



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 19, 2022 – 12:16 PM JST

PDB ID : 7EBY
Title : Crystal structure of D-Succinylase (DSA) from Cupriavidus sp. P4-10-C
Authors : Yamasaki, M.; Sumida, Y.
Deposited on : 2021-03-11
Resolution : 2.00 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 : 2.25
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) : 2.25

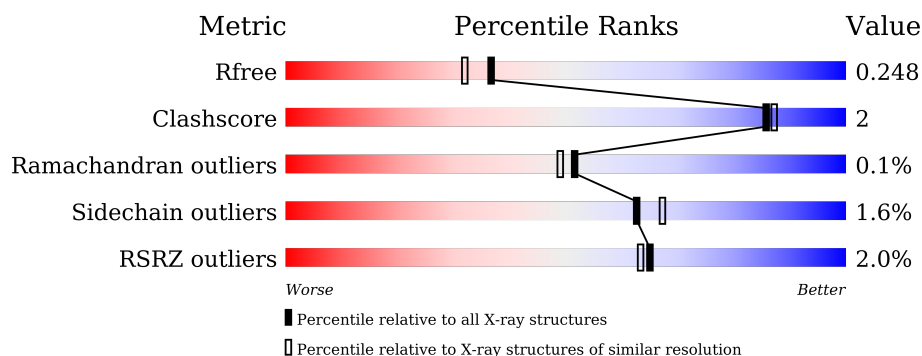
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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	824	<div> <div>2%</div> <div>86%</div> <div>6%</div> <div>8%</div> </div>
1	B	824	<div> <div>%</div> <div>86%</div> <div>6%</div> <div>8%</div> </div>
1	C	824	<div> <div>%</div> <div>86%</div> <div>6%</div> <div>8%</div> </div>
1	D	824	<div> <div>3%</div> <div>87%</div> <div>6%</div> <div>8%</div> </div>
1	E	824	<div> <div>2%</div> <div>84%</div> <div>8%</div> <div>8%</div> </div>
1	F	824	<div> <div>%</div> <div>86%</div> <div>6%</div> <div>8%</div> </div>

2 Entry composition [i](#)

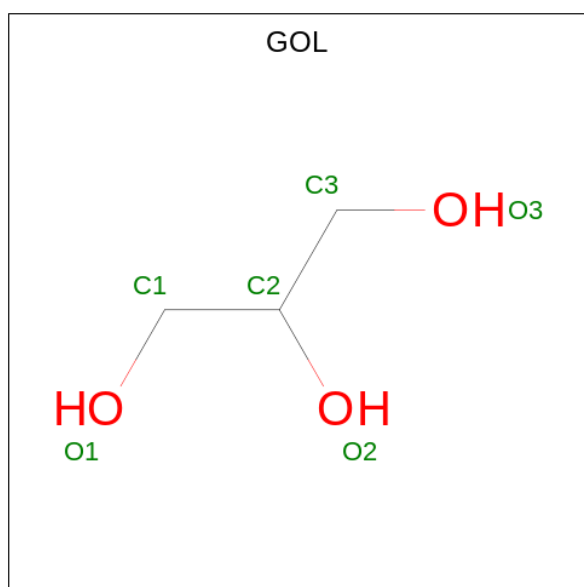
There are 5 unique types of molecules in this entry. The entry contains 38729 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 D-succinylase.

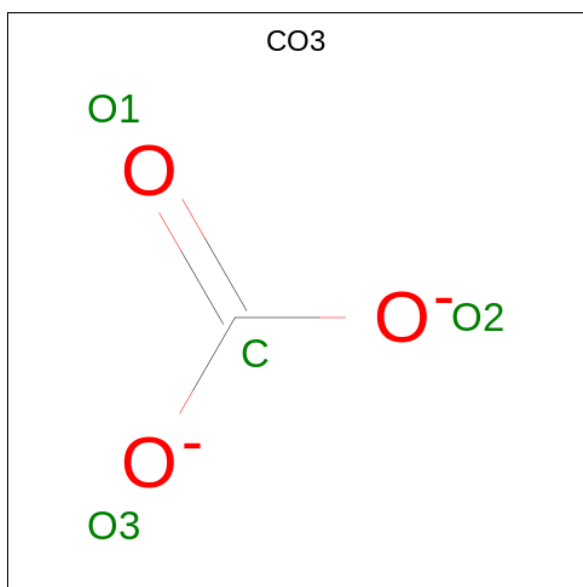
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	761	Total	C	N	O	S	0	4	0
			5970	3769	1101	1082	18			
1	B	761	Total	C	N	O	S	0	2	0
			5973	3770	1097	1088	18			
1	C	762	Total	C	N	O	S	0	5	0
			6003	3787	1103	1095	18			
1	D	762	Total	C	N	O	S	0	1	0
			5960	3765	1092	1085	18			
1	E	762	Total	C	N	O	S	0	4	0
			5997	3784	1102	1093	18			
1	F	761	Total	C	N	O	S	0	3	0
			5971	3770	1098	1085	18			

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

- Molecule 3 is CARBONATE ION (three-letter code: CO3) (formula: CO₃).



