



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:04 AM GMT

PDB ID : 3KRK
Title : X-ray crystal structure of arachidonic acid bound in the cyclooxygenase channel of L531F murine COX-2
Authors : Vecchio, A.J.; Simmons, D.M.; Malkowski, M.G.
Deposited on : 2009-11-18
Resolution : 2.40 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

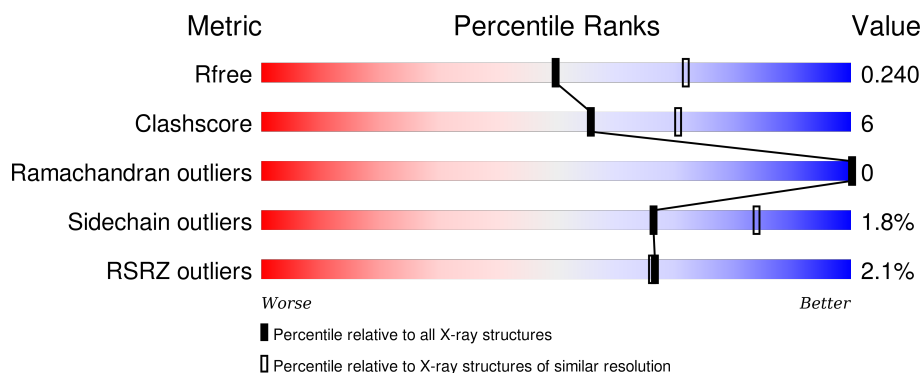
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (2.40-2.40)

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	591	 84% 8% • 7%
1	B	591	 85% 7% • 7%

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	ACD	A	700	-	-	-	X
2	ACD	B	700	-	-	X	X
3	AKR	A	622	-	-	X	-
3	AKR	A	623	-	-	X	-
3	AKR	B	622	-	-	-	X
3	AKR	B	623	-	-	X	-
4	GOL	A	619	-	-	-	X
4	GOL	A	624	-	-	-	X
5	COH	A	625	-	-	-	X
5	COH	B	626	-	-	-	X
6	NAG	A	661	-	-	-	X
6	NAG	B	661	X	-	-	X
7	NAG	A	681	-	-	-	X
8	BOG	A	703	-	-	-	X
8	BOG	B	703	-	-	-	X

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 9919 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.

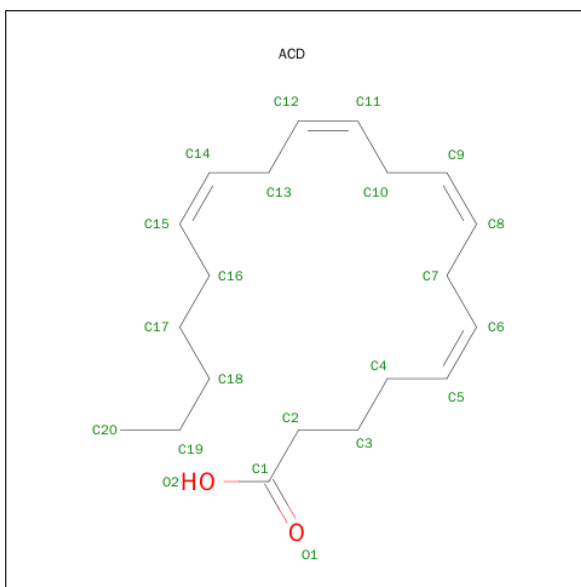
- Molecule 1 is a protein called Prostaglandin G/H synthase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	551	Total	C	N	O	S	0	2	0
			4451	2877	741	808	25			
1	B	552	Total	C	N	O	S	0	4	0
			4477	2893	751	808	25			

There are 16 discrepancies between the modelled and reference sequences:

