



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 10:04 AM UTC

PDB ID : 2F3O / pdb_00002f3o
Title : Crystal Structure of a glycyl radical enzyme from *Archaeoglobus fulgidus*
Authors : Lehtio, L.; Goldman, A.
Deposited on : 2005-11-22
Resolution : 2.90 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 types of validation reports are described at

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

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

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

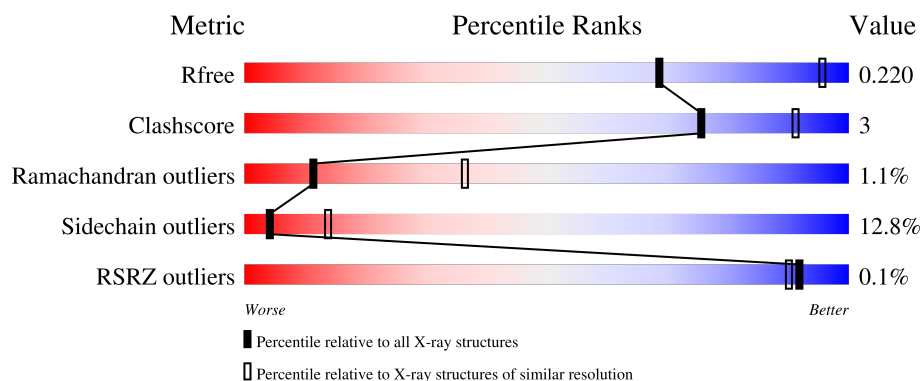
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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}	180053	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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 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	776	 81% 15% . .
1	B	776	 79% 18% .

2 Entry composition [i](#)

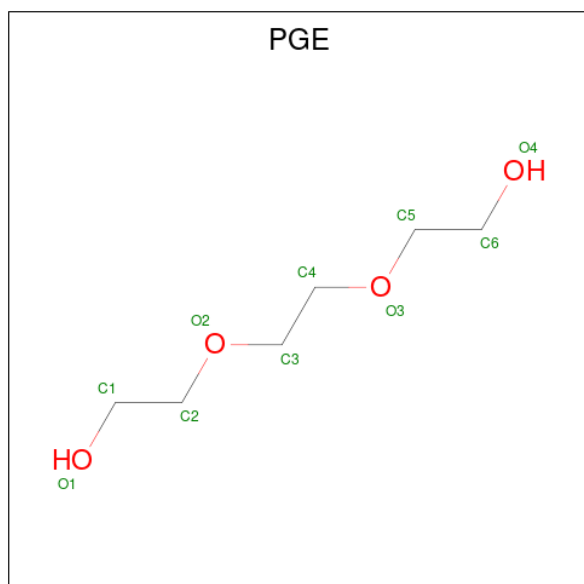
There are 4 unique types of molecules in this entry. The entry contains 12375 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 pyruvate formate-lyase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	767	Total	C	N	O	S	0	0	1
			6065	3853	1033	1155	24			
1	B	773	Total	C	N	O	S	0	0	0
			6111	3882	1040	1164	25			

- Molecule 2 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: C₆H₁₄O₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			10	6	4		
2	B	1	Total	C	O	0	0
			10	6	4		