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

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

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

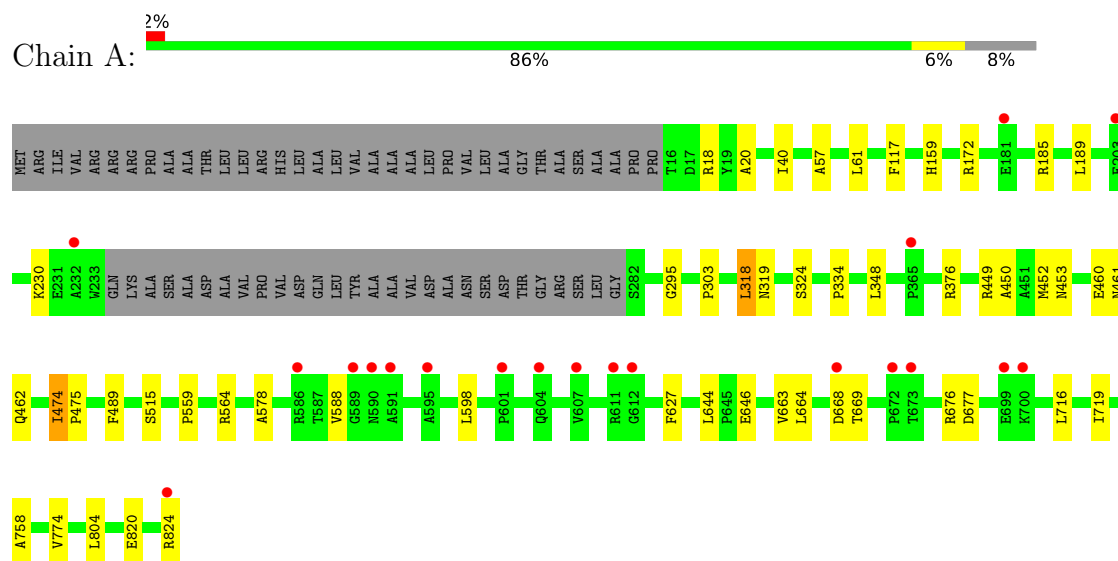
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	397	Total O 397 397	0	0
5	B	475	Total O 475 475	0	0
5	C	461	Total O 461 461	0	0
5	D	449	Total O 449 449	0	0
5	E	414	Total O 414 414	0	0
5	F	455	Total O 455 455	0	2

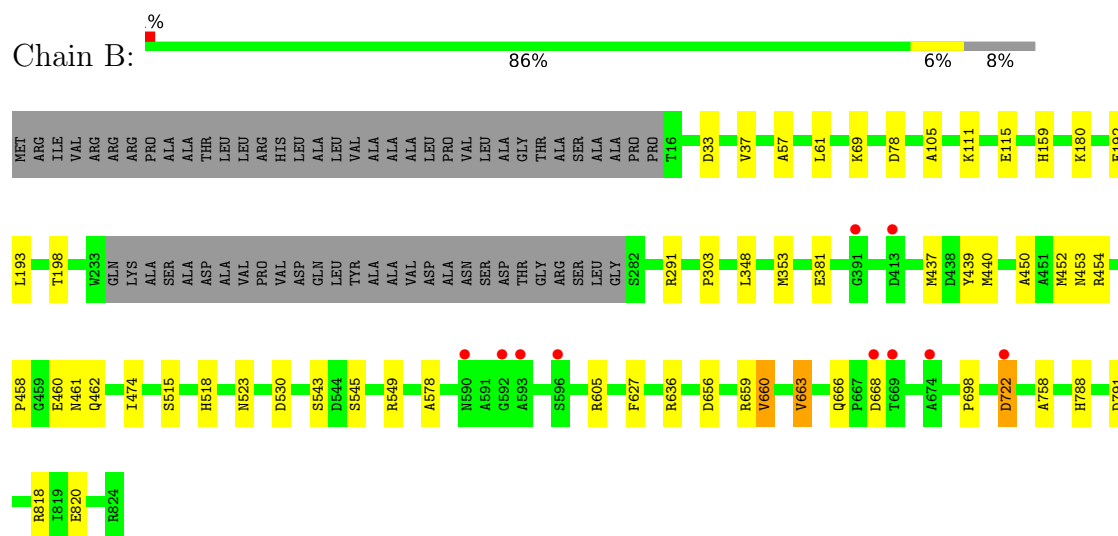
3 Residue-property plots [i](#)

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.

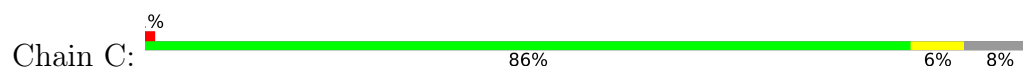
• Molecule 1: D-succinylase

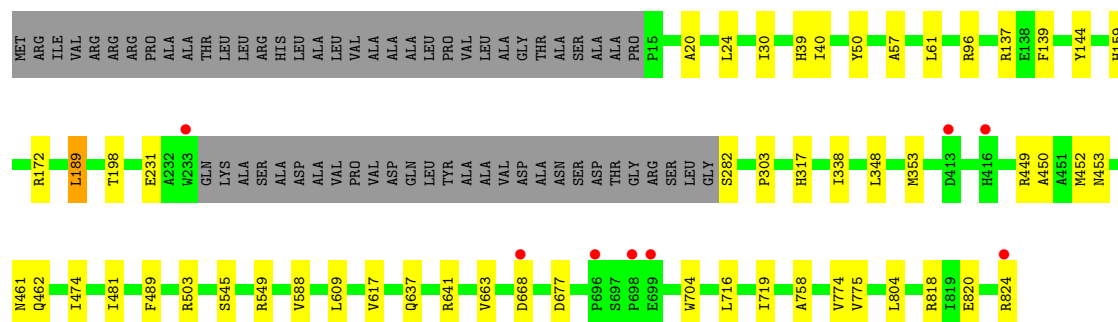


• Molecule 1: D-succinylase

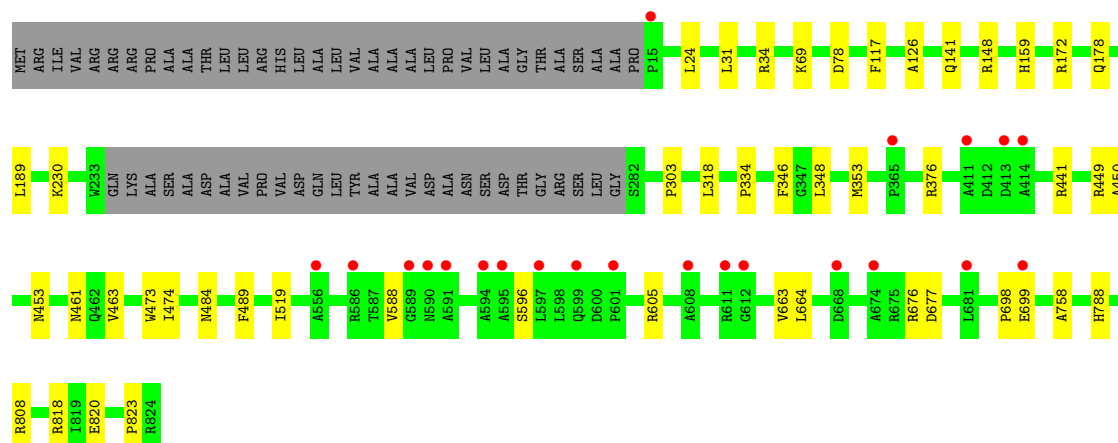
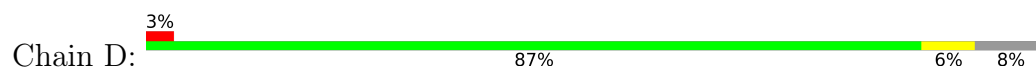


