



# Full wwPDB X-ray Structure Validation Report ⓘ

May 18, 2020 – 09:27 pm BST

PDB ID : 2IGA  
Title : Structure of Homoprotocatechuate 2,3-Dioxygenase from *B. fuscum* in complex with reactive intermediates formed via in crystallo reaction with 4-nitrocatechol at low oxygen concentrations.  
Authors : Kovaleva, E.G.; Lipscomb, J.D.  
Deposited on : 2006-09-22  
Resolution : 1.95 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	:	2.11
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)	:	2.11

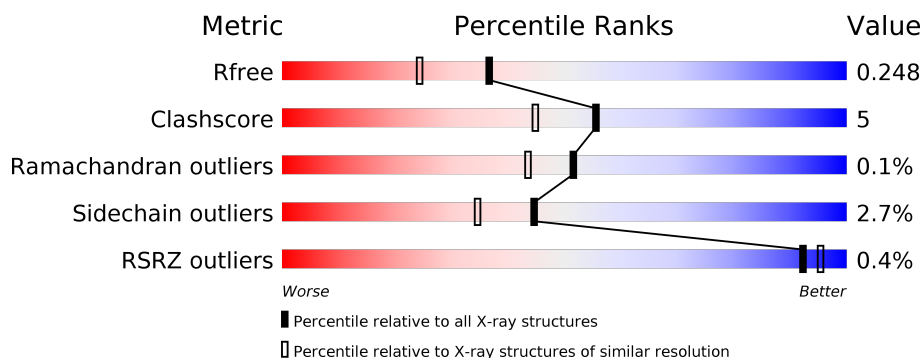
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.95 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	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

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	365	<div> <div>88%</div> <div>10%</div> <div>..</div> </div>
1	B	365	<div> <div>83%</div> <div>15%</div> <div>.</div> </div>
1	C	365	<div> <div>%</div> <div>87%</div> <div>11%</div> <div>.</div> </div>
1	D	365	<div> <div>%</div> <div>87%</div> <div>10%</div> <div>..</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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	XXP	A	600[B]	-	-	X	-
5	GOL	B	804	-	-	X	-
9	OXY	C	600	-	-	X	-

## 2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 12927 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 Homoprotocatechuate 2,3-dioxygenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	359	Total	C	N	O	S	0	11	0
			2951	1863	516	565	7			
1	B	359	Total	C	N	O	S	0	7	0
			2930	1850	512	560	8			
1	C	359	Total	C	N	O	S	0	9	0
			2933	1852	511	563	7			
1	D	359	Total	C	N	O	S	0	8	0
			2932	1854	513	558	7			

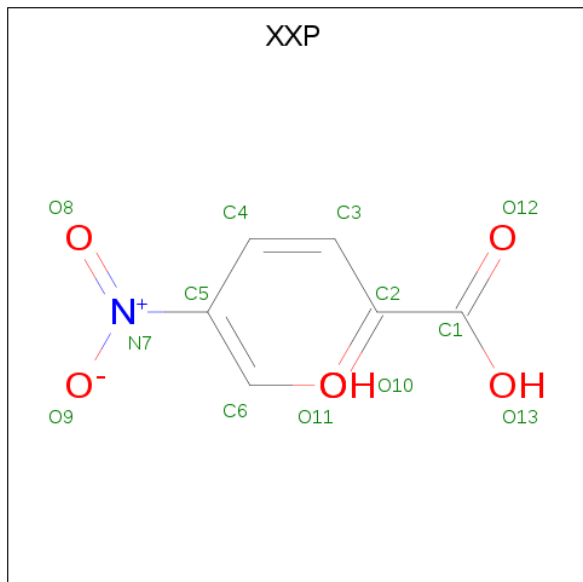
- Molecule 2 is FE (II) ION (three-letter code: FE2) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Fe	0	0
			1	1		
2	A	1	Total	Fe	0	0
			1	1		
2	D	1	Total	Fe	0	0
			1	1		
2	C	1	Total	Fe	0	0
			1	1		

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

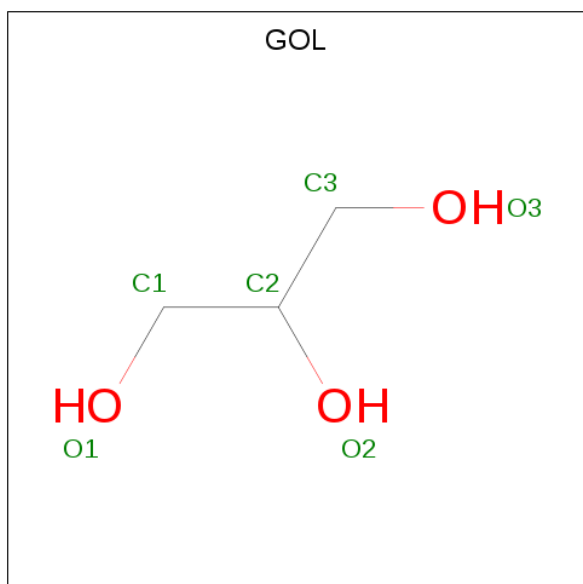
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Cl	0	1
			1	1		
3	A	1	Total	Cl	0	1
			1	1		
3	D	1	Total	Cl	0	1
			1	1		
3	C	1	Total	Cl	0	1
			1	1		