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

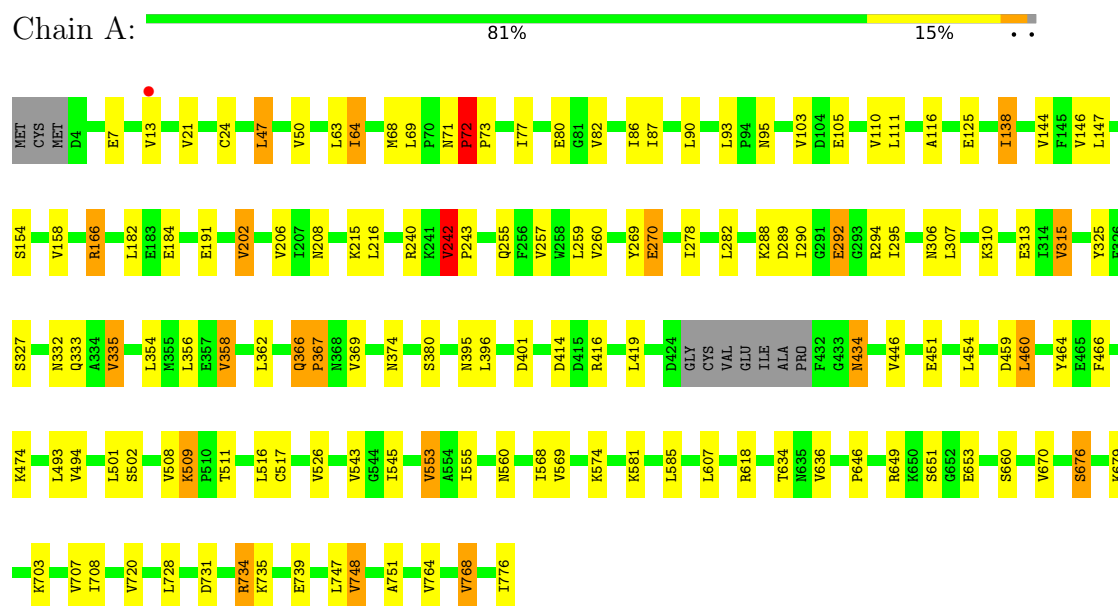
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	100	Total	O	0	0
			100	100		
4	B	67	Total	O	0	0
			67	67		

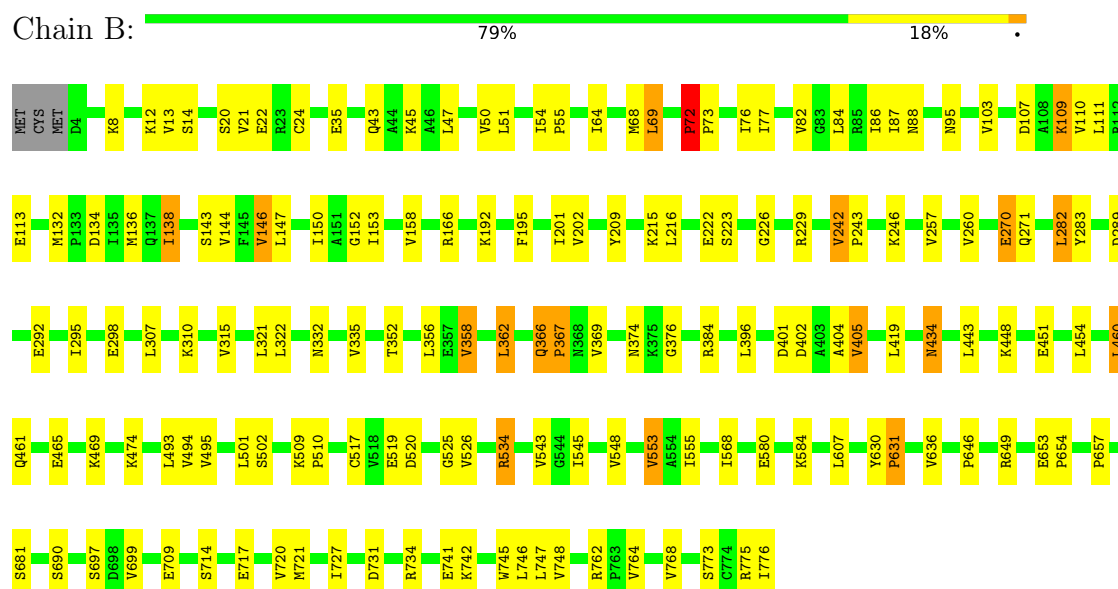
3 Residue-property plots

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: pyruvate formate-lyase 2



• Molecule 1: pyruvate formate-lyase 2



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	167.03Å 174.17Å 162.46Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.69 – 2.90 19.69 – 2.90	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.69-2.90) 99.6 (19.69-2.90)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.14 (at 2.88Å)	Xtriage
Refinement program	REFMAC 5.2.0005, CNS	Depositor
R, R_{free}	0.199 , 0.245 (Not available) , 0.220	Depositor DCC
R_{free} test set	2648 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	58.4	Xtriage
Anisotropy	0.065	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 43.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.023 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	12375	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.34% 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

