



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 10:38 PM UTC

PDB ID : 8GQL / pdb_00008gql
Title : X-ray structure of Thiolase from Pseudomonas aeruginosa PAO1
Authors : Hong, J.; Son, H.F.; Kim, K.J.
Deposited on : 2022-08-30
Resolution : 2.30 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

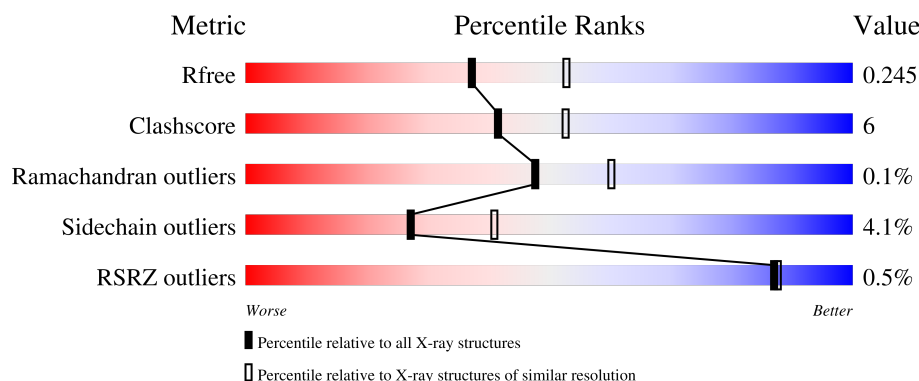
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	399	 86% 11% ..
1	B	399	 79% 16% ..
1	C	399	 78% 18% ..
1	D	399	 80% 16% ..

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11523 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 Thiolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	390	Total	C	N	O	S	0	0	0
			2822	1747	508	546	21			
1	B	387	Total	C	N	O	S	0	0	0
			2796	1732	501	542	21			
1	C	386	Total	C	N	O	S	0	0	0
			2789	1728	500	540	21			
1	D	386	Total	C	N	O	S	0	0	0
			2789	1728	500	540	21			

There are 32 discrepancies between the modelled and reference sequences:

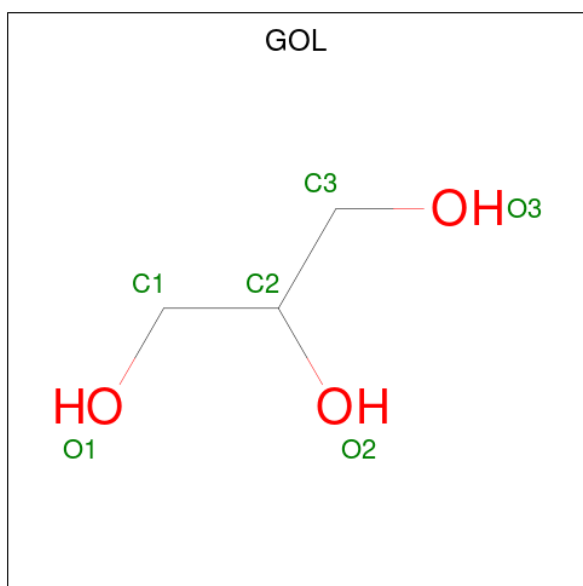
Chain	Residue	Modelled	Actual	Comment	Reference
A	392	LEU	-	expression tag	UNP G3XD40
A	393	GLU	-	expression tag	UNP G3XD40
A	394	HIS	-	expression tag	UNP G3XD40
A	395	HIS	-	expression tag	UNP G3XD40
A	396	HIS	-	expression tag	UNP G3XD40
A	397	HIS	-	expression tag	UNP G3XD40
A	398	HIS	-	expression tag	UNP G3XD40
A	399	HIS	-	expression tag	UNP G3XD40
B	392	LEU	-	expression tag	UNP G3XD40
B	393	GLU	-	expression tag	UNP G3XD40
B	394	HIS	-	expression tag	UNP G3XD40
B	395	HIS	-	expression tag	UNP G3XD40
B	396	HIS	-	expression tag	UNP G3XD40
B	397	HIS	-	expression tag	UNP G3XD40
B	398	HIS	-	expression tag	UNP G3XD40
B	399	HIS	-	expression tag	UNP G3XD40
C	392	LEU	-	expression tag	UNP G3XD40
C	393	GLU	-	expression tag	UNP G3XD40
C	394	HIS	-	expression tag	UNP G3XD40
C	395	HIS	-	expression tag	UNP G3XD40
C	396	HIS	-	expression tag	UNP G3XD40

