2.15	0.46
1:B:295:VAL:HB	1:B:298:LEU:HD22	1.96	0.46
1:A:467:ARG:NH1	1:A:521:THR:OG1	2.49	0.46
1:A:492:LYS:NZ	5:A:973:HOH:O	2.49	0.46
1:C:101:ASN:O	1:C:105:ASN:ND2	2.40	0.46
1:A:179:GLU:OE1	5:A:921:HOH:O	2.21	0.46
1:C:249:ASP:OD1	1:C:317:LYS:HE3	2.15	0.46
1:B:178:LEU:HD11	1:B:445:GLN:HB2	1.97	0.46
1:A:542:PRO:O	1:B:61:ARG:NH1	2.49	0.45
1:D:112:ILE:O	1:D:116:VAL:HG13	2.17	0.45
1:C:543:GLN:HE22	1:D:44:ARG:NH2	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:418:GLY:O	1:B:422:PHE:HB2	2.17	0.45
1:B:271:VAL:HG22	1:B:286:ALA:HB1	1.98	0.44
1:B:276:PRO:HG2	1:B:279:ILE:HG12	1.98	0.44
1:D:470:PHE:CG	1:D:525:LEU:HD22	2.53	0.44
1:D:89:VAL:HG11	4:D:705:BOG:H3'2	1.99	0.44
1:B:101:ASN:O	1:B:105:ASN:ND2	2.37	0.44
1:B:148:TYR:CD1	1:B:377:ILE:HG13	2.53	0.44
1:C:117:LEU:O	1:C:121:SER:OG	2.35	0.44
1:C:462:SER:OG	1:C:465:GLU:HG2	2.17	0.44
1:A:491:LEU:HD11	1:A:509:VAL:HG11	1.99	0.44
1:A:174:SER:OG	1:A:449:LYS:NZ	2.28	0.43
1:A:34:ASN:HB3	1:A:37:CYS:SG	2.58	0.43
1:C:495:TYR:O	1:C:496:SER:C	2.54	0.43
1:C:473:LYS:HA	1:C:474:PRO:HD3	1.88	0.43
1:A:344:VAL:O	1:A:348:TYR:HB3	2.18	0.43
1:C:185:ARG:NH2	4:C:705:BOG:H4'1	2.33	0.43
1:B:539:ILE:HA	1:B:544:TYR:HB3	2.00	0.43
1:C:89:VAL:HG11	4:C:706:BOG:H3'2	2.00	0.43
1:C:119:SER:O	1:C:120:ARG:C	2.55	0.43
1:D:155:VAL:HB	1:D:459:LYS:HE2	2.00	0.43
1:D:389:PRO:HD3	1:D:440:VAL:HG22	2.01	0.43
1:D:226:HIS:HA	1:D:377:ILE:HD13	2.00	0.43
1:A:382:ASN:OD1	1:A:386:HIS:HE1	2.02	0.43
1:C:470:PHE:CG	1:C:525:LEU:HD22	2.54	0.42
1:D:363:PRO:HG2	1:D:545:TRP:CD2	2.53	0.42
1:D:479:GLU:HG2	1:D:480:GLU:H	1.83	0.42
1:A:511:LYS:O	5:A:828:HOH:O	2.21	0.42
1:D:578:THR:HG22	1:D:579:SER:H	1.84	0.42
1:B:173:ASP:HB3	1:B:176:GLU:HB2	2.01	0.42
1:B:65:TYR:O	1:B:71:THR:HG23	2.20	0.42
1:D:465:GLU:OE1	5:D:931:HOH:O	2.22	0.42
1:A:44:ARG:NH2	1:A:125:ASP:OD1	2.48	0.42
1:D:44:ARG:HD2	1:D:469:ARG:HE	1.84	0.42
1:A:334:LEU:HA	1:A:334:LEU:HD23	1.85	0.42
1:C:414:LEU:HA	1:C:422:PHE:CE1	2.54	0.42
1:A:93:LEU:HB3	1:A:355:TYR:CD1	2.54	0.42
1:C:295:VAL:HB	1:C:298:LEU:HD22	2.01	0.42
1:C:229:ASP:HB3	1:D:139:TRP:CZ2	2.54	0.42
4:C:705:BOG:H7'1	4:C:705:BOG:H4'2	1.78	0.42
1:A:473:LYS:HA	1:A:474:PRO:HD3	1.91	0.42
1:C:539:ILE:HA	1:C:544:TYR:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:388:HIS:N	1:A:389:PRO:HD2	2.34	0.42
1:C:230:LEU:HG	1:C:337:ILE:HG12	2.02	0.42
1:A:180:LYS:HD3	1:A:490:GLU:HG3	2.02	0.42
1:A:89:VAL:HG11	4:A:706:BOG:H3'2	2.02	0.41
1:A:456:ARG:HA	5:A:949:HOH:O	2.21	0.41
1:A:363:PRO:HG2	1:A:545:TRP:CD2	2.55	0.41
1:D:414:LEU:HA	1:D:422:PHE:CE1	2.55	0.41
1:B:114:LYS:HE2	1:B:365:LEU:O	2.19	0.41
1:C:172:PRO:HG3	1:C:495:TYR:CD1	2.54	0.41
1:D:295:VAL:HB	1:D:298:LEU:HD22	2.01	0.41
1:B:386:HIS:HB3	1:B:388:HIS:CE1	2.55	0.41
1:C:245:ARG:HD3	1:C:329:PHE:CD1	2.56	0.41
1:B:148:TYR:HD1	1:B:377:ILE:HG13	1.85	0.41
1:C:506:ALA:O	1:C:510:GLU:HB2	2.21	0.41
1:B:530:SER:O	1:B:534:LEU:HD22	2.20	0.41
1:A:206:THR:HG21	1:A:385:TYR:CE1	2.54	0.41
1:C:181:VAL:HG21	1:C:491:LEU:HD21	2.01	0.41
1:A:386:HIS:HB3	1:A:388:HIS:CE1	2.56	0.41
1:D:252:LEU:HD22	1:D:309:HIS:CD2	2.56	0.41
1:A:173:ASP:HB3	1:A:176:GLU:HB2	2.03	0.41
1:C:389:PRO:HB2	1:C:433:ARG:O	2.21	0.41
1:D:230:LEU:HA	1:D:232:HIS:CE1	2.56	0.41
1:B:453:ASP:OD2	5:B:867:HOH:O	2.22	0.41
1:C:183:LEU:HD23	1:C:183:LEU:HA	1.93	0.41
1:A:497:ASP:OD1	1:A:498:ILE:N	2.53	0.40
1:C:230:LEU:HD22	1:C:232:HIS:HE1	1.86	0.40
1:D:148:TYR:CZ	1:D:221:THR:HB	2.56	0.40
1:C:293:GLY:HA2	1:C:299:MET:HE3	2.03	0.40
1:A:139:TRP:CZ2	1:B:229:ASP:HB3	2.57	0.40
1:C:93:LEU:HB3	1:C:355:TYR:CD1	2.57	0.40
1:A:119:SER:O	1:A:122:TYR:HD1	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	550/587 (94%)	528 (96%)	21 (4%)	1 (0%)	52	69
1	B	550/587 (94%)	534 (97%)	14 (2%)	2 (0%)	39	54
1	C	550/587 (94%)	523 (95%)	24 (4%)	3 (0%)	34	47
1	D	550/587 (94%)	533 (97%)	16 (3%)	1 (0%)	52	69
All	All	2200/2348 (94%)	2118 (96%)	75 (3%)	7 (0%)	46	62