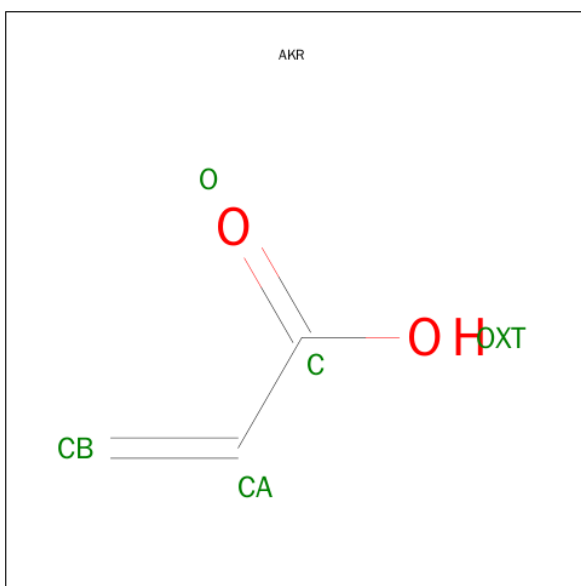
Chain	Residue	Modelled	Actual	Comment	Reference
A	29	HIS	-	EXPRESSION TAG	UNP Q05769
A	30	HIS	-	EXPRESSION TAG	UNP Q05769
A	31	HIS	-	EXPRESSION TAG	UNP Q05769
A	32	HIS	-	EXPRESSION TAG	UNP Q05769
A	33	HIS	-	EXPRESSION TAG	UNP Q05769
A	34	HIS	-	EXPRESSION TAG	UNP Q05769
A	531	PHE	LEU	ENGINEERED	UNP Q05769
A	594	ALA	ASN	ENGINEERED	UNP Q05769
B	29	HIS	-	EXPRESSION TAG	UNP Q05769
B	30	HIS	-	EXPRESSION TAG	UNP Q05769
B	31	HIS	-	EXPRESSION TAG	UNP Q05769
B	32	HIS	-	EXPRESSION TAG	UNP Q05769
B	33	HIS	-	EXPRESSION TAG	UNP Q05769
B	34	HIS	-	EXPRESSION TAG	UNP Q05769
B	531	PHE	LEU	ENGINEERED	UNP Q05769
B	594	ALA	ASN	ENGINEERED	UNP Q05769

- Molecule 2 is ARACHIDONIC ACID (three-letter code: ACD) (formula: C₂₀H₃₂O₂).



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

- Molecule 3 is ACRYLIC ACID (three-letter code: AKR) (formula: $C_3H_4O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			5	3	2		
3	A	1	Total	C	O	0	0
			5	3	2		

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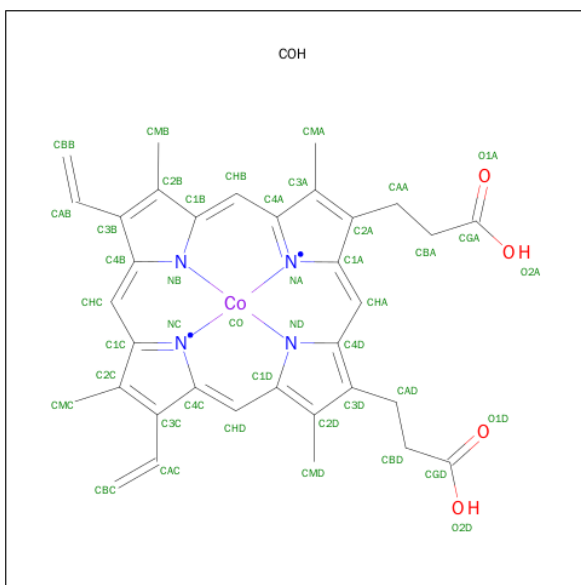
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			5	3	2		
3	B	1	Total	C	O	0	0
			5	3	2		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is PROTOPORPHYRIN IX CONTAINING CO (three-letter code: COH) (formula: $C_{34}H_{32}CoN_4O_4$).



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

- Molecule 6 is a polymer of unknown type called SUGAR (2-MER).

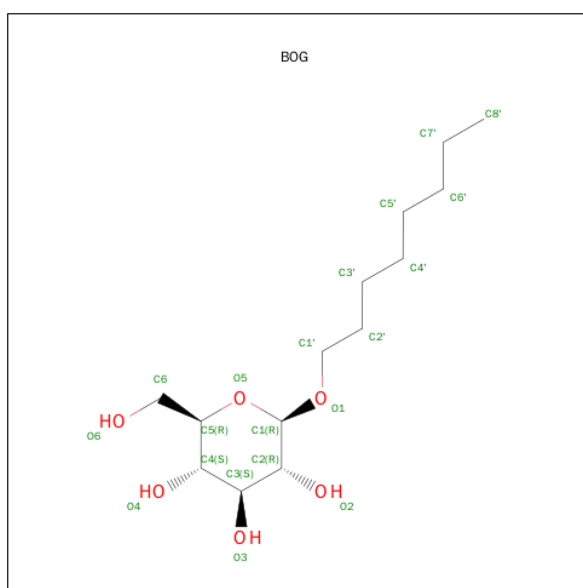
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	2	Total	C	N	O	0	0
			28	16	2	10		
6	A	2	Total	C	N	O	0	0
			28	16	2	10		
6	B	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 7 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 8 is SUGAR (B-OCTYLGLUCOSIDE) (three-letter code: BOG) (formula: $C_{14}H_{28}O_6$).



