



Full wwPDB X-ray Structure Validation Report

Feb 26, 2014 – 06:14 PM GMT

PDB ID : 1FE2
Title : CRYSTAL STRUCTURE OF DIHOMO-GAMMA-LINOLEICACID BOUND
IN THE CYCLOOXYGENASE CHANNEL OF PROSTAGLANDIN EN-
DOPEROXIDE H SYNTHASE-1.
Authors : Thuresson, E.D.; Malkowski, M.G.; Lakkides, K.M.; Smith, W.L.; Garavito,
R.M.
Deposited on : 2000-07-20
Resolution : 3.00 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

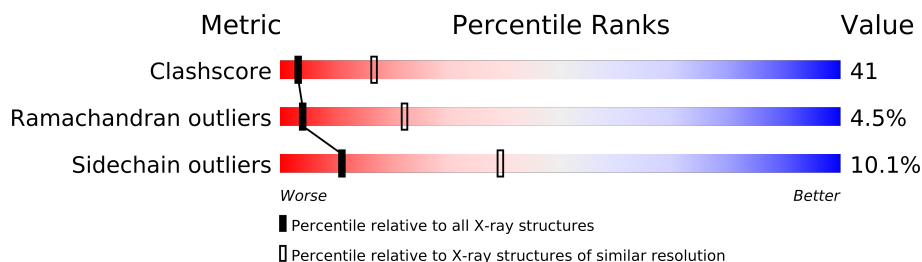
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 21963
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

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))
Clashscore	79885	1594 (3.00-3.00)
Ramachandran outliers	78287	1537 (3.00-3.00)
Sidechain outliers	78261	1540 (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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	576	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 4699 atoms, of which 0 are hydrogen and 0 are deuterium.

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 ENDOPEROXIDE H SYNTHASE-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	553	Total	C	N	O	S	0	0	0
			4397	2855	734	780	28			

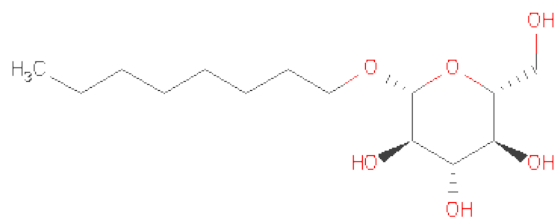
- Molecule 2 is a polymer of unknown type called SUGAR (2-MER).

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

- Molecule 3 is a polymer of unknown type called SUGAR (5-MER).

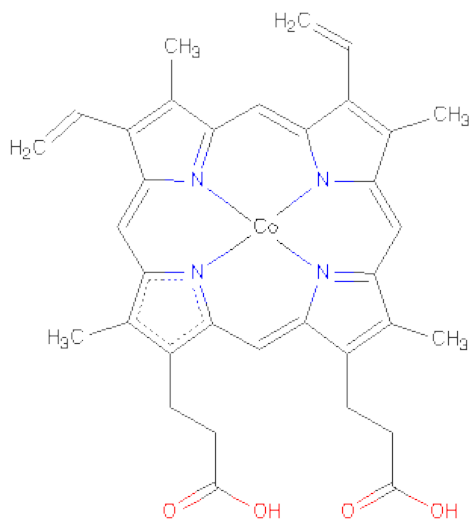
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	5	Total	C	N	O	0	0
			61	34	2	25		

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



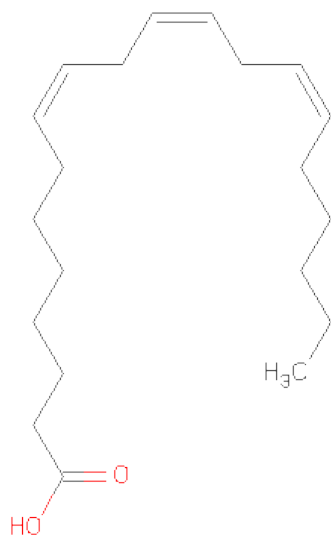
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			20	14	6		
4	A	1	Total	C	O	0	0
			20	14	6		
4	A	1	Total	C	O	0	0
			20	14	6		

- Molecule 5 is PROTOPORPHYRIN IX CONTAINING CO (three-letter code: COH) (formula: C₃₄H₃₂CoN₄O₄).



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

- Molecule 6 is EICOSA-8,11,14-TRIENOICACID (three-letter code: LAX) (formula: $C_{20}H_{34}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			22	20	2		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	60	Total	O	0	0
			60	60		

4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	182.19Å 182.19Å 103.23Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 3.00	Depositor
% Data completeness (in resolution range)	93.4 (20.00-3.00)	Depositor
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 0.9	Depositor
R, R_{free}	0.237 , 0.277	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4699	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: COH, BMA, LAX, 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	0.45	0/4536	0.70	0/6179

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
2	A	1	0
3	A	1	0
All	All	2	0

There are no bond length outliers.

There are no bond angle outliers.

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	662	NAG	C1
3	A	675	BMA	C1

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the

chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4397	0	4203	360	0
2	A	56	0	50	5	0
3	A	61	0	52	3	0
4	A	60	0	84	16	0
5	A	43	0	30	2	0
6	A	22	0	33	22	0
7	A	60	0	0	7	0
All	All	4699	0	4452	370	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 41.