5.1 Standard geometry

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

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	0.69	0/6180	1.11	28/8356 (0.3%)
1	B	0.67	0/6227	1.10	24/8421 (0.3%)
All	All	0.68	0/12407	1.10	52/16777 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	3
All	All	0	6

There are no bond length outliers.

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	71	ASN	CA-C-N	9.91	130.59	120.38
1	A	71	ASN	C-N-CA	9.91	130.59	120.38
1	A	116	ALA	CA-C-N	-7.52	112.05	119.64
1	A	116	ALA	C-N-CA	-7.52	112.05	119.64
1	B	292	GLU	N-CA-C	-7.13	104.73	113.50
1	B	553	VAL	CB-CA-C	-6.89	102.72	112.22
1	B	653	GLU	CA-C-N	6.87	128.43	119.84
1	B	653	GLU	C-N-CA	6.87	128.43	119.84
1	B	509	LYS	CA-C-N	-6.74	113.70	120.31
1	B	509	LYS	C-N-CA	-6.74	113.70	120.31
1	A	242	VAL	CA-C-N	6.68	128.19	119.84
1	A	242	VAL	C-N-CA	6.68	128.19	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	762	ARG	CA-C-N	-6.49	113.03	120.04
1	B	762	ARG	C-N-CA	-6.49	113.03	120.04
1	B	72	PRO	N-CA-C	6.39	118.50	110.70
1	A	292	GLU	N-CA-C	-6.25	104.24	113.61
1	A	553	VAL	CB-CA-C	-6.15	103.83	112.14
1	B	270	GLU	N-CA-C	6.02	120.16	112.34
1	B	242	VAL	N-CA-C	5.87	121.56	108.88
1	B	283	TYR	CA-C-N	-5.84	112.85	119.28
1	B	283	TYR	C-N-CA	-5.84	112.85	119.28
1	B	366	GLN	CA-C-N	5.80	127.09	119.84
1	B	366	GLN	C-N-CA	5.80	127.09	119.84
1	A	72	PRO	CA-C-N	5.70	126.96	119.84
1	A	72	PRO	C-N-CA	5.70	126.96	119.84
1	A	366	GLN	CA-C-N	5.66	126.91	119.84
1	A	366	GLN	C-N-CA	5.66	126.91	119.84
1	A	154	SER	CB-CA-C	-5.61	110.09	116.54
1	B	519	GLU	N-CA-C	5.60	118.77	110.48
1	A	653	GLU	CA-C-N	5.44	125.44	119.89
1	A	653	GLU	C-N-CA	5.44	125.44	119.89
1	A	315	VAL	N-CA-C	-5.41	97.20	108.88
1	B	630	TYR	CA-C-N	-5.41	113.08	119.84
1	B	630	TYR	C-N-CA	-5.41	113.08	119.84
1	A	511	THR	CA-C-N	5.37	125.02	119.05
1	A	511	THR	C-N-CA	5.37	125.02	119.05
1	A	509	LYS	CA-C-N	-5.35	114.45	119.85
1	A	509	LYS	C-N-CA	-5.35	114.45	119.85
1	B	367	PRO	N-CA-C	-5.34	101.46	112.47
1	A	240	ARG	N-CA-C	-5.30	105.96	112.90
1	B	690	SER	N-CA-C	5.24	116.95	108.41
1	B	152	GLY	CA-C-N	-5.22	117.85	122.97
1	B	152	GLY	C-N-CA	-5.22	117.85	122.97
1	A	144	VAL	CB-CA-C	5.20	116.29	111.30
1	B	144	VAL	N-CA-C	5.13	116.43	112.12
1	A	367	PRO	N-CA-C	-5.13	101.91	112.47
1	A	93	LEU	N-CA-C	5.11	120.42	113.16
1	A	660	SER	CA-C-N	5.03	125.30	119.92
1	A	660	SER	C-N-CA	5.03	125.30	119.92
1	A	93	LEU	CA-C-N	-5.02	113.56	119.84
1	A	93	LEU	C-N-CA	-5.02	113.56	119.84
1	B	22	GLU	N-CA-C	5.02	117.14	111.11

