Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 08:25 PM GMT

PDB ID	:	4RUT
Title	:	crystal structure of murine cyclooxygenase-2 with 13-methyl-arachidonic Acid
Authors	:	Xu, S.; Kudalkar, S.N.; Banerjee, S.; Makriyannis, A.; Nikas, S.P.; Marnett, L.J.
Deposited on	:	2014-11-21
Resolution	:	2.16 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

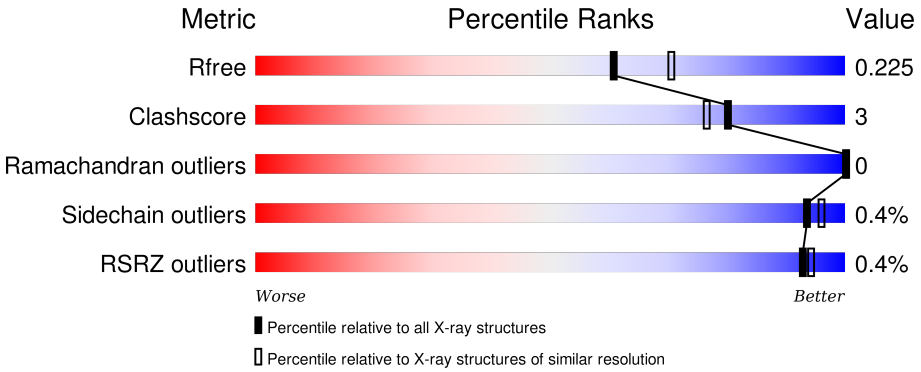
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.16 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	1045 (2.16-2.16)
Clashscore	102246	1152 (2.16-2.16)
Ramachandran outliers	100387	1131 (2.16-2.16)
Sidechain outliers	100360	1131 (2.16-2.16)
RSRZ outliers	91569	1050 (2.16-2.16)

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 <=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	88% 6% 6%
1	B	587	88% 6% 6%
1	C	587	88% 6% 6%
1	D	587	86% 8% 6%

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	COH	A	705	-	-	-	X
4	COH	D	705	-	-	-	X
5	LM8	A	706	-	-	-	X
5	LM8	B	706	-	-	-	X
5	LM8	C	706	-	-	-	X
5	LM8	D	706	-	-	-	X
6	BOG	D	707	-	-	-	X

2 Entry composition

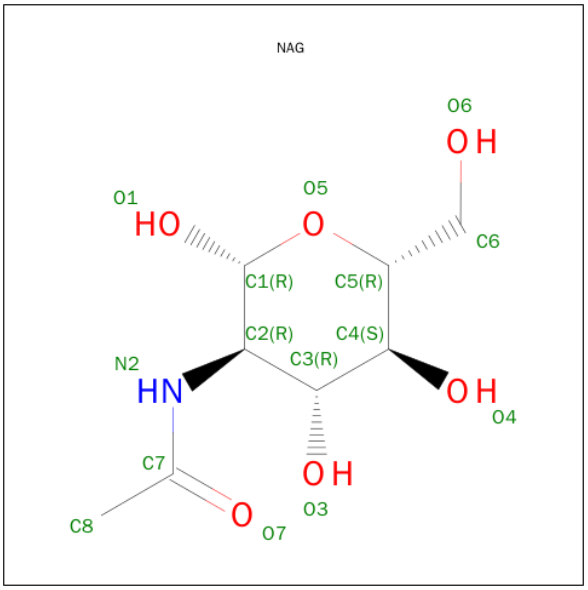
There are 7 unique types of molecules in this entry. The entry contains 19562 atoms, of which 0 are hydrogens and 0 are deuteriums.

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
			4474	2885	750	814	25			
1	B	552	Total	C	N	O	S	0	0	0
			4474	2885	750	814	25			
1	C	552	Total	C	N	O	S	0	0	0
			4474	2885	750	814	25			
1	D	552	Total	C	N	O	S	0	0	0
			4474	2885	750	814	25			

- Molecule 2 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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		

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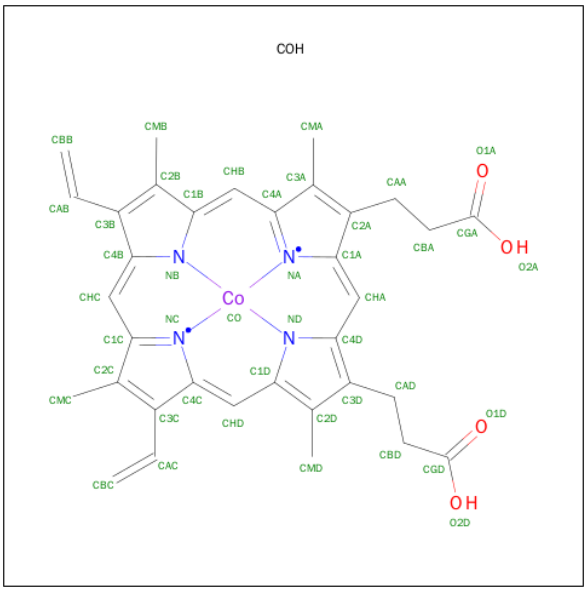
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	D	1	Total	C	N	O	0	0
			14	8	1	5		
2	D	1	Total	C	N	O	0	0
			14	8	1	5		

