



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 20, 2020 – 08:33 PM BST

PDB ID : 4IXS  
Title : Native structure of xometc at ph 5.2  
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Deposited on : 2013-01-28  
Resolution : 2.29 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.13.1  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.13.1

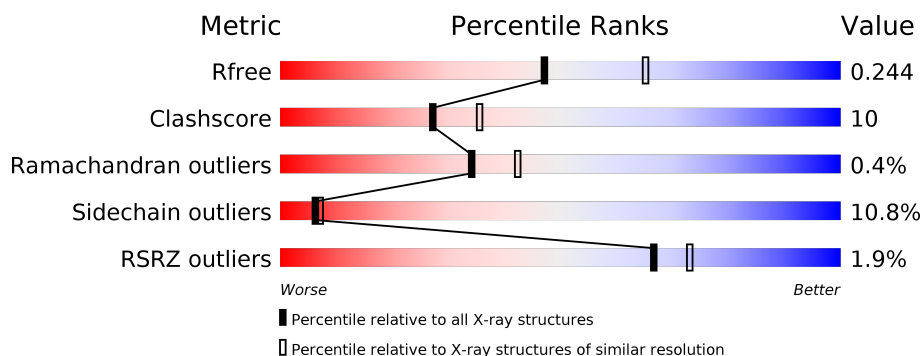
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.29 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))
$R_{free}$	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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 respectively. 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	397	<div> <div>2%</div> <div> <div></div> <div>68%</div> <div>19%</div> <div>•</div> <div>9%</div> </div> </div>
1	B	397	<div> <div>2%</div> <div> <div></div> <div>72%</div> <div>17%</div> <div>• •</div> <div>6%</div> </div> </div>

## 2 Entry composition [i](#)

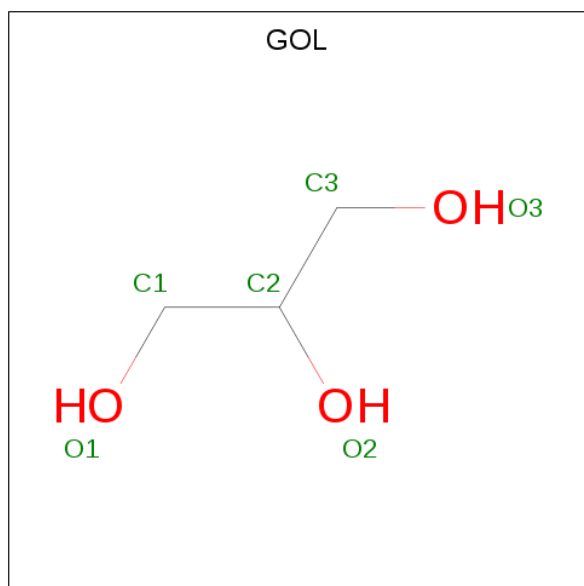
There are 4 unique types of molecules in this entry. The entry contains 5829 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Cystathionine gamma-lyase-like protein.

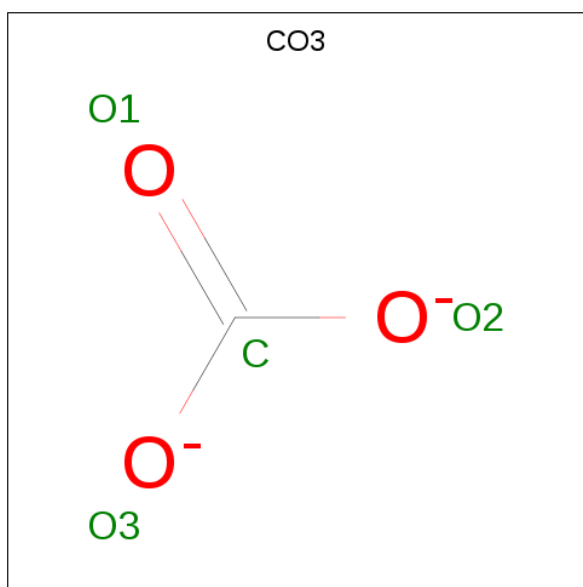
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	361	Total	C	N	O	P	S	0	3	0
			2741	1736	481	508	1	15			
1	B	372	Total	C	N	O	P	S	0	0	0
			2805	1774	494	521	1	15			

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



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

- Molecule 3 is CARBONATE ION (three-letter code: CO3) (formula: CO<sub>3</sub>).