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	242	VAL	Peptide
1	A	366	GLN	Peptide
1	A	72	PRO	Peptide
1	B	242	VAL	Peptide
1	B	366	GLN	Peptide
1	B	72	PRO	Peptide

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	6065	0	6046	35	0
1	B	6111	0	6092	38	0
2	A	10	0	14	0	0
2	B	10	0	14	0	0
3	A	6	0	8	0	0
3	B	6	0	8	1	0
4	A	100	0	0	2	0
4	B	67	0	0	0	0
All	All	12375	0	12182	73	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 3.

All (73) 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:A:63:LEU:H	1:A:306:ASN:ND2	1.80	0.78
1:B:374:ASN:HB3	1:B:401:ASP:HB2	1.78	0.64
1:A:374:ASN:HB3	1:A:401:ASP:HB2	1.86	0.57
1:A:63:LEU:H	1:A:306:ASN:HD21	1.50	0.56
1:A:80:GLU:HG3	1:A:509:LYS:HD3	1.88	0.56
1:A:208:ASN:HB3	4:A:859:HOH:O	2.08	0.54
1:B:158:VAL:HG13	1:B:517:CYS:HB3	1.89	0.53
1:B:555:ILE:HD11	1:B:646:PRO:HG2	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:47:LEU:HD12	1:A:202:VAL:HG22	1.94	0.50
1:B:134:ASP:O	1:B:138:ILE:HG23	2.12	0.50
1:A:255:GLN:HE21	1:A:259:LEU:HG	1.77	0.49
1:A:289:ASP:HB3	1:A:295:ILE:HG12	1.93	0.49
1:A:434:ASN:HD22	1:A:434:ASN:H	1.61	0.48
1:A:731:ASP:HA	1:A:734:ARG:HB2	1.95	0.48
1:B:146:VAL:HG13	1:B:443:LEU:HB2	1.96	0.47
1:A:310:LYS:HE3	1:A:313:GLU:OE2	2.14	0.47
1:A:158:VAL:HG13	1:A:517:CYS:HB3	1.97	0.47
1:B:54:ILE:HG13	1:B:55:PRO:HD2	1.95	0.46
1:B:451:GLU:HG3	1:B:460:LEU:HB2	1.97	0.46
1:B:12:LYS:HD3	1:B:12:LYS:HA	1.82	0.46
1:B:45:LYS:HG3	1:B:201:ILE:HD13	1.97	0.46
1:B:631:PRO:HG3	1:B:657:PRO:HA	1.97	0.46
1:A:64:ILE:H	1:A:306:ASN:ND2	2.14	0.46
1:B:21:VAL:HG11	1:B:107:ASP:HB2	1.97	0.45
1:B:636:VAL:HG21	1:B:764:VAL:HG22	1.98	0.45
1:A:242:VAL:O	1:A:242:VAL:HG23	2.17	0.45
1:A:325:TYR:HB3	1:A:634:THR:HG22	1.98	0.45
1:B:24:CYS:HB2	1:B:77:ILE:HB	1.99	0.45
1:B:109:LYS:HE3	1:B:109:LYS:HB2	1.87	0.45
1:B:51:LEU:HB3	1:B:209:TYR:HB2	1.99	0.45
1:A:451:GLU:HG3	1:A:460:LEU:HB2	1.99	0.45
1:A:270:GLU:HG2	4:A:805:HOH:O	2.16	0.45
