



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 22, 2016 – 06:31 AM EDT

PDB ID : 5F1A  
Title : The Crystal Structure of Salicylate Bound to Human Cyclooxygenase-2  
Authors : Lucido, M.J.; Orlando, B.J.; Malkowski, M.G.  
Deposited on : 2015-11-30  
Resolution : 2.38 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](mailto: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 : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20027107  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0122  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20027107

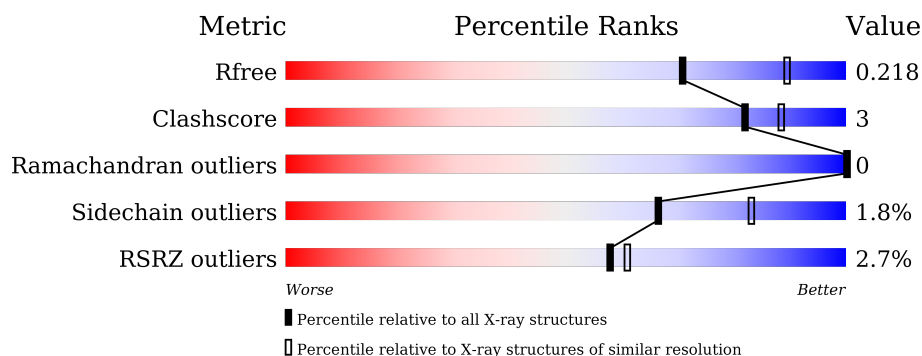
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.38 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	4019 (2.40-2.36)
Clashscore	102246	4595 (2.40-2.36)
Ramachandran outliers	100387	4520 (2.40-2.36)
Sidechain outliers	100360	4522 (2.40-2.36)
RSRZ outliers	91569	4034 (2.40-2.36)

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  $\geq 3$ , 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	553	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 1%, green 98%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>%</span> <span>92%</span> <span>7% .</span> </div> </div>
1	B	553	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 4%, orange 1%, yellow 1%, green 94%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>4%</span> <span>91%</span> <span>8%</span> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SAL	B	601	-	-	X	X
4	NAG	B	603	-	-	-	X
4	NAG	B	607	-	-	-	X
7	EDO	A	610	-	-	-	X
7	EDO	A	611	-	-	-	X
7	EDO	B	611	-	-	-	X
7	EDO	B	612	-	-	-	X

## 2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 9596 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.

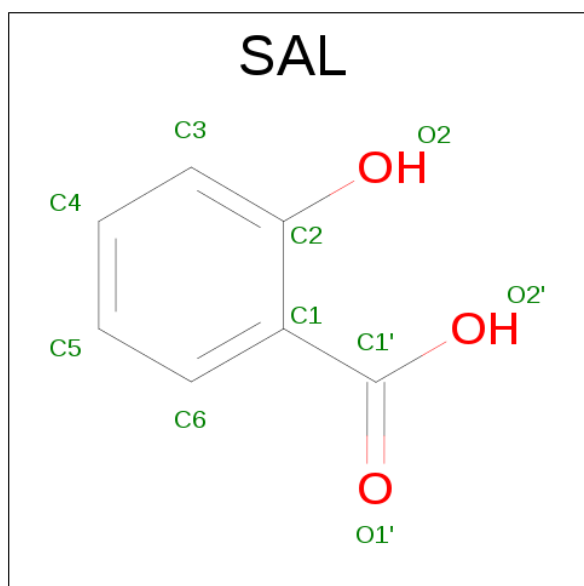
- Molecule 1 is a protein called Prostaglandin G/H synthase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	553	Total	C	N	O	S	0	2	0
			4466	2882	753	805	26			
1	B	552	Total	C	N	O	S	0	2	0
			4447	2865	753	803	26			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	33	LYS	-	expression tag	UNP P35354
B	33	LYS	-	expression tag	UNP P35354

- Molecule 2 is 2-HYDROXYBENZOIC ACID (three-letter code: SAL) (formula: C<sub>7</sub>H<sub>6</sub>O<sub>3</sub>).