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	416	GLU
1	A	398	GLU
1	D	398	GLU
1	C	398	GLU
1	B	398	GLU
1	B	416	GLU
1	C	420	THR

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	493/525 (94%)	460 (93%)	33 (7%)	20	31
1	B	493/525 (94%)	457 (93%)	36 (7%)	17	27
1	C	493/525 (94%)	460 (93%)	33 (7%)	20	31
1	D	493/525 (94%)	457 (93%)	36 (7%)	17	27
All	All	1972/2100 (94%)	1834 (93%)	138 (7%)	19	29

All (138) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	ARG

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Mol	Chain	Res	Type
1	A	71	THR
1	A	75	LEU
1	A	93	LEU
1	A	107	PHE
1	A	116	VAL
1	A	122	TYR
1	A	123	LEU
1	A	137	LYS
1	A	150	ARG
1	A	171	LEU
1	A	176	GLU
1	A	178	LEU
1	A	232	HIS
1	A	248	LYS
1	A	252	LEU
1	A	289	GLN
1	A	298	LEU
1	A	316	LEU
1	A	376	ARG
1	A	385	TYR
1	A	399	ASP
1	A	405	LYS
1	A	422	PHE
1	A	469	ARG
1	A	473	LYS
1	A	479	GLU
1	A	484	GLU
1	A	525	LEU
1	A	532	LYS
1	A	534	LEU
1	A	578	THR
1	A	581	ASN
1	B	71	THR
1	B	75	LEU
1	B	93	LEU
1	B	101	ASN
1	B	107	PHE
1	B	116	VAL
1	B	117	LEU
1	B	122	TYR
1	B	123	LEU
1	B	137	LYS