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

- Molecule 9 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	B	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	327	Total	O	0	0
			327	327		
10	B	305	Total	O	0	0
			305	305		

4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	120.79Å 133.04Å 180.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.92 – 2.40 19.92 – 2.40	Depositor EDS
% Data completeness (in resolution range)	96.6 (19.92-2.40) 96.6 (19.92-2.40)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.11 (at 2.41Å)	Xtriage
Refinement program	REFMAC 5.5.0088	Depositor
R, R_{free}	0.179 , 0.228 0.193 , 0.240	Depositor DCC
R_{free} test set	2794 reflections (5.35%)	DCC
Wilson B-factor (Å ²)	30.0	Xtriage
Anisotropy	0.119	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 43.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	1 of 55045 reflections (0.002%)	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9919	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.27% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 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: GOL, NAG, ACD, AKR, COH, BOG, MAN

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	0.42	0/4588	0.51	0/6231
1	B	0.40	0/4617	0.53	0/6264
All	All	0.41	0/9205	0.52	0/12495

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
6	B	1	0

There are no bond length outliers.

There are no bond angle outliers.

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	B	661	NAG	C5

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	4451	0	4292	52	0
1	B	4477	0	4340	50	0
2	A	22	0	31	6	0
2	B	22	0	31	10	0
3	A	10	0	6	5	0
3	B	10	0	6	3	0
4	A	12	0	16	1	0
4	B	6	0	8	0	0
5	A	43	0	30	9	0
5	B	43	0	30	19	0
6	A	56	0	50	2	0
6	B	28	0	25	0	0
7	A	14	0	13	2	0
7	B	14	0	13	0	0
8	A	20	0	28	7	0
8	B	20	0	28	0	0
9	B	39	0	34	3	0
10	A	327	0	0	4	0
10	B	305	0	0	1	0
All	All	9919	0	8981	113	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (113) 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)
8:A:703:BOG:O2	8:A:703:BOG:H3'1	1.50	1.09
1:A:265:THR:HG22	1:A:268:ASP:H	1.33	0.90
1:A:161:THR:HG21	1:A:166:LYS:O	1.73	0.89
8:A:703:BOG:O2	8:A:703:BOG:C3'	2.29	0.81
1:A:385:TYR:OH	2:A:700:ACD:H14	1.83	0.78
1:B:123:LEU:O	1:B:469:ARG:NH2	2.18	0.75
1:A:386:HIS:NE2	5:A:625:COH:HAD2	2.02	0.74
1:A:478:PHE:HD2	3:A:622:AKR:HA1	1.52	0.73
1:B:216:ARG:NH1	9:B:672:NAG:H83	2.03	0.73
1:A:216:ARG:NH1	6:A:672:NAG:H83	2.06	0.71