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	397	HIS	-	expression tag	UNP G3XD40
C	398	HIS	-	expression tag	UNP G3XD40
C	399	HIS	-	expression tag	UNP G3XD40
D	392	LEU	-	expression tag	UNP G3XD40
D	393	GLU	-	expression tag	UNP G3XD40
D	394	HIS	-	expression tag	UNP G3XD40
D	395	HIS	-	expression tag	UNP G3XD40
D	396	HIS	-	expression tag	UNP G3XD40
D	397	HIS	-	expression tag	UNP G3XD40
D	398	HIS	-	expression tag	UNP G3XD40
D	399	HIS	-	expression tag	UNP G3XD40

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	100	Total	O	0	0
			100	100		
3	B	84	Total	O	0	0
			84	84		
3	C	78	Total	O	0	0
			78	78		

Continued on next page...

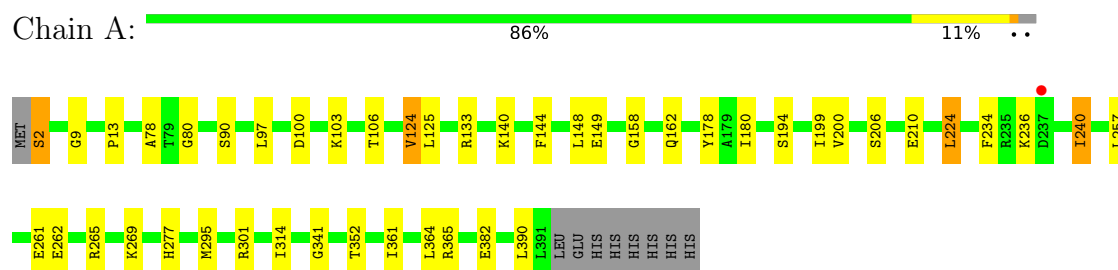
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	59	Total	O	0	0
			59	59		

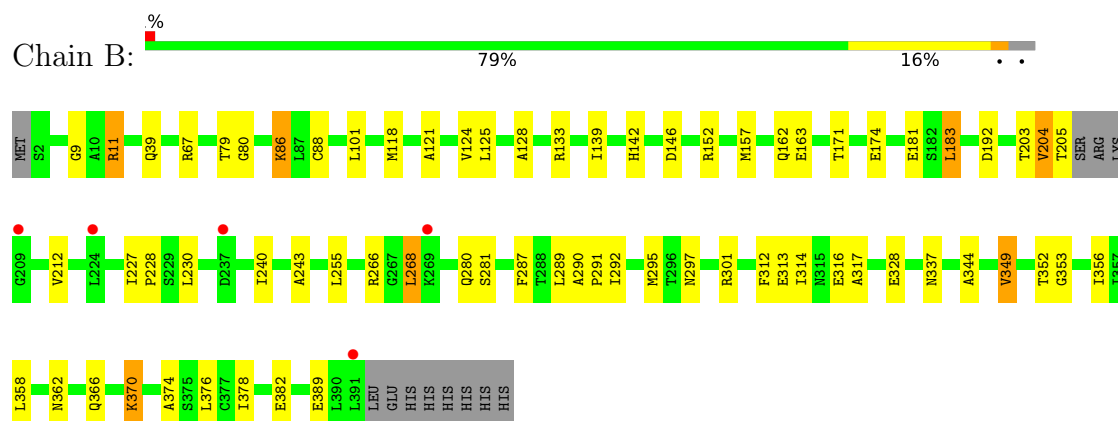
3 Residue-property plots

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.

