



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 14, 2020 – 08:34 pm BST

PDB ID : 3B8I
Title : Crystal Structure of Oxaloacetate Decarboxylase from *Pseudomonas Aeruginosa* (PA4872) in complex with oxalate and Mg²⁺.
Authors : Narayanan, B.C.; Herzberg, O.
Deposited on : 2007-11-01
Resolution : 1.90 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 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

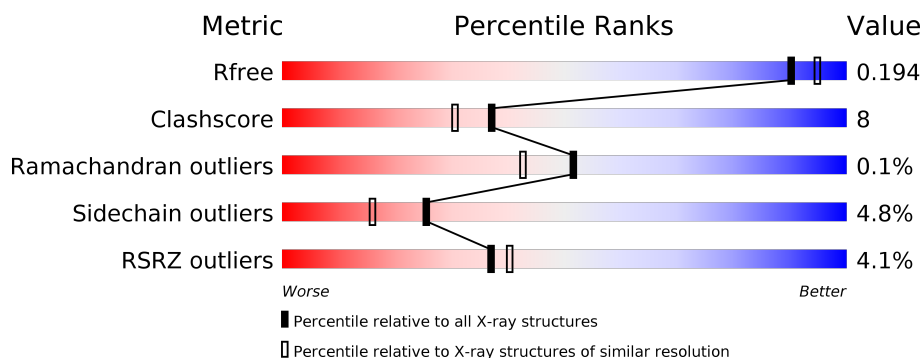
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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 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	287	<div> <div>2%</div> <div> <div></div> <div>84%</div> <div>13%</div> <div>..</div> </div> </div>
1	B	287	<div> <div>3%</div> <div> <div></div> <div>85%</div> <div>13%</div> <div>..</div> </div> </div>
1	C	287	<div> <div>5%</div> <div> <div></div> <div>78%</div> <div>18%</div> <div>..</div> </div> </div>
1	D	287	<div> <div>8%</div> <div> <div></div> <div>77%</div> <div>18%</div> <div>..</div> </div> </div>
1	E	287	<div> <div>%</div> <div> <div></div> <div>86%</div> <div>11%</div> <div>..</div> </div> </div>
1	F	287	<div> <div>6%</div> <div> <div></div> <div>83%</div> <div>13%</div> <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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	GOL	E	291	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 14913 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.

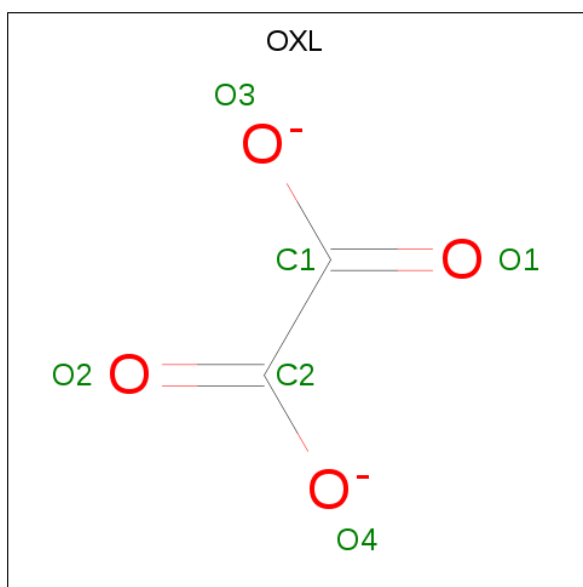
- Molecule 1 is a protein called PA4872 oxaloacetate decarboxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	284	Total	C	N	O	S	0	7	0
			2205	1386	395	414	10			
1	B	283	Total	C	N	O	S	0	1	0
			2153	1359	380	404	10			
1	C	278	Total	C	N	O	S	0	2	0
			2137	1347	380	400	10			
1	D	280	Total	C	N	O	S	0	1	0
			2141	1351	379	401	10			
1	E	283	Total	C	N	O	S	0	1	0
			2163	1364	383	406	10			
1	F	284	Total	C	N	O	S	0	1	0
			2165	1363	387	405	10			

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	1	Total	Mg	0	0
			1	1		
2	E	1	Total	Mg	0	0
			1	1		
2	B	1	Total	Mg	0	0
			1	1		
2	C	1	Total	Mg	0	0
			1	1		
2	A	1	Total	Mg	0	0
			1	1		
2	F	1	Total	Mg	0	0
			1	1		

- Molecule 3 is OXALATE ION (three-letter code: OXL) (formula: C₂O₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	2	4		
3	B	1	Total	C	O	0	0
			6	2	4		
3	C	1	Total	C	O	0	0
			6	2	4		
3	D	1	Total	C	O	0	0
			6	2	4		
3	E	1	Total	C	O	0	0
			6	2	4		
3	F	1	Total	C	O	0	0
			6	2	4		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	381	Total	O	0	0
			381	381		
5	B	291	Total	O	0	0
			291	291		
5	C	323	Total	O	0	0
			323	323		
5	D	223	Total	O	0	0
			223	223		