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

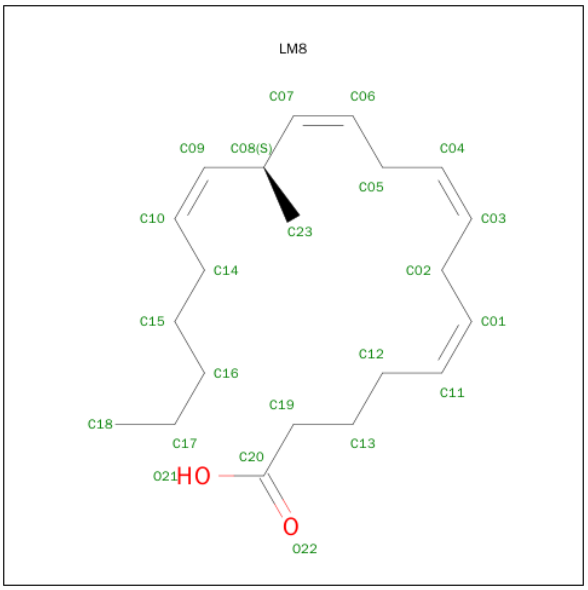
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	2	Total	C	N	O	0	0
			28	16	2	10		
3	B	2	Total	C	N	O	0	0
			28	16	2	10		
3	C	2	Total	C	N	O	0	0
			28	16	2	10		
3	D	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 4 is PROTOPORPHYRIN IX CONTAINING CO (three-letter code: COH) (formula: $C_{34}H_{32}CoN_4O_4$).



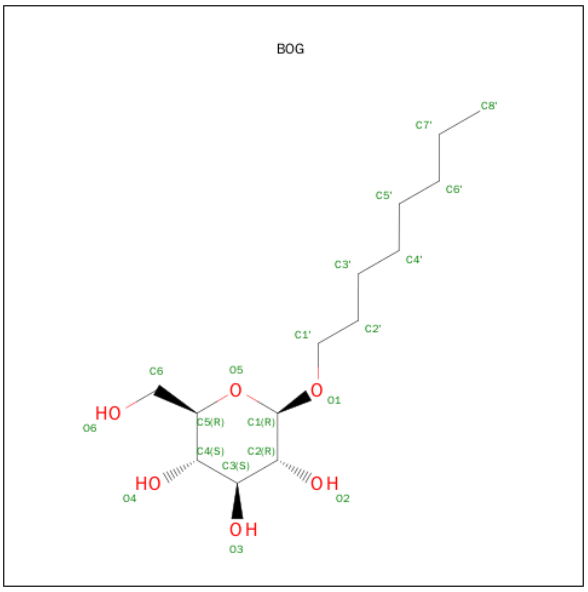
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	Co	N	O	0	0
			43	34	1	4	4		
4	B	1	Total	C	Co	N	O	0	0
			43	34	1	4	4		
4	C	1	Total	C	Co	N	O	0	0
			43	34	1	4	4		
4	D	1	Total	C	Co	N	O	0	0
			43	34	1	4	4		

- Molecule 5 is (5Z,8Z,11Z,13S,14Z)-13-METHYLICOSA-5,8,11,14-TETRAENOIC ACID (three-letter code: LM8) (formula: $C_{21}H_{34}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			23	21	2		
5	B	1	Total	C	O	0	0
			23	21	2		
5	C	1	Total	C	O	0	0
			23	21	2		
5	D	1	Total	C	O	0	0
			23	21	2		

- Molecule 6 is SUGAR (B-OCTYLGLUCOSIDE) (three-letter code: BOG) (formula: $C_{14}H_{28}O_6$).



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

- Molecule 7 is water.

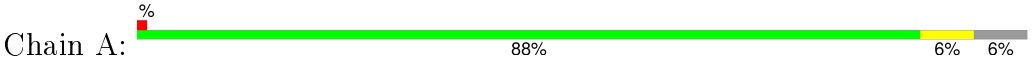
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	276	Total O 276 276	0	0
7	B	306	Total O 306 306	0	0
7	C	288	Total O 288 288	0	0
7	D	268	Total O 268 268	0	0

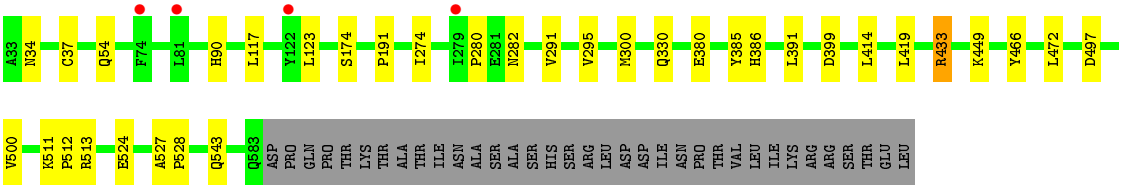
3 Residue-property plots (i)