1:A:391:LEU:HD11	5:A:625:COH:HHC	1.73	0.70
1:A:181:VAL:HG13	1:A:509:VAL:HG11	1.72	0.70
1:B:240:ARG:NH2	1:B:272:GLU:O	2.19	0.69
1:A:391:LEU:CD1	5:A:625:COH:HAB	2.25	0.66
1:B:386:HIS:NE2	5:B:626:COH:HAD2	2.12	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:386:HIS:CE1	5:B:626:COH:HAD1	2.32	0.64
1:B:216:ARG:HH11	9:B:672:NAG:H83	1.62	0.64
5:B:626:COH:HBA1	5:B:626:COH:HHA	1.80	0.62
1:B:205:PHE:HE2	2:B:700:ACD:H15	1.64	0.62
1:A:391:LEU:HD13	5:A:625:COH:HAB	1.82	0.60
1:A:386:HIS:NE2	5:A:625:COH:CAD	2.65	0.59
1:B:205:PHE:CE2	2:B:700:ACD:H15	2.37	0.59
1:B:216:ARG:HG2	9:B:672:NAG:H81	1.84	0.58
1:A:289:GLN:HG2	1:A:292:PHE:CE1	2.40	0.57
1:B:391:LEU:CD2	5:B:626:COH:HAB	2.35	0.56
1:B:203:GLN:HA	5:B:626:COH:HAC	1.87	0.56
1:B:380:GLU:HG2	1:B:466:TYR:CE2	2.41	0.56
1:A:413:ILE:HG12	7:A:681:NAG:H61	1.88	0.55
1:B:391:LEU:CD1	5:B:626:COH:HAB	2.37	0.55
1:A:492:LYS:HD3	3:A:622:AKR:CA	2.36	0.55
5:B:626:COH:HBA1	5:B:626:COH:CHA	2.37	0.54
5:B:626:COH:HHA	5:B:626:COH:CBA	2.37	0.54
1:B:492:LYS:HD3	3:B:622:AKR:HA1	1.88	0.54
1:A:249:ASP:HB3	10:A:750:HOH:O	2.06	0.54
1:B:391:LEU:HD11	5:B:626:COH:HHC	1.89	0.53
1:B:240:ARG:HH21	3:B:623:AKR:HA1	1.74	0.53
1:A:484:GLU:HG2	1:A:485:LYS:H	1.74	0.52
1:A:185:ARG:HH21	8:A:703:BOG:H3	1.74	0.52
1:B:382:ASN:O	1:B:386:HIS:HD2	1.94	0.51
1:B:352[A]:LEU:HD21	1:B:518:PHE:HE2	1.74	0.51
1:A:216:ARG:HG2	6:A:672:NAG:H81	1.91	0.51
1:B:274:ILE:HD12	1:B:291:VAL:HG12	1.91	0.51
1:A:414:LEU:HD11	1:A:419:LEU:HD12	1.93	0.51
1:B:178:LEU:HD21	1:B:445:GLN:HG2	1.92	0.51
1:B:382:ASN:O	1:B:386:HIS:CD2	2.64	0.50
1:B:386:HIS:CE1	5:B:626:COH:CAD	2.94	0.50
1:B:203:GLN:CA	5:B:626:COH:HAC	2.42	0.50
8:A:703:BOG:O2	8:A:703:BOG:H4'2	2.12	0.49
1:A:349:VAL:HG13	2:A:700:ACD:H42	1.94	0.49
1:A:391:LEU:HD11	5:A:625:COH:HAB	1.94	0.49
1:A:181:VAL:HG13	1:A:509:VAL:CG1	2.42	0.49
1:B:289:GLN:HG2	1:B:292:PHE:CE1	2.48	0.49
1:A:472:LEU:HD21	1:A:524:GLU:HG3	1.96	0.48
1:B:352[A]:LEU:HD21	1:B:518:PHE:CE2	2.48	0.48
1:B:280:PRO:HG2	1:B:283:LEU:HD12	1.95	0.48
1:A:161:THR:HG22	1:A:164:GLY:N	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:240:ARG:HH11	3:A:623:AKR:HA1	1.79	0.47
1:A:391:LEU:HD11	5:A:625:COH:CHC	2.41	0.47
1:A:478:PHE:CD2	3:A:622:AKR:HA1	2.40	0.47
1:B:240:ARG:HE	3:B:623:AKR:CA	2.27	0.47
1:A:340:THR:O	1:A:344:VAL:HG23	2.14	0.47
8:A:703:BOG:O2	8:A:703:BOG:C4'	2.62	0.47
1:B:386:HIS:NE2	5:B:626:COH:CAD	2.77	0.47
5:B:626:COH:HHA	5:B:626:COH:HBD1	1.97	0.47
1:B:352[A]:LEU:CD2	2:B:700:ACD:H71	2.44	0.47