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Mol	Chain	Res	Type
1	B	170	GLU
1	B	171	LEU
1	B	176	GLU
1	B	178	LEU
1	B	232	HIS
1	B	238	LEU
1	B	239	ASP
1	B	248	LYS
1	B	252	LEU
1	B	271	VAL
1	B	289	GLN
1	B	298	LEU
1	B	316	LEU
1	B	376	ARG
1	B	377	ILE
1	B	385	TYR
1	B	405	LYS
1	B	409	TYR
1	B	419	LEU
1	B	422	PHE
1	B	484	GLU
1	B	525	LEU
1	B	534	LEU
1	B	556	PHE
1	B	578	THR
1	B	581	ASN
1	C	71	THR
1	C	75	LEU
1	C	93	LEU
1	C	101	ASN
1	C	107	PHE
1	C	108	LEU
1	C	121	SER
1	C	137	LYS
1	C	150	ARG
1	C	165	VAL
1	C	171	LEU
1	C	176	GLU
1	C	178	LEU
1	C	232	HIS
1	C	238	LEU
1	C	239	ASP

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Mol	Chain	Res	Type
1	C	252	LEU
1	C	270	GLN
1	C	298	LEU
1	C	316	LEU
1	C	318	GLN
1	C	376	ARG
1	C	385	TYR
1	C	405	LYS
1	C	422	PHE
1	C	473	LYS
1	C	479	GLU
1	C	484	GLU
1	C	509	VAL
1	C	525	LEU
1	C	534	LEU
1	C	556	PHE
1	C	578	THR
1	D	71	THR
1	D	75	LEU
1	D	93	LEU
1	D	107	PHE
1	D	116	VAL
1	D	122	TYR
1	D	123	LEU
1	D	137	LYS
1	D	150	ARG
1	D	170	GLU
1	D	171	LEU
1	D	178	LEU
1	D	232	HIS
1	D	238	LEU
1	D	239	ASP
1	D	252	LEU
1	D	271	VAL
1	D	289	GLN
1	D	298	LEU
1	D	316	LEU
1	D	317	LYS
1	D	358	LYS
1	D	376	ARG
1	D	377	ILE
1	D	385	TYR

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Mol	Chain	Res	Type
1	D	405	LYS
1	D	409	TYR
1	D	416	GLU
1	D	419	LEU
1	D	422	PHE
1	D	469	ARG
1	D	484	GLU
1	D	509	VAL
1	D	534	LEU
1	D	578	THR
1	D	582	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

8 carbohydrates are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	NAG	A	702	1,3	14,14,15	0.18	0	15,19,21	0.51	0
3	NAG	A	703	3	14,14,15	0.23	0	15,19,21	0.40	0
3	NAG	B	702	1,3	14,14,15	0.34	0	15,19,21	0.40	0
3	NAG	B	703	3	14,14,15	0.24	0	15,19,21	0.36	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	C	702	1,3	14,14,15	0.24	0	15,19,21	0.47	0
3	NAG	C	703	3	14,14,15	0.28	0	15,19,21	0.43	0
3	NAG	D	702	1,3	14,14,15	0.31	0	15,19,21	0.47	0
3	NAG	D	703	3	14,14,15	0.30	0	15,19,21	0.36	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
3	NAG	A	702	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	703	3	-	0/6/23/26	0/1/1/1
3	NAG	B	702	1,3	-	0/6/23/26	0/1/1/1
3	NAG	B	703	3	-	0/6/23/26	0/1/1/1
3	NAG	C	702	1,3	-	0/6/23/26	0/1/1/1
3	NAG	C	703	3	-	0/6/23/26	0/1/1/1
3	NAG	D	702	1,3	-	0/6/23/26	0/1/1/1
3	NAG	D	703	3	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	703	NAG	1	0

5.6 Ligand geometry ⓘ

14 ligands are modelled in this entry.

