



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:01 PM UTC

PDB ID : 7EBY / pdb_00007eby
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 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:

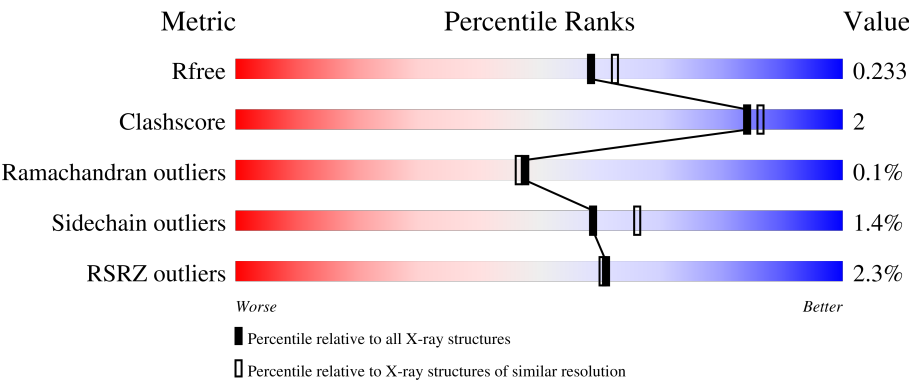
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance i

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}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (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	3% 86% 6% 8%
1	B	824	% 86% 6% 8%
1	C	824	2% 86% 6% 8%
1	D	824	3% 87% 6% 8%
1	E	824	2% 85% 8% 8%

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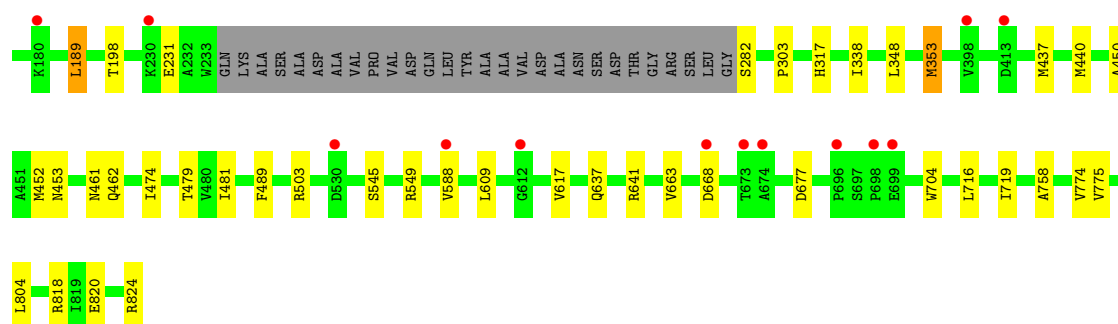
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Mol	Chain	Length	Quality of chain
1	F	824	 2% 86% 6% 8%

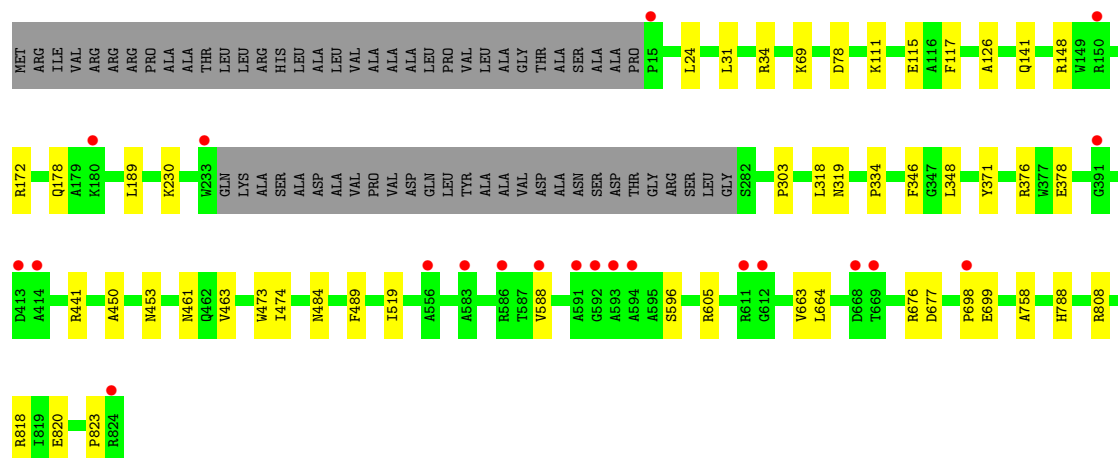
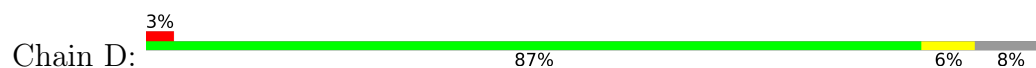
The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	GOL	C	904	-	X	-	-