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

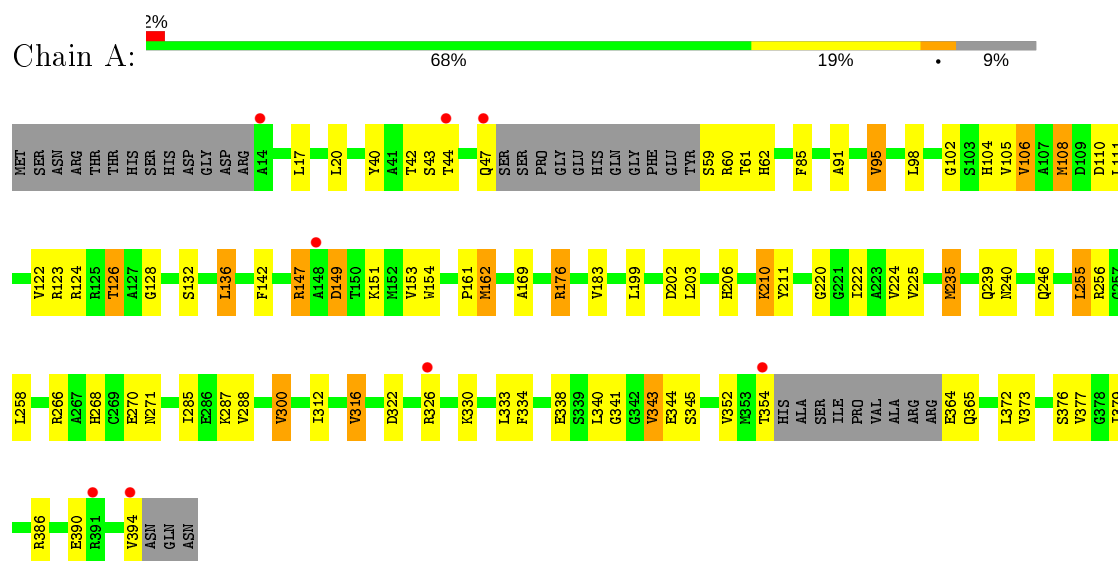
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	123	Total	O	0	0
			123	123		
4	B	150	Total	O	0	0
			150	150		

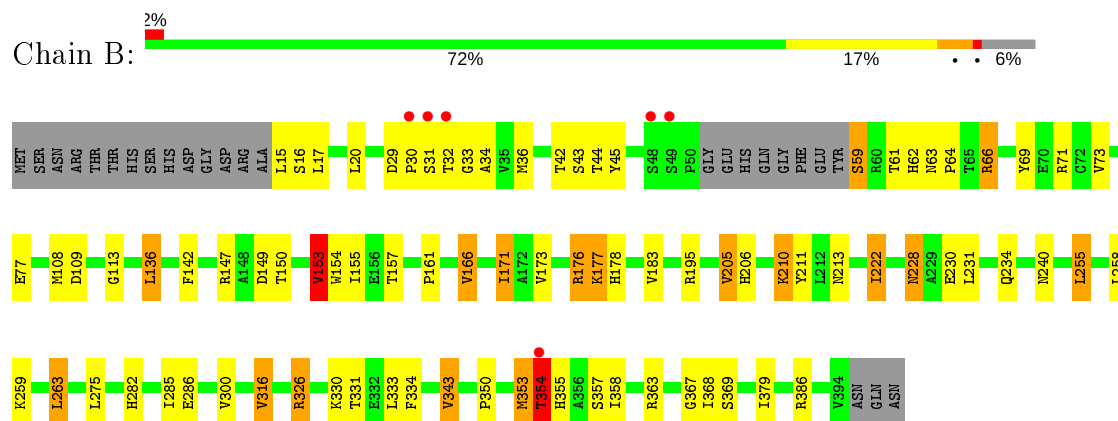
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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: Cystathionine gamma-lyase-like protein