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

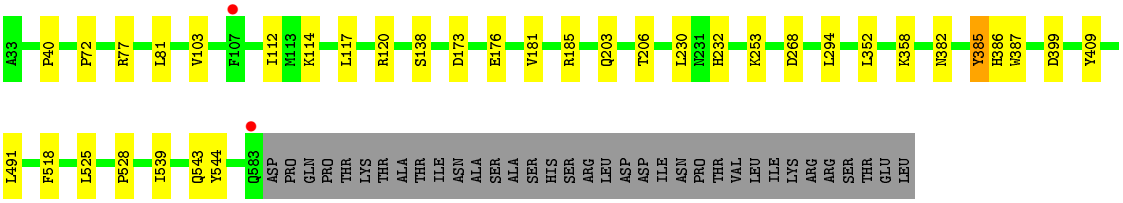
Chain A:





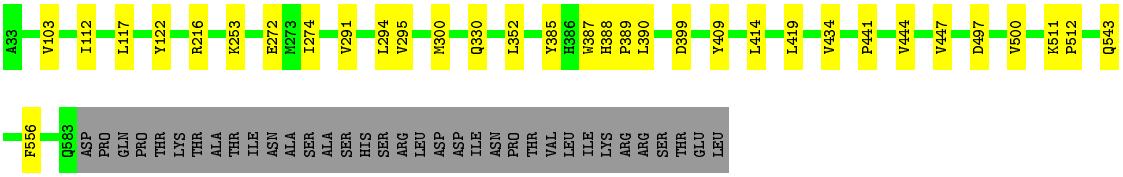
- Molecule 1: Prostaglandin G/H synthase 2

Chain B:



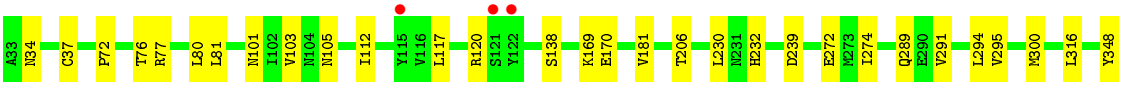
- Molecule 1: Prostaglandin G/H synthase 2

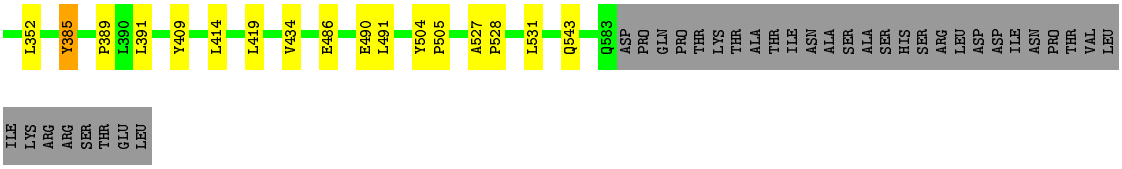
Chain C:



- Molecule 1: Prostaglandin G/H synthase 2

Chain D:




L352
Y385
P389
L390
L391
Y409
L414
L419
V434
E486
E490
L491
Y504
P505
A527
P528
L531
Q543
Q583
ASP
PRO
GLN
PRO
THR
LYS
THR
ALA
THR
ILE
ASN
ALA
SER
ALA
SER
HIS
SER
ARG
LEU
ASP
ASP
ILE
ASN
PRO
THR
VAL
LEU
ILE
LYS
ARG
ARG
SER
THR
GLU
LEU

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	215.80Å 121.54Å 134.94Å 90.00° 123.60° 90.00°	Depositor
Resolution (Å)	112.39 – 2.16 112.40 – 2.16	Depositor EDS
% Data completeness (in resolution range)	98.1 (112.39-2.16) 87.8 (112.40-2.16)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.71 (at 2.16Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.176 , 0.224 0.184 , 0.225	Depositor DCC
R_{free} test set	4543 reflections (3.43%)	DCC
Wilson B-factor (Å^2)	34.4	Xtriage
Anisotropy	0.191	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 45.7	EDS
Estimated twinning fraction	0.009 for 1/2*h-3/2*k,-1/2*h-1/2*k,-1/2*h+1/2*k-l 0.015 for 1/2*h+3/2*k,1/2*h-1/2*k,-1/2*h-1/2*k-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	1 of 152390 reflections (0.001%)	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	19562	wwPDB-VP
Average B, all atoms (Å^2)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.51% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: LM8, COH, 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	0.44	0/4601	0.55	0/6239
1	B	0.45	0/4601	0.56	0/6239
1	C	0.46	0/4601	0.56	0/6239
1	D	0.44	0/4601	0.54	0/6239
All	All	0.45	0/18404	0.55	0/24956

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	4474	0	4373	28	0
1	B	4474	0	4373	32	0
1	C	4474	0	4373	26	0
1	D	4474	0	4373	37	0
2	A	28	0	26	0	0
2	B	28	0	26	1	0
2	C	28	0	26	0	0
2	D	28	0	26	0	0
3	A	28	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	28	0	25	0	0
3	C	28	0	25	1	0
3	D	28	0	25	0	0
4	A	43	0	30	5	0
4	B	43	0	30	2	0
4	C	43	0	30	5	0
4	D	43	0	30	6	0
5	A	23	0	33	3	0
5	B	23	0	33	1	0
5	C	23	0	33	3	0
5	D	23	0	33	3	0
6	B	20	0	28	7	0
6	D	20	0	28	2	0
7	A	276	0	0	3	0
7	B	306	0	0	4	0
7	C	288	0	0	2	0
7	D	268	0	0	1	0
All	All	19562	0	18004	125	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 3.