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
2	NAG	A	701	1	14,14,15	0.34	0	15,19,21	0.48	0
2	NAG	A	704	1	14,14,15	0.24	0	15,19,21	0.18	0
4	BOG	A	705	-	20,20,20	1.06	1 (5%)	25,25,25	1.21	3 (12%)
4	BOG	A	706	-	20,20,20	1.07	1 (5%)	25,25,25	1.18	3 (12%)
2	NAG	B	701	1	14,14,15	0.22	0	15,19,21	0.46	0
2	NAG	B	704	1	14,14,15	0.45	0	15,19,21	0.36	0
4	BOG	B	705	-	20,20,20	1.05	1 (5%)	25,25,25	1.16	3 (12%)
2	NAG	C	701	1	14,14,15	0.22	0	15,19,21	0.39	0
2	NAG	C	704	1	14,14,15	0.34	0	15,19,21	0.16	0
4	BOG	C	705	-	20,20,20	1.02	1 (5%)	25,25,25	1.17	3 (12%)
4	BOG	C	706	-	20,20,20	1.05	1 (5%)	25,25,25	1.16	3 (12%)
2	NAG	D	701	1	14,14,15	0.45	0	15,19,21	0.41	0
2	NAG	D	704	1	14,14,15	0.30	0	15,19,21	0.37	0
4	BOG	D	705	-	20,20,20	1.05	1 (5%)	25,25,25	1.12	3 (12%)

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
2	NAG	A	701	1	-	0/6/23/26	0/1/1/1
2	NAG	A	704	1	-	0/6/23/26	0/1/1/1
4	BOG	A	705	-	-	0/11/31/31	0/1/1/1
4	BOG	A	706	-	-	0/11/31/31	0/1/1/1
2	NAG	B	701	1	-	0/6/23/26	0/1/1/1
2	NAG	B	704	1	-	0/6/23/26	0/1/1/1
4	BOG	B	705	-	-	0/11/31/31	0/1/1/1
2	NAG	C	701	1	-	0/6/23/26	0/1/1/1
2	NAG	C	704	1	-	0/6/23/26	0/1/1/1
4	BOG	C	705	-	-	0/11/31/31	0/1/1/1
4	BOG	C	706	-	-	0/11/31/31	0/1/1/1
2	NAG	D	701	1	-	0/6/23/26	0/1/1/1
2	NAG	D	704	1	-	0/6/23/26	0/1/1/1
4	BOG	D	705	-	-	0/11/31/31	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	705	BOG	O2-C2	-2.53	1.36	1.43
4	A	705	BOG	O2-C2	-2.52	1.36	1.43
4	A	706	BOG	O2-C2	-2.52	1.36	1.43
4	C	706	BOG	O2-C2	-2.50	1.37	1.43
4	D	705	BOG	O2-C2	-2.46	1.37	1.43
4	B	705	BOG	O2-C2	-2.46	1.37	1.43

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	706	BOG	C1-O5-C5	-2.77	108.36	113.75
4	B	705	BOG	C1-O5-C5	-2.64	108.62	113.75
4	A	706	BOG	C1-O5-C5	-2.61	108.67	113.75
4	D	705	BOG	C1-O5-C5	-2.60	108.70	113.75
4	C	705	BOG	C1-O5-C5	-2.25	109.37	113.75
4	A	705	BOG	C1-O5-C5	-2.15	109.57	113.75
4	D	705	BOG	O1-C1-C2	2.12	110.72	108.04
4	B	705	BOG	O1-C1-C2	2.22	110.85	108.04
4	C	705	BOG	O1-C1-C2	2.27	110.90	108.04
4	C	706	BOG	O1-C1-C2	2.34	111.00	108.04
4	A	706	BOG	O1-C1-C2	2.55	111.25	108.04
4	A	705	BOG	C1'-O1-C1	2.57	118.43	113.94
4	A	706	BOG	C1'-O1-C1	3.18	119.51	113.94
4	C	706	BOG	C1'-O1-C1	3.22	119.58	113.94
4	D	705	BOG	C1'-O1-C1	3.29	119.69	113.94
4	B	705	BOG	C1'-O1-C1	3.30	119.71	113.94
4	C	705	BOG	C1'-O1-C1	3.46	119.99	113.94
4	A	705	BOG	O1-C1-C2	3.95	113.03	108.04

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	706	BOG	3	0
4	B	705	BOG	2	0
4	C	705	BOG	2	0
4	C	706	BOG	3	0
4	D	705	BOG	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	552/587 (94%)	-0.17	17 (3%) 52 51	26, 41, 69, 98	0
1	B	552/587 (94%)	-0.11	11 (1%) 68 67	25, 40, 69, 90	0
1	C	552/587 (94%)	-0.02	22 (3%) 42 42	28, 53, 83, 106	0
1	D	552/587 (94%)	0.01	14 (2%) 61 60	27, 48, 77, 95	0
All	All	2208/2348 (94%)	-0.07	64 (2%) 55 54	25, 45, 77, 106	0