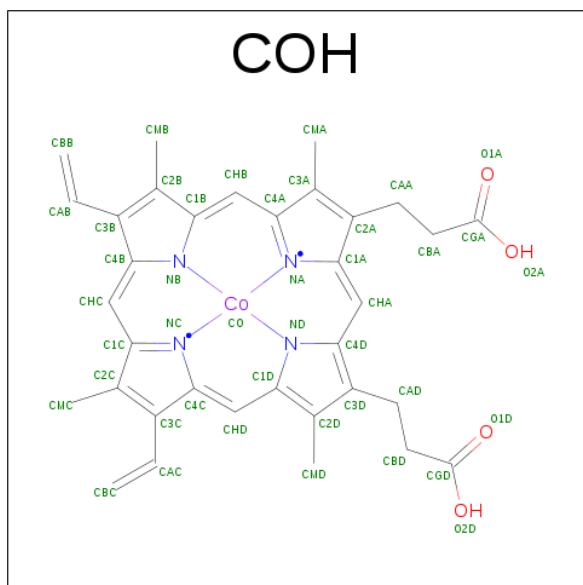
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			10	7	3		

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	C	O	0	0
			10	7	3		

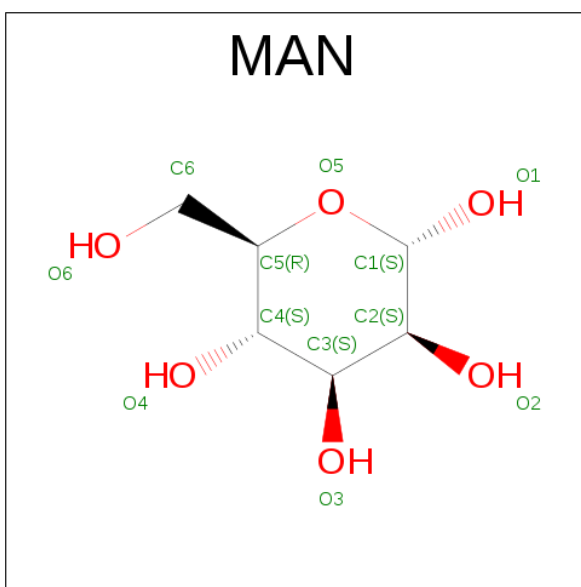
- Molecule 3 is PROTOPORPHYRIN IX CONTAINING CO (three-letter code: COH) (formula:  $C_{34}H_{32}CoN_4O_4$ ).





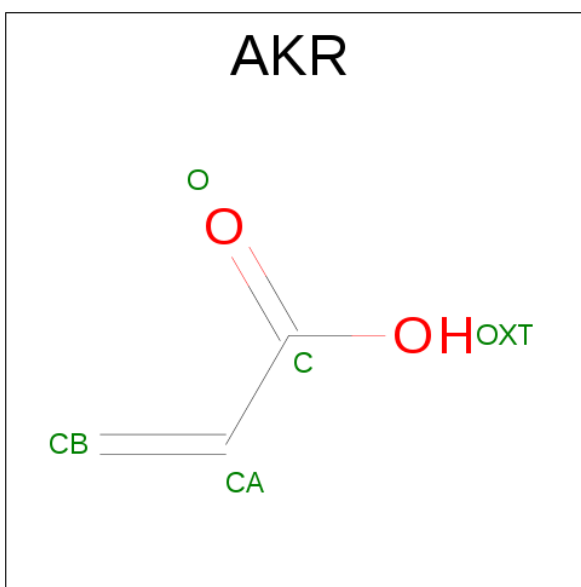
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 5 is ALPHA-D-MANNOSE (three-letter code: MAN) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			11	6	5		
5	A	1	Total	C	O	0	0
			11	6	5		
5	B	1	Total	C	O	0	0
			11	6	5		

- Molecule 6 is ACRYLIC ACID (three-letter code: AKR) (formula:  $C_3H_4O_2$ ).



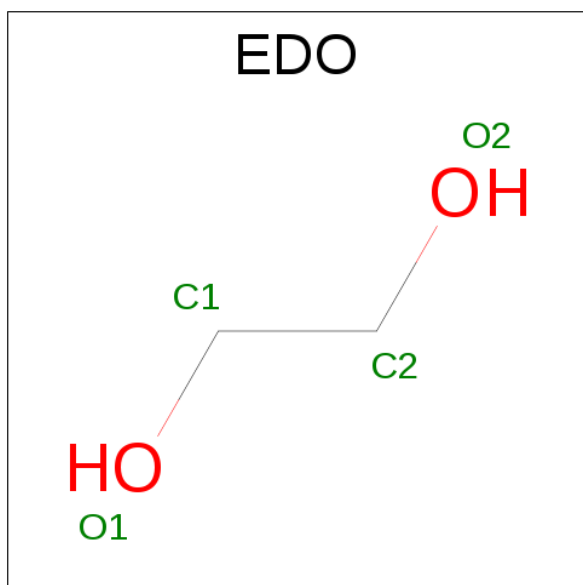
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			5	3	2		

*Continued on next page...*

Continued from previous page...

