Full wwPDB X-ray Structure Validation Report (i)

Oct 18, 2016 – 08:08 AM EDT

PDB ID	:	5JVZ
Title	:	Crystal structure of flurbiprofen bound to S121P murine COX-2 mutant
Authors	:	Malkowski, M.G.; Orlando, B.J.
Deposited on	:	2016-05-11
Resolution	:	2.62 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:

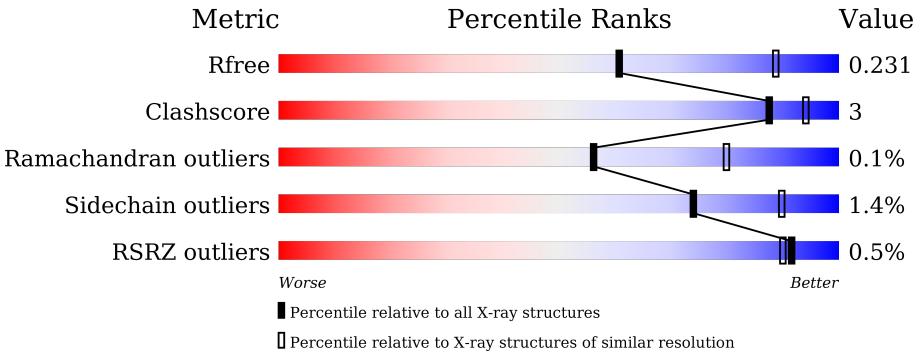
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027939
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027939

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 2.62 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	2700 (2.64-2.60)
Clashscore	102246	3065 (2.64-2.60)
Ramachandran outliers	100387	3015 (2.64-2.60)
Sidechain outliers	100360	3015 (2.64-2.60)
RSRZ outliers	91569	2706 (2.64-2.60)

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	552	93% 7%
1	B	552	93% 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
3	BOG	A	602	-	-	-	X
4	COH	A	603	-	-	-	X
4	COH	B	602	-	-	-	X
5	NAG	A	605	-	-	-	X
5	NAG	A	609	-	-	-	X
5	NAG	B	603	-	-	-	X
7	AKR	A	610	-	-	X	X
7	AKR	A	611	-	-	X	X
7	AKR	B	609	-	-	-	X
8	EDO	B	607	-	-	-	X

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 9431 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.

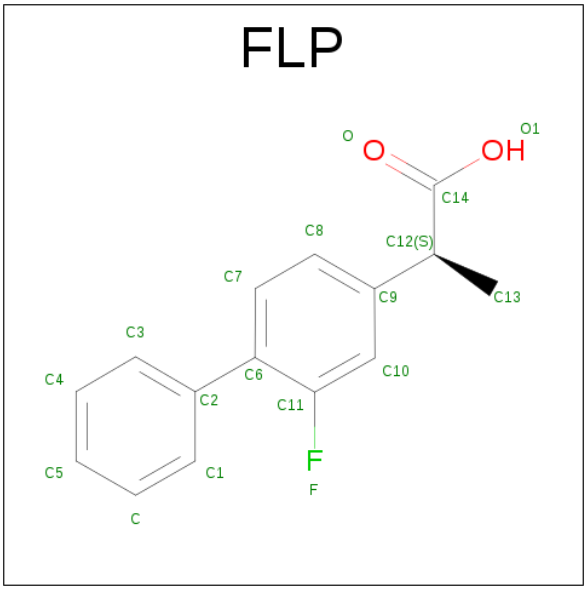
- Molecule 1 is a protein called Prostaglandin G/H synthase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	552	Total	C	N	O	S	6	2	0
			4457	2882	741	809	25			
1	B	551	Total	C	N	O	S	0	1	0
			4442	2871	743	803	25			

There are 6 discrepancies between the modelled and reference sequences:

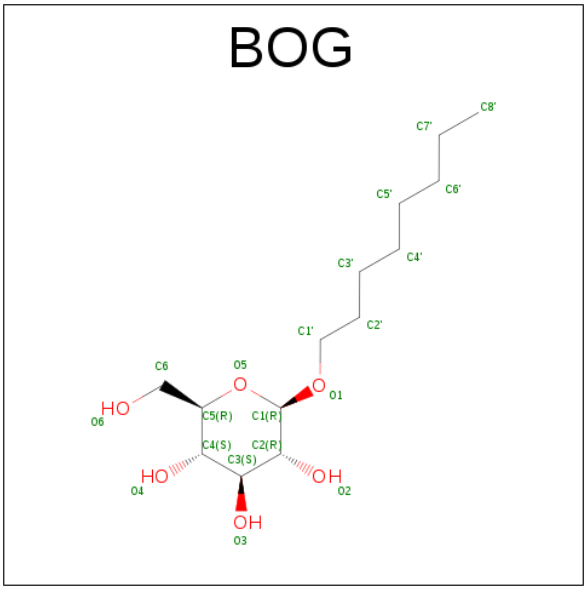
Chain	Residue	Modelled	Actual	Comment	Reference
A	33	HIS	-	expression tag	UNP Q05769
A	34	HIS	-	expression tag	UNP Q05769
A	122	PRO	SER	engineered mutation	UNP Q05769
B	33	HIS	-	expression tag	UNP Q05769
B	34	HIS	-	expression tag	UNP Q05769
B	122	PRO	SER	engineered mutation	UNP Q05769

- Molecule 2 is FLURBIPROFEN (three-letter code: FLP) (formula: $C_{15}H_{13}FO_2$).



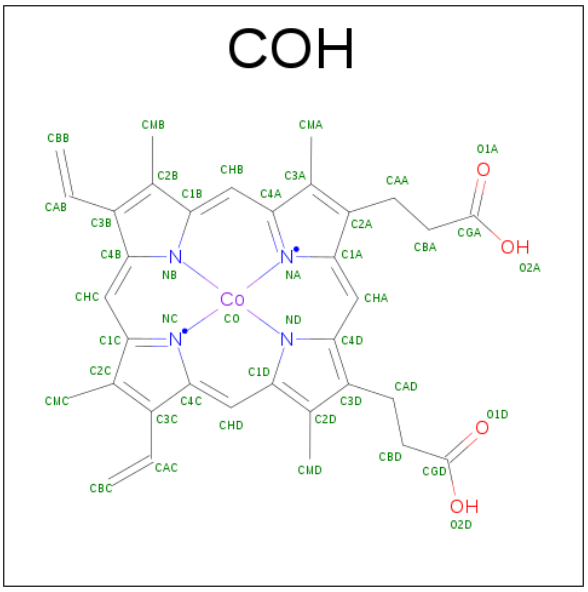
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C F O 18 15 1 2	0	0
2	B	1	Total C F O 18 15 1 2	0	0

- Molecule 3 is B-OCTYLGLUCOSIDE (three-letter code: BOG) (formula: $C_{14}H_{28}O_6$).



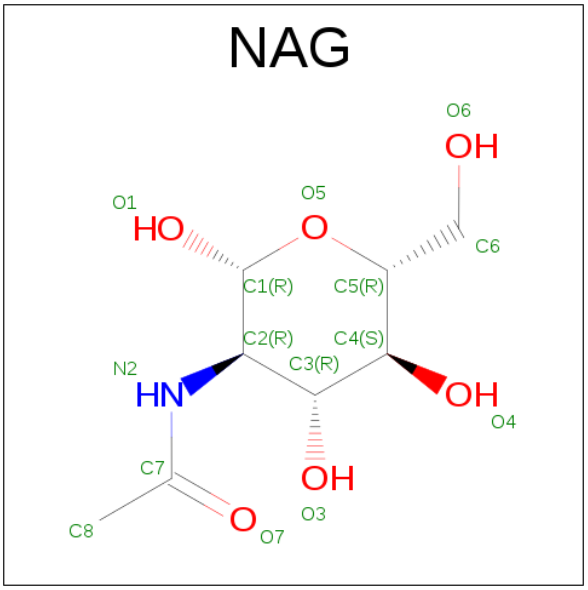
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 20 14 6	0	0
3	A	1	Total C O 20 14 6	0	0