- Molecule 4 is 2-KETO,5-NITRO,6-HYDROXY-3,5-HEXADIENOIC ACID (three-letter code: XXP) (formula:  $C_6H_5NO_6$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	1
			13	6	1	6		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



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

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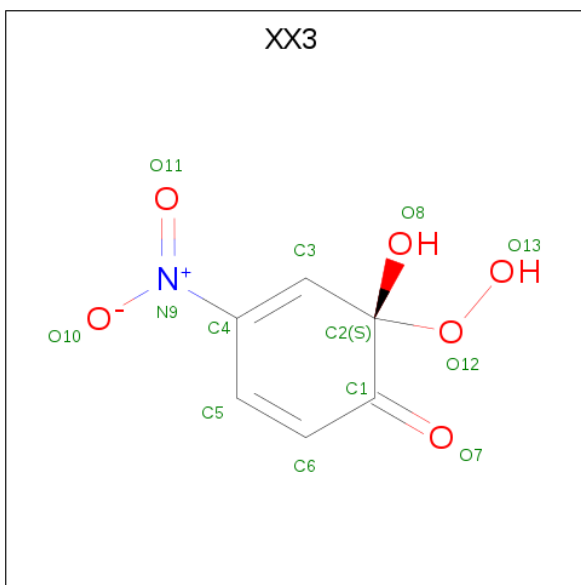
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		
5	C	1	Total	C	O	0	0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

- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

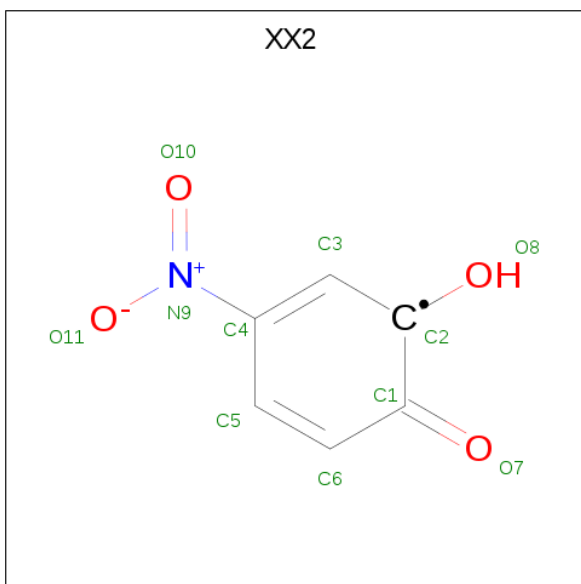
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total	Ca	0	0
			1	1		

- Molecule 7 is (1S)-1-HYDROPEROXY-1-HYDROXY-2-KETO-5-NITROCYCLOHEXA-3, 5-DIENE (three-letter code: XX3) (formula: C<sub>6</sub>H<sub>5</sub>NO<sub>6</sub>).



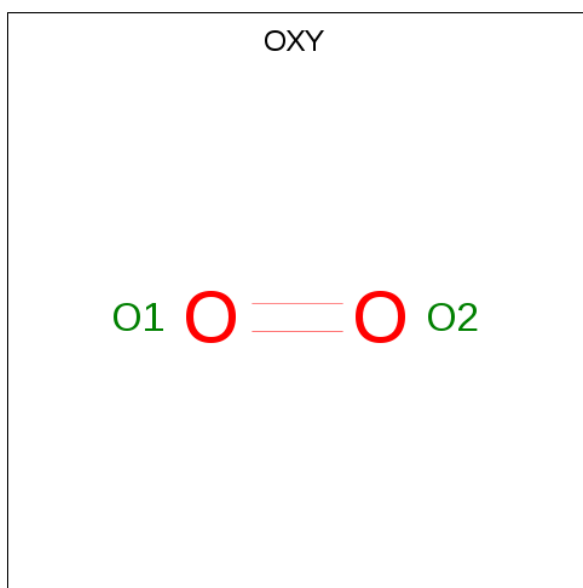
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	B	1	Total	C	N	O	0	1
			13	6	1	6		
7	D	1	Total	C	N	O	0	1
			13	6	1	6		

- Molecule 8 is 1-KETO,2-HYDROXY,4-NITROBENZENE, 1 ELECTRON OXIDIZED (three-letter code: XX2) (formula: C<sub>6</sub>H<sub>4</sub>NO<sub>4</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	C	1	Total	C	N	O	0	1
			11	6	1	4		

- Molecule 9 is OXYGEN MOLECULE (three-letter code: OXY) (formula: O<sub>2</sub>).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	C	1	Total	O	0	0
			2	2		

- Molecule 10 is water.