• Molecule 1: D-succinylase

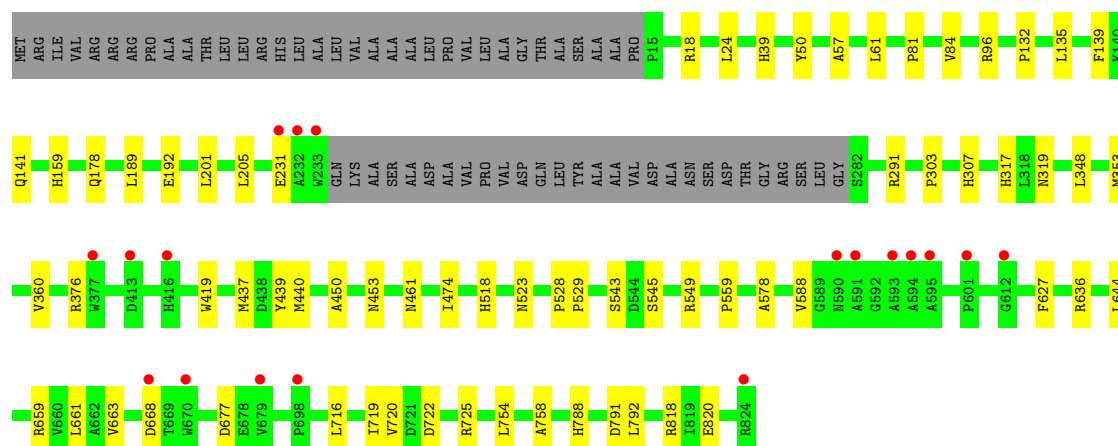
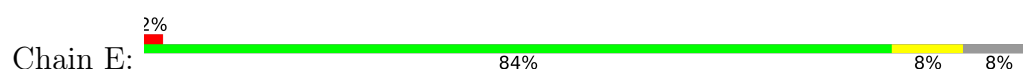




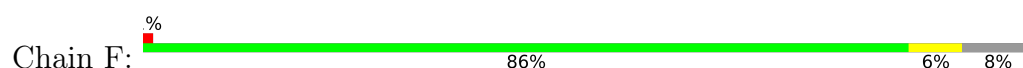
● Molecule 1: D-succinylase



● Molecule 1: D-succinylase



● Molecule 1: D-succinylase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	83.59Å 92.12Å 162.11Å 94.79° 96.31° 104.90°	Depositor
Resolution (Å)	47.63 – 2.00 47.63 – 2.00	Depositor EDS
% Data completeness (in resolution range)	95.8 (47.63-2.00) 95.8 (47.63-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.80 (at 2.00Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.204 , 0.252 0.203 , 0.248	Depositor DCC
R_{free} test set	15045 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	21.8	Xtriage
Anisotropy	0.124	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 44.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	38729	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 45.00 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.4084e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: GOL, CO3, CA

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	0.40	0/6137	0.64	0/8370
1	B	0.39	0/6140	0.65	0/8373
1	C	0.41	0/6171	0.66	0/8415
1	D	0.41	0/6128	0.65	0/8359
1	E	0.39	0/6165	0.65	0/8406
1	F	0.41	0/6138	0.66	0/8371
All	All	0.40	0/36879	0.65	0/50294

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	5970	0	5784	28	0
1	B	5973	0	5790	26	0
1	C	6003	0	5814	25	0
1	D	5960	0	5775	26	0
1	E	5997	0	5816	35	0
1	F	5971	0	5785	23	0
2	A	24	0	31	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	6	0	8	0	0
2	C	24	0	32	0	0
2	D	30	0	39	6	0
2	E	12	0	15	0	0
2	F	30	0	39	0	0
3	A	12	0	0	0	0
3	B	12	0	0	0	0
3	C	12	0	0	1	0
3	D	12	0	0	0	0
3	E	12	0	0	0	0
3	F	12	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
5	A	397	0	0	2	0
5	B	475	0	0	2	0
5	C	461	0	0	1	0
5	D	449	0	0	1	0
5	E	414	0	0	2	0
5	F	455	0	0	3	0
All	All	38729	0	34928	158	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 2.