1:A:533:GLY:HA3	2:A:700:ACD:H191	1.97	0.47
1:A:386:HIS:HB3	1:A:388[B]:HIS:CE1	2.51	0.46
1:B:391:LEU:HD22	5:B:626:COH:HAB	1.96	0.46
1:B:381:PHE:HE1	2:B:700:ACD:H191	1.81	0.46
8:A:703:BOG:H3'1	8:A:703:BOG:C2	2.41	0.46
1:A:161:THR:HG22	1:A:164:GLY:H	1.80	0.46
1:B:414:LEU:HD11	1:B:419:LEU:HD22	1.98	0.46
1:A:274:ILE:HD12	1:A:291:VAL:HG12	1.97	0.46
1:A:229:ASP:HB3	1:B:139:TRP:CZ2	2.51	0.46
8:A:703:BOG:H3'1	8:A:703:BOG:HO2	1.72	0.46
1:B:253:LYS:NZ	10:B:869:HOH:O	2.49	0.45
1:A:198:PHE:CZ	1:A:352:LEU:HD21	2.52	0.45
1:A:198:PHE:HZ	1:A:352:LEU:HD21	1.80	0.45
1:A:348:TYR:HE2	2:A:700:ACD:H12	1.81	0.45
1:B:391:LEU:HD13	5:B:626:COH:HAB	1.99	0.45
1:A:214:HIS:HD2	10:A:828:HOH:O	2.00	0.45
1:A:62:THR:HA	4:A:619:GOL:H12	1.98	0.44
1:A:484:GLU:HG2	1:A:485:LYS:N	2.33	0.44
1:B:442:ILE:O	1:B:445:GLN:HB2	2.18	0.44
1:B:530[A]:SER:HA	2:B:700:ACD:H171	1.99	0.43
1:B:294:LEU:HA	1:B:409:TYR:CE1	2.52	0.43
1:A:391:LEU:HD11	5:A:625:COH:CAB	2.48	0.43
1:A:240:ARG:HH11	3:A:623:AKR:CA	2.30	0.43
1:A:363:PRO:HG2	1:A:545:TRP:CD2	2.53	0.43
1:A:581:ASN:HB2	10:A:781:HOH:O	2.17	0.43
1:A:413:ILE:CG1	7:A:681:NAG:H61	2.49	0.43
1:B:530[B]:SER:HA	2:B:700:ACD:H171	2.00	0.43
1:A:348:TYR:CE2	2:A:700:ACD:H12	2.54	0.42
1:A:459:LYS:HD3	10:A:718:HOH:O	2.18	0.42
1:A:265:THR:HG23	1:A:267:LYS:H	1.83	0.42
1:B:391:LEU:HD11	5:B:626:COH:CHC	2.50	0.42
1:B:348:TYR:CE2	2:B:700:ACD:H14	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:386:HIS:CE1	5:A:625:COH:HAD2	2.55	0.42
1:B:391:LEU:CD2	5:B:626:COH:CAB	2.98	0.42
1:B:533:GLY:HA3	2:B:700:ACD:H192	2.01	0.41
1:B:206:THR:HG21	1:B:385:TYR:CE1	2.55	0.41
1:B:183:LEU:HD21	1:B:445:GLN:HG3	2.03	0.41
1:A:530[A]:SER:OG	2:A:700:ACD:H131	2.21	0.41
5:B:626:COH:CGA	5:B:626:COH:HHA	2.51	0.41
1:B:155:VAL:O	1:B:459:LYS:HE2	2.21	0.41
1:B:363:PRO:HG2	1:B:545:TRP:CD2	2.56	0.41
1:B:526:GLY:HA3	2:B:700:ACD:C9	2.51	0.41
1:B:389:PRO:HB2	1:B:434:VAL:HA	2.02	0.40
5:B:626:COH:CGA	5:B:626:COH:HBD1	2.51	0.40
1:A:575:CYS:O	1:A:575:CYS:SG	2.79	0.40
1:B:352[A]:LEU:HD22	2:B:700:ACD:H71	2.03	0.40
1:A:467:ARG:HG2	1:A:472:LEU:HD12	2.03	0.40
1:A:352:LEU:HD22	1:A:518:PHE:CE2	2.56	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	551/591 (93%)	537 (98%)	14 (2%)	0	100	100
1	B	554/591 (94%)	542 (98%)	12 (2%)	0	100	100
All	All	1105/1182 (94%)	1079 (98%)	26 (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	483/529 (91%)	472 (98%)	11 (2%)	58	78
1	B	486/529 (92%)	480 (99%)	6 (1%)	78	90
All	All	969/1058 (92%)	952 (98%)	17 (2%)	66	84