All (370) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:A:661:NAG:H61	2:A:662:NAG:H82	1.35	1.08
1:A:97:ARG:HH21	1:A:97:ARG:HB2	1.18	1.04
1:A:98:TRP:HB2	4:A:752:BOG:H5'1	1.46	0.95
1:A:251:LYS:HB3	1:A:310:ASN:ND2	1.84	0.93
1:A:97:ARG:NH2	1:A:97:ARG:HB2	1.83	0.92
1:A:243:GLN:HG3	1:A:270:PRO:HG2	1.49	0.92
1:A:294:LEU:O	1:A:295:LEU:HG	1.70	0.90
1:A:239:GLU:CD	1:A:239:GLU:H	1.75	0.89
1:A:501:LEU:HD12	1:A:502:GLU:H	1.38	0.89
1:A:530:SER:OG	6:A:700:LAX:H132	1.76	0.85
1:A:195:ASN:ND2	1:A:427:SER:HA	1.92	0.84
1:A:344:VAL:O	1:A:348:TYR:HB3	1.77	0.84
1:A:272:LEU:HD12	1:A:273:MET:H	1.45	0.80
1:A:87:SER:HB2	4:A:750:BOG:H62	1.63	0.79
1:A:523:ILE:HG23	6:A:700:LAX:H62	1.63	0.79
1:A:533:GLY:HA3	6:A:700:LAX:H203	1.65	0.78
1:A:240:ARG:HG3	1:A:271:VAL:HG21	1.65	0.78
1:A:89:ILE:HG23	4:A:751:BOG:H8'1	1.66	0.78
1:A:208:GLN:NE2	1:A:230:LEU:H	1.84	0.76
1:A:513:HIS:HB2	1:A:516:SER:OG	1.85	0.76
1:A:388:HIS:HB3	1:A:444:ILE:HD12	1.68	0.75
1:A:145:VAL:HG12	1:A:224:LEU:HD22	1.66	0.75
1:A:582:VAL:HG23	1:A:583:PRO:HD2	1.67	0.74
1:A:326:GLU:OE1	1:A:326:GLU:HA	1.88	0.74
1:A:182:LEU:HB3	1:A:440:ILE:HD12	1.68	0.74
1:A:543:GLU:O	1:A:546:LYS:HE3	1.87	0.74

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:120:ARG:NE	4:A:751:BOG:H1	2.03	0.74
1:A:242:TYR:CD2	1:A:247:PHE:HZ	2.06	0.73
1:A:424:ASP:HB2	1:A:576:PRO:HB2	1.70	0.73
1:A:501:LEU:HD12	1:A:502:GLU:N	2.02	0.73
1:A:137:ILE:H	1:A:137:ILE:HD12	1.52	0.73
1:A:156:PRO:HB2	1:A:159:CYS:SG	2.29	0.73
1:A:120:ARG:CZ	4:A:751:BOG:H1	2.18	0.72
1:A:442:HIS:CD2	1:A:443:HIS:H	2.08	0.72
1:A:89:ILE:HG23	4:A:751:BOG:C8'	2.20	0.72
1:A:391:MET:HG3	5:A:601:COH:HAB	1.72	0.71
1:A:462:PRO:HB3	1:A:499:ASP:O	1.91	0.70
1:A:272:LEU:HD12	1:A:273:MET:N	2.06	0.70
1:A:301:TYR:HA	1:A:304:ILE:HD12	1.71	0.70
1:A:263:PRO:HD2	1:A:285:MET:CE	2.20	0.70
1:A:115:LEU:HD23	4:A:751:BOG:H5'2	1.72	0.70
1:A:60:THR:HG22	1:A:61:ARG:HG3	1.74	0.69
1:A:526:GLY:C	6:A:700:LAX:H9	2.13	0.69
1:A:294:LEU:HD22	1:A:409:PHE:CD2	2.28	0.69
1:A:384:LEU:HD23	1:A:384:LEU:C	2.12	0.69
1:A:237:ASN:ND2	1:A:240:ARG:H	1.91	0.68
1:A:130:TYR:HB3	1:A:134:HIS:O	1.92	0.68
1:A:334:LEU:HD23	1:A:337:ILE:HD12	1.75	0.67
1:A:504:TYR:CZ	1:A:508:LEU:HD11	2.29	0.67
1:A:208:GLN:NE2	1:A:228:VAL:HA	2.10	0.67
1:A:150:ARG:NH1	1:A:154:SER:HB3	2.10	0.67
1:A:172:PRO:HB2	1:A:177:LEU:HD13	1.76	0.67
1:A:512:CYS:HA	1:A:519:GLY:HA2	1.75	0.66
1:A:137:ILE:N	1:A:137:ILE:HD12	2.10	0.66
1:A:352:LEU:HD23	6:A:700:LAX:H71	1.78	0.66
1:A:253:LYS:O	1:A:254:TYR:HB3	1.96	0.66
1:A:344:VAL:O	1:A:349:VAL:HG23	1.96	0.65
1:A:172:PRO:CB	1:A:177:LEU:HD13	2.25	0.65
1:A:412:SER:O	1:A:416:ASP:HB2	1.96	0.65
1:A:178:SER:OG	1:A:449:VAL:HG22	1.96	0.65
1:A:89:ILE:HD12	4:A:751:BOG:H8'3	1.78	0.65
1:A:402:TYR:HA	1:A:406:GLN:OE1	1.97	0.65
1:A:163:MET:HB3	1:A:462:PRO:HG3	1.78	0.65
6:A:700:LAX:C8	6:A:700:LAX:H41	2.27	0.65
1:A:334:LEU:HA	1:A:337:ILE:HD12	1.78	0.65
1:A:442:HIS:HD2	1:A:443:HIS:H	1.44	0.64
1:A:527:ALA:HB3	1:A:528:PRO:HD3	1.79	0.64
1:A:279:ILE:HG22	1:A:279:ILE:O	1.98	0.64