All (158) 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:C:189:LEU:HD11	1:C:663:VAL:HG21	1.77	0.67
1:D:484:ASN:ND2	2:D:903:GOL:H12	2.12	0.65
1:C:716:LEU:HD22	1:C:719:ILE:HD11	1.78	0.64
1:D:484:ASN:HD22	2:D:903:GOL:H12	1.62	0.63
1:B:636:ARG:HG2	1:B:660:VAL:HG21	1.79	0.62
1:A:185[B]:ARG:NH2	1:A:669:THR:O	2.29	0.60
1:D:473:TRP:CE3	2:D:905:GOL:H12	2.38	0.59
1:E:716:LEU:HD22	1:E:719:ILE:HD11	1.84	0.58
1:E:231:GLU:N	1:E:231:GLU:OE1	2.36	0.57
1:A:376:ARG:CZ	1:E:559:PRO:HG2	2.33	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:588:VAL:HG13	1:E:677:ASP:HB3	1.86	0.57
1:D:818:ARG:NE	1:D:820:GLU:OE2	2.38	0.57
1:E:57:ALA:O	1:E:61:LEU:HB2	2.05	0.56
1:E:722:ASP:OD1	1:E:725:ARG:NH2	2.38	0.56
1:E:348:LEU:HA	1:E:461:ASN:O	2.05	0.56
1:C:774:VAL:HG13	1:C:804:LEU:HB2	1.88	0.56
1:D:450:ALA:O	1:D:453:ASN:HB2	2.06	0.56
1:B:605:ARG:NH2	1:B:698:PRO:O	2.36	0.55
1:E:545:SER:O	1:E:549:ARG:HG3	2.05	0.55
1:D:31:LEU:HD21	1:D:818:ARG:HH11	1.70	0.55
1:F:111:LYS:NZ	1:F:115:GLU:OE2	2.28	0.55
1:B:437:MET:HA	1:B:440:MET:HE2	1.88	0.55
1:F:374:ARG:NH2	1:F:495:GLY:O	2.40	0.55
1:B:69:LYS:NZ	1:B:78:ASP:OD2	2.34	0.54
1:E:18:ARG:HG2	1:E:820[A]:GLU:HB2	1.88	0.54
1:D:348:LEU:HA	1:D:461:ASN:O	2.07	0.54
1:F:348:LEU:HA	1:F:461:ASN:O	2.07	0.54
1:E:376:ARG:NH2	1:F:379:PRO:HG3	2.23	0.54
1:A:564:ARG:HB2	1:A:564:ARG:NH1	2.23	0.53
1:C:637:GLN:HB3	1:C:641:ARG:HH12	1.75	0.52
1:A:40:ILE:HD12	1:A:318:LEU:HD12	1.91	0.52
1:C:637:GLN:HB3	1:C:641:ARG:NH1	2.25	0.52
1:C:57:ALA:O	1:C:61:LEU:HB2	2.10	0.52
1:F:437:MET:HA	1:F:440:MET:HE2	1.92	0.52
1:E:788:HIS:ND1	1:E:791:ASP:OD2	2.43	0.51
1:B:656:ASP:O	1:B:660:VAL:HG13	2.10	0.51
1:A:450:ALA:O	1:A:453:ASN:HB2	2.10	0.51
1:B:450:ALA:O	1:B:453:ASN:HB2	2.12	0.50
1:B:348:LEU:HA	1:B:461:ASN:O	2.11	0.50
1:E:96[B]:ARG:NH1	5:E:1009:HOH:O	2.42	0.50
1:F:473:TRP:HB2	1:F:519:ILE:HG21	1.92	0.50
1:A:57:ALA:O	1:A:61:LEU:HB2	2.12	0.50
1:F:545:SER:O	1:F:549:ARG:HG3	2.11	0.49
1:F:588:VAL:HG13	1:F:677:ASP:HB3	1.94	0.49
1:E:437:MET:HA	1:E:440:MET:HE2	1.94	0.49
1:C:588:VAL:HG13	1:C:677:ASP:HB3	1.95	0.49
1:A:774:VAL:HG13	1:A:804:LEU:HB2	1.94	0.49
1:C:303:PRO:O	1:C:758:ALA:HA	2.12	0.49
1:F:33:ASP:OD2	1:F:37:VAL:HB	2.11	0.49
1:B:303:PRO:O	1:B:758:ALA:HA	2.13	0.49
1:D:588:VAL:HG13	1:D:677:ASP:HB3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:189:LEU:HD21	1:A:663:VAL:HG21	1.95	0.48
1:B:660:VAL:HA	1:B:663:VAL:HG13	1.94	0.48
1:B:545:SER:O	1:B:549[A]:ARG:HG3	2.14	0.48
1:E:141:GLN:OE1	1:E:720:VAL:HG12	2.13	0.48
1:E:818:ARG:NE	1:E:820[A]:GLU:OE2	2.43	0.48
1:B:722:ASP:OD1	1:B:722:ASP:N	2.40	0.48
1:F:636:ARG:HG2	1:F:660:VAL:HG11	1.96	0.47
1:D:605:ARG:NH2	1:D:698:PRO:O	2.43	0.47
1:E:450:ALA:O	1:E:453:ASN:HB2	2.14	0.47
1:A:449:ARG:HH11	1:A:474:ILE:HD12	1.79	0.47
1:C:348:LEU:HA	1:C:461:ASN:O	2.13	0.47
1:A:319:ASN:ND2	5:A:1017:HOH:O	2.47	0.47
1:D:24:LEU:O	1:D:823:PRO:HB3	2.15	0.47
1:D:441:ARG:NH2	2:D:902:GOL:H32	2.28	0.47
1:F:88:ARG:NH2	5:F:1016:HOH:O	2.47	0.47
1:F:34:ARG:NH2	5:F:1018:HOH:O	2.48	0.47
1:E:189:LEU:HD21	1:E:663:VAL:HG21	1.97	0.47
1:A:324:SER:HB2	5:A:1017:HOH:O	2.15	0.47
1:C:24:LEU:HD13	1:C:50:TYR:CD1	2.50	0.46
1:C:30:ILE:HG12	1:C:40:ILE:HG12	1.97	0.46
1:F:30:ILE:HG12	1:F:40:ILE:HG12	1.97	0.46
1:D:230:LYS:HE3	1:D:230:LYS:HB2	1.70	0.46
1:A:376:ARG:NH2	1:E:559:PRO:HG2	2.31	0.46
1:B:192:GLU:HA	1:B:659:ARG:CZ	2.46	0.46
1:F:450:ALA:O	1:F:453:ASN:HB2	2.16	0.46
1:F:29:SER:OG	1:F:820:GLU:OE2	2.34	0.46
1:D:189:LEU:HA	1:D:189:LEU:HD23	1.79	0.45
1:A:460:GLU:O	1:A:475:PRO:HA	2.17	0.45