All (125) 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:B:72:PRO:HG2	1:B:77:ARG:HE	1.28	0.97
1:B:185:ARG:HE	6:B:707:BOG:C6	1.98	0.77
1:A:295:VAL:HG11	4:A:705:COH:HBB1	1.72	0.70
1:B:185:ARG:HE	6:B:707:BOG:H61	1.55	0.70
1:D:72:PRO:HG2	1:D:77:ARG:HE	1.58	0.69
1:C:295:VAL:HG11	4:C:705:COH:HBB1	1.73	0.69
1:B:185:ARG:HH21	6:B:707:BOG:C6	2.09	0.65
1:C:122:TYR:OH	7:C:945:HOH:O	2.02	0.63
1:C:272:GLU:H	1:C:272:GLU:CD	2.03	0.61
1:D:206:THR:HG21	1:D:385:TYR:CE1	2.35	0.61
1:D:169:LYS:HD2	1:D:170:GLU:HG2	1.82	0.61
1:D:103:VAL:HG11	1:D:112:ILE:HD12	1.84	0.59
4:D:705:COH:HBC1	4:D:705:COH:HMC1	1.88	0.56
1:C:388:HIS:HE1	1:C:447:VAL:HG11	1.69	0.56
1:B:114:LYS:NZ	7:B:929:HOH:O	2.39	0.55
1:A:117:LEU:CD2	5:A:706:LM8:H28	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:120:ARG:NH1	7:B:1037:HOH:O	2.41	0.54
1:C:295:VAL:HG11	4:C:705:COH:CBB	2.37	0.53
4:A:705:COH:HBC1	4:A:705:COH:HMC1	1.90	0.53
1:A:174:SER:OG	1:A:449:LYS:NZ	2.42	0.53
1:C:352:LEU:CD1	5:C:706:LM8:H5	2.39	0.52
1:D:272:GLU:CD	1:D:272:GLU:H	2.12	0.52
1:C:272:GLU:N	1:C:272:GLU:OE1	2.42	0.52
1:D:101:ASN:O	1:D:105:ASN:ND2	2.37	0.52
1:B:294:LEU:HA	1:B:409:TYR:CE1	2.46	0.51
1:B:185:ARG:HH21	6:B:707:BOG:H61	1.74	0.51
1:A:472:LEU:HD21	1:A:524:GLU:HG3	1.93	0.51
1:B:40:PRO:HA	2:B:701:NAG:H82	1.93	0.51
1:C:216:ARG:NH1	3:C:703:NAG:O7	2.44	0.51
1:D:295:VAL:HG11	4:D:705:COH:CBB	2.41	0.51
1:A:295:VAL:HG11	4:A:705:COH:CBB	2.39	0.50
1:A:391:LEU:CD2	4:A:705:COH:HAB	2.41	0.50
1:D:294:LEU:HG	1:D:295:VAL:HG13	1.94	0.50
1:D:294:LEU:HA	1:D:409:TYR:CE1	2.47	0.50
1:C:543:GLN:HA	1:C:543:GLN:OE1	2.12	0.50
1:D:34:ASN:HB3	1:D:37:CYS:SG	2.52	0.49
1:A:391:LEU:HD21	4:A:705:COH:HAB	1.94	0.49
1:A:117:LEU:HD21	5:A:706:LM8:C18	2.42	0.49
1:D:117:LEU:CD2	5:D:706:LM8:H28	2.43	0.49
1:C:103:VAL:HG11	1:C:112:ILE:HD12	1.94	0.49
1:C:497:ASP:HB3	1:C:500:VAL:HG23	1.94	0.49
1:C:352:LEU:CD1	5:C:706:LM8:C04	2.91	0.48
1:B:185:ARG:NE	6:B:707:BOG:C6	2.72	0.48
1:D:348:TYR:OH	1:D:385:TYR:OH	2.24	0.48
1:D:352:LEU:CD1	5:D:706:LM8:H5	2.43	0.48
1:A:280:PRO:HB2	1:A:282:ASN:OD1	2.13	0.48
1:B:77:ARG:O	1:B:81:LEU:HD23	2.14	0.48
1:D:274:ILE:HD12	1:D:291:VAL:HG12	1.94	0.48
1:A:300:MET:HG3	1:A:419:LEU:HD22	1.95	0.48
1:B:382:ASN:O	1:B:386:HIS:HD2	1.97	0.48
1:C:414:LEU:HD11	1:C:419:LEU:HD23	1.96	0.47
1:D:391:LEU:HD21	4:D:705:COH:HAB	1.96	0.47
1:C:441:PRO:HG2	1:C:444:VAL:HG22	1.95	0.47
1:A:386:HIS:HE1	7:A:1010:HOH:O	1.96	0.47
1:A:380:GLU:HG2	1:A:466:TYR:CE1	2.49	0.47
1:D:352:LEU:CD1	5:D:706:LM8:C04	2.93	0.47
1:D:181:VAL:HG21	1:D:491:LEU:HD21	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:117:LEU:CD2	5:C:706:LM8:H28	2.45	0.47
1:A:543:GLN:OE1	1:A:543:GLN:HA	2.15	0.47
4:C:705:COH:HBC1	4:C:705:COH:HMC1	1.97	0.47
1:D:169:LYS:HB3	1:D:169:LYS:HE3	1.63	0.47
1:D:414:LEU:HD11	1:D:419:LEU:HD23	1.97	0.46
1:A:34:ASN:HB3	1:A:37:CYS:SG	2.55	0.46
1:B:268:ASP:OD1	7:B:985:HOH:O	2.21	0.46
1:D:77:ARG:O	1:D:81:LEU:HD23	2.15	0.46
1:A:414:LEU:HD11	1:A:419:LEU:HD23	1.97	0.46
1:D:120:ARG:HB2	1:D:531:LEU:HD22	1.97	0.46