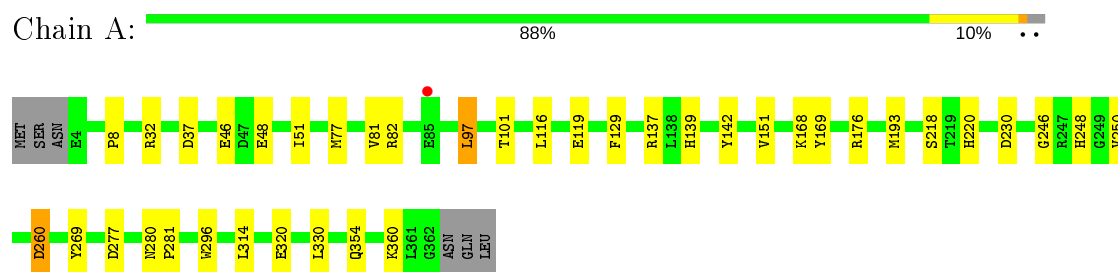
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	275	Total	O	0	0
			275	275		
10	B	299	Total	O	0	0
			299	299		
10	C	229	Total	O	0	0
			229	229		
10	D	239	Total	O	0	0
			239	239		



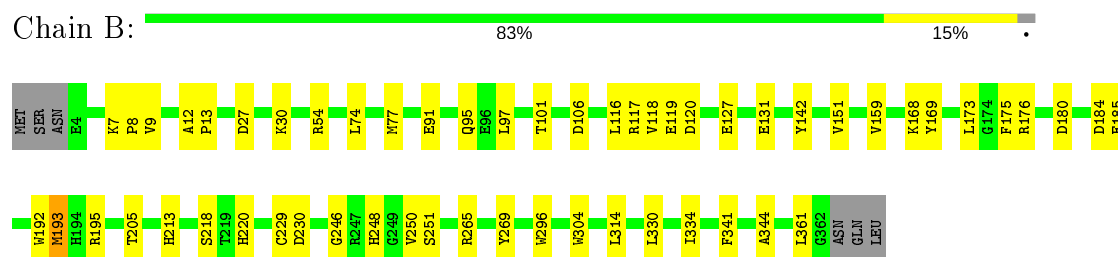
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

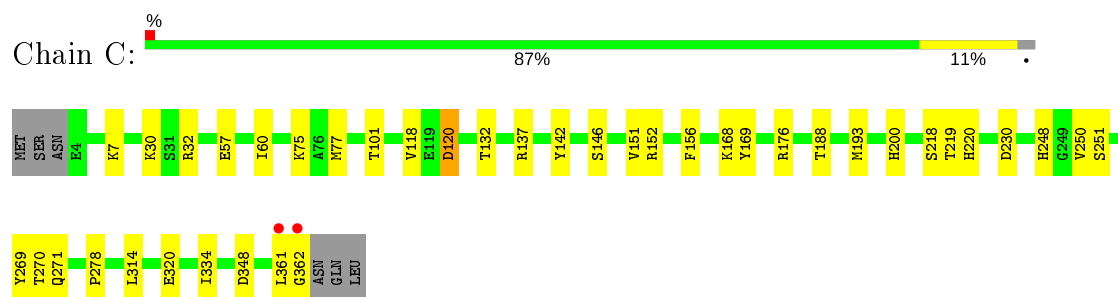
#### • Molecule 1: Homoprotocatechuate 2,3-dioxygenase



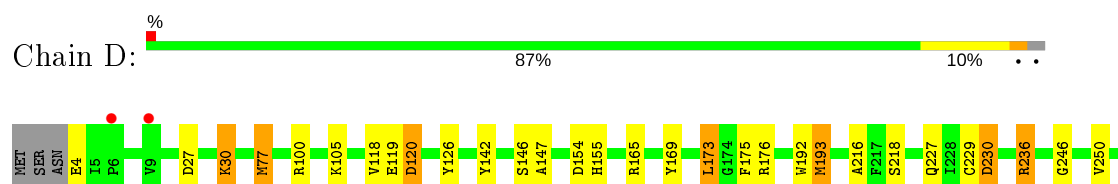
#### • Molecule 1: Homoprotocatechuate 2,3-dioxygenase

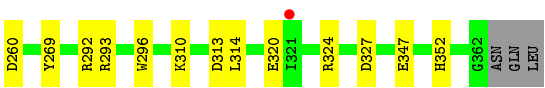


#### • Molecule 1: Homoprotocatechuate 2,3-dioxygenase



#### • Molecule 1: Homoprotocatechuate 2,3-dioxygenase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 2 <sub>1</sub> 2 <sub>1</sub> 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	110.68Å 153.02Å 96.39Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	52.70 – 1.95 52.70 – 1.95	Depositor EDS
% Data completeness (in resolution range)	87.8 (52.70-1.95) 87.8 (52.70-1.95)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.90 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.185 , 0.245 0.189 , 0.248	Depositor DCC
$R_{free}$ test set	5277 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	26.7	Xtriage
Anisotropy	0.144	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 56.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	12927	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.11% 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: XX3, XX2, XXP, OXY, GOL, CA, CL, FE2