1:A:636:VAL:HG21	1:A:764:VAL:HG22	2.00	0.44
1:B:289:ASP:HB3	1:B:295:ILE:HG12	2.00	0.44
1:A:354:LEU:O	1:A:358:VAL:HG12	2.18	0.44
1:A:24:CYS:HB2	1:A:77:ILE:HB	1.99	0.44
1:A:138:ILE:HD13	1:A:138:ILE:HG21	1.68	0.43
1:B:474:LYS:HB2	1:B:474:LYS:HE3	1.63	0.43
1:A:459:ASP:HB2	1:A:464:TYR:HB2	2.00	0.43
1:B:132:MET:HE2	1:B:136:MET:SD	2.58	0.43
1:B:43:GLN:HG3	1:B:510:PRO:HD2	2.00	0.43
1:B:358:VAL:HG23	1:B:362:LEU:HD22	2.00	0.43
1:B:215:LYS:HA	1:B:215:LYS:HD3	1.81	0.43
1:B:584:LYS:HE2	1:B:584:LYS:HB3	1.84	0.43
1:B:520:ASP:OD2	1:B:534:ARG:HG2	2.18	0.43
1:B:87:ILE:HD12	1:B:111:LEU:HB3	2.01	0.43
1:A:676:SER:HA	1:A:679:LYS:HD2	2.01	0.42
1:A:87:ILE:HD12	1:A:111:LEU:HB3	2.00	0.42
1:A:748:VAL:HG21	1:A:768:VAL:HG21	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:271:GLN:HB3	3:B:778:GOL:H32	2.02	0.42
1:B:448:LYS:HD3	1:B:448:LYS:HA	1.80	0.42
1:B:20:SER:HB2	1:B:69:LEU:HD13	2.01	0.42
1:B:68:MET:HE2	1:B:310:LYS:O	2.20	0.42
1:B:404:ALA:HA	1:B:721:MET:HE2	2.02	0.41
1:B:195:PHE:CD2	1:B:525:GLY:HA2	2.55	0.41
1:B:545:ILE:HD13	1:B:607:LEU:HD13	2.02	0.41
1:B:434:ASN:C	1:B:434:ASN:HD22	2.27	0.41
1:A:545:ILE:HD13	1:A:607:LEU:HD13	2.02	0.41
1:A:68:MET:HE1	1:A:333:GLN:HE22	1.85	0.41
1:A:90:LEU:HD23	1:A:90:LEU:HA	1.81	0.41
1:B:246:LYS:HE3	1:B:246:LYS:HB2	1.88	0.41
1:B:746:LEU:HD12	1:B:746:LEU:HA	1.83	0.41
1:A:138:ILE:HB	1:A:466:PHE:CE1	2.56	0.41
1:A:728:LEU:HD21	1:A:748:VAL:HG23	2.03	0.41
1:A:288:LYS:O	1:A:292:GLU:HB2	2.20	0.41
1:B:138:ILE:HD13	1:B:138:ILE:HG21	1.80	0.41
1:A:278:ILE:HG21	1:A:335:VAL:HG22	2.02	0.41
1:B:282:LEU:HD12	1:B:282:LEU:HA	1.82	0.40
1:A:182:LEU:HD23	1:A:182:LEU:HA	1.77	0.40
1:A:555:ILE:HD11	1:A:646:PRO:HG2	2.03	0.40
1:B:401:ASP:O	1:B:405:VAL:HG13	2.21	0.40
1:B:742:LYS:HD3	1:B:742:LYS:HA	1.89	0.40
1:A:166:ARG:HH11	1:A:166:ARG:HD3	1.74	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	764/776 (98%)	718 (94%)	40 (5%)	6 (1%)	16 44

