



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 25, 2026 – 04:55 AM UTC

PDB ID : 2IGA / pdb_00002iga
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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

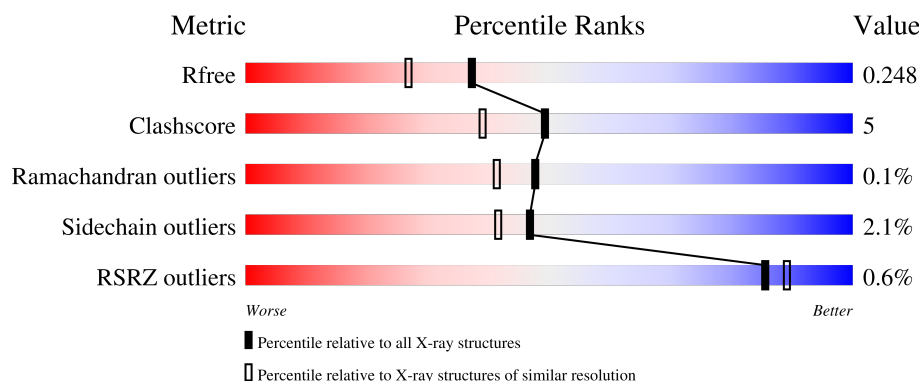
1 Overall quality at a glance

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}	180053	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 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	% 86% 12% ..
1	B	365	82% 16% .
1	C	365	% 86% 12% ..
1	D	365	% 85% 12% ..

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
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			

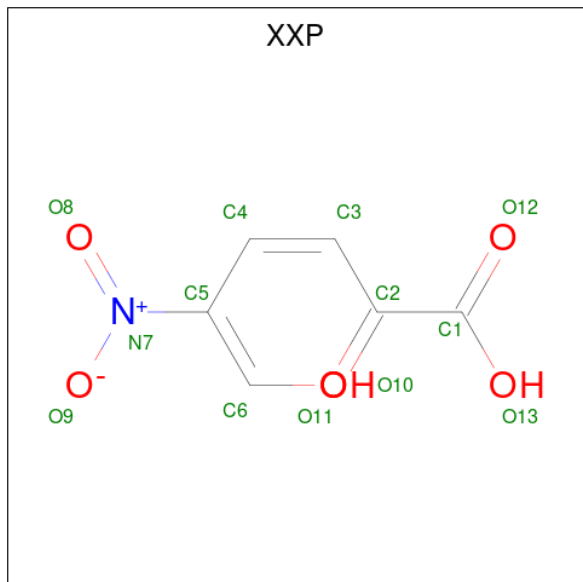
- Molecule 2 is FE (II) ION (CCD ID: FE2) (formula: Fe).

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

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

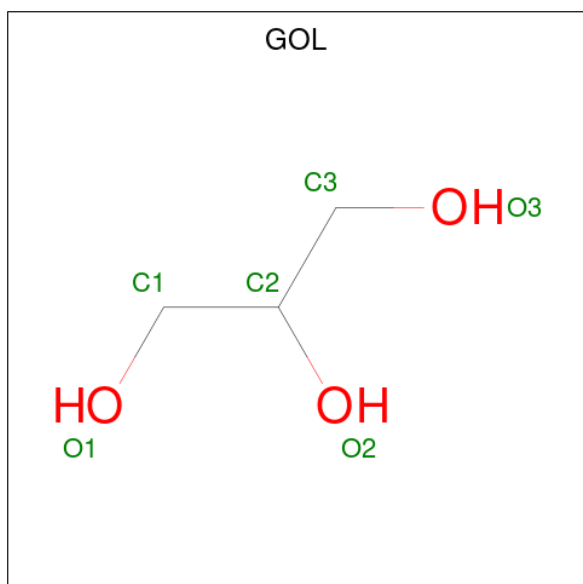
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Cl	0	1
			1	1		
3	B	1	Total	Cl	0	1
			1	1		
3	C	1	Total	Cl	0	1
			1	1		
3	D	1	Total	Cl	0	1
			1	1		