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	161	THR
1	A	174	SER
1	A	181	VAL
1	A	232	HIS
1	A	265	THR
1	A	282	ASN
1	A	318	GLN
1	A	385	TYR
1	A	412	SER
1	A	484	GLU
1	A	556	PHE
1	B	88	THR
1	B	122	TYR
1	B	289	GLN
1	B	385	TYR
1	B	469	ARG
1	B	484	GLU

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

Mol	Chain	Res	Type
1	A	90	HIS

5.3.3 RNA [i](#)

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 ⓘ

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	$\# Z > 2$
6	NAG	A	661	1,6	14,14,15	0.48	0	15,19,21	1.09	1 (6%)
6	NAG	A	662	6	14,14,15	0.51	0	15,19,21	1.64	4 (26%)
6	NAG	A	671	1,6	14,14,15	0.49	0	15,19,21	1.27	2 (13%)
6	NAG	A	672	6	14,14,15	0.46	0	15,19,21	0.71	0
6	NAG	B	661	1,6	14,14,15	0.52	0	15,19,21	0.89	0
6	NAG	B	662	6	14,14,15	0.56	0	15,19,21	1.08	1 (6%)
9	NAG	B	671	1,9	14,14,15	0.53	0	15,19,21	1.01	1 (6%)
9	NAG	B	672	9	14,14,15	0.59	0	15,19,21	1.24	1 (6%)
9	MAN	B	673	9	11,11,12	0.55	0	14,15,17	2.45	5 (35%)

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
6	NAG	A	661	1,6	-	0/6/23/26	0/1/1/1
6	NAG	A	662	6	-	0/6/23/26	0/1/1/1
6	NAG	A	671	1,6	-	0/6/23/26	0/1/1/1
6	NAG	A	672	6	-	0/6/23/26	0/1/1/1
6	NAG	B	661	1,6	1/1/5/7	0/6/23/26	0/1/1/1
6	NAG	B	662	6	-	0/6/23/26	0/1/1/1
9	NAG	B	671	1,9	-	0/6/23/26	0/1/1/1
9	NAG	B	672	9	-	0/6/23/26	0/1/1/1
9	MAN	B	673	9	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	662	NAG	C4-C3-C2	-2.38	107.53	111.23
6	A	671	NAG	C2-N2-C7	-2.25	120.15	123.04
6	A	662	NAG	C3-C2-N2	2.02	115.39	110.56
9	B	673	MAN	O5-C5-C6	2.02	111.73	107.35
9	B	673	MAN	C2-C3-C4	2.07	114.56	111.04
6	B	662	NAG	C4-C3-C2	2.72	115.47	111.23
6	A	661	NAG	C1-O5-C5	2.78	115.77	112.25
9	B	671	NAG	C1-O5-C5	2.83	115.83	112.25
9	B	673	MAN	C3-C4-C5	2.90	115.25	110.20
6	A	662	NAG	C1-O5-C5	3.30	116.44	112.25
6	A	662	NAG	C2-N2-C7	3.38	127.39	123.04
9	B	672	NAG	C4-C3-C2	3.52	116.69	111.23
6	A	671	NAG	C1-O5-C5	3.94	117.25	112.25
9	B	673	MAN	C1-C2-C3	4.60	114.98	109.54
9	B	673	MAN	C1-O5-C5	6.29	120.23	112.25

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	B	661	NAG	C5

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	672	NAG	2	0
9	B	672	NAG	3	0