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	0.91	0/3051	0.84	1/4142 (0.0%)
1	B	0.94	0/3021	0.88	5/4101 (0.1%)
1	C	0.85	0/3024	0.81	3/4106 (0.1%)
1	D	0.84	0/3026	0.81	4/4109 (0.1%)
All	All	0.88	0/12122	0.83	13/16458 (0.1%)

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	230	ASP	CB-CG-OD1	6.05	123.74	118.30
1	B	54	ARG	NE-CZ-NH2	-5.49	117.55	120.30
1	B	106	ASP	CB-CG-OD1	5.49	123.24	118.30
1	B	265	ARG	NE-CZ-NH1	5.48	123.04	120.30
1	A	277	ASP	CB-CG-OD1	5.33	123.10	118.30
1	B	180	ASP	CB-CG-OD1	5.31	123.08	118.30
1	C	32	ARG	NE-CZ-NH1	5.20	122.90	120.30
1	D	173	LEU	CA-CB-CG	5.20	127.25	115.30
1	C	120	ASP	CB-CG-OD1	5.18	122.97	118.30
1	C	137	ARG	NE-CZ-NH2	-5.17	117.71	120.30
1	D	120	ASP	CB-CG-OD1	5.12	122.91	118.30
1	D	236	ARG	NE-CZ-NH2	-5.10	117.75	120.30
1	B	54	ARG	NE-CZ-NH1	5.05	122.82	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	2951	0	2814	25	0
1	B	2930	0	2790	38	0
1	C	2933	0	2789	26	0
1	D	2932	0	2801	27	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	1	0
3	D	1	0	0	0	0
4	A	13	0	3	6	0
5	A	12	0	16	0	0
5	B	36	0	48	6	0
5	C	18	0	24	2	0
5	D	12	0	16	1	0
6	B	1	0	0	0	0
7	B	13	0	3	2	0
7	D	13	0	3	2	0
8	C	11	0	3	3	0
9	C	2	0	0	3	0
10	A	275	0	0	5	0
10	B	299	0	0	5	0
10	C	229	0	0	6	0
10	D	239	0	0	4	0
All	All	12927	0	11310	119	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 5.

All (119) 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)
7:B:600[B]:XX3:O13	7:B:600[B]:XX3:O12	1.53	1.21