- 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		

- Molecule 5 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

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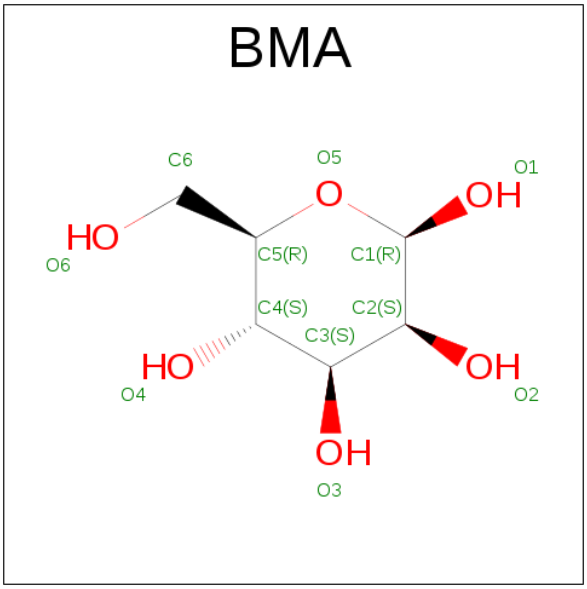
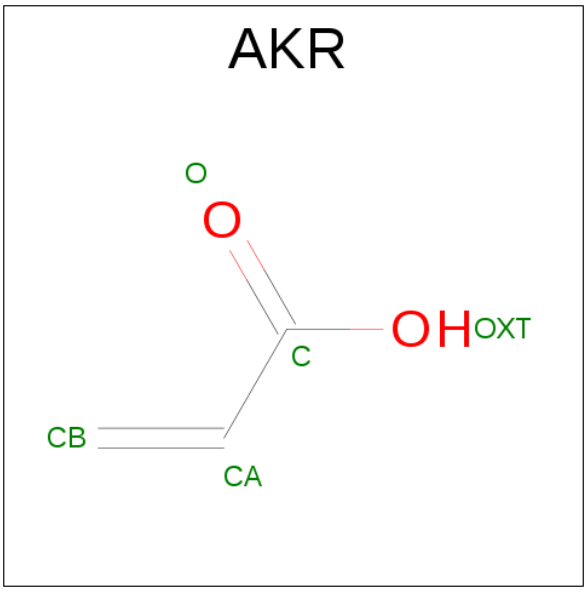
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 6 is BETA-D-MANNOSE (three-letter code: BMA) (formula: $C_6H_{12}O_6$).



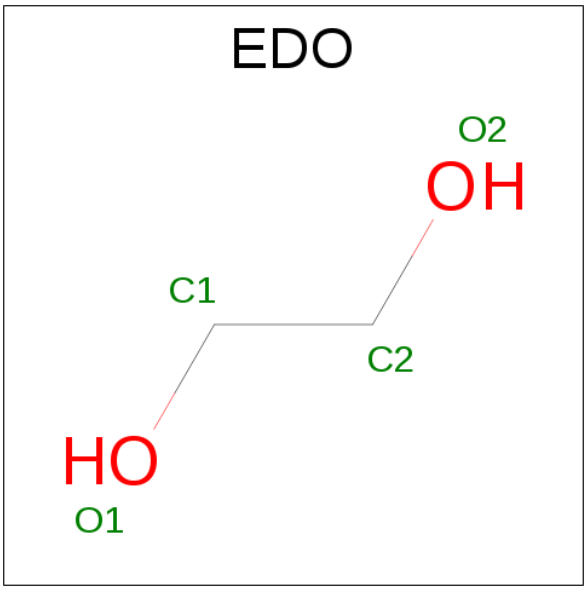
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			11	6	5		

- Molecule 7 is ACRYLIC ACID (three-letter code: AKR) (formula: $C_3H_4O_2$).



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

- Molecule 8 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

- Molecule 9 is water.