- Molecule 4 is 2-KETO,5-NITRO,6-HYDROXY-3,5-HEXADIENOIC ACID (CCD ID: 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 (CCD ID: 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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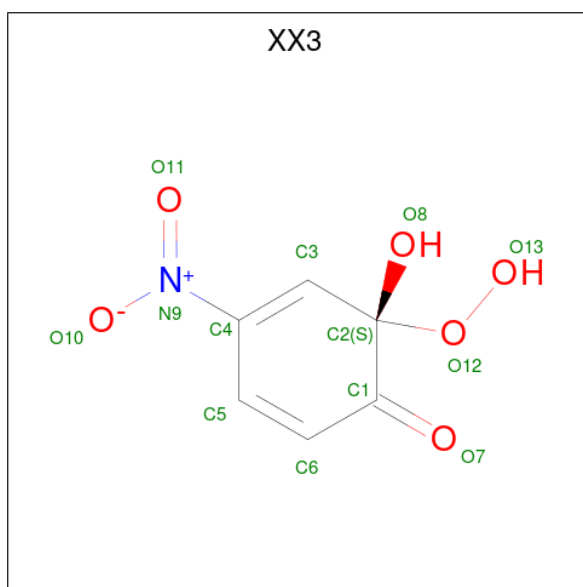
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 6 3 3	0	0
5	B	1	Total C O 6 3 3	0	0
5	B	1	Total C O 6 3 3	0	0
5	B	1	Total C O 6 3 3	0	0
5	B	1	Total C O 6 3 3	0	0
5	B	1	Total C O 6 3 3	0	0
5	B	1	Total C O 6 3 3	0	0
5	C	1	Total C O 6 3 3	0	0
5	C	1	Total C O 6 3 3	0	0
5	C	1	Total C O 6 3 3	0	0
5	D	1	Total C O 6 3 3	0	0
5	D	1	Total C O 6 3 3	0	0

- Molecule 6 is CALCIUM ION (CCD ID: CA) (formula: Ca).

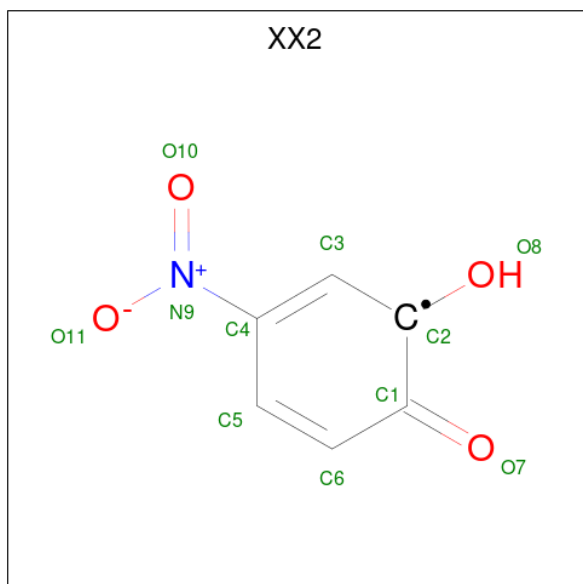
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total Ca 1 1	0	0

- Molecule 7 is (1S)-1-HYDROPEROXY-1-HYDROXY-2-KETO-5-NITROCYCLOHEXA-3,5-DIENE (CCD ID: XX3) (formula: C₆H₅NO₆).



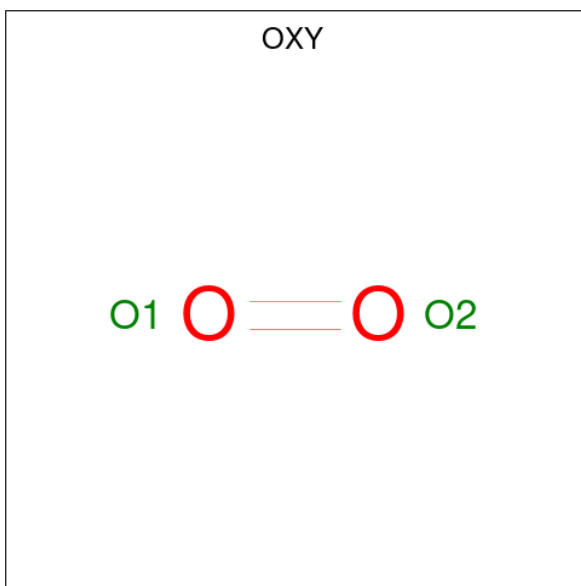
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	B	1	Total	C	N	O	0	1
			13	6	1	6		
7	D	1	Total	C	N	O	0	1
			13	6	1	6		

- Molecule 8 is 1-KETO,2-HYDROXY,4-NITROBENZENE, 1 ELECTRON OXIDIZED (CCD ID: XX2) (formula: C₆H₄NO₄).