#### • Molecule 1: Cystathionine gamma-lyase-like protein



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	85.72Å 124.36Å 146.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.72 – 2.29 48.72 – 2.29	Depositor EDS
% Data completeness (in resolution range)	99.5 (48.72-2.29) 99.5 (48.72-2.29)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.77 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.180 , 0.247 0.179 , 0.244	Depositor DCC
$R_{free}$ test set	1761 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	27.1	Xtriage
Anisotropy	0.108	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 37.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	5829	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.66% 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, 0.333 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: GOL, CO3, LLP

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	1.03	3/2776 (0.1%)	0.97	3/3764 (0.1%)
1	B	1.06	2/2834 (0.1%)	1.00	6/3845 (0.2%)
All	All	1.04	5/5610 (0.1%)	0.99	9/7609 (0.1%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	205	VAL	CB-CG1	-6.64	1.39	1.52
1	A	390	GLU	CG-CD	6.21	1.61	1.51
1	A	344	GLU	CG-CD	5.80	1.60	1.51
1	A	300	VAL	CB-CG2	5.05	1.63	1.52
1	B	211	TYR	N-CA	5.00	1.56	1.46

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	66	ARG	NE-CZ-NH2	-8.85	115.88	120.30
1	B	66	ARG	NE-CZ-NH1	8.79	124.70	120.30
1	A	235	MET	CG-SD-CE	8.30	113.48	100.20
1	B	153	VAL	CB-CA-C	-7.25	97.61	111.40
1	A	255	LEU	CB-CG-CD2	5.53	120.40	111.00
1	B	71	ARG	NE-CZ-NH1	5.48	123.04	120.30
1	B	176	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	B	109	ASP	CB-CG-OD1	5.24	123.02	118.30
1	A	176	ARG	NE-CZ-NH1	5.08	122.84	120.30

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	2741	0	2757	67	0
1	B	2805	0	2819	49	0
2	A	6	0	8	1	0
3	B	4	0	0	1	0
4	A	123	0	0	2	0
4	B	150	0	0	5	0
All	All	5829	0	5584	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 10.