1:D:303:PRO:O	1:D:758:ALA:HA	2.17	0.45
1:B:818:ARG:NE	1:B:820:GLU:OE2	2.32	0.45
1:C:617:VAL:HG12	1:C:704:TRP:CD1	2.51	0.45
1:B:57:ALA:O	1:B:61:LEU:HB2	2.17	0.45
1:C:452:MET:SD	1:C:462:GLN:HG3	2.57	0.45
1:E:201:LEU:HD11	1:E:205:LEU:HD12	1.99	0.45
1:E:291:ARG:NH1	1:E:518:HIS:ND1	2.64	0.45
1:A:559:PRO:HG3	1:D:376:ARG:HH21	1.82	0.45
1:D:189:LEU:HD21	1:D:663:VAL:HG21	1.99	0.45
1:D:473:TRP:HB2	1:D:519:ILE:HG21	1.98	0.45
1:C:39:HIS:HA	1:C:317:HIS:HB3	1.99	0.44
1:A:716:LEU:HD22	1:A:719:ILE:HD11	1.98	0.44
1:C:20:ALA:HB2	1:C:824:ARG:CZ	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:450:ALA:O	1:C:453:ASN:HB2	2.17	0.44
1:C:545:SER:O	1:C:549:ARG:HG3	2.17	0.44
1:A:646:GLU:OE2	1:F:818:ARG:NH1	2.50	0.44
1:B:193:LEU:H	1:B:659:ARG:NH2	2.16	0.44
1:F:361:TYR:OH	1:F:405:HIS:ND1	2.34	0.44
1:A:18:ARG:HG2	1:A:820:GLU:HB3	1.98	0.44
1:A:189:LEU:HA	1:A:189:LEU:HD23	1.79	0.44
1:A:303:PRO:O	1:A:758:ALA:HA	2.18	0.44
1:F:809:LYS:NZ	1:F:813:ARG:HH22	2.15	0.44
1:C:818:ARG:HD3	1:C:820:GLU:OE2	2.17	0.44
1:E:636:ARG:HH11	1:E:636:ARG:HG3	1.83	0.44
1:B:291:ARG:NH1	1:B:518:HIS:ND1	2.67	0.43
1:E:39:HIS:HA	1:E:317:HIS:HB3	1.99	0.43
1:D:126:ALA:HB2	1:D:148:ARG:HH22	1.82	0.43
1:B:788:HIS:ND1	1:B:791:ASP:OD2	2.45	0.43
1:C:172:ARG:HG2	1:C:489:PHE:CE1	2.54	0.43
1:D:69:LYS:NZ	1:D:78:ASP:OD2	2.35	0.43
1:F:285:TRP:HB3	1:F:520:VAL:HG22	2.01	0.43
1:E:528:PRO:HA	1:E:529:PRO:HD3	1.93	0.43
1:E:192:GLU:HA	1:E:659:ARG:CZ	2.49	0.43
1:E:360:VAL:HG22	1:E:419:TRP:CD1	2.54	0.43
1:F:57:ALA:O	1:F:61:LEU:HB2	2.19	0.43
1:E:307:HIS:CD2	1:E:754:LEU:HD21	2.54	0.42
1:B:111:LYS:NZ	1:B:115[A]:GLU:OE2	2.50	0.42
1:B:458:PRO:O	1:B:460:GLU:HG2	2.18	0.42
1:C:481:ILE:HG12	1:C:503:ARG:CZ	2.49	0.42
1:E:81:PRO:HA	1:E:84:VAL:HG23	2.01	0.42
1:B:33:ASP:OD2	1:B:37:VAL:HB	2.19	0.42
1:B:105:ALA:O	1:B:454:ARG:HD3	2.20	0.42
1:E:24:LEU:HD13	1:E:50:TYR:CD1	2.53	0.42
1:F:809:LYS:HB3	1:F:809:LYS:HE3	1.39	0.42
1:E:303:PRO:O	1:E:758:ALA:HA	2.19	0.42
1:A:452:MET:SD	1:A:462:GLN:HG3	2.59	0.42
1:C:139:PHE:HB3	1:C:144:TYR:O	2.20	0.42
1:F:759:SER:HA	1:F:777:THR:HG22	2.02	0.42
1:E:523:ASN:HB2	1:E:543:SER:OG	2.20	0.42
1:D:172:ARG:HG2	1:D:489:PHE:CE1	2.55	0.42
1:A:172:ARG:HG2	1:A:489:PHE:CE1	2.55	0.42
1:A:578:ALA:HA	1:A:627:PHE:CZ	2.54	0.42
1:A:348:LEU:HA	1:A:461:ASN:O	2.19	0.41
1:D:808:ARG:NH1	2:D:904:GOL:H32	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:666:GLN:HB3	5:B:1154:HOH:O	2.18	0.41
1:D:117:PHE:CG	1:D:334:PRO:HG3	2.55	0.41
1:E:132:PRO:HD2	5:E:1052:HOH:O	2.20	0.41
1:F:112:ARG:NH2	5:F:1033:HOH:O	2.53	0.41
1:B:523:ASN:HB2	1:B:543:SER:HB3	2.01	0.41
1:E:189:LEU:HD23	1:E:189:LEU:HA	1.90	0.41
1:C:137[B]:ARG:HG2	5:C:1261:HOH:O	2.21	0.41
1:E:135:LEU:HG	1:E:139:PHE:HB2	2.03	0.41
1:A:664:LEU:O	1:A:676:ARG:NH1	2.52	0.41
1:B:180:LYS:HD2	5:B:1354:HOH:O	2.20	0.41
1:E:317:HIS:NE2	1:E:319:ASN:OD1	2.54	0.41
1:B:452:MET:SD	1:B:462:GLN:HG3	2.61	0.41
1:D:34[B]:ARG:O	1:D:788:HIS:HE1	2.04	0.41
1:E:578:ALA:HA	1:E:627:PHE:CZ	2.56	0.41
1:A:588:VAL:HG13	1:A:677:ASP:HB3	2.02	0.41
1:C:282:SER:N	3:C:905:CO3:O2	2.54	0.41
1:A:20:ALA:HB2	1:A:824:ARG:CZ	2.51	0.40
1:A:117:PHE:CG	1:A:334:PRO:HG3	2.56	0.40
1:C:481:ILE:HG12	1:C:503:ARG:NE	2.35	0.40
1:A:295:GLY:O	2:D:903:GOL:H2	2.21	0.40
1:D:34[A]:ARG:NH2	5:D:1045:HOH:O	2.54	0.40
1:D:346:PHE:HA	1:D:463:VAL:O	2.21	0.40
1:B:578:ALA:HA	1:B:627:PHE:CZ	2.56	0.40
1:C:338:ILE:HD11	1:C:348:LEU:HD11	2.04	0.40
1:D:664:LEU:O	1:D:676:ARG:NH1	2.54	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	761/824 (92%)	741 (97%)	19 (2%)	1 (0%)	51 49