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:D:600[B]:XX3:O13	7:D:600[B]:XX3:O12	1.54	1.21
4:A:600[B]:XXP:C1	4:A:600[B]:XXP:O10	1.87	1.21
1:D:4:GLU:HG2	1:D:165:ARG:HE	1.19	1.01
4:A:600[B]:XXP:O12	4:A:600[B]:XXP:O10	1.88	0.90
1:B:195:ARG:HH22	5:B:812:GOL:H11	1.37	0.90
1:A:8:PRO:HG3	1:A:97:LEU:HD13	1.55	0.89
1:B:344:ALA:H	5:B:804:GOL:H31	1.41	0.86
1:C:7:LYS:HE3	10:C:854:HOH:O	1.76	0.86
4:A:600[B]:XXP:O13	4:A:600[B]:XXP:O10	1.95	0.83
1:B:176:ARG:HG3	10:B:942:HOH:O	1.86	0.75
8:C:601[B]:XX2:C2	9:C:600:OXY:O1	2.35	0.74
1:C:270[B]:THR:HG22	1:C:271:GLN:HG3	1.67	0.74
1:C:75:LYS:NZ	5:C:808:GOL:H32	2.02	0.74
1:B:74:LEU:HD21	1:B:77[A]:MET:HG3	1.72	0.71
1:D:176:ARG:NH1	10:D:981:HOH:O	2.20	0.71
1:D:27:ASP:OD2	1:D:30:LYS:HD3	1.90	0.70
1:A:46:GLU:OE2	10:A:1168:HOH:O	2.10	0.69
1:A:8:PRO:HG3	1:A:97:LEU:CD1	2.22	0.69
4:A:600[B]:XXP:C1	4:A:600[B]:XXP:C6	2.72	0.67
1:A:354[A]:GLN:NE2	10:A:1211:HOH:O	2.28	0.65
1:A:360:LYS:HG3	1:C:362:GLY:HA2	1.79	0.64
1:B:218[A]:SER:HA	1:B:269:TYR:O	1.98	0.63
1:B:218[B]:SER:HA	1:B:269:TYR:O	1.99	0.62
1:B:195:ARG:NH2	5:B:812:GOL:H11	2.11	0.62
1:C:101:THR:HG22	1:C:118:VAL:HG12	1.81	0.62
1:A:137[B]:ARG:NH1	10:A:1243:HOH:O	2.31	0.61
1:C:75:LYS:HZ3	5:C:808:GOL:H32	1.63	0.61
1:C:57:GLU:OE1	10:C:852:HOH:O	2.17	0.58
1:D:4:GLU:HG2	1:D:165:ARG:NE	2.03	0.58
1:D:324[A]:ARG:NH2	10:D:894:HOH:O	2.36	0.58
1:B:334:ILE:HD12	1:B:361:LEU:HD21	1.87	0.57
1:B:74:LEU:HD21	1:B:77[A]:MET:CG	2.35	0.56
1:D:218:SER:HA	1:D:269:TYR:O	2.05	0.56
1:A:151:VAL:HG11	1:A:220:HIS:CE1	2.40	0.56
1:A:218:SER:HA	1:A:269:TYR:O	2.06	0.56
1:A:8:PRO:CG	1:A:97:LEU:HD13	2.33	0.55
1:A:81:VAL:HG22	1:A:129:PHE:O	2.07	0.55
1:C:151:VAL:HG11	1:C:220:HIS:CE1	2.41	0.55
1:A:246:GLY:HA2	1:A:296:TRP:CZ3	2.42	0.55
1:A:119:GLU:HG3	1:A:314:LEU:HG	1.90	0.54
1:C:218[B]:SER:HA	1:C:269:TYR:O	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:176:ARG:HH11	1:C:278:PRO:HA	1.73	0.53
1:B:142:TYR:CG	1:C:230:ASP:HB3	2.44	0.53
1:B:330:LEU:C	1:B:330:LEU:HD23	2.28	0.53
1:B:230:ASP:HB3	1:C:142:TYR:CG	2.44	0.53
1:D:250:VAL:O	7:D:600[B]:XX3:H5	2.08	0.52
1:C:218[A]:SER:HA	1:C:269:TYR:O	2.07	0.52
1:C:219:THR:O	1:C:270[B]:THR:HG23	2.09	0.52
1:B:131:GLU:HG2	10:B:956:HOH:O	2.09	0.52
1:A:32:ARG:HG3	1:A:51:ILE:HD13	1.92	0.50
1:A:248:HIS:HB3	1:A:250:VAL:O	2.11	0.50
1:C:77[A]:MET:HE3	1:C:156:PHE:CD2	2.46	0.50
1:B:184:ASP:OD1	1:B:185:GLU:HG3	2.12	0.50
1:D:147:ALA:CB	1:D:227:GLN:HG2	2.42	0.50
1:B:341:PHE:HE2	5:B:804:GOL:H11	1.76	0.50
4:A:600[B]:XXP:O12	4:A:600[B]:XXP:C6	2.58	0.49
1:A:82:ARG:HD3	10:B:898:HOH:O	2.12	0.49
1:B:175:PHE:HB3	1:B:193:MET:HB2	1.95	0.49
1:D:100:ARG:HG2	1:D:314:LEU:HD12	1.94	0.49
1:A:330:LEU:C	1:A:330:LEU:HD23	2.33	0.49
1:A:101:THR:HB	1:A:116[B]:LEU:HD21	1.95	0.48
5:B:804:GOL:H32	1:D:236:ARG:HD2	1.95	0.48
1:C:250:VAL:O	8:C:601[B]:XX2:H5	2.14	0.48
1:B:101:THR:HG22	1:B:118:VAL:HG12	1.95	0.48
1:D:192:TRP:CE2	1:D:250:VAL:HG11	2.49	0.47
1:D:246:GLY:HA2	1:D:296:TRP:CZ3	2.50	0.47
1:B:119:GLU:HG3	1:B:314:LEU:HG	1.97	0.47
1:B:91:GLU:O	1:B:95[A]:GLN:HG3	2.14	0.47
1:D:324[A]:ARG:NH1	1:D:327:ASP:O	2.48	0.46
1:C:200:HIS:NE2	9:C:600:OXY:O2	2.47	0.46
1:B:192:TRP:HE1	7:B:600[B]:XX3:C6	2.29	0.46
1:B:246:GLY:HA2	1:B:296:TRP:CZ3	2.51	0.46
1:D:292:ARG:HG3	1:D:293:ARG:HG3	1.97	0.46
1:C:188:THR:HG21	10:C:826:HOH:O	2.15	0.46
1:C:176:ARG:HG3	10:C:1029:HOH:O	2.16	0.45
1:B:344:ALA:N	5:B:804:GOL:H31	2.21	0.45
1:B:230:ASP:HB3	1:C:142:TYR:CD2	2.52	0.45
1:B:159:VAL:HA	1:B:205:THR:O	2.16	0.45
1:B:117:ARG:HG2	1:B:127:GLU:HB2	1.99	0.45
1:C:248:HIS:CE1	3:C:700[A]:CL:CL	3.07	0.45
1:D:147:ALA:HB3	1:D:227:GLN:HG2	1.98	0.45
1:D:77:MET:HG3	1:D:126:TYR:CD1	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:192:TRP:CE2	1:B:250:VAL:HG11	2.53	0.44
1:B:176:ARG:NH2	10:B:898:HOH:O	2.50	0.44
1:B:151:VAL:HG11	1:B:220:HIS:CE1	2.52	0.44
1:C:30:LYS:NZ	10:C:893:HOH:O	2.50	0.43
1:D:310:LYS:HD2	10:D:871:HOH:O	2.18	0.43
1:C:248:HIS:HB3	1:C:250:VAL:O	2.19	0.43
1:A:137[B]:ARG:HD2	1:A:139:HIS:ND1	2.34	0.43
1:A:137[B]:ARG:NE	10:A:1243:HOH:O	2.50	0.42
1:D:119:GLU:OE2	1:D:313:ASP:HB2	2.19	0.42
1:A:142:TYR:CG	1:D:230:ASP:HB3	2.54	0.42
1:B:8:PRO:HG3	1:B:97:LEU:CD2	2.49	0.42
1:B:7:LYS:HE2	10:B:892:HOH:O	2.19	0.42
1:B:213:HIS:CE1	1:B:304:TRP:CE2	3.07	0.42
1:C:334:ILE:HD12	1:C:361:LEU:HD21	2.00	0.42
1:A:230:ASP:HB3	1:D:142:TYR:CG	2.55	0.42
1:A:250:VAL:HB	4:A:600[B]:XXP:O9	2.20	0.42
1:A:260:ASP:C	1:A:260:ASP:OD1	2.58	0.42
1:B:296:TRP:CD1	1:D:229:CYS:HB3	2.54	0.42
1:C:152:ARG:NE	10:C:852:HOH:O	2.53	0.42
1:B:12:ALA:HA	1:B:13:PRO:HD2	1.82	0.41
1:B:248:HIS:HB3	1:B:250:VAL:O	2.20	0.41
1:B:229:CYS:HB3	1:D:296:TRP:CD1	2.56	0.41
1:D:347:GLU:OE2	1:D:352:HIS:NE2	2.53	0.41
1:B:101:THR:HB	1:B:116:LEU:HD11	2.01	0.41
1:A:280:ASN:HA	1:A:281:PRO:HD3	1.77	0.41
1:B:77[B]:MET:HB2	1:B:77[B]:MET:HE3	1.95	0.41
1:B:27:ASP:CG	1:B:30:LYS:HG3	2.41	0.40
1:D:155:HIS:CE1	1:D:216:ALA:CB	3.04	0.40
1:C:60:ILE:HB	1:C:132:THR:HG21	2.03	0.40
1:D:100:ARG:O	1:D:118[B]:VAL:HG23	2.21	0.40
1:D:154:ASP:O	1:D:155:HIS:HB3	2.21	0.40
1:D:175:PHE:HB3	1:D:193:MET:HB2	2.03	0.40
5:D:805:GOL:H11	10:D:821:HOH:O	2.21	0.40
8:C:601[B]:XX2:C1	9:C:600:OXY:O1	2.70	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	366/365 (100%)	355 (97%)	11 (3%)	0	100	100
1	B	363/365 (100%)	352 (97%)	10 (3%)	1 (0%)	41	30
1	C	363/365 (100%)	349 (96%)	13 (4%)	1 (0%)	41	30
1	D	363/365 (100%)	352 (97%)	11 (3%)	0	100	100
All	All	1455/1460 (100%)	1408 (97%)	45 (3%)	2 (0%)	51	43