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

- Molecule 9 is OXYGEN MOLECULE (CCD ID: OXY) (formula: O₂).



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

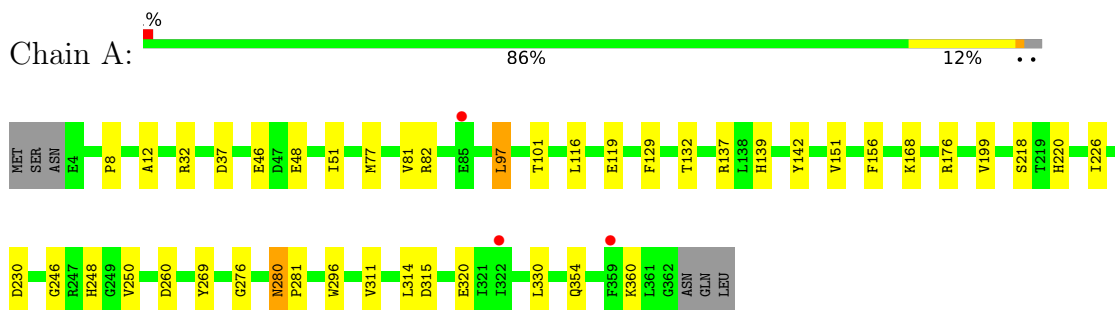
- Molecule 10 is water.

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		

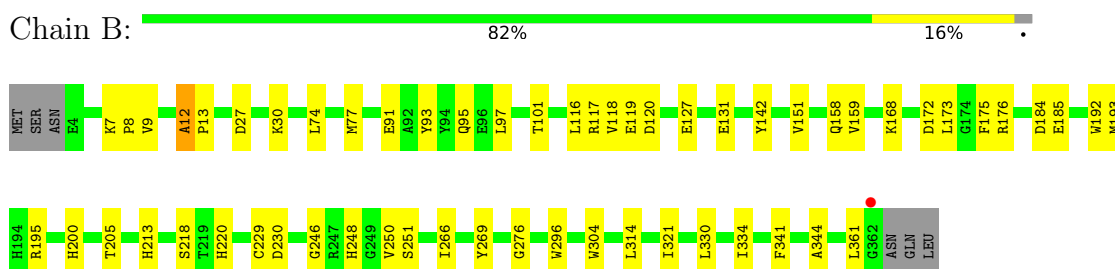
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, 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.

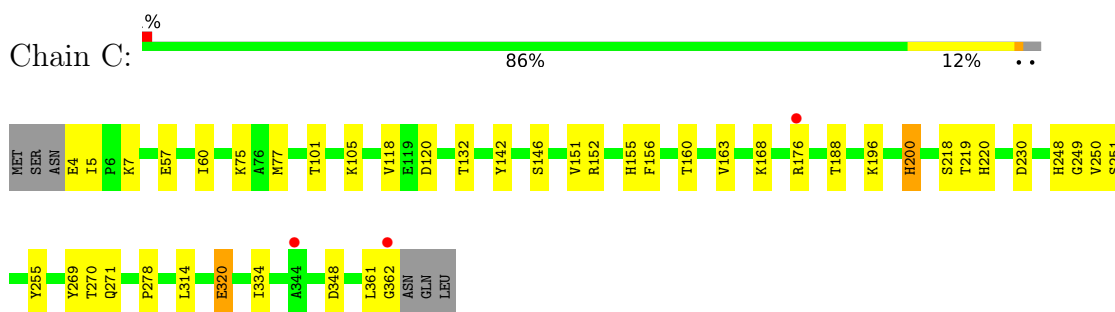
- Molecule 1: Homoprotocatechuate 2,3-dioxygenase



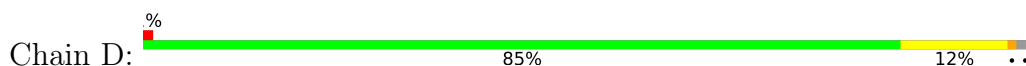
- Molecule 1: Homoprotocatechuate 2,3-dioxygenase