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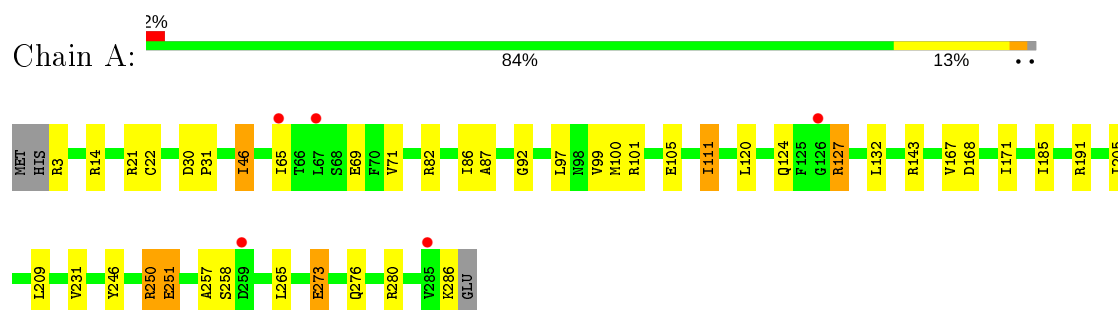
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	E	389	Total	O	0	0
			389	389		
5	F	252	Total	O	0	0
			252	252		

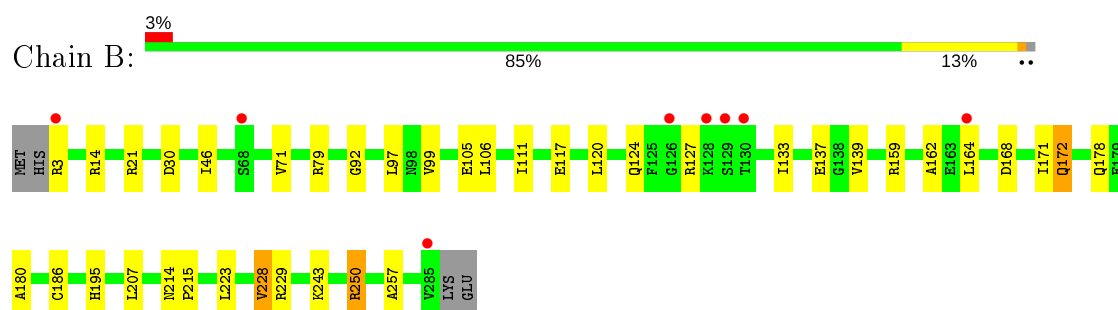
3 Residue-property plots [i](#)

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.

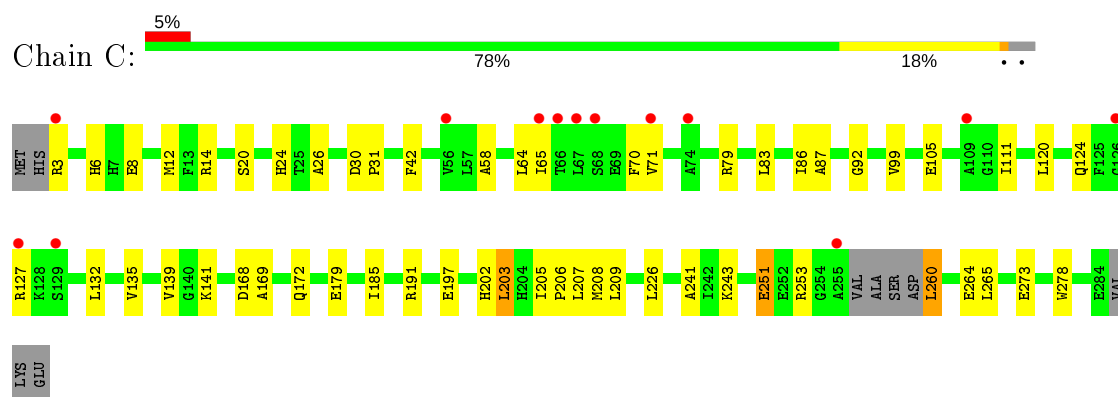
- Molecule 1: PA4872 oxaloacetate decarboxylase



- Molecule 1: PA4872 oxaloacetate decarboxylase

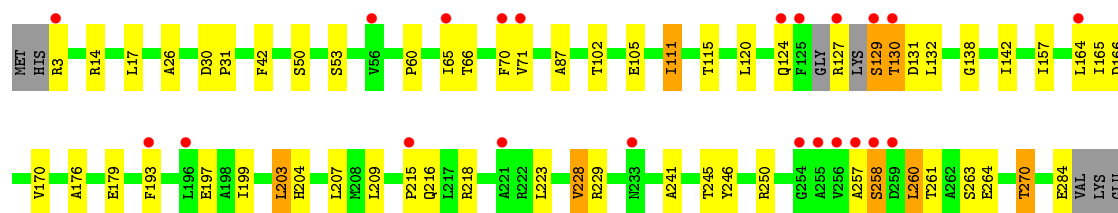


- Molecule 1: PA4872 oxaloacetate decarboxylase

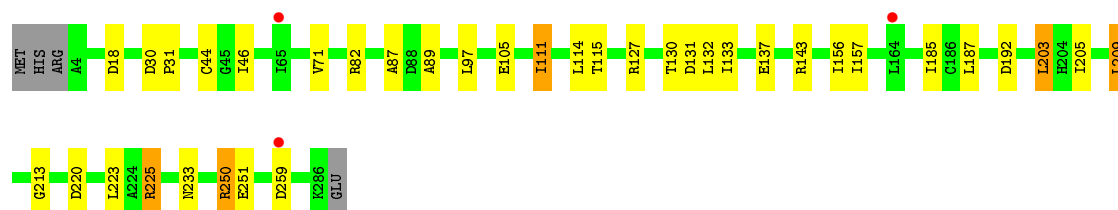
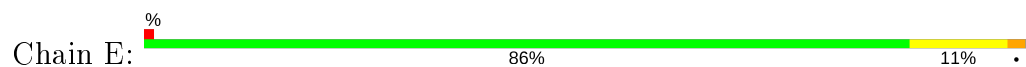