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

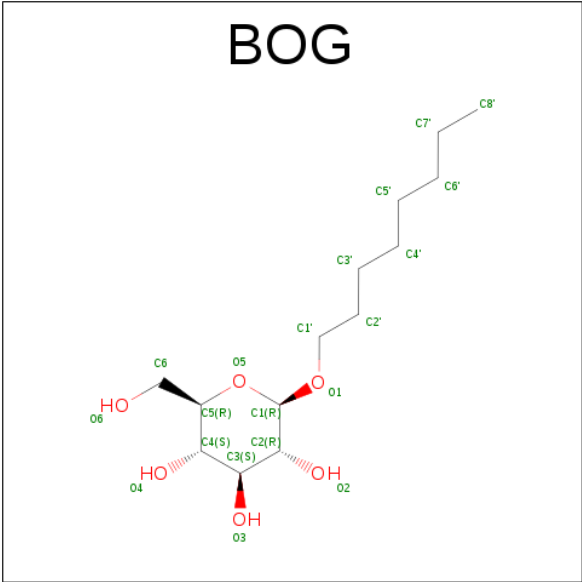
- Molecule 7 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula:  $C_2H_6O_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			4	2	2		
7	A	1	Total	C	O	0	0
			4	2	2		
7	A	1	Total	C	O	0	0
			4	2	2		
7	B	1	Total	C	O	0	0
			4	2	2		
7	B	1	Total	C	O	0	0
			4	2	2		

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





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

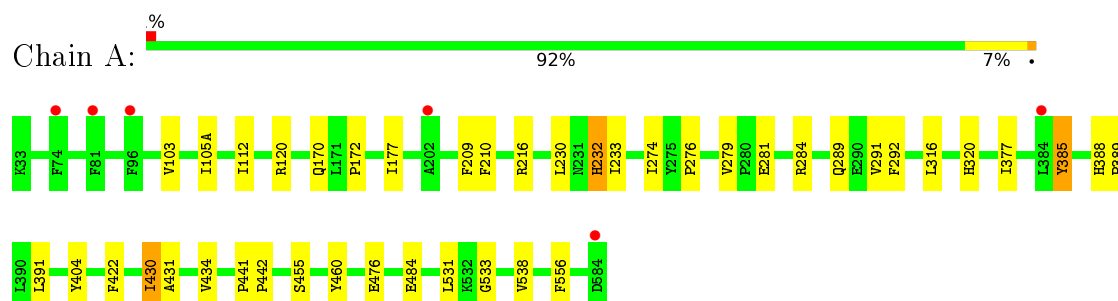
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	212	Total	O	0	0
			212	212		
9	B	179	Total	O	0	0
			179	179		