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	251	SER
1	C	251	SER

### 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	316/313 (101%)	306 (97%)	10 (3%)	39	27
1	B	313/313 (100%)	307 (98%)	6 (2%)	57	50
1	C	313/313 (100%)	304 (97%)	9 (3%)	42	31
1	D	313/313 (100%)	303 (97%)	10 (3%)	39	27
All	All	1255/1252 (100%)	1220 (97%)	35 (3%)	44	33

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48[A]	GLU
1	A	48[B]	GLU
1	A	77	MET
1	A	97	LEU
1	A	168	LYS
1	A	169	TYR
1	A	176	ARG
1	A	193	MET
1	A	260	ASP
1	A	320	GLU
1	B	9	VAL
1	B	120	ASP
1	B	168	LYS
1	B	169	TYR
1	B	173	LEU
1	B	193	MET
1	C	120	ASP
1	C	146[A]	SER
1	C	168	LYS
1	C	169	TYR
1	C	193	MET
1	C	314	LEU
1	C	320[A]	GLU
1	C	320[B]	GLU
1	C	348	ASP
1	D	30	LYS
1	D	77	MET
1	D	105	LYS
1	D	120	ASP
1	D	146	SER
1	D	169	TYR
1	D	173	LEU
1	D	193	MET
1	D	260	ASP
1	D	320	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	C	95	GLN