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	759/824 (92%)	741 (98%)	17 (2%)	1 (0%)	51	49
1	C	763/824 (93%)	744 (98%)	18 (2%)	1 (0%)	51	49
1	D	759/824 (92%)	739 (97%)	20 (3%)	0	100	100
1	E	762/824 (92%)	740 (97%)	21 (3%)	1 (0%)	51	49
1	F	760/824 (92%)	740 (97%)	20 (3%)	0	100	100
All	All	4564/4944 (92%)	4445 (97%)	115 (2%)	4 (0%)	51	49

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	668	ASP
1	E	668	ASP
1	B	668	ASP
1	C	668	ASP

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	592/639 (93%)	584 (99%)	8 (1%)	67	72
1	B	595/639 (93%)	584 (98%)	11 (2%)	59	63
1	C	599/639 (94%)	589 (98%)	10 (2%)	60	65
1	D	593/639 (93%)	584 (98%)	9 (2%)	65	69
1	E	599/639 (94%)	591 (99%)	8 (1%)	69	74
1	F	593/639 (93%)	581 (98%)	12 (2%)	55	58
All	All	3571/3834 (93%)	3513 (98%)	58 (2%)	62	67

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	159	HIS
1	A	230	LYS

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Mol	Chain	Res	Type
1	A	318	LEU
1	A	474	ILE
1	A	515[A]	SER
1	A	515[B]	SER
1	A	598	LEU
1	A	644	LEU
1	B	159	HIS
1	B	198	THR
1	B	353	MET
1	B	381	GLU
1	B	439	TYR
1	B	474	ILE
1	B	515	SER
1	B	530	ASP
1	B	660	VAL
1	B	663	VAL
1	B	722	ASP
1	C	96	ARG
1	C	159	HIS
1	C	189	LEU
1	C	198	THR
1	C	231	GLU
1	C	353	MET
1	C	449	ARG
1	C	474	ILE
1	C	609	LEU
1	C	775	VAL
1	D	141	GLN
1	D	159	HIS
1	D	178	GLN
1	D	318	LEU
1	D	353	MET
1	D	449	ARG
1	D	474	ILE
1	D	596	SER
1	D	699	GLU
1	E	159	HIS
1	E	178	GLN
1	E	353	MET
1	E	439	TYR
1	E	474	ILE
1	E	644	LEU

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Mol	Chain	Res	Type
1	E	661	LEU
1	E	792	LEU
1	F	159	HIS
1	F	189	LEU
1	F	353	MET
1	F	449	ARG
1	F	474	ILE
1	F	582	LEU
1	F	635	LEU
1	F	700	LYS
1	F	808[A]	ARG
1	F	808[B]	ARG
1	F	809	LYS
1	F	821	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 45 ligands modelled in this entry, 6 are monoatomic - leaving 39 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
3	CO3	A	906	-	0,3,3	-	-	0,3,3	-	-
3	CO3	F	908	-	0,3,3	-	-	0,3,3	-	-
3	CO3	E	904	-	0,3,3	-	-	0,3,3	-	-
3	CO3	C	905	-	0,3,3	-	-	0,3,3	-	-
3	CO3	F	907	-	0,3,3	-	-	0,3,3	-	-
2	GOL	F	902	-	5,5,5	1.23	0	5,5,5	1.12	1 (20%)
2	GOL	D	902	-	5,5,5	1.21	1 (20%)	5,5,5	0.82	0
3	CO3	B	904	-	0,3,3	-	-	0,3,3	-	-
2	GOL	C	902	-	5,5,5	1.03	0	5,5,5	0.97	0
2	GOL	D	903	-	5,5,5	1.17	1 (20%)	5,5,5	0.90	0
2	GOL	A	903	-	5,5,5	0.93	0	5,5,5	1.00	0
3	CO3	A	905	-	0,3,3	-	-	0,3,3	-	-
2	GOL	F	905	-	5,5,5	0.85	0	5,5,5	0.94	0
2	GOL	F	903	-	5,5,5	1.28	1 (20%)	5,5,5	0.90	0
2	GOL	D	905	-	5,5,5	1.07	0	5,5,5	1.12	0
2	GOL	C	901	-	5,5,5	0.88	0	5,5,5	1.00	0
3	CO3	E	905	-	0,3,3	-	-	0,3,3	-	-
2	GOL	E	901	-	5,5,5	1.40	1 (20%)	5,5,5	0.94	0
2	GOL	F	904	-	5,5,5	1.15	0	5,5,5	0.91	0
2	GOL	D	904	-	5,5,5	1.02	0	5,5,5	0.90	0
2	GOL	F	901	-	5,5,5	0.92	0	5,5,5	0.77	0
2	GOL	A	902	-	5,5,5	0.78	0	5,5,5	1.08	0
2	GOL	D	901	-	5,5,5	0.81	0	5,5,5	1.24	0
3	CO3	D	908	-	0,3,3	-	-	0,3,3	-	-
3	CO3	D	907	-	0,3,3	-	-	0,3,3	-	-
3	CO3	E	903	-	0,3,3	-	-	0,3,3	-	-
3	CO3	B	902	-	0,3,3	-	-	0,3,3	-	-
3	CO3	C	907	-	0,3,3	-	-	0,3,3	-	-
2	GOL	C	904	-	5,5,5	1.54	1 (20%)	5,5,5	0.56	0
2	GOL	A	901	-	5,5,5	1.33	1 (20%)	5,5,5	0.72	0
3	CO3	C	906	-	0,3,3	-	-	0,3,3	-	-
2	GOL	E	902	-	5,5,5	1.07	0	5,5,5	0.85	0
3	CO3	D	906	-	0,3,3	-	-	0,3,3	-	-
2	GOL	A	904	-	5,5,5	1.00	0	5,5,5	1.01	0
3	CO3	B	903	-	0,3,3	-	-	0,3,3	-	-
2	GOL	B	901	-	5,5,5	0.99	0	5,5,5	1.02	0
3	CO3	F	906	-	0,3,3	-	-	0,3,3	-	-
3	CO3	A	907	-	0,3,3	-	-	0,3,3	-	-
2	GOL	C	903	-	5,5,5	1.08	1 (20%)	5,5,5	1.22	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	F	902	-	-	0/4/4/4	-
2	GOL	D	902	-	-	2/4/4/4	-
2	GOL	C	902	-	-	2/4/4/4	-
2	GOL	D	903	-	-	3/4/4/4	-
2	GOL	A	903	-	-	0/4/4/4	-
2	GOL	F	905	-	-	0/4/4/4	-
2	GOL	F	903	-	-	2/4/4/4	-
2	GOL	D	905	-	-	0/4/4/4	-
2	GOL	C	901	-	-	3/4/4/4	-
2	GOL	E	901	-	-	2/4/4/4	-
2	GOL	F	904	-	-	2/4/4/4	-
2	GOL	D	904	-	-	3/4/4/4	-
2	GOL	F	901	-	-	2/4/4/4	-
2	GOL	A	902	-	-	2/4/4/4	-
2	GOL	D	901	-	-	4/4/4/4	-
2	GOL	C	904	-	-	4/4/4/4	-
2	GOL	A	901	-	-	2/4/4/4	-
2	GOL	E	902	-	-	4/4/4/4	-
2	GOL	A	904	-	-	0/4/4/4	-
2	GOL	B	901	-	-	0/4/4/4	-
2	GOL	C	903	-	-	0/4/4/4	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	901	GOL	O2-C2	-2.79	1.35	1.43
2	F	903	GOL	O2-C2	-2.55	1.35	1.43
2	A	901	GOL	O2-C2	-2.22	1.36	1.43
2	D	902	GOL	O2-C2	-2.20	1.36	1.43
2	D	903	GOL	O2-C2	-2.08	1.37	1.43
2	C	904	GOL	O2-C2	-2.07	1.37	1.43
2	C	903	GOL	C3-C2	2.00	1.60	1.51