1:C:274:ILE:HD12	1:C:291:VAL:HG12	1.98	0.46
1:B:173:ASP:HB3	1:B:176:GLU:HG2	1.97	0.46
1:A:399:ASP:OD1	1:A:399:ASP:N	2.38	0.46
1:C:387:TRP:HB2	4:C:705:COH:CBC	2.45	0.46
1:D:300:MET:HG3	1:D:419:LEU:HD22	1.96	0.45
1:B:399:ASP:OD1	1:B:399:ASP:N	2.37	0.45
1:A:191:PRO:CD	1:A:433:ARG:HD3	2.46	0.45
1:A:54:GLN:HG3	7:A:1021:HOH:O	2.16	0.45
1:B:173:ASP:HB3	1:B:176:GLU:CG	2.47	0.45
1:A:117:LEU:HD21	5:A:706:LM8:H28	1.99	0.44
4:D:705:COH:HBB1	4:D:705:COH:HMB1	2.00	0.44
1:B:206:THR:HG21	1:B:385:TYR:CE1	2.53	0.44
1:D:170:GLU:OE1	7:D:923:HOH:O	2.21	0.44
1:D:272:GLU:N	1:D:272:GLU:OE1	2.47	0.44
1:C:388:HIS:CE1	1:C:447:VAL:HG11	2.50	0.43
1:D:76:THR:O	1:D:80:LEU:HD13	2.17	0.43
1:A:497:ASP:HB3	1:A:500:VAL:HG23	1.99	0.43
1:D:389:PRO:HB2	1:D:434:VAL:HA	2.01	0.43
1:B:185:ARG:NH2	6:B:707:BOG:C6	2.79	0.43
1:D:295:VAL:HG11	4:D:705:COH:HBB1	2.00	0.43
1:D:543:GLN:NE2	1:D:543:GLN:HA	2.34	0.43
1:B:543:GLN:OE1	1:B:543:GLN:HA	2.18	0.43
1:B:539:ILE:HA	1:B:544:TYR:HB3	2.00	0.43
1:A:543:GLN:HB2	7:A:858:HOH:O	2.18	0.43
1:C:253:LYS:NZ	7:C:1008:HOH:O	2.50	0.43
1:B:117:LEU:CD2	5:B:706:LM8:H28	2.49	0.43
1:D:289:GLN:OE1	1:D:291:VAL:HG22	2.19	0.43
1:C:511:LYS:HA	1:C:512:PRO:HD3	1.92	0.43
1:D:486:GLU:OE1	6:D:707:BOG:O4	2.32	0.42
1:B:253:LYS:NZ	7:B:924:HOH:O	2.52	0.42
1:B:525:LEU:O	1:B:528:PRO:HD2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:387:TRP:HB2	4:B:705:COH:HAC	2.02	0.41
1:A:274:ILE:HD12	1:A:291:VAL:HG12	2.02	0.41
1:D:527:ALA:HB3	1:D:528:PRO:HD3	2.02	0.41
1:B:230:LEU:HA	1:B:232:HIS:CE1	2.55	0.41
1:C:389:PRO:HB2	1:C:434:VAL:HA	2.01	0.41
1:A:123:LEU:HA	1:A:123:LEU:HD23	1.87	0.41
1:C:300:MET:HG3	1:C:419:LEU:HD22	2.01	0.41
1:A:330:GLN:HB3	1:B:138:SER:HB2	2.02	0.41
1:B:358:LYS:HB3	1:B:358:LYS:HE3	1.65	0.41
1:B:181:VAL:HG21	1:B:491:LEU:HD21	2.02	0.41
1:C:330:GLN:HB3	1:D:138:SER:HB2	2.01	0.41
1:C:390:LEU:HD12	4:C:705:COH:HBC1	2.03	0.41
1:A:191:PRO:HD2	1:A:433:ARG:HD3	2.02	0.41
1:A:527:ALA:HB3	1:A:528:PRO:HD3	2.03	0.41
1:A:511:LYS:HA	1:A:512:PRO:HD3	1.95	0.41
1:B:103:VAL:HG11	1:B:112:ILE:HD12	2.02	0.41
1:A:90:HIS:CE1	1:A:513:ARG:HG2	2.55	0.41
1:D:316:LEU:HD23	1:D:316:LEU:HA	1.90	0.41
1:B:203:GLN:HA	4:B:705:COH:HBC1	2.02	0.40
1:C:294:LEU:HA	1:C:409:TYR:CE1	2.56	0.40
1:B:352:LEU:HD22	1:B:518:PHE:CE2	2.56	0.40
1:D:230:LEU:HA	1:D:232:HIS:CE1	2.56	0.40
1:B:185:ARG:NE	6:B:707:BOG:H61	2.28	0.40
1:D:490:GLU:OE1	6:D:707:BOG:O2	2.30	0.40
1:D:504:TYR:HB3	1:D:505:PRO:HD3	2.03	0.40
1:D:391:LEU:CD2	4:D:705:COH:HAB	2.52	0.40
1:C:399:ASP:N	1:C:399:ASP:OD1	2.37	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%)	533 (97%)	17 (3%)	0	100	100
1	B	550/587 (94%)	537 (98%)	13 (2%)	0	100	100
1	C	550/587 (94%)	538 (98%)	12 (2%)	0	100	100
1	D	550/587 (94%)	537 (98%)	13 (2%)	0	100	100
All	All	2200/2348 (94%)	2145 (98%)	55 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	493/525 (94%)	491 (100%)	2 (0%)	93	96
1	B	493/525 (94%)	492 (100%)	1 (0%)	95	97
1	C	493/525 (94%)	491 (100%)	2 (0%)	93	96
1	D	493/525 (94%)	491 (100%)	2 (0%)	93	96
All	All	1972/2100 (94%)	1965 (100%)	7 (0%)	93	96