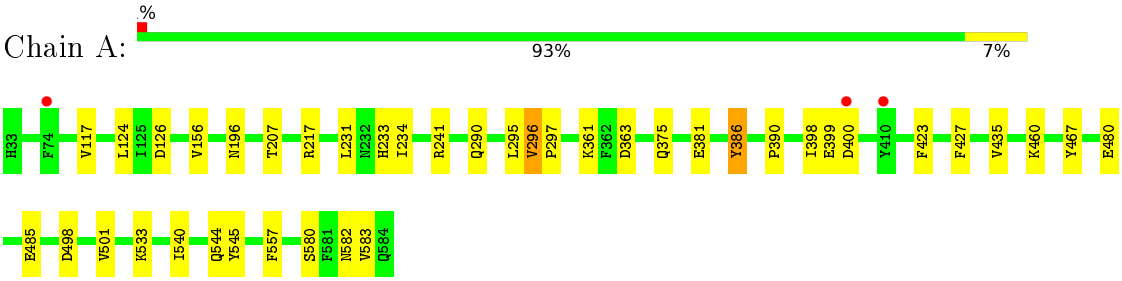
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	123	Total O 123 123	0	0
9	B	100	Total O 100 100	0	0

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.

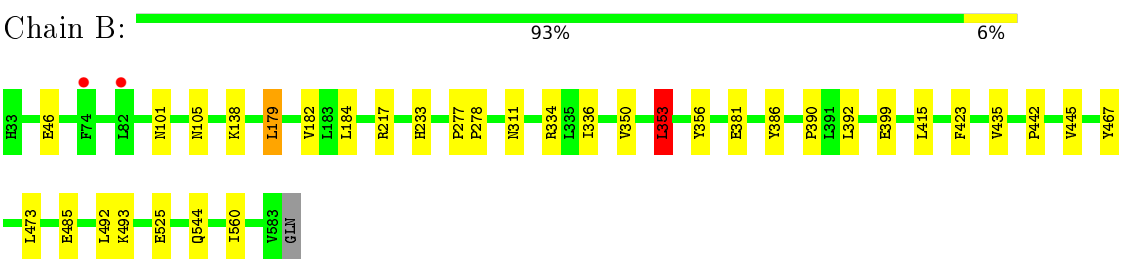
- Molecule 1: Prostaglandin G/H synthase 2

Chain A:



- Molecule 1: Prostaglandin G/H synthase 2

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	119.92Å 131.59Å 179.98Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.62 30.00 – 2.62	Depositor EDS
% Data completeness (in resolution range)	94.1 (30.00-2.62) 88.9 (30.00-2.62)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.38 (at 2.61Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, R_{free}	0.182 , 0.229 0.186 , 0.231	Depositor DCC
R_{free} test set	2061 reflections (5.66%)	DCC
Wilson B-factor (Å^2)	38.8	Xtriage
Anisotropy	0.040	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 28.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	9431	wwPDB-VP
Average B, all atoms (Å^2)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.91% 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, 0.333 respectively for untwinned datasets, and 0.375, 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: BMA, NAG, FLP, EDO, AKR, COH, 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	0.23	0/4593	0.39	0/6237
1	B	0.23	0/4575	0.40	1/6211 (0.0%)
All	All	0.23	0/9168	0.39	1/12448 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	353	LEU	CA-CB-CG	5.41	127.74	115.30