- Molecule 1: PA4872 oxaloacetate decarboxylase

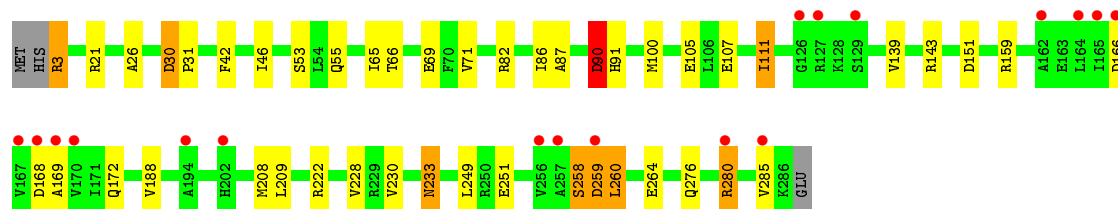
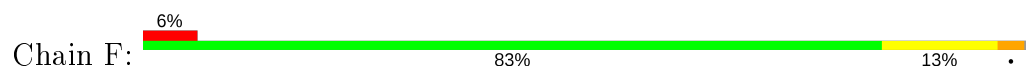




- Molecule 1: PA4872 oxaloacetate decarboxylase



- Molecule 1: PA4872 oxaloacetate decarboxylase



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	260.06 Å 83.83 Å 104.87 Å 90.00° 112.14° 90.00°	Depositor
Resolution (Å)	47.60 – 1.90 43.90 – 1.90	Depositor EDS
% Data completeness (in resolution range)	97.0 (47.60-1.90) 97.0 (43.90-1.90)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.46 (at 1.89 Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.191 , 0.249 0.197 , 0.194	Depositor DCC
R_{free} test set	15883 reflections (9.96%)	wwPDB-VP
Wilson B-factor (Å ²)	29.4	Xtriage
Anisotropy	0.055	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 50.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.000 for -h-2*k,l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	14913	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.91% 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: OXL, GOL, MG

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	0.94	0/2243	0.88	4/3043 (0.1%)
1	B	0.78	0/2191	0.81	4/2976 (0.1%)
1	C	0.83	0/2177	0.85	2/2954 (0.1%)
1	D	0.76	0/2177	0.79	0/2954
1	E	0.97	1/2201 (0.0%)	0.90	4/2989 (0.1%)
1	F	0.79	0/2203	0.81	3/2990 (0.1%)
All	All	0.85	1/13192 (0.0%)	0.84	17/17906 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	44	CYS	CB-SG	-5.77	1.72	1.81

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	225	ARG	NE-CZ-NH2	-7.76	116.42	120.30
1	C	79	ARG	NE-CZ-NH2	-7.75	116.43	120.30
1	A	21	ARG	NE-CZ-NH2	-7.17	116.71	120.30
1	C	79	ARG	NE-CZ-NH1	7.09	123.85	120.30
1	A	21	ARG	NE-CZ-NH1	7.00	123.80	120.30
1	A	143	ARG	NE-CZ-NH1	6.83	123.72	120.30
1	F	30	ASP	CB-CG-OD1	6.26	123.94	118.30
1	A	143	ARG	NE-CZ-NH2	-6.25	117.17	120.30
1	B	79	ARG	NE-CZ-NH1	6.12	123.36	120.30
1	B	79	ARG	NE-CZ-NH2	-5.67	117.47	120.30
1	E	225	ARG	NE-CZ-NH1	5.66	123.13	120.30
1	E	203	LEU	CB-CG-CD1	5.61	120.54	111.00
1	E	97	LEU	CB-CG-CD1	5.52	120.39	111.00
1	F	90	ASP	CB-CG-OD1	5.40	123.16	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	30	ASP	CB-CG-OD1	5.40	123.16	118.30
1	B	250	ARG	NE-CZ-NH1	5.31	122.96	120.30
1	F	151	ASP	CB-CG-OD1	5.03	122.83	118.30

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	2205	0	2206	30	0
1	B	2153	0	2153	22	0
1	C	2137	0	2138	39	0
1	D	2141	0	2140	52	0
1	E	2163	0	2167	30	0
1	F	2165	0	2165	35	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
2	E	1	0	0	0	0
2	F	1	0	0	0	0
3	A	6	0	0	0	0
3	B	6	0	0	0	0
3	C	6	0	0	0	0
3	D	6	0	0	1	0
3	E	6	0	0	0	0
3	F	6	0	0	0	0
4	A	12	0	16	0	0
4	B	12	0	16	1	0
4	D	6	0	8	0	0
4	E	12	0	16	6	0
4	F	6	0	8	1	0
5	A	381	0	0	5	0
5	B	291	0	0	5	0
5	C	323	0	0	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	D	223	0	0	2	0
5	E	389	0	0	9	0
5	F	252	0	0	7	0
All	All	14913	0	13033	204	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 8.