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)
1:B:326:ARG:HH11	1:B:326:ARG:HG2	1.18	1.05
1:B:155:ILE:HD11	1:B:171:ILE:HD11	1.45	0.96
1:A:95:VAL:HA	1:A:235:MET:HE1	1.51	0.92
1:A:222:ILE:HD12	1:A:222:ILE:C	1.99	0.82
1:A:98:LEU:CG	1:A:235:MET:HE2	2.10	0.82
1:B:353:MET:O	1:B:354:THR:HB	1.78	0.81
1:B:77:GLU:OE2	1:B:206:HIS:HE1	1.64	0.79
1:B:350:PRO:O	1:B:354:THR:O	2.01	0.78
1:A:206:HIS:HD2	1:A:222:ILE:HD11	1.48	0.76
1:A:98:LEU:HD11	1:A:235:MET:CE	2.17	0.75
1:B:354:THR:HG23	1:B:355:HIS:ND1	2.03	0.74
1:A:271:ASN:HD21	2:A:401:GOL:H11	1.54	0.73
1:A:95:VAL:HA	1:A:235:MET:CE	2.18	0.73
1:A:220:GLY:HA3	1:A:246:GLN:HE22	1.53	0.72
1:B:59:SER:HA	1:B:62:HIS:O	1.90	0.71
1:B:300:VAL:HG12	4:B:598:HOH:O	1.91	0.71
1:A:124:ARG:HD3	4:A:525:HOH:O	1.91	0.69
1:B:326:ARG:HG2	1:B:326:ARG:NH1	1.98	0.69
1:B:43:SER:O	1:B:59:SER:N	2.25	0.69
1:A:98:LEU:CD1	1:A:235:MET:CE	2.71	0.69
1:A:98:LEU:HG	1:A:235:MET:HE2	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:343:VAL:HG22	1:B:379:ILE:HD13	1.75	0.69
1:A:98:LEU:CD1	1:A:235:MET:HE2	2.24	0.68
1:A:98:LEU:HD11	1:A:235:MET:HE2	1.76	0.68
1:B:286:GLU:HB3	1:B:316:VAL:HG22	1.78	0.66
1:B:32:THR:O	1:B:34:ALA:N	2.27	0.66
1:A:122:VAL:O	1:A:126:THR:HB	1.98	0.64
1:A:61:THR:HG23	1:A:240[B]:ASN:ND2	2.14	0.63
1:A:98:LEU:HG	1:A:235:MET:CE	2.28	0.62
1:A:98:LEU:HD11	1:A:235:MET:HE3	1.83	0.60
1:A:334:PHE:CD2	1:A:345:SER:HB3	2.36	0.60
1:B:77:GLU:OE2	1:B:206:HIS:CE1	2.52	0.59
1:A:40:TYR:O	1:A:42:THR:HG22	2.04	0.57
1:B:155:ILE:HD11	1:B:171:ILE:CD1	2.26	0.57
1:A:287:LYS:HB3	1:A:316:VAL:HG13	1.87	0.56
1:B:343:VAL:HG22	1:B:379:ILE:CD1	2.36	0.56
1:A:98:LEU:CG	1:A:235:MET:CE	2.82	0.56
1:A:206:HIS:HB2	1:A:222:ILE:HG13	1.88	0.56
1:A:222:ILE:HD13	1:A:224:VAL:HG23	1.88	0.55
1:B:228:ASN:C	1:B:228:ASN:HD22	2.09	0.55
1:A:379:ILE:HD12	1:B:263:LEU:HD22	1.88	0.55
1:A:61:THR:HG23	1:A:240[B]:ASN:HD21	1.71	0.55
1:B:73:VAL:HG11	1:B:222:ILE:HG21	1.89	0.55
1:A:285:ILE:HG21	1:A:288:VAL:HG22	1.88	0.55
1:A:222:ILE:O	1:A:222:ILE:HD12	2.07	0.54
1:B:45:TYR:N	1:B:45:TYR:CD1	2.76	0.54
1:A:326:ARG:HH21	1:A:330:LYS:HD2	1.73	0.54
1:B:326:ARG:HH11	1:B:326:ARG:CG	2.06	0.54
1:A:98:LEU:CD2	1:A:235:MET:HE2	2.37	0.54
1:A:256:ARG:NH2	1:B:213:ASN:OD1	2.41	0.53
1:A:98:LEU:CD1	1:A:235:MET:HE3	2.37	0.53
1:A:136:LEU:HD12	1:A:142:PHE:HB2	1.91	0.53
1:A:123:ARG:HD3	1:A:126:THR:HG22	1.90	0.52
1:A:102:GLY:HA2	1:A:128:GLY:O	2.09	0.52
1:A:203:LEU:HD23	1:A:225:VAL:HG12	1.92	0.52
1:B:157:THR:HB	1:B:166:VAL:HG13	1.92	0.52
1:B:108:MET:SD	1:B:136:LEU:HB2	2.50	0.51
1:A:98:LEU:HD21	1:A:235:MET:HE2	1.93	0.51