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	771/776 (99%)	722 (94%)	38 (5%)	11 (1%)	9	30
All	All	1535/1552 (99%)	1440 (94%)	78 (5%)	17 (1%)	11	36

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	73	PRO
1	B	73	PRO
1	B	223	SER
1	A	751	ALA
1	B	226	GLY
1	B	332	ASN
1	B	731	ASP
1	A	243	PRO
1	A	332	ASN
1	B	72	PRO
1	B	376	GLY
1	A	367	PRO
1	B	243	PRO
1	B	367	PRO
1	A	72	PRO
1	B	631	PRO
1	B	654	PRO

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	651/660 (99%)	570 (88%)	81 (12%)	4	15
1	B	656/660 (99%)	570 (87%)	86 (13%)	4	13
All	All	1307/1320 (99%)	1140 (87%)	167 (13%)	4	14

All (167) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	GLU
1	A	13	VAL
1	A	21	VAL
1	A	47	LEU
1	A	50	VAL
1	A	64	ILE
1	A	69	LEU
1	A	82	VAL
1	A	86	ILE
1	A	95	ASN
1	A	103	VAL
1	A	105	GLU
1	A	110	VAL
1	A	125	GLU
1	A	138	ILE
1	A	146	VAL
1	A	147	LEU
1	A	166	ARG
1	A	184	GLU
1	A	191	GLU
1	A	202	VAL
1	A	206	VAL
1	A	215	LYS
1	A	216	LEU
1	A	257	VAL
1	A	260	VAL
1	A	269	TYR
1	A	270	GLU
1	A	282	LEU
1	A	290	ILE
1	A	294	ARG
1	A	307	LEU
1	A	315	VAL
1	A	327	SER
1	A	335	VAL
1	A	356	LEU
1	A	358	VAL
1	A	362	LEU
1	A	369	VAL
1	A	380	SER
1	A	395	ASN
1	A	396	LEU
1	A	414	ASP

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Mol	Chain	Res	Type
1	A	416	ARG
1	A	419	LEU
1	A	434	ASN
1	A	446	VAL
1	A	454	LEU
1	A	460	LEU
1	A	474	LYS
1	A	493	LEU
1	A	494	VAL
1	A	501	LEU
1	A	502	SER
1	A	508	VAL
1	A	516	LEU
1	A	526	VAL
1	A	543	VAL
1	A	553	VAL
1	A	560	ASN
1	A	568	ILE
1	A	569	VAL
1	A	574	LYS
1	A	581	LYS
1	A	585	LEU
1	A	618	ARG
1	A	649	ARG
1	A	651	SER
1	A	670	VAL
1	A	676	SER
1	A	703	LYS
1	A	707	VAL
1	A	708	ILE
1	A	720	VAL
1	A	734	ARG
1	A	735	LYS
1	A	739	GLU
1	A	747	LEU
1	A	748	VAL
1	A	768	VAL
1	A	776	ILE
1	B	8	LYS
1	B	13	VAL
1	B	14	SER
1	B	35	GLU

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Mol	Chain	Res	Type
1	B	47	LEU
1	B	50	VAL
1	B	64	ILE
1	B	69	LEU
1	B	76	ILE
1	B	82	VAL
1	B	84	LEU
1	B	86	ILE
1	B	88	ASN
1	B	95	ASN
1	B	103	VAL
1	B	109	LYS
1	B	110	VAL
1	B	113	GLU
1	B	138	ILE
1	B	143	SER
1	B	146	VAL
1	B	147	LEU
1	B	150	ILE
1	B	153	ILE
1	B	166	ARG
1	B	192	LYS
1	B	202	VAL
1	B	216	LEU
1	B	222	GLU
1	B	229	ARG
1	B	257	VAL
1	B	260	VAL
1	B	270	GLU
1	B	282	LEU
1	B	298	GLU
1	B	307	LEU
1	B	315	VAL
1	B	321	LEU
1	B	322	LEU
1	B	335	VAL
1	B	352	THR
1	B	356	LEU
1	B	358	VAL
1	B	362	LEU
1	B	369	VAL
1	B	384	ARG