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	4457	0	4306	24	0
1	B	4442	0	4293	20	0
2	A	18	0	12	0	0
2	B	18	0	12	1	0
3	A	40	0	56	2	0
4	A	43	0	30	3	0
4	B	43	0	30	4	0
5	A	56	0	50	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	56	0	51	1	0
6	A	11	0	10	0	0
7	A	10	0	6	4	0
7	B	10	0	6	1	0
8	B	4	0	6	1	0
9	A	123	0	0	0	0
9	B	100	0	0	1	0
All	All	9431	0	8868	47	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 (47) 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)
4:A:603:COH:HBC1	4:A:603:COH:HHD	1.68	0.75
4:A:603:COH:HBB1	4:A:603:COH:HMB1	1.68	0.73
1:B:350:VAL:HA	1:B:353:LEU:HD22	1.74	0.70
4:B:602:COH:HHC	4:B:602:COH:HBB1	1.76	0.66
1:A:241:ARG:HH11	7:A:610:AKR:HA1	1.61	0.64
4:B:602:COH:HHD	4:B:602:COH:HBC1	1.78	0.63
1:B:493:LYS:HD3	7:B:609:AKR:HA1	1.84	0.58
1:A:295:LEU:HD21	4:A:603:COH:HMB3	1.86	0.58
1:A:126:ASP:OD1	1:B:544:GLN:NE2	2.36	0.55
1:B:311:ASN:HD22	8:B:607:EDO:H21	1.70	0.55
1:B:336:ILE:HA	1:B:560:ILE:HD11	1.91	0.53
1:A:156:VAL:HB	1:A:460[A]:LYS:HE3	1.90	0.53
1:B:217:ARG:NH1	5:B:605:NAG:O7	2.42	0.52
1:A:390:PRO:HB2	1:A:435:VAL:HA	1.91	0.52
1:A:241:ARG:HH11	7:A:610:AKR:CA	2.23	0.51
1:A:544:GLN:O	1:B:138:LYS:HE2	2.10	0.51
1:B:334:ARG:NH1	9:B:706:HOH:O	2.44	0.51
1:A:217:ARG:NH2	5:A:607:NAG:O7	2.44	0.50
1:A:117:VAL:HG22	3:A:602:BOG:C3'	2.42	0.50
1:A:480:GLU:HG3	7:A:611:AKR:HA1	1.96	0.47
1:B:473:LEU:HD11	1:B:525:GLU:HB2	1.96	0.47
1:B:381:GLU:HG2	1:B:467:TYR:CE2	2.50	0.47
1:A:196:ASN:HB3	1:A:583:VAL:HG13	1.96	0.47
1:A:498:ASP:HB3	1:A:501:VAL:HG22	1.96	0.47
1:B:182:VAL:HG21	1:B:492:LEU:HD21	1.97	0.46
1:A:480:GLU:HG3	7:A:611:AKR:CA	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:375:GLN:O	1:A:533:LYS:NZ	2.43	0.45
1:A:399:GLU:HB3	1:A:400:ASP:H	1.61	0.44
1:A:398:ILE:HD11	1:A:427:PHE:CZ	2.53	0.44
1:B:277:PRO:HA	1:B:278:PRO:HD3	1.90	0.43
1:B:390:PRO:HB2	1:B:435:VAL:HA	1.99	0.43
1:B:356:TYR:CE2	2:B:601:FLP:H12	2.53	0.43
1:A:207:THR:HG21	1:A:386:TYR:CE2	2.53	0.43
1:A:231:LEU:HG	1:A:234:ILE:HD12	2.00	0.43
1:B:442:PRO:HG2	1:B:445:VAL:HG22	2.00	0.43
1:B:179:LEU:HD22	1:B:184:LEU:HG	2.00	0.43
4:B:602:COH:CHD	4:B:602:COH:HBC1	2.46	0.43
1:A:296:VAL:HA	1:A:297:PRO:HD3	1.81	0.42
1:B:392:LEU:HD21	4:B:602:COH:HHC	2.01	0.41
1:A:381:GLU:HG2	1:A:467:TYR:CE2	2.55	0.41
1:A:540:ILE:HA	1:A:545:TYR:HB3	2.03	0.41
1:A:580:SER:OG	1:A:582[A]:ASN:ND2	2.53	0.41
1:B:101:ASN:O	1:B:105:ASN:ND2	2.51	0.41
1:B:184:LEU:HD23	1:B:184:LEU:HA	1.92	0.40
1:B:415:LEU:HA	1:B:423:PHE:CE1	2.56	0.40
1:A:124:LEU:HD21	3:A:602:BOG:H61	2.03	0.40
1:A:361:LYS:HE2	1:A:363:ASP:HB2	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	552/552 (100%)	533 (97%)	19 (3%)	0	100	100
1	B	550/552 (100%)	532 (97%)	17 (3%)	1 (0%)	52	76
All	All	1102/1104 (100%)	1065 (97%)	36 (3%)	1 (0%)	56	80