1:A:266:ARG:O	1:A:270:GLU:HG3	2.11	0.51
1:A:59:SER:O	1:A:60:ARG:HB3	2.11	0.50
1:A:364:GLU:HG3	1:A:365:GLN:H	1.76	0.50
1:A:154:TRP:CZ3	1:A:183:VAL:HG11	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:268:HIS:HD2	1:A:377:VAL:O	1.95	0.50
1:B:228:ASN:ND2	1:B:231:LEU:H	2.10	0.49
1:B:230:GLU:HG2	1:B:234:GLN:HE21	1.77	0.49
1:B:173:VAL:HG22	1:B:176:ARG:HH22	1.78	0.49
1:A:108:MET:SD	1:A:136:LEU:HB2	2.53	0.48
1:A:95:VAL:HB	1:A:235:MET:HE3	1.96	0.48
1:B:142:PHE:CE1	1:B:153:VAL:HG13	2.49	0.48
1:B:367:GLY:O	1:B:369:SER:N	2.44	0.48
1:A:104:HIS:NE2	1:A:132:SER:OG	2.37	0.48
1:B:36:MET:SD	1:B:259:LYS:HE2	2.54	0.48
1:A:206:HIS:CD2	1:A:222:ILE:HD11	2.39	0.47
1:B:177:LYS:HG3	1:B:178:HIS:ND1	2.29	0.47
1:B:171:ILE:C	1:B:171:ILE:HD12	2.35	0.47
1:B:282:HIS:HB3	1:B:285:ILE:HD13	1.97	0.47
1:B:386:ARG:CD	4:B:612:HOH:O	2.62	0.47
1:B:69:TYR:HA	1:B:255:LEU:HG	1.97	0.47
1:A:343:VAL:HG22	1:A:379:ILE:CD1	2.44	0.47
1:A:222:ILE:CD1	1:A:224:VAL:HG23	2.45	0.46
1:B:113:GLY:HA2	1:B:358:ILE:HD11	1.97	0.46
1:B:210:LLP:HE3	3:B:401:CO3:O2	2.15	0.46
1:B:29:ASP:OD1	1:B:30:PRO:HD2	2.15	0.46
1:A:111:LEU:HA	1:A:111:LEU:HD12	1.65	0.45
1:A:285:ILE:HG21	1:A:288:VAL:CG2	2.46	0.45
1:A:176:ARG:NH2	1:A:202:ASP:OD1	2.50	0.45
1:B:363:ARG:NH1	4:B:550:HOH:O	2.33	0.45
1:A:343:VAL:HG22	1:A:379:ILE:HD11	1.98	0.44
1:B:154:TRP:CZ3	1:B:183:VAL:HG11	2.53	0.44
1:B:206:HIS:CD2	4:B:648:HOH:O	2.71	0.44
1:A:61:THR:HG22	1:A:62[B]:HIS:CE1	2.53	0.44
1:A:85:PHE:CE1	1:A:239:GLN:HG3	2.53	0.43
1:A:211:TYR:CE1	1:A:341:GLY:HA2	2.54	0.43
1:A:91:ALA:O	1:A:95:VAL:HG13	2.19	0.42
1:A:162:MET:CE	1:A:372:LEU:CD1	2.97	0.42
1:A:222:ILE:C	1:A:222:ILE:CD1	2.75	0.42
1:A:210:LLP:HD3	1:A:340:LEU:HG	2.02	0.42
1:B:353:MET:O	1:B:354:THR:CB	2.54	0.42
1:A:176:ARG:HB2	1:A:176:ARG:HH11	1.84	0.41
1:B:63:ASN:HA	1:B:64:PRO:HD3	1.91	0.41
1:A:222:ILE:HD13	1:A:224:VAL:CG2	2.51	0.41
1:A:106:VAL:O	1:A:153:VAL:HA	2.20	0.41
1:B:149:ASP:OD2	1:B:149:ASP:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:379:ILE:CD1	1:B:263:LEU:HD22	2.51	0.41
1:A:271:ASN:ND2	4:A:534:HOH:O	2.52	0.41
1:B:147:ARG:H	1:B:150:THR:HG1	1.68	0.41
1:B:331:THR:HB	1:B:334:PHE:HB2	2.02	0.41
1:A:147:ARG:NH1	1:A:149:ASP:HB2	2.36	0.40
1:A:312:ILE:HD13	1:A:376:SER:HA	2.04	0.40
1:A:40:TYR:HB3	1:A:42:THR:CG2	2.50	0.40
1:B:17:LEU:HD23	1:B:17:LEU:HA	1.92	0.40
1:A:169:ALA:HA	1:A:199:LEU:O	2.21	0.40
1:B:206:HIS:HD2	4:B:648:HOH:O	2.03	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	357/397 (90%)	347 (97%)	10 (3%)	0	100	100
1	B	367/397 (92%)	355 (97%)	9 (2%)	3 (1%)	19	23
All	All	724/794 (91%)	702 (97%)	19 (3%)	3 (0%)	34	42