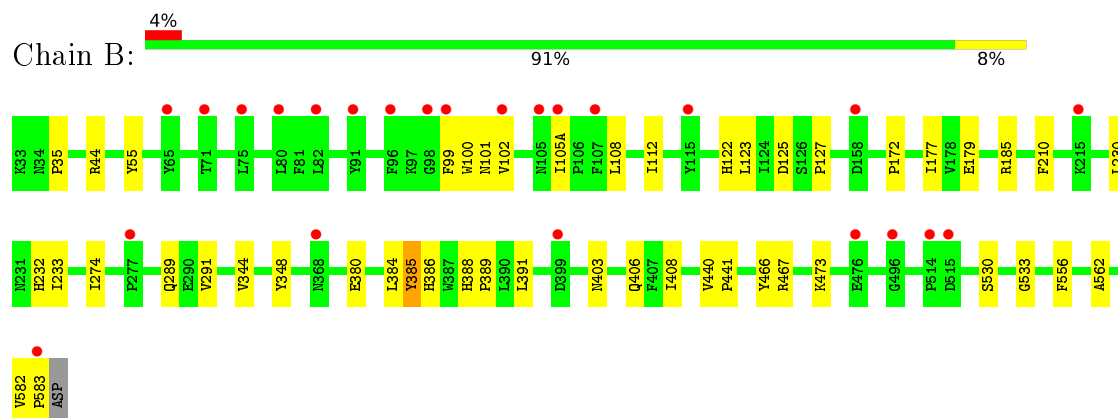
### 3 Residue-property plots

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

- Molecule 1: Prostaglandin G/H synthase 2



- Molecule 1: Prostaglandin G/H synthase 2



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	118.41Å 132.66Å 178.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.32 – 2.38 33.32 – 2.34	Depositor EDS
% Data completeness (in resolution range)	99.5 (33.32-2.38) 99.5 (33.32-2.34)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.30 (at 2.34Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.174 , 0.218 0.179 , 0.218	Depositor DCC
$R_{free}$ test set	5281 reflections (4.96%)	DCC
Wilson B-factor (Å <sup>2</sup> )	34.1	Xtriage
Anisotropy	0.531	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 35.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 59202 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	9596	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.49% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, SAL, AKR, EDO, 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	0.37	0/4605	0.45	0/6252
1	B	0.34	0/4583	0.45	1/6224 (0.0%)
All	All	0.35	0/9188	0.45	1/12476 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	384	LEU	CA-CB-CG	5.25	127.38	115.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4466	0	4317	25	0
1	B	4447	0	4293	28	0
2	A	10	0	4	3	0
2	B	10	0	4	4	0
3	A	43	0	30	4	0
3	B	43	0	30	2	0
4	A	42	0	37	1	0
4	B	56	0	50	1	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	22	0	19	0	0
5	B	11	0	10	0	0
6	A	5	0	3	0	0
6	B	10	0	6	1	0
7	A	12	0	18	3	0
7	B	8	0	12	3	0
8	B	20	0	28	2	0
9	A	212	0	0	2	0
9	B	179	0	0	1	0
All	All	9596	0	8861	57	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 (57) 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:533:GLY:HA3	7:B:612:EDO:H11	1.54	0.87
1:B:385:TYR:CE2	2:B:601:SAL:H3	2.15	0.81
1:B:530:SER:HA	7:B:612:EDO:H21	1.67	0.77
3:A:602:COH:HBB1	3:A:602:COH:HMB1	1.68	0.75
3:A:602:COH:HMC1	3:A:602:COH:HBC1	1.71	0.71
1:B:185:ARG:HE	8:B:608:BOG:H62	1.58	0.69
2:A:601:SAL:O2	9:A:701:HOH:O	2.11	0.68
1:A:385:TYR:CE2	2:A:601:SAL:H3	2.30	0.67
1:A:274:ILE:HD12	1:A:291:VAL:HG12	1.84	0.58
1:B:467:ARG:NH2	1:B:473:LYS:O	2.34	0.58
1:A:281:GLU:HA	1:A:284:ARG:HD2	1.85	0.58
1:A:172:PRO:HG2	1:A:177:ILE:HD11	1.88	0.56