All (204) 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:D:250:ARG:NE	1:D:257:ALA:HB2	1.57	1.17
1:D:250:ARG:CD	1:D:257:ALA:HB2	1.86	1.04
1:C:20:SER:HB2	5:C:591:HOH:O	1.60	1.00
1:D:53:SER:HA	1:D:65[B]:ILE:HD11	1.41	1.00
1:D:250:ARG:HE	1:D:257:ALA:CB	1.74	0.99
1:C:172:GLN:HG2	5:C:480:HOH:O	1.63	0.99
1:F:3:ARG:HG3	1:F:3:ARG:HH11	1.27	0.97
1:B:159:ARG:HB2	1:B:186:CYS:HB3	1.49	0.92
1:F:168:ASP:HB2	5:F:538:HOH:O	1.69	0.92
1:D:250:ARG:HE	1:D:257:ALA:HB2	1.17	0.92
1:D:250:ARG:NE	1:D:257:ALA:CB	2.31	0.90
1:F:3:ARG:HH11	1:F:3:ARG:CG	1.91	0.84
1:E:131:ASP:HB3	4:E:291:GOL:H32	1.61	0.83
1:D:120:LEU:HD21	1:D:124:GLN:HG3	1.59	0.82
1:C:179:GLU:HG2	5:C:515:HOH:O	1.81	0.81
1:A:87:ALA:HB2	1:A:111:ILE:HG12	1.66	0.77
1:F:258:SER:HB3	5:F:447:HOH:O	1.84	0.76
1:E:250:ARG:HD2	1:E:250:ARG:C	2.06	0.76
1:A:280:ARG:HG3	1:A:280:ARG:HH11	1.50	0.76
1:C:251:GLU:HG3	5:C:578:HOH:O	1.86	0.75
1:A:124:GLN:OE1	1:A:127[A]:ARG:HG2	1.88	0.74
1:D:17:LEU:HA	1:D:229:ARG:HG2	1.71	0.72
1:E:131:ASP:CB	4:E:291:GOL:H32	2.19	0.72
1:D:223:LEU:HB3	1:D:228:VAL:CG2	2.21	0.70
1:A:276:GLN:NE2	5:A:618:HOH:O	2.23	0.70
1:B:133:ILE:HD12	1:B:137:GLU:HG2	1.74	0.70
1:F:280:ARG:HH11	1:F:280:ARG:HG2	1.56	0.70
1:D:127:ARG:C	1:D:129:SER:N	2.45	0.69
1:C:197:GLU:HG2	1:C:226:LEU:HD21	1.76	0.68
1:C:71:VAL:HG21	1:C:105:GLU:HB3	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:213:GLY:HA2	5:E:932:HOH:O	1.93	0.67
1:D:65[A]:ILE:HD12	1:D:70:PHE:HB2	1.77	0.66
1:F:107:GLU:OE1	4:F:290:GOL:H11	1.96	0.66
1:F:3:ARG:NH1	1:F:3:ARG:CG	2.57	0.66
1:D:250:ARG:CG	1:D:257:ALA:HB2	2.25	0.66
1:E:71:VAL:HG21	1:E:105:GLU:HB3	1.76	0.66
1:D:127:ARG:CB	1:D:129:SER:N	2.60	0.65
1:D:120:LEU:HD21	1:D:124:GLN:CG	2.26	0.65
1:C:251:GLU:HG2	5:C:580:HOH:O	1.96	0.64
1:D:130:THR:O	1:D:130:THR:HG23	1.96	0.64
1:F:71:VAL:HG21	1:F:105:GLU:HB3	1.78	0.64
1:D:246:TYR:HE2	1:D:257:ALA:HB1	1.62	0.64
1:F:3:ARG:NH1	1:F:3:ARG:HG3	2.08	0.64
1:D:223:LEU:HB3	1:D:228:VAL:HG22	1.81	0.63
1:F:139:VAL:O	1:F:143:ARG:HG3	1.99	0.62
1:A:273:GLU:CD	1:A:273:GLU:H	2.03	0.62
1:C:273:GLU:HB2	5:C:556:HOH:O	1.98	0.62
1:C:92:GLY:HA3	1:C:99:VAL:HG22	1.82	0.62
1:A:82:ARG:HD2	5:A:591:HOH:O	2.00	0.61
1:C:87:ALA:HB2	1:C:111:ILE:HG12	1.83	0.61
4:B:290:GOL:H32	1:C:6:HIS:ND1	2.16	0.60
1:E:127:ARG:HH11	1:E:131:ASP:CG	2.03	0.60
1:E:30:ASP:HB2	1:E:31:PRO:HD2	1.81	0.60
1:C:30:ASP:HB2	1:C:31:PRO:CD	2.32	0.60
1:A:124:GLN:CB	1:A:127[A]:ARG:HB3	2.31	0.60
1:B:223:LEU:HB3	1:B:228:VAL:CG2	2.32	0.59
1:D:261:THR:OG1	1:D:264:GLU:HG3	2.02	0.59
1:F:166:ASP:HB2	5:F:474:HOH:O	2.02	0.59
1:E:87:ALA:HB2	1:E:111:ILE:HG12	1.85	0.58
1:B:207:LEU:HB2	1:B:228:VAL:HA	1.86	0.57
1:D:30:ASP:HB2	1:D:31:PRO:HD2	1.86	0.57
1:F:233:ASN:OD1	1:F:233:ASN:N	2.37	0.57
1:B:71:VAL:HG21	1:B:105:GLU:HB3	1.87	0.57
1:C:30:ASP:HB2	1:C:31:PRO:HD2	1.86	0.57
1:F:30:ASP:HB2	1:F:31:PRO:HD2	1.86	0.57
1:C:203:LEU:HD23	1:C:207:LEU:CD2	2.34	0.57
1:A:124:GLN:HB2	1:A:127[A]:ARG:HB3	1.86	0.56
1:D:223:LEU:HB3	1:D:228:VAL:HG21	1.85	0.56
1:A:286:LYS:HE2	5:A:407:HOH:O	2.05	0.56
1:F:260:LEU:HG	1:F:264:GLU:HB3	1.87	0.56