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:48:VAL:HG22	7:A:852:HOH:O	1.97	0.64
1:A:495:TYR:OH	1:A:502:GLU:HG3	1.98	0.64
1:A:260:GLU:HB2	1:A:262:TYR:HE1	1.61	0.64
1:A:102:PHE:O	1:A:106:THR:HG23	1.98	0.63
1:A:126:SER:HA	1:A:127:PRO:C	2.19	0.63
1:A:530:SER:OG	6:A:700:LAX:H101	1.98	0.63
1:A:258:ASN:HD21	1:A:415:VAL:HG12	1.62	0.63
1:A:414:LEU:HD12	1:A:414:LEU:O	1.99	0.63
1:A:39:TYR:OH	1:A:155:VAL:HG22	1.99	0.63
1:A:463:PHE:HB2	1:A:502:GLU:O	1.98	0.63
1:A:226:HIS:HB3	1:A:377:ILE:HG12	1.81	0.63
1:A:287:VAL:HG23	1:A:289:GLN:H	1.64	0.62
1:A:202:ALA:O	1:A:206:THR:HG23	1.98	0.62
1:A:442:HIS:CD2	1:A:443:HIS:N	2.66	0.62
2:A:661:NAG:H61	2:A:662:NAG:C8	2.22	0.62
1:A:388:HIS:HB3	1:A:444:ILE:CD1	2.28	0.62
1:A:88:PHE:O	1:A:91:PHE:HB3	1.99	0.62
1:A:88:PHE:CZ	1:A:92:LEU:HD11	2.34	0.62
1:A:258:ASN:ND2	1:A:415:VAL:HG12	2.15	0.62
1:A:263:PRO:HD2	1:A:285:MET:HE1	1.81	0.61
1:A:40:PRO:HB3	2:A:661:NAG:H62	1.82	0.61
1:A:207:HIS:HB3	1:A:289:GLN:HE21	1.65	0.61
1:A:364:GLU:HG2	1:A:367:PHE:CE1	2.36	0.61
1:A:237:ASN:HB2	1:A:239:GLU:OE1	2.01	0.61
1:A:444:ILE:O	1:A:447:VAL:HG23	2.00	0.61
1:A:424:ASP:O	1:A:428:ARG:HD2	2.01	0.61
1:A:255:GLN:HE21	1:A:264:PRO:HA	1.65	0.60
1:A:265:SER:HA	1:A:285:MET:HA	1.82	0.60
1:A:564:LEU:HD22	1:A:578:VAL:CG2	2.32	0.60
1:A:352:LEU:HD23	6:A:700:LAX:C7	2.31	0.60
1:A:97:ARG:O	1:A:101:ASP:OD2	2.19	0.60
1:A:582:VAL:HG22	1:A:583:PRO:O	2.02	0.60
1:A:463:PHE:HE1	1:A:507:LEU:HG	1.66	0.60
1:A:179:ARG:HA	1:A:183:LEU:HB2	1.84	0.60
1:A:412:SER:O	1:A:416:ASP:N	2.31	0.59
1:A:196:LEU:HD11	1:A:429:GLN:NE2	2.16	0.59
1:A:109:ARG:NH2	1:A:360:LYS:HB2	2.18	0.59
1:A:120:ARG:HD2	4:A:751:BOG:O2	2.02	0.59
1:A:257:LEU:O	1:A:258:ASN:HB2	2.01	0.59
1:A:204:HIS:CD2	1:A:232:HIS:CD2	2.91	0.59
1:A:182:LEU:HB3	1:A:440:ILE:CD1	2.33	0.59
1:A:245:ARG:NH2	1:A:325:ASP:OD2	2.36	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:230:LEU:HA	1:A:232:HIS:CE1	2.38	0.58
1:A:263:PRO:HD2	1:A:285:MET:HE2	1.84	0.58
1:A:577:TYR:CE2	1:A:583:PRO:HD3	2.38	0.58
1:A:243:GLN:HG3	1:A:270:PRO:CG	2.29	0.58
1:A:234:TYR:CE2	1:A:333:ARG:HG3	2.39	0.58
1:A:279:ILE:C	1:A:281:PRO:CD	2.72	0.58
1:A:237:ASN:HD21	1:A:240:ARG:HB2	1.69	0.58
1:A:86:PRO:HA	4:A:751:BOG:H62	1.84	0.58
1:A:163:MET:HE2	1:A:163:MET:HA	1.85	0.58
1:A:566:LYS:O	1:A:570:LEU:HB2	2.04	0.58
1:A:96:GLY:O	1:A:98:TRP:N	2.36	0.57
1:A:292:PHE:CD1	1:A:298:LEU:HD23	2.40	0.57
1:A:185:ARG:HD2	1:A:185:ARG:N	2.18	0.57
1:A:337:ILE:O	1:A:341:ILE:HG13	2.04	0.57
1:A:246:LEU:O	1:A:246:LEU:HG	2.04	0.57
1:A:216:MET:HG2	3:A:672:NAG:C8	2.33	0.57
1:A:230:LEU:C	1:A:232:HIS:H	2.07	0.57
1:A:77:TRP:O	1:A:81:THR:HG23	2.04	0.57
1:A:333:ARG:O	1:A:337:ILE:HG13	2.05	0.57
1:A:185:ARG:NH1	1:A:438:ARG:NH1	2.53	0.57
1:A:319:GLU:HB3	1:A:320:HIS:ND1	2.20	0.57
1:A:523:ILE:CG2	6:A:700:LAX:H62	2.34	0.56
1:A:279:ILE:N	1:A:280:PRO:HD3	2.20	0.56
1:A:280:PRO:N	1:A:281:PRO:HD3	2.19	0.56
1:A:415:VAL:HG23	7:A:857:HOH:O	2.05	0.56
1:A:243:GLN:CG	1:A:270:PRO:HG2	2.31	0.56
1:A:204:HIS:CD2	1:A:232:HIS:HD2	2.23	0.56
1:A:115:LEU:O	1:A:119:VAL:HG23	2.05	0.55
1:A:403:SER:N	1:A:406:GLN:OE1	2.38	0.55
1:A:484:GLU:OE2	1:A:487:MET:N	2.39	0.55
1:A:216:MET:HG2	3:A:672:NAG:H82	1.88	0.55
1:A:388:HIS:N	1:A:389:PRO:HD2	2.22	0.55
1:A:109:ARG:HH21	1:A:360:LYS:HB2	1.71	0.55
1:A:242:TYR:CD2	1:A:247:PHE:CZ	2.93	0.55