5.6 Ligand geometry [i](#)

15 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
4	GOL	A	619	-	5,5,5	0.26	0	5,5,5	0.28	0
3	AKR	A	622	-	1,4,4	1.53	0	0,4,4	0.00	-
3	AKR	A	623	-	1,4,4	1.13	0	0,4,4	0.00	-
4	GOL	A	624	-	5,5,5	0.31	0	5,5,5	0.23	0
5	COH	A	625	-	28,50,50	2.39	10 (35%)	19,82,82	3.18	9 (47%)
7	NAG	A	681	1	14,14,15	1.48	1 (7%)	15,19,21	1.36	2 (13%)
2	ACD	A	700	-	18,21,21	0.42	0	18,21,21	0.58	0
8	BOG	A	703	-	20,20,20	0.70	1 (5%)	25,25,25	0.80	1 (4%)
3	AKR	B	622	-	1,4,4	1.41	0	0,4,4	0.00	-
3	AKR	B	623	-	1,4,4	1.47	0	0,4,4	0.00	-
4	GOL	B	624	-	5,5,5	0.26	0	5,5,5	0.24	0
5	COH	B	626	-	28,50,50	2.42	9 (32%)	19,82,82	2.78	8 (42%)
7	NAG	B	681	1	14,14,15	0.55	0	15,19,21	0.65	0
2	ACD	B	700	-	18,21,21	0.45	0	18,21,21	0.44	0
8	BOG	B	703	-	20,20,20	0.80	2 (10%)	25,25,25	1.59	4 (16%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	A	619	-	-	0/4/4/4	0/0/0/0
3	AKR	A	622	-	-	0/0/2/2	0/0/0/0
3	AKR	A	623	-	-	0/0/2/2	0/0/0/0
4	GOL	A	624	-	-	0/4/4/4	0/0/0/0
5	COH	A	625	-	-	0/6/54/54	0/0/8/8
7	NAG	A	681	1	-	0/6/23/26	0/1/1/1
2	ACD	A	700	-	-	0/17/19/19	0/0/0/0
8	BOG	A	703	-	-	0/11/31/31	0/1/1/1
3	AKR	B	622	-	-	0/0/2/2	0/0/0/0
3	AKR	B	623	-	-	0/0/2/2	0/0/0/0
4	GOL	B	624	-	-	0/4/4/4	0/0/0/0
5	COH	B	626	-	-	0/6/54/54	0/0/8/8
7	NAG	B	681	1	-	0/6/23/26	0/1/1/1
2	ACD	B	700	-	-	0/17/19/19	0/0/0/0
8	BOG	B	703	-	-	0/11/31/31	0/1/1/1

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	681	NAG	O5-C1	-5.36	1.34	1.43
8	B	703	BOG	O5-C1	2.01	1.47	1.41
5	B	626	COH	C4C-CHD	2.02	1.45	1.39
5	A	625	COH	C4C-CHD	2.03	1.45	1.39
5	A	625	COH	C4B-CHC	2.18	1.45	1.39
8	B	703	BOG	O1-C1	2.39	1.44	1.40
8	A	703	BOG	O1-C1	2.45	1.44	1.40
5	A	625	COH	C4B-NB	3.51	1.46	1.36
5	A	625	COH	C3D-C2D	3.51	1.48	1.37
5	A	625	COH	C4D-ND	3.71	1.46	1.36
5	A	625	COH	C2A-C3A	3.83	1.49	1.37
5	B	626	COH	C3D-C2D	3.84	1.49	1.37
5	B	626	COH	C2A-C3A	3.86	1.49	1.37
5	B	626	COH	C4D-ND	3.91	1.47	1.36
5	B	626	COH	C4B-NB	3.93	1.47	1.36
5	A	625	COH	C4C-NC	4.18	1.48	1.36
5	B	626	COH	C1B-NB	4.19	1.48	1.36
5	B	626	COH	C4C-NC	4.19	1.48	1.36
5	A	625	COH	C1B-NB	4.47	1.48	1.36
5	A	625	COH	C3B-C2B	4.96	1.46	1.40
5	B	626	COH	C3B-C2B	5.01	1.46	1.40
5	B	626	COH	C3C-C2C	5.28	1.47	1.40
5	A	625	COH	C3C-C2C	5.32	1.47	1.40

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	681	NAG	C1-O5-C5	-4.18	106.94	112.25
5	B	626	COH	C3C-CAC-CBC	-3.62	118.91	126.32
5	A	625	COH	C3C-CAC-CBC	-3.44	119.28	126.32
5	A	625	COH	C3B-CAB-CBB	-3.26	119.65	126.32
5	B	626	COH	C3B-CAB-CBB	-3.20	119.78	126.32
5	A	625	COH	C1D-ND-C4D	-2.56	96.85	105.58
8	B	703	BOG	C1'-O1-C1	-2.47	109.62	113.94
5	A	625	COH	CBA-CAA-C2A	-2.44	108.15	112.53
5	B	626	COH	C1C-NC-C4C	-2.32	97.67	105.58
8	A	703	BOG	C1'-O1-C1	-2.23	110.05	113.94
5	A	625	COH	C1C-NC-C4C	-2.15	98.23	105.58
5	A	625	COH	CBD-CAD-C3D	-2.02	108.92	112.53
5	A	625	COH	CMB-C2B-C3B	2.03	129.07	125.09
5	B	626	COH	CMB-C2B-C3B	2.08	129.15	125.09
7	A	681	NAG	O5-C5-C6	2.34	112.41	107.35
5	B	626	COH	CAD-CBD-CGD	2.43	117.19	112.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	626	COH	CAA-C2A-C1A	2.77	130.01	127.01
8	B	703	BOG	O5-C1-C2	3.24	116.92	110.28
8	B	703	BOG	O5-C5-C4	4.23	117.63	109.68
8	B	703	BOG	C1-O5-C5	4.59	122.66	113.75
5	B	626	COH	C3D-C4D-ND	6.30	114.38	108.74
5	A	625	COH	C2A-C1A-NA	6.45	114.47	108.70
5	B	626	COH	C2A-C1A-NA	6.71	114.71	108.70
5	A	625	COH	C3D-C4D-ND	9.79	117.51	108.74