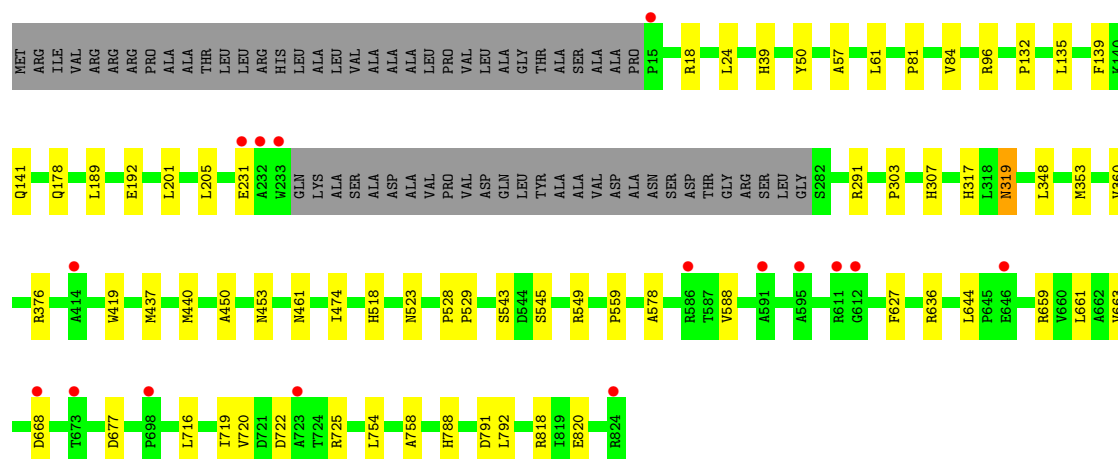
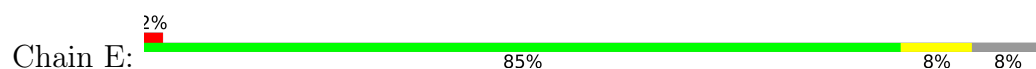
ENTRY-COMPOSITION INFOmissingINFO