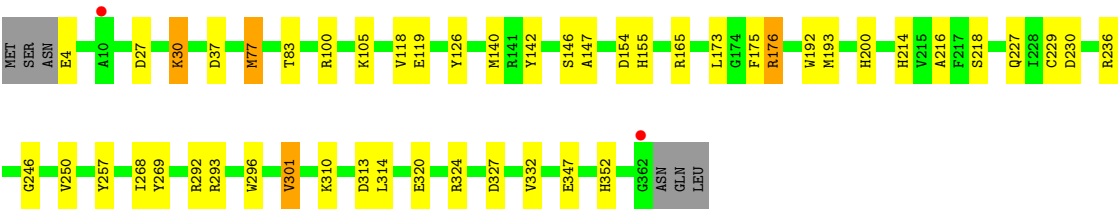


- Molecule 1: Homoprotocatechuate 2,3-dioxygenase



- Molecule 1: Homoprotocatechuate 2,3-dioxygenase





4 Data and refinement statistics

Property	Value	Source
Space group	P 2 ₁ 2 ₁ 2	Depositor
Cell constants a, b, c, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	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 (4.41%)	wwPDB-VP
Wilson B-factor (Å ²)	26.7	Xtriage
Anisotropy	0.144	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 50.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	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 ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: FE2, CL, XXP, OXY, CA, XX3, GOL, XX2

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	1.08	3/3051 (0.1%)	1.04	7/4142 (0.2%)
1	B	1.12	1/3021 (0.0%)	1.04	5/4101 (0.1%)
1	C	1.05	2/3024 (0.1%)	1.03	7/4106 (0.2%)
1	D	1.03	4/3026 (0.1%)	1.01	4/4109 (0.1%)
All	All	1.07	10/12122 (0.1%)	1.03	23/16458 (0.1%)

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	160	THR	CA-CB	6.79	1.65	1.53
1	C	163	VAL	CA-CB	5.53	1.57	1.54
1	D	83	THR	N-CA	5.51	1.50	1.45
1	D	301[A]	VAL	CA-C	5.49	1.59	1.52
1	B	266	ILE	CA-CB	5.49	1.61	1.54
1	A	226	ILE	CA-CB	5.46	1.61	1.54
1	D	268	ILE	CA-CB	5.40	1.61	1.54
1	A	199	VAL	CA-CB	5.27	1.61	1.54
1	D	332	VAL	CA-CB	5.23	1.60	1.54
1	A	132	THR	CA-CB	5.03	1.62	1.53

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	4	GLU	CA-C-N	-7.44	117.54	122.60
1	C	4	GLU	C-N-CA	-7.44	117.54	122.60
1	C	200	HIS	N-CA-C	7.09	119.30	108.52
1	C	5	ILE	CA-C-N	-6.87	113.58	120.31
1	C	5	ILE	C-N-CA	-6.87	113.58	120.31
1	A	276	GLY	N-CA-C	6.52	121.84	114.67
1	D	301[A]	VAL	N-CA-CB	-6.31	103.17	110.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	12	ALA	CA-C-N	6.17	126.53	119.93
1	B	12	ALA	C-N-CA	6.17	126.53	119.93
1	C	155	HIS	N-CA-C	6.07	117.46	108.60
1	B	93	TYR	N-CA-C	-5.92	104.75	111.14
1	B	200	HIS	N-CA-C	5.68	117.70	109.07
1	A	280	ASN	CA-C-N	5.66	127.19	120.23
1	A	280	ASN	C-N-CA	5.66	127.19	120.23
1	D	214	HIS	N-CA-C	5.21	116.21	108.60
1	C	196	LYS	N-CA-C	5.17	119.46	113.20
1	D	200	HIS	N-CA-C	5.17	116.70	108.79
1	A	156	PHE	N-CA-C	-5.16	101.70	109.85
1	D	37	ASP	N-CA-C	5.15	116.97	111.36
1	B	276	GLY	N-CA-C	5.15	120.39	114.16
1	A	315	ASP	N-CA-C	-5.13	106.70	113.17
1	A	12	ALA	CA-C-N	-5.11	114.65	119.76
1	A	12	ALA	C-N-CA	-5.11	114.65	119.76