1:B:223:LEU:HB3	1:B:228:VAL:HG22	1.86	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:259:ASP:HB2	5:F:404:HOH:O	2.06	0.55
1:B:250:ARG:HD2	1:B:257:ALA:HA	1.88	0.55
1:C:24:HIS:HD2	5:C:583:HOH:O	1.89	0.55
1:A:191:ARG:NH1	5:A:516:HOH:O	2.35	0.55
1:D:246:TYR:CE2	1:D:257:ALA:HB1	2.43	0.54
1:E:225:ARG:NH2	5:E:948:HOH:O	2.41	0.54
1:D:138:GLY:O	1:D:142:ILE:HG12	2.07	0.54
1:D:30:ASP:HB2	1:D:31:PRO:CD	2.37	0.54
1:D:71:VAL:HG21	1:D:105:GLU:HB3	1.88	0.54
1:B:164:LEU:N	5:B:420:HOH:O	2.28	0.54
1:F:86:ILE:HD13	1:F:208:MET:CE	2.37	0.54
1:F:276:GLN:HG3	1:F:280:ARG:HH21	1.73	0.54
1:A:280:ARG:CG	1:A:280:ARG:HH11	2.19	0.53
1:D:129:SER:O	1:D:131:ASP:N	2.41	0.53
1:D:87:ALA:HB2	1:D:111:ILE:HG12	1.91	0.53
1:C:253:ARG:NH1	5:C:455:HOH:O	2.41	0.53
1:C:86:ILE:HG21	1:C:208:MET:HE1	1.91	0.53
1:D:127:ARG:HB3	1:D:129:SER:N	2.23	0.53
1:F:100:MET:CE	5:F:480:HOH:O	2.57	0.53
1:E:114:LEU:HD21	1:E:156:ILE:CD1	2.39	0.53
1:F:55:GLN:HB3	5:F:450:HOH:O	2.09	0.52
1:C:203:LEU:HD23	1:C:207:LEU:HD21	1.90	0.52
1:D:204:HIS:HD2	5:D:413:HOH:O	1.92	0.52
1:F:86:ILE:HD13	1:F:208:MET:HE1	1.92	0.52
1:B:168:ASP:HA	1:B:171:ILE:HD12	1.91	0.52
1:A:14[B]:ARG:HD3	1:A:14[B]:ARG:O	2.10	0.52
1:A:30:ASP:HB2	1:A:31:PRO:HD2	1.92	0.52
1:F:87:ALA:HB2	1:F:111:ILE:HG13	1.92	0.52
1:E:250:ARG:HD2	1:E:251:GLU:N	2.24	0.52
1:A:185:ILE:HG12	1:A:205:ILE:HD11	1.92	0.51
1:B:139:VAL:HG13	1:B:180:ALA:HB2	1.91	0.51
1:D:250:ARG:HD3	1:D:257:ALA:N	2.25	0.51
1:C:20:SER:CB	5:C:591:HOH:O	2.37	0.51
1:D:60:PRO:HG3	1:D:270:THR:HG23	1.92	0.51
1:C:168[B]:ASP:OD1	1:C:169:ALA:N	2.44	0.50
1:E:220:ASP:HA	1:E:223:LEU:HD12	1.94	0.50
1:D:250:ARG:CD	1:D:257:ALA:CB	2.75	0.50
1:A:167:VAL:O	1:A:171:ILE:HG13	2.12	0.50
1:A:92:GLY:HA3	1:A:99:VAL:HG22	1.94	0.50
1:C:99:VAL:HG21	1:C:141:LYS:HD3	1.93	0.49
1:A:251:GLU:HG3	5:A:445:HOH:O	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:191:ARG:NH1	5:C:507:HOH:O	2.45	0.49
1:C:135:VAL:O	1:C:139:VAL:HG23	2.12	0.49
1:C:185:ILE:HG12	1:C:205:ILE:HD11	1.94	0.49
1:E:132:LEU:H	4:E:291:GOL:H2	1.78	0.49
1:D:164:LEU:HB2	5:D:486:HOH:O	2.13	0.48
1:A:120:LEU:HD13	1:A:124:GLN:OE1	2.12	0.48
1:E:132:LEU:H	4:E:291:GOL:C3	2.27	0.48
1:E:82:ARG:NH2	5:E:1007:HOH:O	2.41	0.48
1:A:65[B]:ILE:HG12	1:A:69:GLU:HB2	1.96	0.48
1:C:127:ARG:HD3	5:C:439:HOH:O	2.13	0.48
1:C:241:ALA:HB1	1:D:241:ALA:HB1	1.95	0.48
1:B:172:GLN:NE2	5:B:555:HOH:O	2.47	0.47
1:B:162:ALA:O	1:B:195:HIS:HE1	1.97	0.47
1:A:124:GLN:HB3	1:A:127[A]:ARG:HB3	1.95	0.47
1:D:165:ILE:HG13	1:D:170:VAL:HG23	1.96	0.47
1:C:58:ALA:HB2	1:D:31:PRO:HB2	1.95	0.47
1:E:82:ARG:HD3	5:E:897:HOH:O	2.15	0.47
1:D:250:ARG:HG3	1:D:257:ALA:HB2	1.97	0.47
1:E:233:ASN:HB3	5:E:932:HOH:O	2.14	0.47
1:E:187:LEU:HB2	1:E:209:LEU:HD12	1.96	0.47
1:E:185:ILE:HG12	1:E:205:ILE:HD11	1.96	0.46
1:D:176:ALA:O	1:D:179:GLU:HB3	2.14	0.46
1:F:53:SER:HA	1:F:65[B]:ILE:HD11	1.98	0.46
1:D:26:ALA:HB2	1:D:42:PHE:CD1	2.51	0.46
1:D:50:SER:OG	3:D:288:OXL:O3	2.32	0.46
1:F:65[A]:ILE:HG12	1:F:69:GLU:HB2	1.98	0.45
1:E:233:ASN:ND2	5:E:932:HOH:O	2.48	0.45
1:D:258:SER:HB3	1:D:260:LEU:H	1.82	0.45
1:F:21:ARG:HE	1:F:21:ARG:HB3	1.24	0.45
1:A:46:ILE:HD12	1:A:86:ILE:HB	1.99	0.45