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	902	GOL	C3-C2-C1	-2.16	103.32	111.70

There are no chirality outliers.

All (37) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	901	GOL	O1-C1-C2-O2
2	A	901	GOL	O1-C1-C2-C3
2	C	901	GOL	C1-C2-C3-O3
2	C	901	GOL	O2-C2-C3-O3
2	C	902	GOL	O1-C1-C2-C3
2	C	904	GOL	C1-C2-C3-O3
2	D	901	GOL	O1-C1-C2-C3
2	D	901	GOL	C1-C2-C3-O3
2	D	901	GOL	O2-C2-C3-O3
2	D	903	GOL	C1-C2-C3-O3
2	D	904	GOL	C1-C2-C3-O3
2	E	901	GOL	C1-C2-C3-O3
2	F	903	GOL	C1-C2-C3-O3
2	F	904	GOL	C1-C2-C3-O3
2	D	901	GOL	O1-C1-C2-O2
2	F	903	GOL	O2-C2-C3-O3
2	A	902	GOL	C1-C2-C3-O3
2	E	902	GOL	O1-C1-C2-C3
2	E	902	GOL	C1-C2-C3-O3
2	F	901	GOL	C1-C2-C3-O3
2	A	902	GOL	O2-C2-C3-O3
2	E	901	GOL	O2-C2-C3-O3
2	E	902	GOL	O2-C2-C3-O3
2	F	904	GOL	O2-C2-C3-O3
2	C	902	GOL	O1-C1-C2-O2
2	C	904	GOL	O2-C2-C3-O3
2	D	904	GOL	O2-C2-C3-O3
2	F	901	GOL	O2-C2-C3-O3
2	D	902	GOL	O2-C2-C3-O3
2	D	903	GOL	O2-C2-C3-O3
2	E	902	GOL	O1-C1-C2-O2
2	C	904	GOL	O1-C1-C2-C3
2	D	904	GOL	O1-C1-C2-C3
2	C	901	GOL	O1-C1-C2-O2
2	D	903	GOL	O1-C1-C2-O2
2	D	902	GOL	C1-C2-C3-O3
2	C	904	GOL	O1-C1-C2-O2

There are no ring outliers.

5 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	905	CO3	1	0
2	D	902	GOL	1	0
2	D	903	GOL	3	0
2	D	905	GOL	1	0
2	D	904	GOL	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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	761/824 (92%)	0.04	20 (2%) 56 54	12, 23, 45, 72	0
1	B	761/824 (92%)	-0.06	10 (1%) 77 76	13, 21, 37, 55	0
1	C	762/824 (92%)	-0.14	8 (1%) 82 81	11, 20, 36, 62	0
1	D	762/824 (92%)	0.04	22 (2%) 51 50	11, 21, 42, 62	0
1	E	762/824 (92%)	0.04	18 (2%) 59 57	12, 23, 41, 60	0
1	F	761/824 (92%)	-0.06	12 (1%) 72 70	12, 20, 39, 58	0
All	All	4569/4944 (92%)	-0.02	90 (1%) 65 63	11, 21, 40, 72	0

All (90) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	593	ALA	4.7
1	E	668	ASP	4.4
1	D	414	ALA	4.4
1	A	824	ARG	4.3
1	F	414	ALA	4.2
1	A	591	ALA	4.2
1	F	233	TRP	4.2
1	C	668	ASP	4.0
1	D	556	ALA	3.9
1	D	611	ARG	3.8
1	E	698	PRO	3.8
1	A	699	GLU	3.7
1	A	590	ASN	3.6
1	F	413	ASP	3.5
1	E	824	ARG	3.5
1	B	391	GLY	3.5
1	A	611	ARG	3.5
1	D	674	ALA	3.5
1	D	601	PRO	3.3