1:A:254:TYR:CD1	1:A:261:VAL:HG13	2.41	0.54
1:A:340:THR:O	1:A:344:VAL:HG23	2.08	0.54
1:A:87:SER:CB	4:A:750:BOG:H62	2.33	0.54
1:A:149:THR:O	1:A:378:ALA:HA	2.05	0.54
1:A:335:ILE:O	1:A:339:GLU:HG3	2.07	0.54
1:A:381:PHE:HB2	1:A:529:PHE:CD1	2.43	0.54
1:A:564:LEU:HD22	1:A:578:VAL:HG21	1.88	0.54
1:A:287:VAL:HG21	1:A:292:PHE:HB2	1.88	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:151:ILE:HG23	1:A:469:ARG:NH1	2.23	0.54
1:A:391:MET:HA	1:A:391:MET:CE	2.37	0.54
1:A:254:TYR:HD1	1:A:261:VAL:HG13	1.73	0.53
1:A:414:LEU:HD12	1:A:414:LEU:C	2.28	0.53
1:A:452:ILE:O	1:A:456:ARG:HG3	2.08	0.53
1:A:470:PHE:CD1	1:A:525:MET:HA	2.43	0.53
1:A:152:LEU:HD12	1:A:466:TYR:CE1	2.43	0.53
1:A:245:ARG:HB2	1:A:247:PHE:CE1	2.43	0.53
1:A:513:HIS:CE1	1:A:523:ILE:HD11	2.43	0.53
1:A:238:LEU:O	1:A:241:GLN:HB3	2.08	0.53
1:A:308:GLU:O	1:A:311:ARG:HB3	2.09	0.53
1:A:408:LEU:HB3	1:A:409:PHE:CE1	2.44	0.53
1:A:134:HIS:HB3	1:A:136:TYR:CE1	2.44	0.53
1:A:320:HIS:O	1:A:323:TRP:HB2	2.08	0.53
1:A:298:LEU:N	1:A:298:LEU:HD12	2.24	0.53
1:A:40:PRO:O	1:A:68:ASN:HB3	2.08	0.53
1:A:181:PHE:O	1:A:438:ARG:N	2.42	0.53
1:A:226:HIS:HB3	1:A:377:ILE:H	1.74	0.52
1:A:210:PHE:CE1	1:A:382:ASN:HA	2.44	0.52
1:A:195:ASN:HD22	1:A:427:SER:HA	1.73	0.52
1:A:201:PHE:C	1:A:201:PHE:CD2	2.81	0.52
1:A:142:PHE:O	1:A:376:ARG:NH2	2.43	0.52
1:A:408:LEU:HB3	1:A:409:PHE:CD1	2.44	0.52
1:A:64:TYR:CE1	1:A:76:THR:HG21	2.45	0.52
1:A:258:ASN:ND2	1:A:415:VAL:CG1	2.73	0.52
1:A:201:PHE:HD2	1:A:201:PHE:C	2.12	0.52
1:A:348:TYR:CE2	6:A:700:LAX:H14	2.46	0.52
1:A:384:LEU:HD23	1:A:384:LEU:O	2.10	0.52
1:A:295:LEU:HD21	1:A:408:LEU:HD23	1.92	0.51
1:A:537:ASN:OD1	1:A:539:ILE:HG23	2.11	0.51
1:A:380:GLU:HG2	1:A:466:TYR:CZ	2.46	0.51
1:A:261:VAL:HB	1:A:307:ARG:HD2	1.93	0.51
1:A:291:VAL:CG2	1:A:294:LEU:HD12	2.41	0.51
1:A:163:MET:HA	1:A:163:MET:CE	2.40	0.51
1:A:530:SER:OG	6:A:700:LAX:H161	2.11	0.51
1:A:201:PHE:HD2	1:A:201:PHE:O	1.94	0.51
4:A:752:BOG:C4'	4:A:752:BOG:H8'2	2.40	0.51
1:A:513:HIS:HB2	1:A:516:SER:CB	2.41	0.51
1:A:413:MET:HE3	7:A:856:HOH:O	2.10	0.51
1:A:218:PRO:HB3	1:A:454:GLU:HG3	1.92	0.51
1:A:89:ILE:CD1	4:A:751:BOG:H8'3	2.41	0.51
1:A:403:SER:OG	1:A:405:GLU:HG2	2.11	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:A:752:BOG:H4'1	4:A:752:BOG:H8'2	1.93	0.51
1:A:306:LEU:HD23	1:A:306:LEU:C	2.32	0.50
1:A:530:SER:O	1:A:534:LEU:HD22	2.11	0.50
1:A:278:GLY:C	1:A:280:PRO:HD3	2.32	0.50
1:A:289:GLN:HG3	1:A:292:PHE:CE1	2.47	0.50
1:A:185:ARG:HH11	1:A:185:ARG:HG2	1.75	0.50
1:A:413:MET:HA	2:A:681:NAG:O6	2.11	0.50
1:A:75:TRP:CE3	1:A:78:LEU:HD12	2.46	0.50
1:A:238:LEU:HB3	1:A:239:GLU:OE2	2.11	0.50
1:A:568:VAL:HG12	1:A:569:CYS:N	2.25	0.50
1:A:518:PHE:HZ	6:A:700:LAX:H72	1.76	0.50
1:A:228:VAL:O	1:A:337:ILE:HG23	2.12	0.49
1:A:201:PHE:HB2	1:A:301:TYR:CZ	2.47	0.49
1:A:137:ILE:CD1	1:A:137:ILE:H	2.21	0.49
1:A:157:ARG:NH1	1:A:459:ARG:HD2	2.26	0.49
1:A:204:HIS:ND1	1:A:301:TYR:CB	2.76	0.49
1:A:120:ARG:NH1	6:A:700:LAX:O2	2.45	0.49
1:A:289:GLN:HB3	1:A:292:PHE:CD1	2.47	0.49
1:A:43:HIS:O	1:A:44:GLN:HB2	2.12	0.49
1:A:287:VAL:HG23	1:A:288:GLY:N	2.27	0.49
1:A:478:PHE:CE1	1:A:498:ILE:HA	2.48	0.49
1:A:498:ILE:HG23	1:A:499:ASP:N	2.26	0.49
1:A:504:TYR:HB3	1:A:505:PRO:HD3	1.95	0.48
1:A:289:GLN:HG3	1:A:292:PHE:CZ	2.49	0.48
1:A:373:TYR:CZ	1:A:541:SER:HA	2.48	0.48