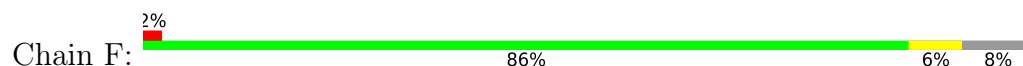
• Molecule 1: D-succinylase

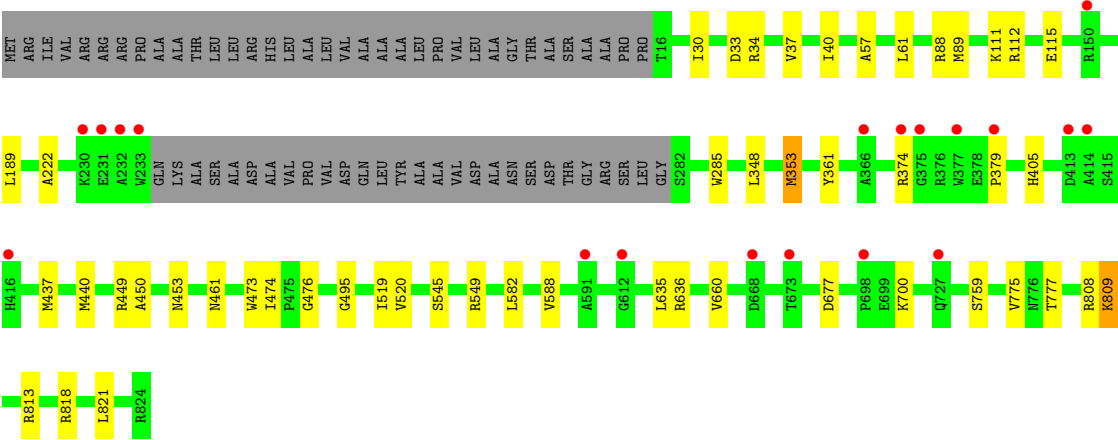


• Molecule 1: D-succinylase



• Molecule 1: D-succinylase





3 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) 96.0 (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 (Not available) , 0.233	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 , 39.3	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	0.93	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.

4 Model quality [i](#)

4.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CA, GOL, CO3

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	0.33	0/6137	0.52	0/8370
1	B	0.33	0/6140	0.53	0/8373
1	C	0.34	0/6171	0.54	0/8415
1	D	0.35	0/6128	0.55	0/8359
1	E	0.32	0/6165	0.54	0/8406
1	F	0.34	0/6138	0.54	0/8371
All	All	0.33	0/36879	0.54	0/50294

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

4.2 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	30	0
1	B	5973	0	5790	26	0
1	C	6003	0	5814	27	0
1	D	5960	0	5775	28	0
1	E	5997	0	5816	36	0
1	F	5971	0	5785	24	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	166	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 (166) 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:A:353:MET:HE1	1:A:476:GLY:C	2.24	0.63
1:B:636:ARG:HG2	1:B:660:VAL:HG21	1.79	0.62
1:B:69:LYS:NZ	1:B:78:ASP:OD2	2.34	0.60
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:E:588:VAL:HG13	1:E:677:ASP:HB3	1.86	0.57
1:F:437:MET:HA	1:F:440:MET:HE2	1.87	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:F:374:ARG:NH2	1:F:495:GLY:O	2.40	0.55
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:B:437:MET:HA	1:B:440:MET:HE2	1.90	0.52
1:D:111:LYS:NZ	1:D:115:GLU:OE2	2.43	0.52
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:E:437:MET:HA	1:E:440:MET:HE2	1.92	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:D:371:TYR:OH	1:D:378:GLU:OE2	2.32	0.46
1:C:24:LEU:HD13	1:C:50:TYR:CD1	2.50	0.46
1:C:353:MET:HE2	1:C:479:THR:OG1	2.15	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:F:361:TYR:OH	1:F:405:HIS:ND1	2.34	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:D:189:LEU:HA	1:D:189:LEU:HD23	1.79	0.45
1:F:353:MET:HE1	1:F:476:GLY:C	2.41	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:89:MET:HE3	1:F:222:ALA:HB2	1.99	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:A:353:MET:HE1	1:A:476:GLY:O	2.17	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:C:437:MET:HA	1:C:440:MET:HE2	1.99	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
1:E:440:MET:HE3	1:E:440:MET:HB2	1.99	0.40

There are no symmetry-related clashes.