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

11 monomers are involved in 62 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	619	GOL	1	0
3	A	622	AKR	3	0
3	A	623	AKR	2	0
5	A	625	COH	9	0
7	A	681	NAG	2	0
2	A	700	ACD	6	0
8	A	703	BOG	7	0
3	B	622	AKR	1	0
3	B	623	AKR	2	0
5	B	626	COH	19	0
2	B	700	ACD	10	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	551/591 (93%)	-0.33	7 (1%) 79 79	12, 27, 42, 49	0
1	B	552/591 (93%)	-0.13	16 (2%) 55 54	15, 29, 43, 47	0
All	All	1103/1182 (93%)	-0.23	23 (2%) 67 66	12, 28, 43, 49	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	583	GLN	4.4
1	B	82	LEU	4.2
1	B	91	TYR	3.4
1	A	399	ASP	3.3
1	A	74	PHE	3.2
1	B	74	PHE	2.8
1	A	278	HIS	2.7
1	B	53	ASP	2.6
1	A	122	TYR	2.5
1	B	214	HIS	2.5
1	B	157	ASP	2.5
1	B	78	ILE	2.4
1	B	428	ARG	2.4
1	A	115	TYR	2.3
1	B	278	HIS	2.3
1	B	122	TYR	2.3
1	A	239	ASP	2.2
1	A	81	LEU	2.1
1	B	101	ASN	2.1
1	B	399	ASP	2.1
1	B	102	ILE	2.1
1	B	81	LEU	2.0
1	B	514	PRO	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
6	NAG	B	661	14/15	0.84	0.32	7.03	44,51,53,58	0
6	NAG	A	661	14/15	0.87	0.25	4.76	41,44,47,51	0
6	NAG	A	671	14/15	0.93	0.13	0.20	22,26,29,33	0
9	NAG	B	671	14/15	0.97	0.10	-1.16	27,31,34,40	0
9	MAN	B	673	11/12	0.60	0.51	-	58,60,60,61	0
6	NAG	A	662	14/15	0.78	0.48	-	54,56,57,58	0
6	NAG	B	662	14/15	0.81	0.48	-	61,63,64,64	0
9	NAG	B	672	14/15	0.76	0.30	-	44,48,51,55	0
6	NAG	A	672	14/15	0.93	0.19	-	36,38,40,40	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	COH	A	625	43/43	0.65	0.38	7.14	83,86,86,87	0
2	ACD	A	700	22/22	0.87	0.23	4.57	47,48,50,51	0
5	COH	B	626	43/43	0.64	0.37	4.25	77,79,80,81	0
2	ACD	B	700	22/22	0.84	0.26	3.90	42,52,57,58	0
4	GOL	A	624	6/6	0.93	0.19	3.64	38,39,40,40	0
4	GOL	A	619	6/6	0.71	0.30	2.82	77,78,78,78	0
3	AKR	B	622	5/5	0.85	0.27	2.50	61,61,61,61	0
8	BOG	A	703	20/20	0.90	0.21	2.49	71,72,73,73	20
7	NAG	A	681	14/15	0.91	0.28	2.40	40,43,46,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
8	BOG	B	703	20/20	0.88	0.20	2.16	18,20,21,21	20
3	AKR	A	622	5/5	0.86	0.25	1.79	52,52,52,52	0
3	AKR	B	623	5/5	0.82	0.26	1.51	52,52,52,52	0
3	AKR	A	623	5/5	0.94	0.25	1.39	45,45,45,45	0
7	NAG	B	681	14/15	0.90	0.24	1.09	39,42,44,45	0
4	GOL	B	624	6/6	0.96	0.14	0.62	40,41,41,41	0

6.5 Other polymers [i](#)

There are no such residues in this entry.