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	385	TYR
1	A	433	ARG
1	B	385	TYR
1	C	385	TYR
1	C	556	PHE
1	D	239	ASP
1	D	385	TYR

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

Mol	Chain	Res	Type
1	D	543	GLN

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	0.27	0	15,19,21	0.87	1 (6%)
3	NAG	A	703	3	14,14,15	0.72	1 (7%)	15,19,21	0.41	0
3	NAG	B	702	1,3	14,14,15	0.51	0	15,19,21	0.92	1 (6%)
3	NAG	B	703	3	14,14,15	0.38	0	15,19,21	0.52	0
3	NAG	C	702	1,3	14,14,15	0.36	0	15,19,21	0.66	1 (6%)
3	NAG	C	703	3	14,14,15	0.61	0	15,19,21	0.41	0
3	NAG	D	702	1,3	14,14,15	0.35	0	15,19,21	0.82	1 (6%)
3	NAG	D	703	3	14,14,15	0.64	0	15,19,21	0.48	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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	703	NAG	C1-C2	2.47	1.55	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	702	NAG	C1-O5-C5	2.12	114.94	112.25
3	D	702	NAG	C1-O5-C5	2.94	115.98	112.25
3	A	702	NAG	C1-O5-C5	3.00	116.05	112.25
3	B	702	NAG	C1-O5-C5	3.39	116.55	112.25

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	C	703	NAG	1	0

5.6 Ligand geometry (i)

18 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	0.91	1 (7%)	15,19,21	0.52	0
2	NAG	A	704	1	14,14,15	0.39	0	15,19,21	0.50	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	COH	A	705	1	28,50,50	1.63	6 (21%)	19,82,82	4.33	8 (42%)
5	LM8	A	706	-	19,22,22	0.40	0	17,23,23	0.87	1 (5%)
2	NAG	B	701	1	14,14,15	0.44	0	15,19,21	0.42	0
2	NAG	B	704	1	14,14,15	0.36	0	15,19,21	0.35	0
4	COH	B	705	1	28,50,50	1.62	6 (21%)	19,82,82	4.22	8 (42%)
5	LM8	B	706	-	19,22,22	0.41	0	17,23,23	0.87	1 (5%)
6	BOG	B	707	-	20,20,20	0.71	0	25,25,25	1.95	7 (28%)
2	NAG	C	701	1	14,14,15	0.46	0	15,19,21	0.42	0
2	NAG	C	704	1	14,14,15	0.55	0	15,19,21	0.67	0
4	COH	C	705	1	28,50,50	1.72	5 (17%)	19,82,82	4.18	8 (42%)
5	LM8	C	706	-	19,22,22	0.41	0	17,23,23	0.87	1 (5%)
2	NAG	D	701	1	14,14,15	0.69	0	15,19,21	0.44	0
2	NAG	D	704	1	14,14,15	0.20	0	15,19,21	0.38	0
4	COH	D	705	1	28,50,50	1.63	6 (21%)	19,82,82	4.30	8 (42%)
5	LM8	D	706	-	19,22,22	0.40	0	17,23,23	0.87	1 (5%)
6	BOG	D	707	-	20,20,20	0.45	0	25,25,25	0.62	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
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	COH	A	705	1	-	0/6/54/54	0/0/8/8
5	LM8	A	706	-	-	0/19/21/21	0/0/0/0
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	COH	B	705	1	-	0/6/54/54	0/0/8/8
5	LM8	B	706	-	-	0/19/21/21	0/0/0/0
6	BOG	B	707	-	-	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	COH	C	705	1	-	0/6/54/54	0/0/8/8
5	LM8	C	706	-	-	0/19/21/21	0/0/0/0
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	COH	D	705	1	-	0/6/54/54	0/0/8/8
5	LM8	D	706	-	-	0/19/21/21	0/0/0/0
6	BOG	D	707	-	-	0/11/31/31	0/1/1/1