4.3 Torsion angles

4.3.1 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%)	48	46
1	B	759/824 (92%)	741 (98%)	17 (2%)	1 (0%)	48	46
1	C	763/824 (93%)	744 (98%)	18 (2%)	1 (0%)	48	46
1	D	759/824 (92%)	739 (97%)	20 (3%)	0	100	100
1	E	762/824 (92%)	740 (97%)	21 (3%)	1 (0%)	48	46
1	F	760/824 (92%)	740 (97%)	20 (3%)	0	100	100
All	All	4564/4944 (92%)	4445 (97%)	115 (2%)	4 (0%)	48	46

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

4.3.2 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%)	59	66
1	B	595/639 (93%)	586 (98%)	9 (2%)	57	64
1	C	599/639 (94%)	591 (99%)	8 (1%)	61	68

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	593/639 (93%)	586 (99%)	7 (1%)	63	70
1	E	599/639 (94%)	592 (99%)	7 (1%)	63	70
1	F	593/639 (93%)	581 (98%)	12 (2%)	48	54
All	All	3571/3834 (93%)	3520 (99%)	51 (1%)	59	66

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	230	LYS
1	A	318	LEU
1	A	353	MET
1	A	474	ILE
1	A	515[A]	SER
1	A	515[B]	SER
1	A	598	LEU
1	A	644	LEU
1	B	198	THR
1	B	353	MET
1	B	381	GLU
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	189	LEU
1	C	198	THR
1	C	231	GLU
1	C	353	MET
1	C	474	ILE
1	C	609	LEU
1	C	775	VAL
1	D	141	GLN
1	D	178	GLN
1	D	318	LEU
1	D	319	ASN
1	D	474	ILE
1	D	596	SER
1	D	699	GLU
1	E	178	GLN

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Mol	Chain	Res	Type
1	E	319	ASN
1	E	353	MET
1	E	474	ILE
1	E	644	LEU
1	E	661	LEU
1	E	792	LEU
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	775	VAL
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. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	416	HIS
1	A	504	ASN
1	B	227	ASN
1	B	504	ASN
1	B	727	GLN
1	C	131	GLN
1	C	301	ASN
1	D	504	ASN
1	E	178	GLN
1	E	727	GLN
1	F	131	GLN
1	F	753	HIS

4.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

4.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

4.6 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	$\# Z > 2$
2	GOL	A	903	-	5,5,5	0.99	1 (20%)	5,5,5	1.07	0
3	CO3	F	906	-	3,3,3	0.89	0	2,3,3	0.14	0
2	GOL	A	902	-	5,5,5	0.80	0	5,5,5	1.16	0
3	CO3	A	905	-	3,3,3	1.25	1 (33%)	2,3,3	0.71	0
2	GOL	D	901	-	5,5,5	0.85	0	5,5,5	1.34	1 (20%)
2	GOL	F	904	-	5,5,5	1.21	0	5,5,5	0.98	0
2	GOL	D	904	-	5,5,5	1.05	1 (20%)	5,5,5	0.97	0
3	CO3	C	905	-	3,3,3	1.02	0	2,3,3	0.38	0
2	GOL	C	904	-	5,5,5	1.62	2 (40%)	5,5,5	0.61	0
3	CO3	E	904	-	3,3,3	0.89	0	2,3,3	0.63	0
2	GOL	B	901	-	5,5,5	1.03	0	5,5,5	1.10	1 (20%)
2	GOL	C	901	-	5,5,5	0.92	0	5,5,5	1.07	0
3	CO3	D	907	-	3,3,3	0.99	0	2,3,3	0.47	0
3	CO3	C	907	-	3,3,3	0.87	0	2,3,3	0.20	0
3	CO3	D	906	-	3,3,3	0.79	0	2,3,3	0.15	0
2	GOL	C	902	-	5,5,5	1.08	0	5,5,5	1.04	0
3	CO3	E	905	-	3,3,3	1.01	0	2,3,3	0.89	0
2	GOL	A	901	-	5,5,5	1.38	1 (20%)	5,5,5	0.78	0
2	GOL	D	905	-	5,5,5	1.14	1 (20%)	5,5,5	1.20	0
3	CO3	A	907	-	3,3,3	0.64	0	2,3,3	0.14	0
3	CO3	E	903	-	3,3,3	1.00	0	2,3,3	0.07	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	CO3	D	908	-	3,3,3	0.66	0	2,3,3	0.24	0
3	CO3	F	908	-	3,3,3	0.95	0	2,3,3	0.27	0
2	GOL	D	903	-	5,5,5	1.21	1 (20%)	5,5,5	0.96	0
2	GOL	F	901	-	5,5,5	0.95	0	5,5,5	0.84	0
2	GOL	C	903	-	5,5,5	1.14	1 (20%)	5,5,5	1.30	0
3	CO3	C	906	-	3,3,3	1.01	0	2,3,3	0.55	0
2	GOL	D	902	-	5,5,5	1.25	1 (20%)	5,5,5	0.88	0
2	GOL	F	903	-	5,5,5	1.32	1 (20%)	5,5,5	0.97	0
3	CO3	B	904	-	3,3,3	1.16	0	2,3,3	0.61	0
3	CO3	A	906	-	3,3,3	0.83	0	2,3,3	0.13	0
3	CO3	B	903	-	3,3,3	0.77	0	2,3,3	0.18	0
3	CO3	B	902	-	3,3,3	0.74	0	2,3,3	0.18	0
2	GOL	A	904	-	5,5,5	1.04	0	5,5,5	1.09	0
2	GOL	F	902	-	5,5,5	1.26	0	5,5,5	1.20	1 (20%)
3	CO3	F	907	-	3,3,3	0.93	0	2,3,3	0.18	0
2	GOL	E	902	-	5,5,5	1.12	0	5,5,5	0.91	0
2	GOL	E	901	-	5,5,5	1.44	1 (20%)	5,5,5	1.02	0
2	GOL	F	905	-	5,5,5	0.88	0	5,5,5	1.01	0