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	40	0
1	C	2933	0	2789	28	0
1	D	2932	0	2801	30	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	3	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	5	0
10	D	239	0	0	4	0
All	All	12927	0	11310	125	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 (125) 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
4:A:600[B]:XXP:O10	4:A:600[B]:XXP:C1	1.87	1.21
7:D:600[B]:XX3:O13	7:D:600[B]:XX3:O12	1.54	1.21
1:D:4:GLU:HG2	1:D:165:ARG:HE	1.19	1.01
4:A:600[B]:XXP:O10	4:A:600[B]:XXP:O12	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:O10	4:A:600[B]:XXP:O13	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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	1.65	0.60
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:330:LEU:C	1:B:330:LEU:HD23	2.28	0.57
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
1:A:330:LEU:C	1:A:330:LEU:HD23	2.33	0.53
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: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:C:77[A]:MET:HE3	1:C:156:PHE:CD2	2.46	0.50
1:A:248:HIS:HB3	1:A:250:VAL:O	2.11	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:91:GLU:O	1:B:95[A]:GLN:HG3	2.14	0.47
1:B:119:GLU:HG3	1:B:314:LEU:HG	1.97	0.47
1:A:260:ASP:C	1:A:260:ASP:OD1	2.58	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:27:ASP:CG	1:B:30:LYS:HG3	2.41	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
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:249:GLY:HA2	1:D:140:MET:HE1	2.00	0.44
1:C:255:TYR:CD2	1:C:255:TYR:C	2.96	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:77[A]:MET:HE1	1:B:158:GLN:OE1	2.19	0.42
1:D:27:ASP:CG	1:D:30:LYS:HD3	2.45	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:C:320[B]:GLU:H	1:C:320[B]:GLU:CD	2.28	0.41
1:D:257:TYR:OH	7:D:600[B]:XX3:O8	2.37	0.41
1:A:280:ASN:HA	1:A:281:PRO:HD3	1.77	0.41
1:B:168:LYS:NZ	1:B:172:ASP:OD2	2.48	0.41
1:B:74:LEU:CD2	1:B:77[B]:MET:HE2	2.51	0.41
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%)	36	28
1	C	363/365 (100%)	349 (96%)	13 (4%)	1 (0%)	36	28
1	D	363/365 (100%)	352 (97%)	11 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1455/1460 (100%)	1408 (97%)	45 (3%)	2 (0%)	48	41

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%)	308 (98%)	8 (2%)	42	34
1	B	313/313 (100%)	309 (99%)	4 (1%)	61	58
1	C	313/313 (100%)	305 (97%)	8 (3%)	40	33
1	D	313/313 (100%)	305 (97%)	8 (3%)	40	33
All	All	1255/1252 (100%)	1227 (98%)	28 (2%)	47	40

All (28) 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	176	ARG
1	A	311	VAL
1	A	320	GLU
1	B	9	VAL
1	B	120	ASP
1	B	173	LEU
1	B	321	ILE
1	C	105	LYS

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Mol	Chain	Res	Type
1	C	120	ASP
1	C	146[A]	SER
1	C	168	LYS
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	146	SER
1	D	173	LEU
1	D	176	ARG
1	D	301[A]	VAL
1	D	320	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	33	ASN
1	C	157	ASN
1	C	290	ASN
1	C	352	HIS
1	D	290	ASN
1	D	319	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 oligosaccharides 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	802	-	5,5,5	0.40	0	5,5,5	1.12	0
5	GOL	C	808	-	5,5,5	0.36	0	5,5,5	1.02	0
5	GOL	B	806	-	5,5,5	0.48	0	5,5,5	0.35	0
5	GOL	D	803	-	5,5,5	0.59	0	5,5,5	0.73	0
8	XX2	C	601[B]	-	8,11,11	5.68	5 (62%)	6,15,15	1.81	2 (33%)
5	GOL	B	812	-	5,5,5	0.33	0	5,5,5	0.40	0
9	OXY	C	600	-	1,1,1	0.34	0	-		
5	GOL	D	805	-	5,5,5	0.41	0	5,5,5	0.40	0
5	GOL	C	807	-	5,5,5	0.47	0	5,5,5	1.16	0
5	GOL	A	811	-	5,5,5	0.32	0	5,5,5	0.39	0
7	XX3	B	600[B]	-	10,13,13	2.78	6 (60%)	6,19,19	2.21	2 (33%)
4	XXP	A	600[B]	-	9,12,12	4.58	3 (33%)	4,15,15	1.91	1 (25%)
7	XX3	D	600[B]	-	10,13,13	2.59	5 (50%)	6,19,19	2.23	1 (16%)
5	GOL	A	801	-	5,5,5	0.52	0	5,5,5	1.10	0
5	GOL	C	810	-	5,5,5	0.30	0	5,5,5	0.94	0
5	GOL	B	813	-	5,5,5	0.25	0	5,5,5	0.69	0
5	GOL	B	804	-	5,5,5	0.28	0	5,5,5	0.45	0
5	GOL	B	809	-	5,5,5	0.25	0	5,5,5	1.92	2 (40%)