1:A:100:MET:HE1	1:C:278:TRP:HB3	1.99	0.45
1:A:250:ARG:NH1	1:A:257:ALA:HA	2.32	0.45
1:C:120:LEU:HD22	1:C:124:GLN:HG3	1.98	0.45
1:D:193:PHE:O	1:D:197:GLU:HB2	2.16	0.45
1:C:241:ALA:HB2	1:D:245:THR:OG1	2.17	0.45
1:D:127:ARG:HD2	1:D:131:ASP:OD2	2.17	0.44
1:B:214:ASN:HA	1:B:215:PRO:HD3	1.88	0.44
1:E:133:ILE:HD12	1:E:137:GLU:HG2	2.00	0.44
1:A:71:VAL:HG21	1:A:105:GLU:HB3	1.98	0.44
1:D:199:ILE:O	1:D:203:LEU:HD22	2.18	0.44
1:B:14:ARG:HB3	5:B:506:HOH:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:101:ARG:O	1:A:105:GLU:HG2	2.18	0.44
1:A:246:TYR:CE2	1:A:258:SER:HB2	2.53	0.44
1:D:250:ARG:NE	1:D:257:ALA:HB3	2.30	0.43
1:C:202:HIS:HB2	5:C:453:HOH:O	2.19	0.43
1:A:111:ILE:HA	1:A:111:ILE:HD12	1.86	0.43
1:C:8:GLU:O	1:C:12:MET:HG3	2.18	0.43
1:D:215:PRO:HA	1:D:218:ARG:CZ	2.48	0.43
1:E:131:ASP:CA	4:E:291:GOL:H32	2.48	0.43
1:E:46:ILE:HG23	1:E:46:ILE:O	2.19	0.43
1:B:178:GLN:O	5:B:439:HOH:O	2.21	0.43
1:E:143:ARG:HD3	5:E:731:HOH:O	2.18	0.43
1:D:127:ARG:HB2	1:D:129:SER:N	2.33	0.43
1:E:115:THR:HG22	1:E:157:ILE:HB	2.01	0.43
1:E:259:ASP:HB2	5:E:992:HOH:O	2.17	0.43
1:F:26:ALA:HB2	1:F:42:PHE:CD1	2.53	0.43
1:B:243:LYS:NZ	5:B:408:HOH:O	2.23	0.42
1:F:280:ARG:HH11	1:F:280:ARG:CG	2.26	0.42
1:B:117:GLU:CB	1:B:159:ARG:HG2	2.49	0.42
1:D:115:THR:HA	1:D:157:ILE:O	2.19	0.42
1:D:250:ARG:HD3	1:D:257:ALA:HB2	1.89	0.42
1:F:276:GLN:HG3	1:F:280:ARG:NH2	2.33	0.42
1:A:22:CYS:SG	1:A:231:VAL:HG23	2.59	0.42
1:B:21:ARG:HE	1:B:21:ARG:HB3	1.58	0.42
1:F:30:ASP:HB2	1:F:31:PRO:CD	2.48	0.42
1:F:169:ALA:O	1:F:172:GLN:HB3	2.20	0.41
1:F:208:MET:HE2	1:F:230:VAL:HG11	2.00	0.41
1:F:65[B]:ILE:HG22	1:F:66:THR:O	2.20	0.41
1:A:246:TYR:CB	1:A:265:LEU:HD21	2.51	0.41
1:B:106:LEU:O	1:B:111:ILE:HG13	2.20	0.41
1:B:92:GLY:HA3	1:B:99:VAL:HG22	2.01	0.41
1:D:203:LEU:HD23	1:D:207:LEU:HD21	2.02	0.41
1:E:132:LEU:H	4:E:291:GOL:C2	2.33	0.41
1:F:82:ARG:HD2	5:F:334:HOH:O	2.20	0.41
1:C:203:LEU:HD23	1:C:207:LEU:HD22	2.03	0.41
1:C:65[B]:ILE:HD12	1:C:70:PHE:HB2	2.02	0.41
1:C:83:LEU:HD23	1:C:83:LEU:H	1.85	0.41
1:C:243:LYS:HA	1:C:265:LEU:HD23	2.02	0.41
1:F:159:ARG:CZ	1:F:188:VAL:HG21	2.51	0.41
1:A:280:ARG:CG	1:A:280:ARG:NH1	2.83	0.40
1:E:89:ALA:HB3	1:E:115:THR:O	2.20	0.40
1:B:223:LEU:HB3	1:B:228:VAL:HG21	2.01	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:130:THR:CG2	1:D:130:THR:O	2.60	0.40
1:D:65[B]:ILE:HG22	1:D:66:THR:O	2.22	0.40
1:F:249:LEU:HA	1:F:249:LEU:HD23	1.91	0.40
1:C:260:LEU:HG	1:C:264:GLU:HB3	2.02	0.40
1:E:127:ARG:NH1	1:E:131:ASP:CG	2.73	0.40
1:E:192:ASP:HB2	5:E:702:HOH:O	2.21	0.40
1:B:21:ARG:O	1:B:229:ARG:HD3	2.21	0.40
1:C:3:ARG:HD2	5:C:577:HOH:O	2.21	0.40
1:C:26:ALA:HB2	1:C:42:PHE:CD1	2.57	0.40
1:F:90:ASP:HB3	1:F:91:HIS:H	1.70	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	288/287 (100%)	285 (99%)	3 (1%)	0	100	100
1	B	282/287 (98%)	273 (97%)	8 (3%)	1 (0%)	34	24
1	C	276/287 (96%)	272 (99%)	4 (1%)	0	100	100
1	D	276/287 (96%)	266 (96%)	9 (3%)	1 (0%)	34	24
1	E	282/287 (98%)	275 (98%)	7 (2%)	0	100	100
1	F	283/287 (99%)	279 (99%)	4 (1%)	0	100	100
All	All	1687/1722 (98%)	1650 (98%)	35 (2%)	2 (0%)	51	43