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

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	D	902	-	-	1/4/4/4	-
2	GOL	F	903	-	-	2/4/4/4	-
2	GOL	A	904	-	-	0/4/4/4	-
2	GOL	F	902	-	-	0/4/4/4	-
2	GOL	E	902	-	-	4/4/4/4	-
2	GOL	E	901	-	-	2/4/4/4	-
2	GOL	F	905	-	-	0/4/4/4	-

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	901	GOL	O2-C2	-2.85	1.35	1.43
2	F	903	GOL	O2-C2	-2.61	1.35	1.43
2	A	901	GOL	O2-C2	-2.27	1.36	1.43
2	D	902	GOL	O2-C2	-2.25	1.36	1.43
2	C	903	GOL	C3-C2	2.15	1.60	1.51
2	D	905	GOL	C1-C2	2.13	1.59	1.51
3	A	905	CO3	O1-C	2.13	1.33	1.25
2	D	903	GOL	O2-C2	-2.13	1.37	1.43
2	C	904	GOL	O2-C2	-2.12	1.37	1.43
2	C	904	GOL	C3-C2	2.09	1.59	1.51
2	D	904	GOL	O2-C2	-2.01	1.37	1.43
2	A	903	GOL	C1-C2	2.00	1.59	1.51

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	902	GOL	C3-C2-C1	-2.31	103.32	111.80
2	B	901	GOL	C3-C2-C1	-2.03	104.35	111.80
2	D	901	GOL	C3-C2-C1	-2.02	104.38	111.80

There are no chirality outliers.

All (36) 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

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Mol	Chain	Res	Type	Atoms
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	C	901	GOL	O1-C1-C2-O2
2	D	903	GOL	O1-C1-C2-O2
2	C	904	GOL	O1-C1-C2-O2
2	D	904	GOL	O1-C1-C2-C3

There are no ring outliers.

5 monomers are involved in 7 short contacts:

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

4.7 Other polymers [i](#)

There are no such residues in this entry.