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	701	NAG	O5-C1	-2.93	1.38	1.43
4	A	705	COH	C4C-CHD	2.08	1.45	1.39
4	D	705	COH	C1B-CHB	2.09	1.45	1.39
4	D	705	COH	C4B-CHC	2.11	1.45	1.39
4	B	705	COH	C4C-CHD	2.12	1.45	1.39
4	B	705	COH	C1B-CHB	2.14	1.45	1.39
4	A	705	COH	C1B-CHB	2.27	1.46	1.39
4	C	705	COH	C1B-CHB	2.29	1.46	1.39
4	A	705	COH	C2A-C3A	2.78	1.45	1.37
4	D	705	COH	C2A-C3A	2.81	1.46	1.37
4	B	705	COH	C2A-C3A	2.91	1.46	1.37
4	B	705	COH	C3D-C2D	2.92	1.46	1.37
4	D	705	COH	C3D-C2D	2.98	1.46	1.37
4	A	705	COH	C3D-C2D	3.01	1.46	1.37
4	C	705	COH	C2A-C3A	3.02	1.46	1.37
4	C	705	COH	C3D-C2D	3.26	1.47	1.37
4	A	705	COH	C3B-C2B	3.99	1.45	1.40
4	B	705	COH	C3B-C2B	4.07	1.45	1.40
4	D	705	COH	C3B-C2B	4.43	1.46	1.40
4	D	705	COH	C3C-C2C	4.46	1.46	1.40
4	B	705	COH	C3C-C2C	4.49	1.46	1.40
4	C	705	COH	C3C-C2C	4.67	1.46	1.40
4	C	705	COH	C3B-C2B	4.74	1.46	1.40
4	A	705	COH	C3C-C2C	4.77	1.46	1.40

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	705	COH	CBD-CAD-C3D	-5.13	103.33	112.53
4	D	705	COH	CBD-CAD-C3D	-5.07	103.44	112.53
4	B	705	COH	CBD-CAD-C3D	-5.04	103.50	112.53
4	C	705	COH	CBD-CAD-C3D	-4.46	104.54	112.53
4	A	705	COH	CAA-CBA-CGA	-3.07	107.12	112.75
6	B	707	BOG	O1-C1-C2	-3.04	104.20	108.04
4	C	705	COH	CAA-CBA-CGA	-2.80	107.61	112.75
6	B	707	BOG	O4-C4-C3	-2.71	104.23	110.34
4	D	705	COH	C3C-CAC-CBC	-2.47	121.26	126.32
5	C	706	LM8	C23-C08-C09	-2.42	104.91	110.63
5	D	706	LM8	C23-C08-C09	-2.42	104.91	110.63
5	B	706	LM8	C23-C08-C09	-2.42	104.91	110.63
4	B	705	COH	C3B-CAB-CBB	-2.40	121.40	126.32
5	A	706	LM8	C23-C08-C09	-2.39	104.96	110.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	705	COH	CBA-CAA-C2A	-2.26	108.48	112.53
4	B	705	COH	CBA-CAA-C2A	-2.07	108.81	112.53
6	B	707	BOG	O5-C1-O1	-2.05	105.11	110.05
4	A	705	COH	C1D-ND-C4D	-2.04	98.63	105.58
4	D	705	COH	CBA-CAA-C2A	-2.03	108.89	112.53
4	D	705	COH	CMD-C2D-C3D	2.00	129.42	125.24
4	B	705	COH	CMB-C2B-C3B	2.19	129.37	125.09
4	A	705	COH	CMB-C2B-C3B	2.24	129.48	125.09
4	A	705	COH	CAA-C2A-C1A	2.46	129.67	127.01
4	C	705	COH	CMD-C2D-C3D	2.49	130.44	125.24
4	C	705	COH	CMB-C2B-C3B	2.53	130.03	125.09
6	B	707	BOG	O5-C1-C2	2.63	115.68	110.28
6	B	707	BOG	C3-C4-C5	2.72	114.94	110.20
4	B	705	COH	CAA-C2A-C1A	2.93	130.19	127.01
4	D	705	COH	CMB-C2B-C3B	3.11	131.16	125.09
4	B	705	COH	CMC-C2C-C3C	3.11	131.17	125.09
4	C	705	COH	CMC-C2C-C3C	3.55	132.04	125.09
4	A	705	COH	CMC-C2C-C3C	3.64	132.20	125.09
4	D	705	COH	CMC-C2C-C3C	3.81	132.53	125.09
6	B	707	BOG	O5-C5-C4	3.96	117.11	109.68
6	B	707	BOG	C1-O5-C5	4.84	123.14	113.75
4	C	705	COH	C2A-C1A-NA	10.68	118.26	108.70
4	A	705	COH	C2A-C1A-NA	11.16	118.69	108.70
4	B	705	COH	C3D-C4D-ND	11.35	118.91	108.74
4	D	705	COH	C2A-C1A-NA	11.50	118.99	108.70
4	B	705	COH	C2A-C1A-NA	11.52	119.01	108.70
4	D	705	COH	C3D-C4D-ND	11.65	119.17	108.74
4	C	705	COH	C3D-C4D-ND	11.74	119.26	108.74
4	A	705	COH	C3D-C4D-ND	12.07	119.55	108.74