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	399	GLU

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	483/494 (98%)	476 (99%)	7 (1%)	74 90
1	B	480/494 (97%)	474 (99%)	6 (1%)	76 91
All	All	963/988 (98%)	950 (99%)	13 (1%)	74 91

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	233	HIS
1	A	290	GLN
1	A	296	VAL
1	A	386	TYR
1	A	423	PHE
1	A	485	GLU
1	A	557	PHE
1	B	46	GLU
1	B	179	LEU
1	B	233	HIS
1	B	353	LEU
1	B	386	TYR
1	B	485	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	271	GLN
1	B	401	GLN
1	B	582	ASN

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

20 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	FLP	A	601	-	16,19,19	1.58	1 (6%)	22,26,26	1.12	2 (9%)
3	BOG	A	602	-	20,20,20	0.91	1 (5%)	25,25,25	0.86	0
4	COH	A	603	-	27,50,50	4.50	19 (70%)	23,82,82	4.36	10 (43%)
3	BOG	A	604	-	20,20,20	0.89	1 (5%)	25,25,25	0.91	0
5	NAG	A	605	1	14,14,15	0.28	0	15,19,21	0.47	0
5	NAG	A	606	1,5	14,14,15	0.24	0	15,19,21	0.46	0
5	NAG	A	607	5,6	14,14,15	0.49	0	15,19,21	0.37	0
6	BMA	A	608	5	11,11,12	0.71	0	15,15,17	1.13	1 (6%)
5	NAG	A	609	1	14,14,15	0.29	0	15,19,21	0.39	0
7	AKR	A	610	-	1,4,4	0.90	0	0,4,4	0.00	-
7	AKR	A	611	-	1,4,4	0.91	0	0,4,4	0.00	-
2	FLP	B	601	-	16,19,19	1.59	1 (6%)	22,26,26	1.25	2 (9%)
4	COH	B	602	-	27,50,50	4.52	19 (70%)	23,82,82	4.31	7 (30%)
5	NAG	B	603	1	14,14,15	0.27	0	15,19,21	0.39	0
5	NAG	B	604	1,5	14,14,15	0.32	0	15,19,21	0.35	0
5	NAG	B	605	5	14,14,15	0.30	0	15,19,21	0.29	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	NAG	B	606	1	14,14,15	0.23	0	15,19,21	0.33	0
8	EDO	B	607	-	3,3,3	0.45	0	2,2,2	0.29	0
7	AKR	B	608	-	1,4,4	0.91	0	0,4,4	0.00	-
7	AKR	B	609	-	1,4,4	0.90	0	0,4,4	0.00	-

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	FLP	A	601	-	-	0/8/12/12	0/2/2/2
3	BOG	A	602	-	-	0/11/31/31	0/1/1/1
4	COH	A	603	-	-	0/8/94/94	0/0/8/8
3	BOG	A	604	-	-	0/11/31/31	0/1/1/1
5	NAG	A	605	1	-	0/6/23/26	0/1/1/1
5	NAG	A	606	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	607	5,6	-	0/6/23/26	0/1/1/1
6	BMA	A	608	5	-	0/2/19/22	0/1/1/1
5	NAG	A	609	1	-	0/6/23/26	0/1/1/1
7	AKR	A	610	-	-	0/0/2/2	0/0/0/0
7	AKR	A	611	-	-	0/0/2/2	0/0/0/0
2	FLP	B	601	-	-	0/8/12/12	0/2/2/2
4	COH	B	602	-	-	0/8/94/94	0/0/8/8
5	NAG	B	603	1	-	0/6/23/26	0/1/1/1
5	NAG	B	604	1,5	-	0/6/23/26	0/1/1/1
5	NAG	B	605	5	-	0/6/23/26	0/1/1/1
5	NAG	B	606	1	-	0/6/23/26	0/1/1/1
8	EDO	B	607	-	-	0/1/1/1	0/0/0/0
7	AKR	B	608	-	-	0/0/2/2	0/0/0/0
7	AKR	B	609	-	-	0/0/2/2	0/0/0/0