1:B:230:LEU:HD13	1:B:233:ILE:HD12	1.90	0.54
1:B:179:GLU:HB3	8:B:608:BOG:H4'2	1.89	0.54
1:A:388[B]:HIS:HE1	3:A:602:COH:ND	2.05	0.54
2:B:601:SAL:O2	9:B:702:HOH:O	2.19	0.54
3:B:602:COH:HHC	3:B:602:COH:HBB1	1.90	0.53
1:B:172:PRO:HG2	1:B:177:ILE:HD11	1.90	0.53
1:B:44:ARG:NH2	1:B:125:ASP:OD1	2.42	0.53
1:B:389:PRO:HD3	1:B:440:VAL:HG22	1.90	0.52
1:A:391:LEU:HB3	1:A:404:TYR:OH	2.11	0.51
1:A:216:ARG:HB2	4:A:604:NAG:H81	1.92	0.50
1:B:274:ILE:HD12	1:B:291:VAL:HG12	1.93	0.48
1:A:276:PRO:HG2	1:A:279:VAL:HG23	1.94	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:562:ALA:HA	7:B:611:EDO:H21	1.96	0.47
1:A:230:LEU:HG	1:A:233:ILE:HD12	1.96	0.47
1:A:430:ILE:HG13	1:A:431:ALA:N	2.30	0.47
1:A:170:GLN:NE2	9:A:714:HOH:O	2.48	0.46
1:B:210:PHE:HB3	3:B:602:COH:HBD1	1.97	0.46
1:B:344:VAL:HA	1:B:348:TYR:HB3	1.97	0.46
1:A:533:GLY:HA3	7:A:611:EDO:H22	1.98	0.46
1:A:538:VAL:HG23	1:B:127:PRO:HB2	1.99	0.45
1:B:385:TYR:CZ	2:B:601:SAL:H3	2.50	0.45
1:A:389:PRO:HB2	1:A:434:VAL:HA	1.98	0.45
1:A:385:TYR:CZ	2:A:601:SAL:H3	2.52	0.44
1:A:120:ARG:HG3	1:A:531:LEU:HD12	2.00	0.44
1:B:35:PRO:HB2	1:B:55:TYR:HB3	1.98	0.44
1:B:406:GLN:HB3	4:B:607:NAG:H62	2.00	0.42
1:A:209:PHE:HB2	1:A:377:ILE:HG13	2.02	0.42
1:B:100:TRP:HZ3	1:B:112:ILE:HD13	1.83	0.42
1:A:316:LEU:O	1:A:320:HIS:N	2.53	0.42
1:B:582:VAL:HA	1:B:583:PRO:HD3	1.91	0.42
1:B:403:ASN:HB2	6:B:610:AKR:O	2.20	0.41
1:B:385:TYR:HE2	2:B:601:SAL:H3	1.75	0.41
1:B:99:PHE:O	1:B:102:VAL:HG12	2.20	0.41
1:A:232:HIS:HB2	1:A:292:PHE:CE2	2.56	0.41
1:A:103:VAL:HG11	1:A:112:ILE:HD12	2.02	0.41
1:A:120:ARG:HH21	7:A:610:EDO:C2	2.34	0.41
1:A:441:PRO:HA	1:A:442:PRO:HD3	1.98	0.41
1:A:455[A]:SER:HB2	1:A:460:TYR:CD2	2.56	0.41
1:A:120:ARG:HH21	7:A:610:EDO:H21	1.86	0.41
1:B:380:GLU:HG2	1:B:466:TYR:CE1	2.55	0.41
1:B:391:LEU:HB2	1:B:441:PRO:HG2	2.02	0.40
1:A:210:PHE:HB3	3:A:602:COH:HBD1	2.03	0.40
1:B:386:HIS:HB3	1:B:388[A]:HIS:NE2	2.36	0.40
1:B:105(A):ILE:HD13	1:B:108:LEU:HD12	2.03	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	553/553 (100%)	536 (97%)	17 (3%)	0	100	100
1	B	552/553 (100%)	536 (97%)	16 (3%)	0	100	100
All	All	1105/1106 (100%)	1072 (97%)	33 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	485/492 (99%)	476 (98%)	9 (2%)	65	82
1	B	482/492 (98%)	474 (98%)	8 (2%)	68	84
All	All	967/984 (98%)	950 (98%)	17 (2%)	66	83