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

11 monomers are involved in 38 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	705	COH	5	0
5	A	706	LM8	3	0
2	B	701	NAG	1	0
4	B	705	COH	2	0
5	B	706	LM8	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	707	BOG	7	0
4	C	705	COH	5	0
5	C	706	LM8	3	0
4	D	705	COH	6	0
5	D	706	LM8	3	0
6	D	707	BOG	2	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, 95^{th} 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%)	-0.19	4 (0%) 89 91	27, 43, 72, 102	0
1	B	552/587 (94%)	-0.20	2 (0%) 93 94	24, 40, 67, 96	0
1	C	552/587 (94%)	-0.19	0 100 100	25, 40, 66, 97	0
1	D	552/587 (94%)	-0.10	3 (0%) 91 93	26, 45, 71, 98	0
All	All	2208/2348 (94%)	-0.17	9 (0%) 93 94	24, 42, 69, 102	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	122	TYR	2.5
1	B	583	GLN	2.4
1	A	122	TYR	2.3
1	B	107	PHE	2.3
1	A	74	PHE	2.1
1	A	81	LEU	2.1
1	A	279	ILE	2.0
1	D	115	TYR	2.0
1	D	121	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

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, 95^{th} 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	C	702	14/15	0.97	0.11	1.46	32,44,51,58	0
3	NAG	A	702	14/15	0.94	0.12	0.78	36,40,50,55	0
3	NAG	B	702	14/15	0.96	0.11	0.24	30,38,41,49	0
3	NAG	D	702	14/15	0.97	0.09	-1.48	31,40,44,45	0
3	NAG	A	703	14/15	0.92	0.10	-	47,65,80,85	0
3	NAG	C	703	14/15	0.89	0.12	-	37,66,74,83	0
3	NAG	D	703	14/15	0.92	0.13	-	50,66,75,76	0
3	NAG	B	703	14/15	0.95	0.10	-	43,52,66,74	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
5	LM8	B	706	23/23	0.86	0.24	8.09	46,56,70,72	0
6	BOG	D	707	20/20	0.81	0.23	7.68	59,71,85,90	0
5	LM8	C	706	23/23	0.88	0.25	6.30	43,55,73,77	0
5	LM8	D	706	23/23	0.86	0.25	5.68	51,61,69,71	0
5	LM8	A	706	23/23	0.91	0.20	4.45	50,57,66,68	0
2	NAG	B	701	14/15	0.84	0.18	3.53	61,77,91,92	0
4	COH	A	705	43/43	0.94	0.16	2.71	33,51,71,84	0
4	COH	D	705	43/43	0.75	0.17	2.04	37,49,89,252	0
4	COH	B	705	43/43	0.94	0.15	1.47	35,46,83,103	0
4	COH	C	705	43/43	0.97	0.14	1.45	29,41,69,90	0
2	NAG	D	704	14/15	0.90	0.16	0.68	52,69,79,89	0
2	NAG	B	704	14/15	0.90	0.15	0.61	49,64,75,77	0
2	NAG	A	704	14/15	0.90	0.17	0.51	48,69,89,91	0
6	BOG	B	707	20/20	0.93	0.13	0.28	44,72,79,83	0
2	NAG	C	704	14/15	0.89	0.10	-0.98	39,57,67,75	0
2	NAG	C	701	14/15	0.84	0.18	-	66,82,88,94	0
2	NAG	A	701	14/15	0.76	0.20	-	59,83,97,97	0
2	NAG	D	701	14/15	0.82	0.18	-	61,79,87,89	0

6.5 Other polymers (i)

There are no such residues in this entry.