4.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

5 Fit of model and data ⓘ

5.1 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%)	0.23	28 (3%)	45	44	9, 23, 45, 72	4 (0%)
1	B	761/824 (92%)	0.02	5 (0%)	84	84	9, 21, 37, 55	2 (0%)
1	C	762/824 (92%)	-0.04	14 (1%)	67	67	9, 20, 36, 62	5 (0%)
1	D	762/824 (92%)	0.10	21 (2%)	55	54	11, 21, 42, 62	1 (0%)
1	E	762/824 (92%)	0.16	16 (2%)	63	63	10, 23, 41, 60	4 (0%)
1	F	761/824 (92%)	0.03	19 (2%)	58	58	12, 20, 39, 58	3 (0%)
All	All	4569/4944 (92%)	0.08	103 (2%)	61	60	9, 21, 40, 72	19 (0%)

All (103) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	414	ALA	4.4
1	E	233	TRP	4.0
1	E	231	GLU	3.8
1	C	698	PRO	3.6
1	A	699	GLU	3.3
1	D	594	ALA	3.2
1	A	608	ALA	3.2
1	A	591	ALA	3.1
1	C	668	ASP	3.1
1	F	668	ASP	3.1
1	D	612	GLY	3.1
1	D	391	GLY	3.1
1	D	414	ALA	3.1
1	C	612	GLY	3.1
1	D	15	PRO	3.1
1	A	612	GLY	3.0
1	A	611	ARG	3.0
1	E	232	ALA	3.0
1	F	612	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	586	ARG	2.9
1	A	181	GLU	2.9
1	F	233	TRP	2.9
1	F	366	ALA	2.9
1	A	592	GLY	2.9
1	F	413	ASP	2.8
1	A	588	VAL	2.8
1	C	699	GLU	2.8
1	A	595	ALA	2.8
1	A	824	ARG	2.8
1	E	646	GLU	2.8
1	A	589	GLY	2.8
1	D	413	ASP	2.7
1	A	601	PRO	2.7
1	A	698	PRO	2.7
1	D	592	GLY	2.7
1	B	591	ALA	2.7
1	D	556	ALA	2.7
1	A	598	LEU	2.7
1	A	203	GLU	2.7
1	E	591	ALA	2.7
1	D	591	ALA	2.6
1	B	722	ASP	2.6
1	E	15	PRO	2.6
1	E	668	ASP	2.5
1	C	696	PRO	2.5
1	F	231	GLU	2.5
1	C	588	VAL	2.5
1	A	673	THR	2.5
1	E	612	GLY	2.5
1	D	611	ARG	2.5
1	B	612	GLY	2.5
1	A	179	ALA	2.4
1	F	232	ALA	2.4
1	E	611	ARG	2.4
1	F	150[A]	ARG	2.4
1	F	416	HIS	2.4
1	F	375	GLY	2.4
1	A	696	PRO	2.4
1	A	180	LYS	2.4
1	A	674	ALA	2.4
1	A	604	GLN	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	824	ARG	2.4
1	A	593	ALA	2.4
1	C	230	LYS	2.4
1	B	669	THR	2.4
1	C	15	PRO	2.4
1	F	377	TRP	2.4
1	A	606	ALA	2.3
1	D	593	ALA	2.3
1	E	595	ALA	2.3
1	A	605	ARG	2.3
1	D	588	VAL	2.3
1	C	673	THR	2.3
1	D	233	TRP	2.3
1	E	824	ARG	2.3
1	D	180	LYS	2.3
1	B	668	ASP	2.3
1	C	413	ASP	2.3
1	E	414	ALA	2.3
1	C	674	ALA	2.2
1	F	727	GLN	2.2
1	F	374	ARG	2.2
1	E	586	ARG	2.2
1	F	698	PRO	2.2
1	C	530	ASP	2.2
1	C	180	LYS	2.2
1	D	150	ARG	2.1
1	A	231	GLU	2.1
1	D	668	ASP	2.1
1	A	233	TRP	2.1
1	F	230	LYS	2.1
1	A	590	ASN	2.1
1	D	698	PRO	2.1
1	E	673	THR	2.1
1	F	673	THR	2.1
1	A	607	VAL	2.1
1	D	583	ALA	2.1
1	F	591	ALA	2.1
1	D	669	THR	2.1
1	E	698	PRO	2.0
1	C	398	VAL	2.0
1	E	723	ALA	2.0
1	F	379	PRO	2.0