1:A:209:PHE:HB2	1:A:377:ILE:HG13	1.95	0.48
1:A:582:VAL:CG2	1:A:583:PRO:HD2	2.39	0.48
1:A:266:VAL:HG21	1:A:284:GLN:HE22	1.78	0.48
1:A:392:PRO:HG3	1:A:429:GLN:NE2	2.29	0.48
1:A:149:THR:HG22	1:A:377:ILE:O	2.13	0.48
1:A:200:PHE:O	1:A:203:GLN:N	2.47	0.48
1:A:257:LEU:O	1:A:258:ASN:CB	2.61	0.48
3:A:673:BMA:O6	3:A:674:BMA:H62	2.13	0.48
1:A:145:VAL:HG13	1:A:226:HIS:HE2	1.78	0.47
1:A:458:LEU:O	1:A:459:ARG:HB2	2.13	0.47
1:A:384:LEU:C	1:A:384:LEU:CD2	2.82	0.47
1:A:490:GLU:O	1:A:493:GLU:HB3	2.14	0.47
1:A:241:GLN:O	1:A:245:ARG:HG3	2.13	0.47
1:A:74:ILE:CG2	1:A:75:TRP:N	2.77	0.47
6:A:700:LAX:C11	6:A:700:LAX:H71	2.44	0.47
1:A:419:VAL:O	1:A:420:GLU:C	2.52	0.47
1:A:478:PHE:CE2	1:A:491:LEU:HB3	2.50	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:448:ALA:O	1:A:452:ILE:HG13	2.14	0.47
1:A:305:TRP:O	1:A:308:GLU:HB3	2.15	0.47
1:A:433:ARG:NH1	1:A:436:GLY:HA3	2.29	0.47
1:A:208:GLN:HB3	1:A:232:HIS:ND1	2.28	0.47
1:A:272:LEU:O	1:A:273:MET:HG2	2.13	0.47
1:A:527:ALA:N	6:A:700:LAX:H9	2.29	0.47
1:A:208:GLN:HE22	1:A:230:LEU:H	1.61	0.47
1:A:151:ILE:CG2	1:A:469:ARG:NH1	2.78	0.47
1:A:103:VAL:HG13	1:A:108:ILE:CG2	2.45	0.47
1:A:294:LEU:HD22	1:A:409:PHE:CE2	2.50	0.47
1:A:200:PHE:O	1:A:201:PHE:C	2.54	0.47
1:A:333:ARG:HG2	1:A:337:ILE:HD11	1.97	0.47
1:A:523:ILE:HA	6:A:700:LAX:H8	1.96	0.46
1:A:239:GLU:CD	1:A:239:GLU:N	2.56	0.46
1:A:88:PHE:CE2	1:A:92:LEU:HD11	2.50	0.46
1:A:441:ASP:OD2	1:A:442:HIS:HD2	1.97	0.46
1:A:267:GLU:O	1:A:268:GLU:HB2	2.14	0.46
1:A:245:ARG:HD2	1:A:329:PHE:CZ	2.50	0.46
1:A:204:HIS:ND1	1:A:301:TYR:HB2	2.30	0.46
1:A:461:GLN:HB3	1:A:462:PRO:CD	2.45	0.46
1:A:323:TRP:CE3	1:A:327:GLN:HG2	2.50	0.46
1:A:42:GLN:NE2	7:A:827:HOH:O	2.49	0.46
1:A:74:ILE:HG22	1:A:75:TRP:N	2.30	0.45
1:A:239:GLU:OE2	1:A:239:GLU:N	2.48	0.45
1:A:345:ILE:HG22	1:A:346:GLU:N	2.30	0.45
1:A:183:LEU:HB2	1:A:445:LEU:HD22	1.97	0.45
1:A:490:GLU:HG3	7:A:835:HOH:O	2.15	0.45
1:A:237:ASN:OD1	1:A:240:ARG:HB3	2.17	0.45
1:A:245:ARG:HD2	1:A:329:PHE:CE2	2.52	0.45
1:A:253:LYS:O	1:A:254:TYR:CB	2.63	0.45
1:A:274:HIS:CD2	1:A:290:GLU:HB2	2.52	0.45
1:A:309:HIS:CD2	1:A:309:HIS:C	2.89	0.45
1:A:145:VAL:HG11	1:A:224:LEU:HB3	1.98	0.45
1:A:246:LEU:HD12	1:A:253:LYS:HG2	1.98	0.45
1:A:181:PHE:HZ	1:A:490:GLU:HG2	1.82	0.45
1:A:117:LEU:O	1:A:118:THR:C	2.54	0.45
1:A:269:ALA:O	1:A:271:VAL:N	2.49	0.44
1:A:500:ALA:O	1:A:501:LEU:C	2.56	0.44
1:A:280:PRO:N	1:A:281:PRO:CD	2.80	0.44
1:A:503:PHE:CZ	1:A:507:LEU:HD11	2.53	0.44
1:A:208:GLN:HG2	1:A:209:PHE:CD1	2.52	0.44
1:A:107:PHE:CD2	1:A:107:PHE:N	2.85	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:352:LEU:HD21	1:A:387:TRP:CH2	2.53	0.44
1:A:34:ASN:HB2	1:A:158:ASP:OD2	2.17	0.44
1:A:116:VAL:O	1:A:120:ARG:HB2	2.17	0.44
1:A:523:ILE:HG22	6:A:700:LAX:C3	2.47	0.44
1:A:200:PHE:HE2	1:A:426:PHE:CE1	2.35	0.44
1:A:338:GLY:O	1:A:339:GLU:C	2.55	0.44
1:A:152:LEU:HD12	1:A:466:TYR:CD1	2.53	0.44
1:A:191:PRO:HG2	1:A:515:ASN:O	2.17	0.44
1:A:381:PHE:HB2	1:A:529:PHE:CG	2.52	0.44
1:A:442:HIS:HE2	1:A:443:HIS:CE1	2.34	0.44
1:A:134:HIS:HB3	1:A:136:TYR:CD1	2.52	0.44
1:A:512:CYS:HA	1:A:519:GLY:CA	2.45	0.44
1:A:151:ILE:HG13	1:A:529:PHE:CZ	2.52	0.44
1:A:252:LEU:HD11	1:A:329:PHE:HE1	1.83	0.44
1:A:84:PRO:HB2	1:A:88:PHE:HD1	1.83	0.44
1:A:144:ASN:HB3	1:A:147:TYR:HD2	1.82	0.44
1:A:292:PHE:O	1:A:299:MET:HE2	2.18	0.43
1:A:486:GLU:O	1:A:487:MET:C	2.56	0.43