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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	B	802	-	-	4/4/4/4	-
5	GOL	C	808	-	-	2/4/4/4	-
5	GOL	B	806	-	-	2/4/4/4	-
5	GOL	D	803	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	XX2	C	601[B]	-	-	0/2/17/17	0/1/1/1
5	GOL	B	812	-	-	2/4/4/4	-
5	GOL	D	805	-	-	2/4/4/4	-
5	GOL	C	807	-	-	0/4/4/4	-
5	GOL	A	811	-	-	2/4/4/4	-
7	XX3	B	600[B]	-	-	0/2/23/23	0/1/1/1
4	XXP	A	600[B]	-	-	5/9/15/15	-
7	XX3	D	600[B]	-	-	0/2/23/23	0/1/1/1
5	GOL	A	801	-	-	1/4/4/4	-
5	GOL	C	810	-	-	2/4/4/4	-
5	GOL	B	813	-	-	2/4/4/4	-
5	GOL	B	804	-	-	2/4/4/4	-
5	GOL	B	809	-	-	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	13.84	1.46	1.22
4	A	600[B]	XXP	O8-N7	12.92	1.45	1.22
7	B	600[B]	XX3	C2-C3	-5.31	1.43	1.50
8	C	601[B]	XX2	C3-C4	5.02	1.41	1.33
7	D	600[B]	XX3	C3-C4	4.76	1.42	1.33
8	C	601[B]	XX2	C6-C1	-4.52	1.40	1.46
7	D	600[B]	XX3	C2-C3	-4.01	1.45	1.50
7	B	600[B]	XX3	C3-C4	3.91	1.40	1.33
4	A	600[B]	XXP	C4-C5	3.48	1.51	1.44
8	C	601[B]	XX2	O7-C1	3.20	1.27	1.22
7	D	600[B]	XX3	C6-C1	-2.99	1.40	1.46
7	B	600[B]	XX3	C6-C1	-2.90	1.40	1.46
7	B	600[B]	XX3	O7-C1	2.79	1.28	1.22
8	C	601[B]	XX2	C6-C5	2.65	1.41	1.35
7	B	600[B]	XX3	C5-C6	2.40	1.41	1.35
7	D	600[B]	XX3	O13-O12	2.34	1.54	1.46
7	B	600[B]	XX3	O13-O12	2.13	1.53	1.46
7	D	600[B]	XX3	C5-C6	2.03	1.40	1.35
4	A	600[B]	XXP	O12-C1	2.03	1.27	1.22

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	D	600[B]	XX3	C5-C6-C1	-4.85	116.02	122.27
7	B	600[B]	XX3	C5-C6-C1	-4.51	116.46	122.27
5	B	809	GOL	C3-C2-C1	-3.62	98.52	111.80
8	C	601[B]	XX2	C5-C6-C1	-3.47	118.52	122.08
4	A	600[B]	XXP	C3-C4-C5	3.41	132.84	124.51
5	B	809	GOL	O1-C1-C2	-2.21	100.43	110.38
8	C	601[B]	XX2	C5-C4-N9	2.17	122.43	118.85
7	B	600[B]	XX3	C5-C4-C3	-2.00	120.03	123.01

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	600[B]	XXP	C3-C4-C5-N7
4	A	600[B]	XXP	C1-C2-C3-C4
4	A	600[B]	XXP	O12-C1-C2-C3
5	B	802	GOL	O1-C1-C2-C3
5	B	804	GOL	O1-C1-C2-C3
5	B	806	GOL	O1-C1-C2-C3
5	B	809	GOL	O1-C1-C2-C3
5	B	812	GOL	O2-C2-C3-O3
5	B	813	GOL	O1-C1-C2-C3
5	C	808	GOL	O1-C1-C2-C3
5	C	810	GOL	C1-C2-C3-O3
5	A	811	GOL	O1-C1-C2-C3
5	B	802	GOL	C1-C2-C3-O3
5	B	812	GOL	C1-C2-C3-O3
5	D	805	GOL	O1-C1-C2-C3
5	B	806	GOL	O1-C1-C2-O2
5	B	809	GOL	O1-C1-C2-O2
5	B	813	GOL	O1-C1-C2-O2
5	C	810	GOL	O2-C2-C3-O3
5	B	804	GOL	O1-C1-C2-O2
5	C	808	GOL	O1-C1-C2-O2
5	D	805	GOL	O1-C1-C2-O2
5	A	811	GOL	O1-C1-C2-O2
5	B	802	GOL	O2-C2-C3-O3
4	A	600[B]	XXP	O11-C2-C3-C4
5	B	802	GOL	O1-C1-C2-O2
5	A	801	GOL	C1-C2-C3-O3
5	D	803	GOL	O1-C1-C2-O2
4	A	600[B]	XXP	C2-C3-C4-C5
5	D	803	GOL	O1-C1-C2-C3