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	130	THR
1	B	127	ARG

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	224/224 (100%)	212 (95%)	12 (5%)	22	13
1	B	218/224 (97%)	211 (97%)	7 (3%)	39	30
1	C	217/224 (97%)	209 (96%)	8 (4%)	34	25
1	D	217/224 (97%)	201 (93%)	16 (7%)	13	6
1	E	220/224 (98%)	214 (97%)	6 (3%)	44	38
1	F	219/224 (98%)	205 (94%)	14 (6%)	17	8
All	All	1315/1344 (98%)	1252 (95%)	63 (5%)	25	16

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ARG
1	A	46	ILE
1	A	97	LEU
1	A	111	ILE
1	A	127[A]	ARG
1	A	127[B]	ARG
1	A	132	LEU
1	A	168	ASP
1	A	209	LEU
1	A	250	ARG
1	A	251	GLU
1	A	273	GLU
1	B	3	ARG
1	B	46	ILE
1	B	97	LEU
1	B	120	LEU
1	B	124	GLN
1	B	172	GLN
1	B	228	VAL
1	C	14	ARG
1	C	64	LEU
1	C	132	LEU

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Mol	Chain	Res	Type
1	C	203	LEU
1	C	206	PRO
1	C	209	LEU
1	C	251	GLU
1	C	260	LEU
1	D	3	ARG
1	D	14	ARG
1	D	102	THR
1	D	111	ILE
1	D	129	SER
1	D	132	LEU
1	D	166	ASP
1	D	203	LEU
1	D	209	LEU
1	D	216	GLN
1	D	228	VAL
1	D	258	SER
1	D	260	LEU
1	D	263	SER
1	D	270	THR
1	D	284	GLU
1	E	18	ASP
1	E	111	ILE
1	E	130	THR
1	E	203	LEU
1	E	209	LEU
1	E	250	ARG
1	F	3	ARG
1	F	46	ILE
1	F	90	ASP
1	F	111	ILE
1	F	209	LEU
1	F	222	ARG
1	F	228	VAL
1	F	233	ASN
1	F	251	GLU
1	F	258	SER
1	F	259	ASP
1	F	260	LEU
1	F	280	ARG
1	F	285	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such

sidechains are listed below:

Mol	Chain	Res	Type
1	D	204	HIS
1	F	216	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 20 ligands modelled in this entry, 6 are monoatomic - leaving 14 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	$\# Z > 2$
4	GOL	B	290	-	5,5,5	0.42	0	5,5,5	0.96	0
4	GOL	D	290	-	5,5,5	0.46	0	5,5,5	1.00	0
4	GOL	B	291	-	5,5,5	0.36	0	5,5,5	0.29	0
4	GOL	F	290	-	5,5,5	0.37	0	5,5,5	0.51	0
4	GOL	A	291	-	5,5,5	0.48	0	5,5,5	0.90	0
3	OXL	F	288	2	0,5,5	0.00	-	0,6,6	0.00	-
3	OXL	E	288	2	0,5,5	0.00	-	0,6,6	0.00	-
3	OXL	D	288	2	0,5,5	0.00	-	0,6,6	0.00	-
3	OXL	C	288	2	0,5,5	0.00	-	0,6,6	0.00	-
3	OXL	B	288	2	0,5,5	0.00	-	0,6,6	0.00	-
3	OXL	A	288	2	0,5,5	0.00	-	0,6,6	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	GOL	A	290	-	5,5,5	0.43	0	5,5,5	1.08	0
4	GOL	E	290	-	5,5,5	0.42	0	5,5,5	0.86	0
4	GOL	E	291	-	5,5,5	0.30	0	5,5,5	0.92	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
4	GOL	B	290	-	-	4/4/4/4	-
4	GOL	D	290	-	-	2/4/4/4	-
4	GOL	B	291	-	-	2/4/4/4	-
4	GOL	F	290	-	-	1/4/4/4	-
4	GOL	A	291	-	-	2/4/4/4	-
3	OXL	F	288	2	-	0/0/4/4	-
3	OXL	E	288	2	-	0/0/4/4	-
3	OXL	D	288	2	-	0/0/4/4	-
3	OXL	C	288	2	-	0/0/4/4	-
3	OXL	B	288	2	-	0/0/4/4	-
3	OXL	A	288	2	-	0/0/4/4	-
4	GOL	A	290	-	-	2/4/4/4	-
4	GOL	E	290	-	-	2/4/4/4	-
4	GOL	E	291	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	290	GOL	C1-C2-C3-O3
4	A	291	GOL	O1-C1-C2-C3
4	A	290	GOL	O1-C1-C2-C3
4	D	290	GOL	O1-C1-C2-C3
4	E	291	GOL	O1-C1-C2-O2
4	E	291	GOL	O1-C1-C2-C3
4	E	290	GOL	C1-C2-C3-O3
4	E	290	GOL	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
4	B	290	GOL	O1-C1-C2-O2
4	B	290	GOL	O2-C2-C3-O3
4	A	291	GOL	O1-C1-C2-O2
4	A	290	GOL	O1-C1-C2-O2
4	B	290	GOL	O1-C1-C2-C3
4	D	290	GOL	O1-C1-C2-O2
4	B	291	GOL	C1-C2-C3-O3
4	B	291	GOL	O2-C2-C3-O3
4	F	290	GOL	O1-C1-C2-C3

There are no ring outliers.