1:A:123:LEU:O	1:A:469:ARG:NH2	2.50	0.43
1:A:433:ARG:HH11	1:A:433:ARG:HG2	1.82	0.43
1:A:349:VAL:CG1	6:A:700:LAX:H51	2.48	0.43
1:A:103:VAL:HG13	1:A:108:ILE:HG22	2.00	0.43
1:A:276:PRO:HA	7:A:842:HOH:O	2.18	0.43
1:A:201:PHE:CD2	1:A:201:PHE:O	2.71	0.43
1:A:256:MET:SD	1:A:261:VAL:HG22	2.59	0.43
1:A:107:PHE:C	1:A:109:ARG:N	2.71	0.43
1:A:96:GLY:C	1:A:98:TRP:H	2.21	0.43
1:A:156:PRO:HD2	1:A:159:CYS:SG	2.59	0.43
1:A:106:THR:OG1	1:A:108:ILE:HG13	2.18	0.43
1:A:550:PHE:O	1:A:551:GLY:O	2.36	0.43
1:A:204:HIS:ND1	1:A:301:TYR:HB3	2.34	0.43
1:A:176:PHE:O	1:A:180:ARG:HB2	2.19	0.43
1:A:87:SER:HB2	4:A:750:BOG:C6	2.42	0.43
1:A:96:GLY:C	1:A:98:TRP:N	2.72	0.43
1:A:198:PHE:CZ	1:A:352:LEU:HD13	2.54	0.43
1:A:185:ARG:HD3	1:A:438:ARG:HD3	2.01	0.43
1:A:321:PRO:C	1:A:323:TRP:H	2.22	0.42
1:A:64:TYR:CZ	1:A:76:THR:HG21	2.54	0.42
1:A:237:ASN:HD21	1:A:240:ARG:H	1.65	0.42
1:A:294:LEU:HD22	1:A:409:PHE:HD2	1.76	0.42
6:A:700:LAX:C4	6:A:700:LAX:C8	2.96	0.42
1:A:246:LEU:O	1:A:248:LYS:N	2.52	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:553:GLU:O	1:A:557:ASN:ND2	2.52	0.42
1:A:523:ILE:H	1:A:523:ILE:HG13	1.56	0.42
1:A:208:GLN:HB3	1:A:232:HIS:CG	2.54	0.42
1:A:230:LEU:HA	1:A:232:HIS:ND1	2.34	0.42
1:A:461:GLN:HB3	1:A:462:PRO:HD2	2.02	0.42
1:A:145:VAL:HG13	1:A:226:HIS:NE2	2.34	0.42
1:A:502:GLU:HB2	1:A:505:PRO:HD2	2.01	0.42
1:A:179:ARG:O	1:A:183:LEU:HB3	2.20	0.42
1:A:568:VAL:O	1:A:570:LEU:N	2.53	0.42
1:A:394:SER:C	1:A:395:PHE:CD1	2.93	0.42
1:A:352:LEU:CD2	6:A:700:LAX:H11	2.50	0.42
1:A:75:TRP:O	1:A:78:LEU:N	2.52	0.42
1:A:510:GLU:HG2	1:A:511:LYS:O	2.20	0.42
1:A:271:VAL:HG22	1:A:272:LEU:N	2.35	0.42
1:A:34:ASN:HA	1:A:35:PRO:HD2	1.77	0.42
1:A:527:ALA:HB2	6:A:700:LAX:C4	2.50	0.41
1:A:390:LEU:HD21	1:A:434:ILE:HD11	2.02	0.41
1:A:86:PRO:HA	4:A:751:BOG:C6	2.50	0.41
1:A:178:SER:HB3	1:A:445:LEU:HD11	2.02	0.41
1:A:266:VAL:CG2	1:A:284:GLN:NE2	2.83	0.41
1:A:290:GLU:H	1:A:290:GLU:CD	2.21	0.41
1:A:464:ASN:OD1	1:A:475:TYR:N	2.52	0.41
1:A:492:GLU:O	1:A:496:GLY:N	2.44	0.41
1:A:107:PHE:HD2	1:A:107:PHE:H	1.65	0.41
1:A:295:LEU:HD11	5:A:601:COH:HBB1	2.03	0.41
1:A:304:ILE:CG2	1:A:567:LEU:HG	2.51	0.41
1:A:184:ARG:NH1	1:A:187:PHE:HD2	2.19	0.41
1:A:179:ARG:HA	1:A:183:LEU:CB	2.49	0.41
1:A:83:ARG:HA	1:A:84:PRO:HD2	1.97	0.41
1:A:266:VAL:CG2	1:A:284:GLN:HE22	2.33	0.41
1:A:53:ASP:OD2	1:A:54:ARG:HG3	2.20	0.41
1:A:375:ASN:HD22	1:A:375:ASN:HA	1.71	0.41
1:A:251:LYS:HD3	1:A:310:ASN:HD22	1.85	0.41
1:A:500:ALA:O	1:A:501:LEU:O	2.39	0.41
1:A:442:HIS:NE2	1:A:443:HIS:CE1	2.89	0.40
1:A:279:ILE:C	1:A:281:PRO:HD3	2.41	0.40
1:A:299:MET:HG3	1:A:414:LEU:HD23	2.03	0.40
1:A:275:TYR:CG	1:A:284:GLN:HG2	2.55	0.40
1:A:289:GLN:HB3	1:A:292:PHE:CG	2.56	0.40
1:A:196:LEU:HD21	1:A:392:PRO:HD3	2.03	0.40
1:A:255:GLN:NE2	1:A:265:SER:N	2.68	0.40
1:A:303:THR:O	1:A:307:ARG:HB2	2.22	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:279:ILE:N	1:A:280:PRO:CD	2.85	0.40
1:A:260:GLU:HB2	1:A:262:TYR:CE1	2.48	0.40
2:A:682:NAG:H2	7:A:850:HOH:O	2.21	0.40
6:A:700:LAX:H101	6:A:700:LAX:H132	1.79	0.40
1:A:35:PRO:C	1:A:37:CYS:H	2.25	0.40
1:A:165:THR:HG22	1:A:166:LYS:HG2	2.03	0.40
1:A:284:GLN:HE21	1:A:284:GLN:HB3	1.53	0.40
1:A:50:PHE:CE2	1:A:56:GLN:NE2	2.89	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	551/576 (96%)	430 (78%)	96 (17%)	25 (4%)	4	22