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	583	GLN	7.1
1	C	409	TYR	4.8
1	C	81	LEU	4.3
1	C	82	LEU	4.0
1	C	215	LYS	4.0
1	A	75	LEU	3.8
1	D	82	LEU	3.5
1	C	74	PHE	3.4
1	A	82	LEU	3.3
1	C	105(A)	ILE	3.1
1	A	583	GLN	3.1
1	C	80	LEU	3.0
1	D	278	HIS	3.0
1	A	79	LYS	3.0
1	D	409	TYR	3.0
1	A	107	PHE	3.0
1	A	115	TYR	3.0
1	A	80	LEU	2.9
1	C	90	TRP	2.9
1	C	399	ASP	2.9
1	C	53	ASP	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	74	PHE	2.8
1	B	583	GLN	2.8
1	A	81	LEU	2.8
1	C	52	PHE	2.8
1	B	81	LEU	2.7
1	D	77	ARG	2.7
1	C	416	GLU	2.7
1	B	82	LEU	2.7
1	C	405	LYS	2.7
1	B	409	TYR	2.6
1	D	91	TYR	2.6
1	C	421	GLN	2.6
1	A	215	LYS	2.5
1	B	377	ILE	2.5
1	C	33	ALA	2.5
1	D	493	ALA	2.5
1	A	540	CYS	2.5
1	B	169	LYS	2.5
1	D	74	PHE	2.4
1	A	258	GLY	2.4
1	D	168	ASN	2.4
1	B	74	PHE	2.3
1	A	78	ILE	2.3
1	B	53	ASP	2.3
1	A	122	TYR	2.3
1	B	122	TYR	2.3
1	B	170	GLU	2.2
1	A	214	HIS	2.2
1	C	107	PHE	2.2
1	C	495	TYR	2.2
1	C	79	LYS	2.2
1	D	81	LEU	2.2
1	D	514	PRO	2.2
1	A	399	ASP	2.1
1	C	54	GLN	2.1
1	D	122	TYR	2.1
1	C	418	GLY	2.1
1	D	239	ASP	2.1
1	A	83	LYS	2.0
1	B	77	ARG	2.0
1	C	415	LEU	2.0
1	D	540	CYS	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	171	LEU	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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	NAG	B	702	14/15	0.96	0.12	-0.80	30,39,47,59	0
3	NAG	A	702	14/15	0.95	0.11	-1.64	28,36,42,53	0
3	NAG	C	702	14/15	0.96	0.10	-1.92	31,44,49,51	0
3	NAG	D	702	14/15	0.95	0.10	-2.21	27,38,45,55	0
3	NAG	B	703	14/15	0.92	0.14	-	48,66,73,78	0
3	NAG	C	703	14/15	0.93	0.21	-	54,59,69,72	0
3	NAG	A	703	14/15	0.90	0.20	-	56,66,73,76	0
3	NAG	D	703	14/15	0.93	0.16	-	52,60,69,71	0

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
4	BOG	D	705	20/20	0.58	0.54	6.67	139,147,151,151	0
4	BOG	C	706	20/20	0.59	0.45	6.24	133,145,148,150	0
4	BOG	A	706	20/20	0.47	0.57	5.40	134,147,150,153	0
4	BOG	B	705	20/20	0.69	0.40	5.09	137,142,147,147	0
2	NAG	B	701	14/15	0.72	0.29	3.90	68,79,86,91	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	BOG	A	705	20/20	0.88	0.21	2.68	44,58,97,99	0
4	BOG	C	705	20/20	0.84	0.27	2.51	59,72,86,87	0
2	NAG	D	701	14/15	0.75	0.17	1.87	63,74,82,85	0
2	NAG	A	701	14/15	0.83	0.18	1.80	61,72,88,90	0
2	NAG	A	704	14/15	0.89	0.24	0.56	58,68,76,77	0
2	NAG	D	704	14/15	0.83	0.16	0.25	56,62,73,75	0
2	NAG	C	704	14/15	0.78	0.24	-0.10	63,72,85,92	0
2	NAG	B	704	14/15	0.91	0.13	-0.47	46,55,62,68	0
2	NAG	C	701	14/15	0.86	0.25	-	63,80,87,88	0

6.5 Other polymers [i](#)

There are no such residues in this entry.