5.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.4 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
2	GOL	D	905	6/6	0.75	0.17	26,27,33,37	0
2	GOL	E	902	6/6	0.79	0.18	33,35,39,41	0
2	GOL	A	901	6/6	0.82	0.15	22,30,35,44	0
2	GOL	C	904	6/6	0.82	0.17	19,24,35,39	0
3	CO3	C	907	4/4	0.82	0.14	30,36,36,37	0
3	CO3	D	907	4/4	0.82	0.11	30,34,36,36	0
3	CO3	B	904	4/4	0.83	0.11	28,30,31,43	0
2	GOL	D	903	6/6	0.83	0.16	25,31,36,39	0
3	CO3	A	906	4/4	0.83	0.13	29,29,32,38	0
3	CO3	E	903	4/4	0.83	0.11	29,29,31,36	0
2	GOL	F	905	6/6	0.85	0.19	27,30,31,35	0
2	GOL	E	901	6/6	0.86	0.15	19,25,28,36	0
2	GOL	A	903	6/6	0.86	0.12	22,23,27,32	0
3	CO3	A	907	4/4	0.87	0.11	24,26,28,39	0
2	GOL	D	904	6/6	0.87	0.13	29,34,39,39	0
2	GOL	F	904	6/6	0.87	0.13	29,33,38,40	0
2	GOL	A	902	6/6	0.87	0.11	23,27,32,39	0
2	GOL	C	903	6/6	0.87	0.11	20,24,28,29	0
3	CO3	F	907	4/4	0.87	0.13	27,32,34,35	0
3	CO3	D	906	4/4	0.89	0.12	20,22,26,35	0
2	GOL	D	901	6/6	0.90	0.11	25,29,33,36	0
3	CO3	C	905	4/4	0.91	0.12	20,24,26,33	0
3	CO3	B	903	4/4	0.91	0.10	18,26,29,34	0
3	CO3	F	906	4/4	0.91	0.13	22,25,25,35	0
2	GOL	C	901	6/6	0.91	0.09	26,29,34,36	0
2	GOL	F	901	6/6	0.92	0.09	21,29,33,41	0
2	GOL	B	901	6/6	0.92	0.10	20,25,25,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	CO3	A	905	4/4	0.94	0.07	14,16,25,26	0
2	GOL	A	904	6/6	0.94	0.08	26,27,31,31	0
3	CO3	C	906	4/4	0.94	0.07	13,14,17,21	0
3	CO3	E	904	4/4	0.95	0.08	17,23,29,37	0
2	GOL	F	903	6/6	0.95	0.08	17,19,26,28	0
2	GOL	C	902	6/6	0.95	0.09	16,22,23,32	0
2	GOL	D	902	6/6	0.96	0.07	20,23,27,27	0
3	CO3	D	908	4/4	0.96	0.07	11,11,14,22	0
3	CO3	B	902	4/4	0.96	0.06	13,14,19,23	0
3	CO3	F	908	4/4	0.96	0.06	10,14,16,21	0
3	CO3	E	905	4/4	0.97	0.05	12,16,18,21	0
2	GOL	F	902	6/6	0.97	0.07	20,21,22,23	0
4	CA	A	908	1/1	0.99	0.02	18,18,18,18	0
4	CA	B	905	1/1	0.99	0.03	15,15,15,15	0
4	CA	C	908	1/1	0.99	0.01	14,14,14,14	0
4	CA	D	909	1/1	0.99	0.05	18,18,18,18	0
4	CA	E	906	1/1	0.99	0.02	18,18,18,18	0
4	CA	F	909	1/1	0.99	0.03	13,13,13,13	0

5.5 Other polymers [i](#)

There are no such residues in this entry.