There are no ring outliers.

9 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	808	GOL	2	0
8	C	601[B]	XX2	3	0
5	B	812	GOL	2	0
9	C	600	OXY	3	0
5	D	805	GOL	1	0
7	B	600[B]	XX3	2	0
4	A	600[B]	XXP	6	0
7	D	600[B]	XX3	3	0
5	B	804	GOL	4	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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	359/365 (98%)	0.20	3 (0%) 82 86	16, 30, 43, 58	9 (2%)
1	B	359/365 (98%)	-0.04	1 (0%) 90 92	13, 28, 38, 49	6 (1%)
1	C	359/365 (98%)	0.20	3 (0%) 82 86	18, 33, 44, 57	6 (1%)
1	D	359/365 (98%)	0.18	2 (0%) 85 89	15, 32, 46, 59	6 (1%)
All	All	1436/1460 (98%)	0.13	9 (0%) 85 89	13, 31, 43, 59	27 (1%)

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	362	GLY	4.3
1	D	10	ALA	3.7
1	C	362	GLY	3.3
1	A	85	GLU	2.8
1	C	344	ALA	2.5
1	A	322	ILE	2.4
1	A	359	PHE	2.3
1	C	176	ARG	2.1
1	D	362	GLY	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 oligosaccharides 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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	GOL	D	805	6/6	0.78	0.15	66,68,68,68	0
5	GOL	C	810	6/6	0.81	0.17	52,52,52,54	0
5	GOL	A	811	6/6	0.83	0.17	57,58,60,61	0
7	XX3	B	600[B]	13/13	0.83	0.19	28,37,43,45	13
5	GOL	B	813	6/6	0.84	0.14	41,52,55,60	0
5	GOL	B	809	6/6	0.85	0.16	47,49,50,51	0
5	GOL	B	812	6/6	0.85	0.12	45,49,50,51	0
5	GOL	B	806	6/6	0.85	0.12	53,55,55,55	0
7	XX3	D	600[B]	13/13	0.86	0.18	20,35,39,42	13
5	GOL	C	808	6/6	0.88	0.12	55,55,56,56	0
5	GOL	D	803	6/6	0.89	0.12	37,38,39,40	0
4	XXP	A	600[B]	13/13	0.89	0.18	15,27,44,45	13
8	XX2	C	601[B]	11/11	0.89	0.13	19,30,38,41	11
5	GOL	C	807	6/6	0.90	0.12	35,44,45,46	0
5	GOL	A	801	6/6	0.91	0.11	29,35,38,40	0
5	GOL	B	804	6/6	0.91	0.12	48,50,51,54	0
5	GOL	B	802	6/6	0.95	0.08	30,36,38,39	0
9	OXY	C	600	2/2	0.95	0.10	35,35,35,39	0
3	CL	A	700[A]	1/1	0.96	0.11	13,13,13,13	1
3	CL	D	700[A]	1/1	0.97	0.11	6,6,6,6	1
6	CA	B	701	1/1	0.97	0.07	18,18,18,18	1
3	CL	C	700[A]	1/1	0.97	0.10	11,11,11,11	1
3	CL	B	700[A]	1/1	0.98	0.13	6,6,6,6	1
2	FE2	C	500	1/1	0.99	0.04	32,32,32,32	0
2	FE2	A	500	1/1	0.99	0.02	31,31,31,31	0
2	FE2	D	500	1/1	1.00	0.02	32,32,32,32	0
2	FE2	B	500	1/1	1.00	0.02	29,29,29,29	0

6.5 Other polymers [i](#)

There are no such residues in this entry.