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Mol	Chain	Res	Type
1	B	396	LEU
1	B	402	ASP
1	B	405	VAL
1	B	419	LEU
1	B	434	ASN
1	B	454	LEU
1	B	460	LEU
1	B	461	GLN
1	B	465	GLU
1	B	469	LYS
1	B	493	LEU
1	B	494	VAL
1	B	495	VAL
1	B	501	LEU
1	B	502	SER
1	B	526	VAL
1	B	534	ARG
1	B	543	VAL
1	B	548	VAL
1	B	553	VAL
1	B	568	ILE
1	B	580	GLU
1	B	649	ARG
1	B	681	SER
1	B	697	SER
1	B	699	VAL
1	B	709	GLU
1	B	714	SER
1	B	717	GLU
1	B	720	VAL
1	B	727	ILE
1	B	734	ARG
1	B	741	GLU
1	B	745	TRP
1	B	747	LEU
1	B	748	VAL
1	B	768	VAL
1	B	773	SER
1	B	775	ARG
1	B	776	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	43	GLN
1	A	71	ASN
1	A	137	GLN
1	A	261	GLN
1	A	306	ASN
1	A	312	ASN
1	A	333	GLN
1	A	395	ASN
1	A	434	ASN
1	A	455	ASN
1	A	461	GLN
1	A	687	ASN
1	B	33	GLN
1	B	43	GLN
1	B	71	ASN
1	B	88	ASN
1	B	261	GLN
1	B	333	GLN
1	B	374	ASN
1	B	455	ASN
1	B	461	GLN
1	B	583	HIS
1	B	617	HIS
1	B	687	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

4 ligands are modelled in this entry.

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	GOL	B	778	-	5,5,5	0.41	0	5,5,5	0.84	0
2	PGE	A	777	-	9,9,9	0.56	0	8,8,8	0.27	0
3	GOL	A	778	-	5,5,5	0.36	0	5,5,5	1.05	0
2	PGE	B	777	-	9,9,9	0.58	0	8,8,8	0.20	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
3	GOL	B	778	-	-	2/4/4/4	-
2	PGE	A	777	-	-	5/7/7/7	-
3	GOL	A	778	-	-	1/4/4/4	-
2	PGE	B	777	-	-	4/7/7/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	777	PGE	O1-C1-C2-O2
3	B	778	GOL	C1-C2-C3-O3
2	A	777	PGE	O3-C5-C6-O4
2	B	777	PGE	O2-C3-C4-O3
2	A	777	PGE	O1-C1-C2-O2
3	A	778	GOL	O1-C1-C2-O2
2	A	777	PGE	C3-C4-O3-C5
2	A	777	PGE	O2-C3-C4-O3
2	B	777	PGE	C1-C2-O2-C3
2	B	777	PGE	C6-C5-O3-C4

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Mol	Chain	Res	Type	Atoms
3	B	778	GOL	O2-C2-C3-O3
2	A	777	PGE	C1-C2-O2-C3

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	778	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	765/776 (98%)	-0.37	1 (0%) 92 90	33, 53, 75, 85	0
1	B	773/776 (99%)	-0.21	0 100 100	42, 60, 82, 91	0
All	All	1538/1552 (99%)	-0.29	1 (0%) 92 90	33, 56, 80, 91	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	13	VAL	2.3

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	GOL	B	778	6/6	0.83	0.15	56,58,58,59	0
2	PGE	B	777	10/10	0.89	0.14	73,76,76,76	0
2	PGE	A	777	10/10	0.90	0.12	57,61,64,64	0
3	GOL	A	778	6/6	0.94	0.11	39,41,42,42	0

6.5 Other polymers [i](#)

There are no such residues in this entry.