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	603	COH	CHA-C1A	-7.98	1.38	1.53
4	B	602	COH	CHD-C4C	-7.92	1.38	1.53
4	B	602	COH	CHA-C1A	-7.91	1.38	1.53
4	A	603	COH	CHB-C4A	-7.89	1.38	1.53
4	B	602	COH	CHB-C4A	-7.89	1.38	1.53
4	A	603	COH	CHC-C1C	-7.82	1.38	1.53
4	A	603	COH	CHD-C4C	-7.80	1.38	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	602	COH	CHC-C1C	-7.64	1.38	1.53
2	B	601	FLP	C6-C2	-6.13	1.39	1.49
2	A	601	FLP	C6-C2	-6.05	1.39	1.49
4	B	602	COH	C3B-C2B	-5.12	1.33	1.40
4	B	602	COH	CHD-C1D	-4.98	1.38	1.51
4	B	602	COH	CHB-C1B	-4.95	1.38	1.51
4	A	603	COH	CHB-C1B	-4.95	1.38	1.51
4	B	602	COH	CHA-C4D	-4.88	1.38	1.51
4	A	603	COH	CHA-C4D	-4.85	1.38	1.51
4	A	603	COH	CHD-C1D	-4.84	1.38	1.51
4	A	603	COH	CHC-C4B	-4.84	1.38	1.51
4	B	602	COH	CHC-C4B	-4.76	1.38	1.51
4	A	603	COH	C3B-C2B	-4.09	1.35	1.40
4	B	602	COH	C4C-C3C	-3.32	1.45	1.50
4	A	603	COH	C4C-C3C	-3.12	1.46	1.50
4	A	603	COH	CMC-C2C	2.45	1.54	1.50
4	B	602	COH	CMC-C2C	2.46	1.54	1.50
4	B	602	COH	CMA-C3A	2.61	1.55	1.50
3	A	604	BOG	O5-C1	2.64	1.48	1.41
4	A	603	COH	CMA-C3A	2.68	1.55	1.50
4	B	602	COH	CAA-C2A	2.73	1.54	1.51
3	A	602	BOG	O5-C1	2.74	1.48	1.41
4	A	603	COH	CAA-C2A	3.28	1.55	1.51
4	B	602	COH	C3B-CAB	3.52	1.55	1.47
4	A	603	COH	C3B-CAB	3.74	1.55	1.47
4	A	603	COH	C4D-C3D	4.84	1.44	1.38
4	B	602	COH	C1D-C2D	4.89	1.44	1.38
4	A	603	COH	C1D-C2D	4.94	1.45	1.38
4	B	602	COH	CAC-C3C	4.96	1.55	1.45
4	B	602	COH	C1B-C2B	5.08	1.45	1.38
4	A	603	COH	CAC-C3C	5.08	1.55	1.45
4	B	602	COH	C4D-C3D	5.10	1.45	1.38
4	A	603	COH	C1B-C2B	5.20	1.45	1.38
4	A	603	COH	C3D-C2D	5.46	1.53	1.37
4	B	602	COH	C3D-C2D	5.46	1.53	1.37