4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	290	GOL	1	0
4	F	290	GOL	1	0
3	D	288	OXL	1	0
4	E	291	GOL	6	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	284/287 (98%)	-0.20	5 (1%) 68 71	18, 25, 39, 56	0
1	B	283/287 (98%)	0.01	8 (2%) 53 56	21, 36, 56, 67	0
1	C	278/287 (96%)	0.08	13 (4%) 31 34	20, 33, 46, 58	0
1	D	280/287 (97%)	0.38	22 (7%) 12 14	23, 39, 55, 68	0
1	E	283/287 (98%)	-0.25	3 (1%) 80 82	15, 24, 39, 49	0
1	F	284/287 (98%)	0.16	18 (6%) 20 22	18, 35, 64, 69	0
All	All	1692/1722 (98%)	0.03	69 (4%) 37 40	15, 31, 54, 69	0

All (69) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	256	VAL	8.6
1	D	257	ALA	7.0
1	B	126	GLY	4.6
1	B	129	SER	4.4
1	B	285	VAL	4.2
1	D	259	ASP	4.2
1	D	129	SER	4.1
1	A	126[A]	GLY	4.1
1	D	164	LEU	4.0
1	D	255	ALA	4.0
1	C	56	VAL	3.8
1	D	258	SER	3.7
1	F	285	VAL	3.7
1	F	259	ASP	3.6
1	D	127	ARG	3.6
1	F	257	ALA	3.5
1	B	164	LEU	3.4
1	B	128	LYS	3.4
1	F	256	VAL	3.4

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Mol	Chain	Res	Type	RSRZ
1	D	130	THR	3.3
1	C	129	SER	3.2
1	B	130	THR	3.2
1	D	56	VAL	3.1
1	D	65[A]	ILE	3.1
1	F	194	ALA	3.1
1	C	65[A]	ILE	3.1
1	A	285	VAL	3.0
1	C	71	VAL	3.0
1	F	165	ILE	3.0
1	F	167	VAL	2.9
1	F	168	ASP	2.8
1	F	126	GLY	2.8
1	D	233	ASN	2.8
1	A	65[A]	ILE	2.8
1	D	193	PHE	2.7
1	F	164	LEU	2.5
1	C	255	ALA	2.5
1	C	67	LEU	2.5
1	F	170	VAL	2.5
1	C	109	ALA	2.4
1	C	127	ARG	2.4
1	C	3	ARG	2.4
1	C	126	GLY	2.4
1	F	166	ASP	2.4
1	B	3	ARG	2.4
1	B	68	SER	2.4
1	D	71	VAL	2.4
1	D	196	LEU	2.4
1	C	68	SER	2.3
1	C	66	THR	2.3
1	D	254	GLY	2.3
1	F	129	SER	2.3
1	D	3	ARG	2.2
1	F	127	ARG	2.2
1	D	221	ALA	2.2
1	F	162	ALA	2.2
1	E	65[A]	ILE	2.2
1	D	125	PHE	2.2
1	F	202	HIS	2.1
1	A	67	LEU	2.1
1	E	164	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	F	280	ARG	2.1
1	E	259	ASP	2.1
1	D	124	GLN	2.1
1	A	259	ASP	2.0
1	D	70	PHE	2.0
1	C	74	ALA	2.0
1	D	215	PRO	2.0
1	F	169	ALA	2.0

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. 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
4	GOL	A	291	6/6	0.76	0.19	43,51,52,52	0
4	GOL	B	290	6/6	0.78	0.17	51,52,53,55	0
4	GOL	E	291	6/6	0.84	0.19	38,41,45,48	0
2	MG	F	289	1/1	0.85	0.06	49,49,49,49	0
3	OXL	F	288	6/6	0.85	0.12	42,44,46,46	0
3	OXL	D	288	6/6	0.87	0.10	48,51,52,53	0
3	OXL	B	288	6/6	0.92	0.10	47,48,52,52	0
4	GOL	A	290	6/6	0.92	0.10	31,36,38,41	0
3	OXL	E	288	6/6	0.93	0.09	27,34,37,40	0
4	GOL	B	291	6/6	0.93	0.09	37,39,39,45	0
4	GOL	F	290	6/6	0.94	0.11	34,37,39,41	0
2	MG	B	289	1/1	0.95	0.03	37,37,37,37	0
3	OXL	C	288	6/6	0.95	0.07	39,45,48,51	0
4	GOL	D	290	6/6	0.95	0.09	32,37,39,40	0
2	MG	D	289	1/1	0.96	0.08	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	OXL	A	288	6/6	0.96	0.08	29,32,36,38	0
4	GOL	E	290	6/6	0.96	0.12	28,33,35,39	0
2	MG	C	289	1/1	0.98	0.11	39,39,39,39	0
2	MG	A	289	1/1	0.99	0.05	27,27,27,27	0
2	MG	E	289	1/1	0.99	0.08	29,29,29,29	0

6.5 Other polymers [i](#)

There are no such residues in this entry.