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

Mol	Chain	Res	Type
1	A	105(A)	ILE
1	A	232	HIS
1	A	289	GLN
1	A	385	TYR
1	A	422	PHE
1	A	430	ILE
1	A	476	GLU
1	A	484	GLU
1	A	556	PHE
1	B	101	ASN
1	B	122	HIS
1	B	123	LEU
1	B	232	HIS
1	B	289	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	385	TYR
1	B	408	ILE
1	B	556	PHE

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

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

23 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	SAL	A	601	-	7,10,10	1.71	2 (28%)	10,13,13	1.14	1 (10%)
3	COH	A	602	1	27,50,50	4.58	20 (74%)	23,82,82	4.51	7 (30%)
4	NAG	A	603	1,4	14,14,15	0.19	0	15,19,21	0.54	0
4	NAG	A	604	5,4	14,14,15	0.49	0	15,19,21	0.70	0
5	MAN	A	605	5,4	11,11,12	1.28	2 (18%)	15,15,17	1.63	3 (20%)
5	MAN	A	606	5	11,11,12	0.80	0	15,15,17	0.85	1 (6%)
4	NAG	A	607	1	14,14,15	0.18	0	15,19,21	0.40	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	AKR	A	608	-	1,4,4	0.55	0	0,4,4	0.00	-
7	EDO	A	609	-	3,3,3	0.45	0	2,2,2	0.38	0
7	EDO	A	610	-	3,3,3	0.24	0	2,2,2	0.78	0
7	EDO	A	611	-	3,3,3	0.41	0	2,2,2	0.42	0
2	SAL	B	601	-	7,10,10	1.36	1 (14%)	10,13,13	1.36	1 (10%)
3	COH	B	602	1	27,50,50	4.49	20 (74%)	23,82,82	4.47	7 (30%)
4	NAG	B	603	1	14,14,15	0.74	1 (7%)	15,19,21	0.58	0
4	NAG	B	604	1,4	14,14,15	0.29	0	15,19,21	0.41	0
4	NAG	B	605	5,4	14,14,15	0.69	1 (7%)	15,19,21	0.50	0
5	MAN	B	606	4	11,11,12	0.91	1 (9%)	15,15,17	1.39	1 (6%)
4	NAG	B	607	1	14,14,15	1.22	1 (7%)	15,19,21	1.54	1 (6%)
8	BOG	B	608	-	20,20,20	0.48	0	25,25,25	0.94	2 (8%)
6	AKR	B	609	-	1,4,4	0.57	0	0,4,4	0.00	-
6	AKR	B	610	-	1,4,4	0.54	0	0,4,4	0.00	-
7	EDO	B	611	-	3,3,3	0.48	0	2,2,2	0.38	0
7	EDO	B	612	-	3,3,3	0.40	0	2,2,2	0.28	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	SAL	A	601	-	-	0/0/4/4	0/1/1/1
3	COH	A	602	1	-	0/8/94/94	0/0/8/8
4	NAG	A	603	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	604	5,4	-	0/6/23/26	0/1/1/1
5	MAN	A	605	5,4	-	0/2/19/22	1/1/1/1
5	MAN	A	606	5	-	0/2/19/22	0/1/1/1
4	NAG	A	607	1	-	0/6/23/26	0/1/1/1
6	AKR	A	608	-	-	0/0/2/2	0/0/0/0
7	EDO	A	609	-	-	0/1/1/1	0/0/0/0
7	EDO	A	610	-	-	0/1/1/1	0/0/0/0
7	EDO	A	611	-	-	0/1/1/1	0/0/0/0
2	SAL	B	601	-	-	0/0/4/4	0/1/1/1
3	COH	B	602	1	-	0/8/94/94	0/0/8/8
4	NAG	B	603	1	-	0/6/23/26	0/1/1/1
4	NAG	B	604	1,4	-	0/6/23/26	0/1/1/1
4	NAG	B	605	5,4	-	0/6/23/26	0/1/1/1
5	MAN	B	606	4	-	0/2/19/22	1/1/1/1
4	NAG	B	607	1	-	0/6/23/26	0/1/1/1

Continued on next page...

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	BOG	B	608	-	-	0/11/31/31	0/1/1/1
6	AKR	B	609	-	-	0/0/2/2	0/0/0/0
6	AKR	B	610	-	-	0/0/2/2	0/0/0/0
7	EDO	B	611	-	-	0/1/1/1	0/0/0/0
7	EDO	B	612	-	-	0/1/1/1	0/0/0/0