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	33	GLY
1	B	368	ILE
1	B	354	THR

### 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	284/312 (91%)	254 (89%)	30 (11%)	6	7
1	B	291/312 (93%)	259 (89%)	32 (11%)	6	7
All	All	575/624 (92%)	513 (89%)	62 (11%)	6	7

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	LEU
1	A	20	LEU
1	A	43	SER
1	A	44	THR
1	A	47	GLN
1	A	95	VAL
1	A	105	VAL
1	A	106	VAL
1	A	108	MET
1	A	110	ASP
1	A	126	THR
1	A	136	LEU
1	A	147	ARG
1	A	149	ASP
1	A	151	LYS
1	A	161	PRO
1	A	162	MET
1	A	255	LEU
1	A	258	LEU
1	A	300	VAL
1	A	316	VAL
1	A	322	ASP
1	A	333	LEU
1	A	338	GLU
1	A	343	VAL
1	A	352	VAL
1	A	354	THR

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Mol	Chain	Res	Type
1	A	373	VAL
1	A	386	ARG
1	A	394	VAL
1	B	15	LEU
1	B	16	SER
1	B	20	LEU
1	B	31	SER
1	B	42	THR
1	B	44	THR
1	B	59	SER
1	B	61	THR
1	B	66	ARG
1	B	136	LEU
1	B	153	VAL
1	B	161	PRO
1	B	166	VAL
1	B	171	ILE
1	B	177	LYS
1	B	195	ARG
1	B	205	VAL
1	B	222	ILE
1	B	228	ASN
1	B	240	ASN
1	B	255	LEU
1	B	258	LEU
1	B	263	LEU
1	B	275	LEU
1	B	316	VAL
1	B	326	ARG
1	B	330	LYS
1	B	333	LEU
1	B	343	VAL
1	B	353	MET
1	B	354	THR
1	B	357	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	246	GLN
1	A	268	HIS
1	A	271	ASN

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Mol	Chain	Res	Type
1	B	26	GLN
1	B	62	HIS
1	B	206	HIS
1	B	228	ASN
1	B	234	GLN
1	B	348	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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	$\# Z  > 2$
1	LLP	B	210	1	23,24,25	3.53	11 (47%)	25,32,34	2.69	7 (28%)
1	LLP	A	210	1	23,24,25	3.06	10 (43%)	25,32,34	2.11	8 (32%)

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
1	LLP	B	210	1	-	4/16/17/19	0/1/1/1
1	LLP	A	210	1	-	6/16/17/19	0/1/1/1

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	210	LLP	CB-CA	8.10	1.64	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	210	LLP	C3-C2	7.98	1.48	1.40
1	A	210	LLP	C3-C2	7.19	1.48	1.40
1	A	210	LLP	O-C	-7.03	0.91	1.19
1	B	210	LLP	O-C	-5.75	0.96	1.19
1	A	210	LLP	CB-CA	5.35	1.60	1.53
1	B	210	LLP	C4-C5	5.32	1.48	1.42
1	B	210	LLP	C4-C3	5.31	1.48	1.40
1	A	210	LLP	C4-C5	5.23	1.48	1.42
1	B	210	LLP	P-OP2	-4.63	1.37	1.54
1	B	210	LLP	P-OP4	-3.68	1.48	1.60
1	A	210	LLP	P-OP3	-3.59	1.41	1.54
1	A	210	LLP	C4-C3	3.44	1.46	1.40
1	B	210	LLP	P-OP3	-3.35	1.41	1.54
1	A	210	LLP	P-OP2	-3.33	1.42	1.54
1	B	210	LLP	O3-C3	-2.39	1.31	1.37
1	A	210	LLP	P-OP4	-2.20	1.53	1.60
1	A	210	LLP	P-OP1	-2.17	1.43	1.50
1	B	210	LLP	OP4-C5'	-2.17	1.36	1.45
1	B	210	LLP	P-OP1	-2.07	1.43	1.50
1	A	210	LLP	CE-NZ	-2.02	1.42	1.46