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	117	LEU
1	A	247	PHE
1	A	281	PRO
1	A	97	ARG
1	A	178	SER
1	A	268	GLU
1	A	277	ARG
1	A	292	PHE
1	A	501	LEU
1	A	551	GLY
1	A	569	CYS
1	A	272	LEU
1	A	278	GLY
1	A	486	GLU
1	A	254	TYR

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Mol	Chain	Res	Type
1	A	118	THR
1	A	160	PRO
1	A	400	GLN
1	A	401	ASP
1	A	576	PRO
1	A	280	PRO
1	A	392	PRO
1	A	481	LEU
1	A	145	VAL
1	A	270	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	466/506 (92%)	419 (90%)	47 (10%)	11	39

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	VAL
1	A	49	ARG
1	A	70	THR
1	A	74	ILE
1	A	80	THR
1	A	87	SER
1	A	97	ARG
1	A	99	LEU
1	A	106	THR
1	A	120	ARG
1	A	130	TYR
1	A	136	TYR
1	A	180	ARG
1	A	185	ARG
1	A	201	PHE
1	A	209	PHE
1	A	239	GLU
1	A	252	LEU

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Mol	Chain	Res	Type
1	A	272	LEU
1	A	283	SER
1	A	284	GLN
1	A	289	GLN
1	A	290	GLU
1	A	307	ARG
1	A	326	GLU
1	A	374	ARG
1	A	375	ASN
1	A	376	ARG
1	A	384	LEU
1	A	385	TYR
1	A	405	GLU
1	A	414	LEU
1	A	416	ASP
1	A	433	ARG
1	A	442	HIS
1	A	469	ARG
1	A	484	GLU
1	A	518	PHE
1	A	523	ILE
1	A	534	LEU
1	A	554	VAL
1	A	556	PHE
1	A	564	LEU
1	A	570	LEU
1	A	574	THR
1	A	578	VAL
1	A	584	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	42	GLN
1	A	43	HIS
1	A	56	GLN
1	A	203	GLN
1	A	208	GLN
1	A	232	HIS
1	A	241	GLN
1	A	255	GLN
1	A	258	ASN

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Mol	Chain	Res	Type
1	A	274	HIS
1	A	284	GLN
1	A	310	ASN
1	A	375	ASN
1	A	443	HIS
1	A	557	ASN

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

9 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	$\# Z > 2$
2	NAG	A	661	1,2	12,14,15	0.63	0	15,19,21	1.00	1 (6%)
2	NAG	A	662	2	12,14,15	0.71	0	15,19,21	1.10	1 (6%)
3	NAG	A	671	1,3	12,14,15	0.59	0	15,19,21	0.75	0
3	NAG	A	672	3	12,14,15	1.11	1 (8%)	15,19,21	0.98	1 (6%)
3	BMA	A	673	3	10,11,12	0.63	0	11,15,17	0.58	0
3	BMA	A	674	3	10,11,12	0.86	0	11,15,17	0.94	1 (9%)
3	BMA	A	675	3	10,11,12	0.53	0	11,15,17	0.61	0
2	NAG	A	681	1,2	12,14,15	0.46	0	15,19,21	0.77	0
2	NAG	A	682	2	12,14,15	0.53	0	15,19,21	0.99	1 (6%)