All (49) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	602	COH	CHA-C1A	-8.18	1.37	1.53
3	B	602	COH	CHB-C4A	-7.87	1.38	1.53
3	B	602	COH	CHA-C1A	-7.81	1.38	1.53
3	A	602	COH	CHD-C4C	-7.79	1.38	1.53
3	A	602	COH	CHC-C1C	-7.77	1.38	1.53
3	A	602	COH	CHB-C4A	-7.67	1.38	1.53
3	B	602	COH	CHC-C1C	-7.57	1.38	1.53
3	B	602	COH	CHD-C4C	-7.17	1.39	1.53
3	A	602	COH	CHA-C4D	-5.19	1.37	1.51
3	B	602	COH	C3B-C2B	-5.16	1.33	1.40
3	B	602	COH	CHA-C4D	-4.91	1.38	1.51
3	A	602	COH	CHD-C1D	-4.87	1.38	1.51
3	B	602	COH	CHB-C1B	-4.86	1.38	1.51
3	A	602	COH	CHC-C4B	-4.79	1.38	1.51
3	B	602	COH	CHC-C4B	-4.77	1.38	1.51
3	A	602	COH	CHB-C1B	-4.73	1.38	1.51
3	B	602	COH	CHD-C1D	-4.46	1.39	1.51
3	A	602	COH	C4C-C3C	-3.93	1.44	1.50
3	A	602	COH	C3B-C2B	-3.78	1.35	1.40
2	A	601	SAL	C6-C1	-2.86	1.35	1.40
3	B	602	COH	C4C-C3C	-2.76	1.46	1.50
2	B	601	SAL	C6-C1	-2.56	1.35	1.40
4	B	605	NAG	O5-C1	-2.53	1.39	1.43
2	A	601	SAL	C3-C2	-2.39	1.35	1.39
3	A	602	COH	CAD-C3D	2.02	1.55	1.52
5	A	605	MAN	C2-C3	2.04	1.55	1.52
5	B	606	MAN	O5-C5	2.20	1.48	1.43
4	B	603	NAG	C1-C2	2.53	1.56	1.52
3	B	602	COH	CMA-C3A	2.54	1.54	1.50
3	B	602	COH	CAD-C3D	2.57	1.56	1.52
5	A	605	MAN	C4-C5	2.57	1.58	1.53
3	A	602	COH	CMA-C3A	2.61	1.55	1.50
3	B	602	COH	CMC-C2C	2.62	1.55	1.50

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	602	COH	CMC-C2C	2.81	1.55	1.50
3	B	602	COH	CAA-C2A	2.92	1.55	1.51
3	A	602	COH	CAA-C2A	3.08	1.55	1.51
3	B	602	COH	C3B-CAB	3.54	1.55	1.47
3	A	602	COH	C3B-CAB	3.79	1.55	1.47
4	B	607	NAG	O5-C1	4.24	1.50	1.43
3	B	602	COH	CAC-C3C	4.91	1.55	1.45
3	A	602	COH	CAC-C3C	4.94	1.55	1.45
3	B	602	COH	C4D-C3D	5.00	1.45	1.38
3	A	602	COH	C4D-C3D	5.09	1.45	1.38
3	B	602	COH	C1B-C2B	5.14	1.45	1.38
3	A	602	COH	C1D-C2D	5.62	1.45	1.38
3	A	602	COH	C1B-C2B	5.62	1.45	1.38
3	B	602	COH	C1D-C2D	5.65	1.45	1.38
3	A	602	COH	C3D-C2D	5.66	1.54	1.37
3	B	602	COH	C3D-C2D	5.80	1.54	1.37

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	602	COH	CMB-C2B-C1B	-3.58	123.48	127.13
3	A	602	COH	CHC-C4B-C3B	-3.11	125.75	129.66
3	B	602	COH	CBC-CAC-C3C	-3.10	121.81	126.34
2	B	601	SAL	C2-C1-C1'	-2.75	118.84	121.64
5	A	605	MAN	O2-C2-C3	-2.55	105.05	110.19
5	A	606	MAN	O2-C2-C3	-2.26	105.63	110.19
8	B	608	BOG	O5-C1-O1	-2.23	104.65	109.99
3	B	602	COH	C3B-CAB-CBB	-2.10	122.17	126.40
2	A	601	SAL	C2-C1-C1'	-2.09	119.52	121.64
8	B	608	BOG	C1-O5-C5	2.38	118.42	113.74
5	A	605	MAN	O2-C2-C1	2.39	114.02	109.23
3	A	602	COH	C4B-C3B-C2B	2.52	107.62	104.44
3	B	602	COH	C4B-C3B-C2B	2.80	107.97	104.44
5	A	605	MAN	C1-O5-C5	3.46	117.23	112.14
5	B	606	MAN	C1-O5-C5	4.24	118.38	112.14
4	B	607	NAG	C1-O5-C5	5.73	120.56	112.14
3	B	602	COH	CHD-C4C-NC	9.49	124.67	110.12
3	A	602	COH	CHB-C4A-NA	9.80	125.14	110.12
3	A	602	COH	CHC-C1C-NC	10.03	125.50	110.12
3	B	602	COH	CHB-C4A-NA	10.11	125.61	110.12
3	A	602	COH	CHA-C1A-NA	10.55	126.29	110.12
3	B	602	COH	CHA-C1A-NA	10.57	126.32	110.12

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	602	COH	CHD-C4C-NC	10.74	126.58	110.12
3	B	602	COH	CHC-C1C-NC	10.91	126.83	110.12

There are no chirality outliers.