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	210	LLP	OP4-C5'-C5	8.35	125.25	109.35
1	B	210	LLP	C4-C3-C2	-6.48	116.18	120.19
1	A	210	LLP	C4-C3-C2	-6.42	116.22	120.19
1	B	210	LLP	CD-CE-NZ	-4.25	100.52	110.93
1	B	210	LLP	OP2-P-OP4	-4.06	95.94	106.73
1	A	210	LLP	OP4-C5'-C5	3.96	116.89	109.35
1	B	210	LLP	CD-CG-CB	2.61	122.86	113.62
1	A	210	LLP	C3-C4-C4'	-2.52	115.72	120.41
1	A	210	LLP	OP2-P-OP1	2.31	119.71	110.68
1	A	210	LLP	C5-C4-C4'	2.26	125.27	121.56
1	B	210	LLP	OP3-P-OP1	2.24	119.46	110.68
1	A	210	LLP	O3-C3-C2	2.23	122.35	117.49
1	B	210	LLP	C6-N1-C2	2.22	123.28	119.17
1	A	210	LLP	C2'-C2-C3	-2.16	118.22	120.89
1	A	210	LLP	C6-N1-C2	2.07	123.01	119.17

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	210	LLP	O-C-CA-CB
1	A	210	LLP	N-CA-CB-CG
1	A	210	LLP	O-C-CA-CB
1	A	210	LLP	CG-CD-CE-NZ
1	B	210	LLP	CA-CB-CG-CD
1	B	210	LLP	CG-CD-CE-NZ
1	A	210	LLP	CA-CB-CG-CD
1	B	210	LLP	C3-C4-C4'-NZ
1	A	210	LLP	C3-C4-C4'-NZ
1	A	210	LLP	CD-CE-NZ-C4'

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	210	LLP	1	0
1	A	210	LLP	1	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

2 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	$\# Z  > 2$
3	CO3	B	401	-	0,3,3	0.00	-	0,3,3	0.00	-
2	GOL	A	401	-	5,5,5	0.47	0	5,5,5	0.53	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	GOL	A	401	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	401	CO3	1	0
2	A	401	GOL	1	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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	360/397 (90%)	-0.34	8 (2%) 62 69	13, 23, 43, 67	0
1	B	371/397 (93%)	-0.28	6 (1%) 72 77	13, 24, 47, 53	0
All	All	731/794 (92%)	-0.31	14 (1%) 66 73	13, 24, 45, 67	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	48	SER	4.0
1	A	326	ARG	3.8
1	B	49	SER	3.2
1	A	47	GLN	2.8
1	A	354	THR	2.8
1	A	394	VAL	2.7
1	B	30	PRO	2.6
1	A	148	ALA	2.5
1	B	32	THR	2.5
1	B	31	SER	2.5
1	A	14	ALA	2.4
1	B	354	THR	2.2
1	A	391	ARG	2.2
1	A	44	THR	2.1

### 6.2 Non-standard residues in protein, DNA, RNA chains [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. 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	B-factors( $\text{\AA}^2$ )	Q<0.9
1	LLP	B	210	24/25	0.96	0.12	13,16,21,22	0
1	LLP	A	210	24/25	0.98	0.10	14,21,25,25	0

### 6.3 Carbohydrates [i](#)

There are no monosaccharides 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. 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	B-factors( $\text{\AA}^2$ )	Q<0.9
2	GOL	A	401	6/6	0.89	0.17	38,42,44,46	0
3	CO3	B	401	4/4	0.92	0.19	46,48,48,49	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.