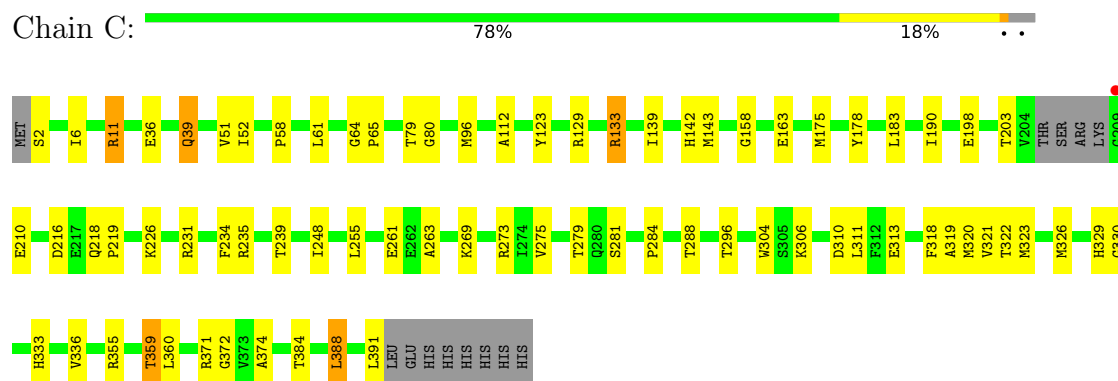
• Molecule 1: Thiolase



• Molecule 1: Thiolase



• Molecule 1: Thiolase



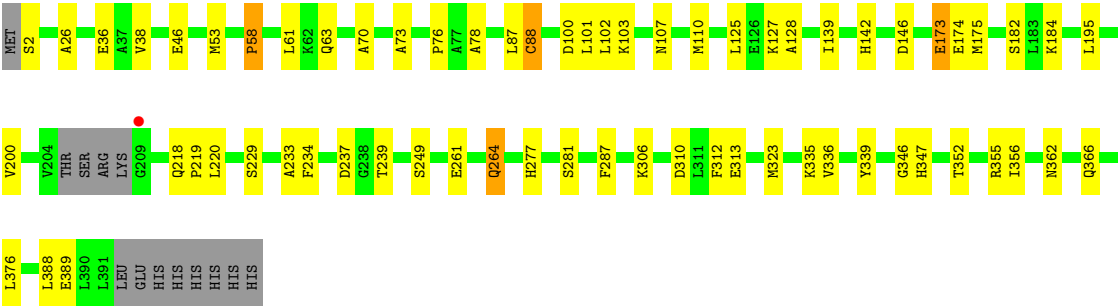
• Molecule 1: Thiolase

Chain D:

80%

16%

• •



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	74.10Å 93.75Å 111.53Å 90.00° 108.29° 90.00°	Depositor
Resolution (Å)	34.47 – 2.30 34.47 – 2.30	Depositor EDS
% Data completeness (in resolution range)	97.9 (34.47-2.30) 98.2 (34.47-2.30)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.83 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.191 , 0.265 (Not available) , 0.245	Depositor DCC
R_{free} test set	3092 reflections (4.77%)	wwPDB-VP
Wilson B-factor (Å ²)	27.3	Xtriage
Anisotropy	0.076	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 32.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.023 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11523	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.53% 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: 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	1.20	2/2855 (0.1%)	1.56	7/3854 (0.2%)
1	B	1.17	1/2828 (0.0%)	1.55	7/3818 (0.2%)
1	C	1.18	2/2821 (0.1%)	1.58	11/3808 (0.3%)
1	D	1.14	0/2821	1.58	10/3808 (0.3%)
All	All	1.18	5/11325 (0.0%)	1.57	35/15288 (0.2%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	353	GLY	C-O	6.22	1.31	1.23
1	C	248	ILE	C-O	5.71	1.29	1.24
1	C	142	HIS	CE1-NE2	5.66	1.38	1.32
1	A	9	GLY	C-O	5.54	1.29	1.23
1	A	199	ILE	C-O	-5.26	1.17	1.24

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	53	MET	CA-C-N	8.72	128.29	119.92
1	D	53	MET	C-N-CA	8.72	128.29	119.92
1	B	192	ASP	CA-CB-CG	7.09	119.69	112.60
1	C	11	ARG	NE-CZ-NH2	6.35	124.92	119.20
1	C	80	GLY	CA-C-O	-6.29	115.92	121.58
1	D	346	GLY	CA-C-O	-6.16	118.22	122.22
1	B	352	THR	CA-CB-OG1	-5.98	100.63	109.60
1	C	275	VAL	N-CA-C	-5.95	105.92	111.45
1	A	106	THR	CA-CB-OG1	-5.87	100.80	109.60
1	A	341	GLY	CA-C-N	5.84	128.90	120.38
1	A	341	GLY	C-N-CA	5.84	128.90	120.38
1	C	11	ARG	NE-CZ-NH1	-5.80	115.70	121.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	121	ALA	O-C-N	-5.72	117.01	121.47
1	A	90	SER	CA-C-N	5.69	126.41	120.03
1	A	90	SER	C-N-CA	5.69	126.41	120.03
1	D	26	ALA	CA-C-N	5.67	127.91	120.60
1	D	26	ALA	C-N-CA	5.67	127.91	120.60
1	C	269	LYS	CB-CA-C	5.67	115.78	110.17
1	C	190	ILE	CA-C-N	5.65	127.78	120.44
1	C	190	ILE	C-N-CA	5.65	127.78	120.44
1	C	263	ALA	CA-C-N	5.54	128.02	120.54
1	C	263	ALA	C-N-CA	5.54	128.02	120.54
1	D	287	PHE	CA-C-O	-5.47	114.75	120.55
1	A	352	THR	CA-C-N	5.43	125.86	119.94
1	A	352	THR	C-N-CA	5.43	125.86	119.94
1	D	264	GLN	CA-C-O	-5.39	115.16	120.82
1	B	11	ARG	CG-CD-NE	5.27	123.59	112.00
1	C	359	THR	CA-CB-OG1	-5.27	101.70	109.60
1	D	313	GLU	CB-CG-CD	5.26	121.54	112.60
1	B	152	ARG	CA-C-O	-5.21	114.90	120.42
1	D	38	VAL	CA-C-N	5.16	127.50	120.54
1	D	38	VAL	C-N-CA	5.16	127.50	120.54
1	C	388	LEU	N-CA-CB	-5.08	101.94	111.13
1	B	181	GLU	CA-C-N	5.08	127.04	120.44
1	B	181	GLU	C-N-CA	5.08	127.04	120.44