There are no torsion outliers.

All (2) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	605	MAN	C1-C2-C3-C4-C5-O5
5	B	606	MAN	C1-C2-C3-C4-C5-O5

12 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	SAL	3	0
3	A	602	COH	4	0
4	A	604	NAG	1	0
7	A	610	EDO	2	0
7	A	611	EDO	1	0
2	B	601	SAL	4	0
3	B	602	COH	2	0
4	B	607	NAG	1	0
8	B	608	BOG	2	0
6	B	610	AKR	1	0
7	B	611	EDO	1	0
7	B	612	EDO	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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	553/553 (100%)	-0.10	6 (1%) 82 84	22, 39, 63, 83	0
1	B	552/553 (99%)	0.10	24 (4%) 39 44	23, 43, 75, 94	0
All	All	1105/1106 (99%)	-0.00	30 (2%) 58 61	22, 41, 69, 94	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	215	LYS	3.8
1	A	81	PHE	3.7
1	B	75	LEU	3.6
1	A	74	PHE	3.5
1	B	98	GLY	3.4
1	B	96	PHE	3.1
1	B	105(A)	ILE	3.0
1	B	99	PHE	3.0
1	B	102	VAL	2.9
1	B	158	ASP	2.9
1	B	65	TYR	2.8
1	B	80	LEU	2.7
1	B	107	PHE	2.6
1	B	496	GLY	2.5
1	B	115	TYR	2.5
1	B	71	THR	2.5
1	B	476	GLU	2.5
1	B	515	ASP	2.4
1	B	583	PRO	2.3
1	B	368	ASN	2.2
1	A	96	PHE	2.2
1	B	105	ASN	2.2
1	A	202	ALA	2.2
1	B	82	LEU	2.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	584	ASP	2.1
1	B	91	TYR	2.1
1	A	384	LEU	2.1
1	B	277	PRO	2.1
1	B	514	PRO	2.1
1	B	399	ASP	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](#)

There are no carbohydrates in this entry.

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
4	NAG	B	603	14/15	0.69	0.43	3.81	53,84,89,89	0
7	EDO	A	611	4/4	0.95	0.29	3.48	47,47,48,48	0
7	EDO	A	610	4/4	0.89	0.20	2.62	63,63,63,63	0
2	SAL	B	601	10/10	0.88	0.25	2.39	83,83,84,84	0
7	EDO	B	612	4/4	0.95	0.23	2.27	45,46,47,47	0
4	NAG	B	607	14/15	0.82	0.32	2.26	61,70,74,77	0
7	EDO	B	611	4/4	0.91	0.19	2.21	43,43,45,45	0
8	BOG	B	608	20/20	0.84	0.20	1.82	50,69,74,74	0
3	COH	B	602	43/43	0.82	0.23	1.70	48,72,83,91	0
7	EDO	A	609	4/4	0.95	0.16	1.68	47,48,49,50	0
3	COH	A	602	43/43	0.84	0.22	1.60	51,61,78,83	0
6	AKR	B	609	5/5	0.94	0.18	1.43	48,48,49,50	0
6	AKR	A	608	5/5	0.92	0.21	1.06	51,51,55,58	0
4	NAG	A	607	14/15	0.93	0.18	0.59	57,59,64,67	0
6	AKR	B	610	5/5	0.87	0.18	0.34	67,67,67,68	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	SAL	A	601	10/10	0.94	0.17	0.14	54,55,57,57	0
4	NAG	B	604	14/15	0.96	0.13	-0.02	30,35,40,44	0
4	NAG	A	603	14/15	0.96	0.11	-0.45	28,30,31,34	0
5	MAN	A	606	11/12	0.54	0.28	-	86,93,100,103	0
4	NAG	A	604	14/15	0.95	0.16	-	33,39,47,57	0
4	NAG	B	605	14/15	0.89	0.24	-	44,54,63,64	0
5	MAN	B	606	11/12	0.81	0.34	-	66,73,76,76	0
5	MAN	A	605	11/12	0.72	0.17	-	63,68,85,86	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.