### 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 ⓘ

Of 27 ligands modelled in this entry, 9 are monoatomic - leaving 18 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
5	GOL	B	804	-	5,5,5	0.28	0	5,5,5	0.43	0
5	GOL	B	802	-	5,5,5	0.40	0	5,5,5	1.07	0
7	XX3	B	600[B]	-	10,13,13	2.80	6 (60%)	6,19,19	2.52	1 (16%)
5	GOL	B	813	-	5,5,5	0.24	0	5,5,5	0.64	0
5	GOL	C	807	-	5,5,5	0.45	0	5,5,5	1.10	0
5	GOL	C	810	-	5,5,5	0.30	0	5,5,5	0.86	0
5	GOL	B	809	-	5,5,5	0.24	0	5,5,5	1.79	2 (40%)
5	GOL	D	805	-	5,5,5	0.39	0	5,5,5	0.39	0
5	GOL	B	806	-	5,5,5	0.47	0	5,5,5	0.34	0
5	GOL	B	812	-	5,5,5	0.32	0	5,5,5	0.36	0
7	XX3	D	600[B]	-	10,13,13	2.74	6 (60%)	6,19,19	2.57	1 (16%)
8	XX2	C	601[B]	-	7,11,11	6.06	5 (71%)	6,15,15	1.89	2 (33%)
5	GOL	A	811	-	5,5,5	0.31	0	5,5,5	0.34	0
4	XXP	A	600[B]	-	6,12,12	5.97	2 (33%)	4,15,15	1.85	1 (25%)
5	GOL	A	801	-	5,5,5	0.51	0	5,5,5	1.06	0
5	GOL	D	803	-	5,5,5	0.57	0	5,5,5	0.71	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
9	OXY	C	600	-	1,1,1	0.43	0	-		
5	GOL	C	808	-	5,5,5	0.34	0	5,5,5	0.98	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
5	GOL	B	804	-	-	2/4/4/4	-
5	GOL	B	802	-	-	4/4/4/4	-
7	XX3	B	600[B]	-	-	0/2/23/23	0/1/1/1
5	GOL	B	813	-	-	2/4/4/4	-
5	GOL	C	807	-	-	0/4/4/4	-
5	GOL	C	810	-	-	2/4/4/4	-
5	GOL	B	809	-	-	2/4/4/4	-
5	GOL	D	805	-	-	2/4/4/4	-
5	GOL	B	806	-	-	2/4/4/4	-
5	GOL	B	812	-	-	2/4/4/4	-
7	XX3	D	600[B]	-	-	0/2/23/23	0/1/1/1
8	XX2	C	601[B]	-	-	0/2/17/17	0/1/1/1
5	GOL	A	811	-	-	2/4/4/4	-
4	XXP	A	600[B]	-	-	2/3/15/15	-
5	GOL	A	801	-	-	1/4/4/4	-
5	GOL	D	803	-	-	2/4/4/4	-
5	GOL	C	808	-	-	2/4/4/4	-

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	C	601[B]	XX2	O10-N9	14.04	1.46	1.22
4	A	600[B]	XXP	O8-N7	13.12	1.45	1.22
4	A	600[B]	XXP	C4-C5	6.37	1.51	1.44
7	B	600[B]	XX3	C2-C3	-5.31	1.43	1.50
8	C	601[B]	XX2	C3-C4	4.61	1.41	1.33
7	D	600[B]	XX3	C3-C4	4.46	1.42	1.33
8	C	601[B]	XX2	C6-C1	-4.34	1.40	1.46
7	D	600[B]	XX3	C2-C3	-4.01	1.45	1.50
7	B	600[B]	XX3	C3-C4	3.65	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	D	600[B]	XX3	C6-C1	-3.57	1.40	1.46
7	B	600[B]	XX3	C6-C1	-3.46	1.40	1.46
7	D	600[B]	XX3	O8-C2	3.23	1.45	1.39
8	C	601[B]	XX2	O7-C1	2.97	1.27	1.22
7	B	600[B]	XX3	O7-C1	2.77	1.28	1.22
8	C	601[B]	XX2	C6-C5	2.77	1.41	1.35
7	B	600[B]	XX3	C5-C6	2.51	1.41	1.35
7	D	600[B]	XX3	O13-O12	2.22	1.54	1.45
7	D	600[B]	XX3	C5-C6	2.12	1.40	1.35
7	B	600[B]	XX3	O13-O12	2.02	1.53	1.45

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	D	600[B]	XX3	C5-C6-C1	-5.81	116.02	122.20
7	B	600[B]	XX3	C5-C6-C1	-5.39	116.46	122.20
8	C	601[B]	XX2	C5-C6-C1	-3.57	118.52	122.06
4	A	600[B]	XXP	C3-C4-C5	3.57	132.84	124.36
5	B	809	GOL	C3-C2-C1	-3.39	98.52	111.70
8	C	601[B]	XX2	C5-C4-N9	2.22	122.43	118.77
5	B	809	GOL	O1-C1-C2	-2.04	100.43	110.20