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Mol	Chain	Res	Type	RSRZ
1	C	696	PRO	3.2
1	F	668	ASP	3.2
1	E	233	TRP	3.2
1	B	668	ASP	3.2
1	D	594	ALA	3.1
1	D	586	ARG	3.1
1	A	673	THR	3.1
1	E	231	GLU	3.1
1	B	722	ASP	3.0
1	B	596	SER	3.0
1	A	607	VAL	3.0
1	D	365	PRO	3.0
1	D	681	LEU	3.0
1	D	590	ASN	3.0
1	A	601	PRO	2.9
1	A	595	ALA	2.9
1	F	612	GLY	2.9
1	E	590	ASN	2.9
1	E	594	ALA	2.8
1	D	612	GLY	2.8
1	D	413	ASP	2.8
1	C	698	PRO	2.8
1	A	589	GLY	2.8
1	B	590	ASN	2.8
1	A	700	LYS	2.8
1	A	612	GLY	2.8
1	B	413	ASP	2.7
1	D	15	PRO	2.7
1	A	604	GLN	2.6
1	D	599	GLN	2.6
1	D	591	ALA	2.6
1	B	674	ALA	2.6
1	F	231	GLU	2.6
1	E	591	ALA	2.5
1	D	699	GLU	2.5
1	F	599	GLN	2.5
1	A	586	ARG	2.5
1	F	611	ARG	2.5
1	A	232	ALA	2.5
1	D	608	ALA	2.5
1	D	668	ASP	2.5
1	E	679	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	699	GLU	2.5
1	A	203	GLU	2.5
1	F	366	ALA	2.4
1	A	365	PRO	2.4
1	E	595	ALA	2.4
1	E	413	ASP	2.4
1	D	595	ALA	2.4
1	E	593	ALA	2.4
1	F	593	ALA	2.4
1	B	592	GLY	2.4
1	C	413	ASP	2.4
1	E	601	PRO	2.3
1	D	589	GLY	2.3
1	E	232	ALA	2.3
1	C	233	TRP	2.2
1	E	377	TRP	2.2
1	F	592	GLY	2.2
1	C	824	ARG	2.2
1	E	416	HIS	2.2
1	A	181	GLU	2.2
1	A	668	ASP	2.2
1	C	416	HIS	2.2
1	E	670	TRP	2.2
1	F	698	PRO	2.2
1	B	669	THR	2.1
1	E	612	GLY	2.1
1	A	672	PRO	2.1
1	D	411	ALA	2.0
1	D	597	LEU	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 monosaccharides 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
3	CO3	B	904	4/4	0.68	0.16	28,30,31,43	0
2	GOL	D	905	6/6	0.75	0.18	26,27,33,37	0
2	GOL	E	902	6/6	0.77	0.16	33,35,39,41	0
3	CO3	F	907	4/4	0.77	0.15	27,32,34,35	0
3	CO3	C	907	4/4	0.80	0.18	30,36,36,37	0
3	CO3	A	906	4/4	0.80	0.17	29,29,32,38	0
3	CO3	E	903	4/4	0.82	0.14	29,29,31,36	0
2	GOL	D	903	6/6	0.82	0.21	25,31,36,39	0
2	GOL	F	904	6/6	0.84	0.15	29,33,38,40	0
2	GOL	A	901	6/6	0.85	0.20	22,30,35,44	0
2	GOL	E	901	6/6	0.86	0.20	19,25,28,36	0
3	CO3	D	907	4/4	0.87	0.15	30,34,36,36	0
2	GOL	F	905	6/6	0.87	0.25	27,30,31,35	0
2	GOL	C	904	6/6	0.87	0.18	19,24,35,39	0
2	GOL	A	903	6/6	0.88	0.14	22,23,27,32	0
2	GOL	C	903	6/6	0.89	0.14	20,24,28,29	0
2	GOL	C	901	6/6	0.89	0.10	26,29,34,36	0
2	GOL	D	901	6/6	0.90	0.11	25,29,33,36	0
2	GOL	A	902	6/6	0.91	0.09	23,27,32,39	0
2	GOL	F	901	6/6	0.92	0.16	21,29,33,41	0
2	GOL	B	901	6/6	0.93	0.12	20,25,25,28	0
2	GOL	D	904	6/6	0.93	0.19	29,34,39,39	0
2	GOL	F	903	6/6	0.94	0.10	17,19,26,28	0
3	CO3	D	906	4/4	0.94	0.11	20,22,26,35	0
3	CO3	B	903	4/4	0.94	0.11	18,26,29,34	0
3	CO3	A	905	4/4	0.94	0.14	14,16,25,26	0
3	CO3	C	905	4/4	0.94	0.10	20,24,26,33	0
2	GOL	D	902	6/6	0.95	0.13	20,23,27,27	0
2	GOL	C	902	6/6	0.95	0.13	16,22,23,32	0
2	GOL	A	904	6/6	0.95	0.12	26,27,31,31	0
3	CO3	F	906	4/4	0.95	0.10	22,25,25,35	0
3	CO3	A	907	4/4	0.95	0.11	24,26,28,39	0
3	CO3	E	904	4/4	0.96	0.10	17,23,29,37	0
3	CO3	E	905	4/4	0.96	0.20	12,16,18,21	0
3	CO3	B	902	4/4	0.96	0.14	13,14,19,23	0
3	CO3	C	906	4/4	0.96	0.19	13,14,17,21	0
3	CO3	F	908	4/4	0.96	0.14	10,14,16,21	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	GOL	F	902	6/6	0.97	0.09	20,21,22,23	0
3	CO3	D	908	4/4	0.97	0.17	11,11,14,22	0
4	CA	A	908	1/1	0.99	0.10	18,18,18,18	0
4	CA	D	909	1/1	0.99	0.06	18,18,18,18	0
4	CA	F	909	1/1	0.99	0.05	13,13,13,13	0
4	CA	B	905	1/1	1.00	0.10	15,15,15,15	0
4	CA	E	906	1/1	1.00	0.07	18,18,18,18	0
4	CA	C	908	1/1	1.00	0.08	14,14,14,14	0

6.5 Other polymers [i](#)

There are no such residues in this entry.