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	603	COH	CMB-C2B-C1B	-3.97	123.08	127.13
2	B	601	FLP	C10-C11-C6	-3.18	120.05	124.18
2	A	601	FLP	C10-C11-C6	-3.02	120.26	124.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	608	BMA	O2-C2-C3	-2.85	104.44	110.19
4	A	603	COH	CHC-C4B-C3B	-2.85	126.08	129.66
4	B	602	COH	CBC-CAC-C3C	-2.47	122.74	126.34
4	A	603	COH	CAD-CBD-CGD	-2.42	108.08	112.78
4	A	603	COH	CBC-CAC-C3C	-2.30	122.99	126.34
4	B	602	COH	CAD-CBD-CGD	-2.10	108.69	112.78
4	A	603	COH	CMB-C2B-C3B	2.04	129.08	125.09
4	A	603	COH	C4B-C3B-C2B	2.43	107.51	104.44
4	B	602	COH	C4B-C3B-C2B	2.65	107.78	104.44
2	A	601	FLP	C7-C6-C11	3.18	119.45	115.99
2	B	601	FLP	C7-C6-C11	3.27	119.56	115.99
4	B	602	COH	CHD-C4C-NC	9.31	124.39	110.12
4	A	603	COH	CHA-C1A-NA	9.45	124.61	110.12
4	A	603	COH	CHD-C4C-NC	9.58	124.80	110.12
4	A	603	COH	CHB-C4A-NA	9.68	124.96	110.12
4	B	602	COH	CHB-C4A-NA	9.70	124.99	110.12
4	B	602	COH	CHA-C1A-NA	10.10	125.60	110.12
4	A	603	COH	CHC-C1C-NC	10.41	126.08	110.12
4	B	602	COH	CHC-C1C-NC	10.45	126.14	110.12

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

10 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	602	BOG	2	0
4	A	603	COH	3	0
5	A	607	NAG	1	0
7	A	610	AKR	2	0
7	A	611	AKR	2	0
2	B	601	FLP	1	0
4	B	602	COH	4	0
5	B	605	NAG	1	0
8	B	607	EDO	1	0
7	B	609	AKR	1	0

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

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	552/552 (100%)	-0.41	3 (0%)	91	90	28, 37, 52, 74	0
1	B	551/552 (99%)	-0.47	2 (0%)	93	91	28, 38, 56, 79	0
All	All	1103/1104 (99%)	-0.44	5 (0%)	91	90	28, 37, 54, 79	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	82	LEU	3.5
1	A	400	ASP	3.1
1	A	74	PHE	2.9
1	B	74	PHE	2.4
1	A	410	TYR	2.2

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

There are no carbohydrates in this entry.

6.4 Ligands

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
8	EDO	B	607	4/4	0.95	0.28	10.88	31,33,34,37	0
3	BOG	A	602	20/20	0.82	0.38	5.92	47,79,94,96	0
7	AKR	A	610	5/5	0.92	0.35	4.97	51,55,60,67	0
4	COH	B	602	43/43	0.83	0.29	4.33	49,85,109,111	0
5	NAG	A	605	14/15	0.90	0.28	3.59	43,55,64,67	0
4	COH	A	603	43/43	0.77	0.32	3.44	52,96,105,147	0
5	NAG	A	609	14/15	0.89	0.24	2.99	45,53,62,66	0
7	AKR	A	611	5/5	0.95	0.32	2.86	53,56,60,61	0
7	AKR	B	609	5/5	0.87	0.29	2.67	55,57,61,61	0
5	NAG	B	603	14/15	0.88	0.25	2.64	45,64,74,82	0
5	NAG	B	606	14/15	0.88	0.28	1.97	61,68,77,79	0
5	NAG	B	604	14/15	0.96	0.21	1.71	25,32,39,40	0
7	AKR	B	608	5/5	0.91	0.22	0.80	58,59,63,66	0
2	FLP	B	601	18/18	0.96	0.14	0.56	24,38,52,63	0
5	NAG	A	606	14/15	0.96	0.15	-0.11	19,31,41,43	0
2	FLP	A	601	18/18	0.95	0.14	-0.16	25,31,47,57	0
3	BOG	A	604	20/20	0.95	0.14	-0.22	35,51,70,73	0
5	NAG	B	605	14/15	0.84	0.33	-	39,69,76,77	0
6	BMA	A	608	11/12	0.87	0.23	-	70,76,84,90	0
5	NAG	A	607	14/15	0.94	0.26	-	47,52,61,77	0

6.5 Other polymers (i)

There are no such residues in this entry.