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	804	GOL	O1-C1-C2-C3
5	B	813	GOL	O1-C1-C2-C3
5	B	802	GOL	O1-C1-C2-C3
4	A	600[B]	XXP	C1-C2-C3-C4
5	C	810	GOL	C1-C2-C3-O3
5	B	812	GOL	O2-C2-C3-O3
5	B	809	GOL	O1-C1-C2-C3
5	B	806	GOL	O1-C1-C2-C3
5	C	808	GOL	O1-C1-C2-C3
4	A	600[B]	XXP	O11-C2-C3-C4
5	D	805	GOL	O1-C1-C2-C3
5	B	802	GOL	C1-C2-C3-O3
5	B	812	GOL	C1-C2-C3-O3
5	A	811	GOL	O1-C1-C2-C3
5	B	813	GOL	O1-C1-C2-O2
5	C	810	GOL	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
5	B	809	GOL	O1-C1-C2-O2
5	B	806	GOL	O1-C1-C2-O2
5	B	804	GOL	O1-C1-C2-O2
5	D	805	GOL	O1-C1-C2-O2
5	C	808	GOL	O1-C1-C2-O2
5	B	802	GOL	O2-C2-C3-O3
5	A	811	GOL	O1-C1-C2-O2
5	A	801	GOL	C1-C2-C3-O3
5	B	802	GOL	O1-C1-C2-O2
5	D	803	GOL	O1-C1-C2-O2
5	D	803	GOL	O1-C1-C2-C3

There are no ring outliers.

9 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	804	GOL	4	0
7	B	600[B]	XX3	2	0
5	D	805	GOL	1	0
5	B	812	GOL	2	0
7	D	600[B]	XX3	2	0
8	C	601[B]	XX2	3	0
4	A	600[B]	XXP	6	0
9	C	600	OXY	3	0
5	C	808	GOL	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 [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	359/365 (98%)	-0.31	1 (0%) 94 96	24, 31, 43, 58	0
1	B	359/365 (98%)	-0.41	0 100 100	22, 28, 38, 49	0
1	C	359/365 (98%)	-0.23	2 (0%) 89 93	23, 33, 44, 57	0
1	D	359/365 (98%)	-0.15	3 (0%) 86 90	23, 32, 46, 59	0
All	All	1436/1460 (98%)	-0.27	6 (0%) 92 95	22, 31, 43, 59	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	362	GLY	2.8
1	A	85	GLU	2.8
1	D	321	ILE	2.4
1	D	9	VAL	2.3
1	D	6	PRO	2.1
1	C	361	LEU	2.1

### 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. 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(Å <sup>2</sup> )	Q<0.9
5	GOL	D	805	6/6	0.75	0.24	66,68,68,68	0
5	GOL	B	804	6/6	0.82	0.18	48,50,51,54	0
7	XX3	D	600[B]	13/13	0.83	0.20	20,35,39,42	13
8	XX2	C	601[B]	11/11	0.84	0.20	19,30,38,41	11
5	GOL	C	810	6/6	0.85	0.15	52,52,52,54	0
5	GOL	C	808	6/6	0.85	0.22	55,55,56,56	0
7	XX3	B	600[B]	13/13	0.86	0.23	28,37,43,45	13
5	GOL	D	803	6/6	0.87	0.14	37,38,39,40	0
5	GOL	B	806	6/6	0.88	0.25	53,55,55,55	0
5	GOL	B	813	6/6	0.89	0.21	41,52,55,60	0
5	GOL	A	811	6/6	0.90	0.16	57,58,60,61	0
5	GOL	B	812	6/6	0.90	0.22	45,49,50,51	0
5	GOL	B	809	6/6	0.90	0.14	47,49,50,51	0
5	GOL	B	802	6/6	0.91	0.12	30,36,38,39	0
5	GOL	A	801	6/6	0.91	0.09	29,35,38,40	0
4	XXP	A	600[B]	13/13	0.91	0.24	15,27,44,45	13
5	GOL	C	807	6/6	0.91	0.15	35,44,45,46	0
3	CL	D	700[A]	1/1	0.94	0.21	6,6,6,6	1
3	CL	B	700[A]	1/1	0.95	0.21	6,6,6,6	1
9	OXY	C	600	2/2	0.97	0.13	35,35,35,39	0
3	CL	C	700[A]	1/1	0.97	0.15	11,11,11,11	1
3	CL	A	700[A]	1/1	0.97	0.19	13,13,13,13	1
6	CA	B	701	1/1	0.98	0.12	18,18,18,18	1
2	FE2	D	500	1/1	1.00	0.08	32,32,32,32	0
2	FE2	A	500	1/1	1.00	0.07	31,31,31,31	0
2	FE2	B	500	1/1	1.00	0.07	29,29,29,29	0
2	FE2	C	500	1/1	1.00	0.03	32,32,32,32	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.