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	661	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	662	2	1/1/5/7	0/6/23/26	0/1/1/1
3	NAG	A	671	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	672	3	-	0/6/23/26	0/1/1/1
3	BMA	A	673	3	-	0/2/19/22	0/1/1/1
3	BMA	A	674	3	-	0/2/19/22	0/1/1/1
3	BMA	A	675	3	1/1/4/5	0/2/19/22	0/1/1/1
2	NAG	A	681	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	682	2	-	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	672	NAG	O4-C4	2.26	1.48	1.43

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	682	NAG	C2-N2-C7	-2.69	118.57	123.09
3	A	674	BMA	O3-C3-C2	2.36	114.26	109.94
2	A	661	NAG	C4-C3-C2	-2.19	105.95	111.32
3	A	672	NAG	C4-C3-C2	-2.17	106.01	111.32
2	A	662	NAG	C3-C2-N2	-2.15	108.48	111.76

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	662	NAG	C1
3	A	675	BMA	C1

There are no torsion outliers.

There are no ring outliers.

5.6 Ligand geometry ⓘ

5 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	$\# Z > 2$
5	COH	A	601	1	50,50,50	2.61	15 (30%)	60,82,82	2.53	22 (36%)
6	LAX	A	700	-	21,21,21	0.69	0	21,21,21	1.10	2 (9%)
4	BOG	A	750	-	20,20,20	0.54	0	25,25,25	0.58	1 (4%)
4	BOG	A	751	-	20,20,20	0.48	0	25,25,25	0.96	2 (8%)
4	BOG	A	752	-	20,20,20	0.67	0	25,25,25	0.75	1 (4%)

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
5	COH	A	601	1	-	0/10/54/54	0/0/8/8
6	LAX	A	700	-	-	0/19/19/19	0/0/0/0
4	BOG	A	750	-	-	0/11/31/31	0/1/1/1
4	BOG	A	751	-	-	0/11/31/31	0/1/1/1
4	BOG	A	752	-	-	0/11/31/31	0/1/1/1

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	601	COH	C4D-ND	9.00	1.44	1.36
5	A	601	COH	C1B-C2B	5.85	1.47	1.40
5	A	601	COH	C3B-C4B	5.39	1.48	1.40
5	A	601	COH	C1B-NB	5.14	1.41	1.36
5	A	601	COH	C3C-CAC	-4.65	1.45	1.49
5	A	601	COH	C4B-NB	4.57	1.40	1.36
5	A	601	COH	CAA-C2A	4.40	1.61	1.52
5	A	601	COH	C1A-NA	4.14	1.43	1.36
5	A	601	COH	C1D-C2D	3.78	1.56	1.43
5	A	601	COH	C4A-C3A	3.52	1.55	1.43
5	A	601	COH	C1A-C2A	3.23	1.54	1.43
5	A	601	COH	CAD-C3D	2.66	1.56	1.52
5	A	601	COH	C2A-C3A	2.60	1.44	1.37
5	A	601	COH	C3B-C2B	-2.49	1.36	1.41
5	A	601	COH	CBC-CAC	2.12	1.44	1.28

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	601	COH	C3A-C4A-NA	6.33	114.68	108.60
5	A	601	COH	C2B-C1B-NB	6.25	114.47	109.32
5	A	601	COH	C3C-C4C-NC	5.90	114.38	108.64
5	A	601	COH	C4A-C3A-C2A	-5.80	103.21	106.89
5	A	601	COH	CMD-C2D-C3D	4.76	133.91	124.94
5	A	601	COH	C3B-C4B-NB	4.62	113.13	108.64
5	A	601	COH	C1D-C2D-C3D	-4.59	103.97	106.89
5	A	601	COH	C4B-NB-C1B	-4.06	100.98	108.54
5	A	601	COH	C2D-C1D-ND	3.86	112.31	108.60
5	A	601	COH	C3B-C2B-C1B	-3.30	105.07	107.00
5	A	601	COH	CAA-C2A-C1A	3.04	130.16	124.67
4	A	751	BOG	C1'-O1-C1	3.02	119.39	113.96
5	A	601	COH	CBA-CAA-C2A	2.89	117.76	112.35
5	A	601	COH	C1D-ND-C4D	-2.76	103.41	108.54
5	A	601	COH	C2A-C1A-NA	2.64	111.50	109.48
5	A	601	COH	CMA-C3A-C2A	2.64	129.91	124.94
4	A	751	BOG	O1-C1-C2	2.59	111.48	108.18
5	A	601	COH	CMB-C2B-C3B	2.34	128.66	124.97
5	A	601	COH	CMC-C2C-C3C	2.29	128.58	124.97
5	A	601	COH	C1C-NC-C4C	-2.25	104.36	108.54
4	A	752	BOG	O1-C1-C2	2.23	111.02	108.18
5	A	601	COH	C2C-C1C-NC	2.21	110.73	108.60
5	A	601	COH	C2C-C3C-CAC	2.13	131.69	127.33
6	A	700	LAX	C17-C16-C15	2.09	122.56	112.50
4	A	750	BOG	O1-C1-C2	2.08	110.83	108.18
5	A	601	COH	CMD-C2D-C1D	-2.05	122.11	126.16
6	A	700	LAX	C14-C13-C12	2.04	118.74	111.65
5	A	601	COH	C1D-CHD-C4C	-2.01	124.82	127.47

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.