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	2822	0	2869	25	0
1	B	2796	0	2837	39	0
1	C	2789	0	2830	52	0
1	D	2789	0	2830	36	0
2	C	6	0	8	1	0
3	A	100	0	0	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	84	0	0	0	0
3	C	78	0	0	2	0
3	D	59	0	0	1	0
All	All	11523	0	11374	144	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 6.

All (144) 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:101:LEU:HB3	1:D:110:MET:HE1	1.51	0.92
1:C:326:MET:HE1	1:C:333:HIS:HA	1.51	0.91
1:D:102:LEU:HG	1:D:110:MET:HE3	1.55	0.89
1:C:58:PRO:HA	1:C:61:LEU:HD12	1.63	0.77
1:C:326:MET:CE	1:C:333:HIS:HA	2.15	0.76
1:C:175:MET:HG2	1:C:323:MET:HE1	1.68	0.75
1:C:39:GLN:OE1	1:C:39:GLN:C	2.29	0.75
2:C:401:GOL:O1	1:D:63:GLN:HB3	1.89	0.73
1:D:101:LEU:CB	1:D:110:MET:HE1	2.21	0.71
1:D:107:ASN:HB2	1:D:110:MET:HE2	1.74	0.70
1:C:296:THR:HG22	1:C:329:HIS:CE1	2.29	0.68
1:B:313:GLU:HG2	1:B:356:ILE:HB	1.77	0.65
1:A:364:LEU:HB3	1:A:390:LEU:HD11	1.79	0.65
1:A:180:ILE:HG23	1:A:224:LEU:HD21	1.77	0.65
1:C:273:ARG:HG2	1:C:391:LEU:HD21	1.79	0.65
1:C:320:MET:HA	1:C:323:MET:HE3	1.79	0.64
1:C:360:LEU:HD22	1:C:388:LEU:HD13	1.81	0.63
1:D:107:ASN:HD22	1:D:110:MET:HE2	1.64	0.63
1:C:360:LEU:C	1:C:360:LEU:HD23	2.24	0.62
1:B:370:LYS:O	1:B:389:GLU:HA	1.99	0.62
1:A:269:LYS:O	1:A:269:LYS:HG3	2.00	0.62
1:A:210:GLU:HG2	3:A:459:HOH:O	2.01	0.61
1:C:279:THR:HG22	1:C:384:THR:HG22	1.82	0.60
1:B:314:ILE:H	1:B:337:ASN:HD21	1.50	0.60
1:B:142:HIS:HD2	1:B:146:ASP:OD2	1.86	0.59
1:D:362:ASN:HD21	1:D:366:GLN:NE2	1.99	0.59
1:D:142:HIS:HD2	1:D:146:ASP:OD2	1.85	0.59
1:B:86:LYS:HD3	1:B:378:ILE:HD13	1.86	0.58
1:C:326:MET:HE3	1:C:336:VAL:HB	1.85	0.58
1:C:319:ALA:HB1	1:C:323:MET:HE2	1.85	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:233:ALA:HB3	1:D:234:PHE:CD2	2.38	0.58
1:B:362:ASN:HD21	1:B:366:GLN:NE2	2.01	0.58
1:C:175:MET:HE1	1:C:239:THR:OG1	2.03	0.57
1:A:162:GLN:HE22	1:A:240:ILE:H	1.52	0.57
1:B:227:ILE:HB	1:B:228:PRO:HD3	1.86	0.57
1:C:288:THR:HB	1:C:321:VAL:HG22	1.87	0.56
1:C:326:MET:HE1	1:C:333:HIS:CA	2.31	0.56
1:C:326:MET:HE3	1:C:336:VAL:CB	2.35	0.56
1:B:9:GLY:HA3	1:B:358:LEU:HD21	1.87	0.56
1:C:296:THR:HG21	3:C:506:HOH:O	2.05	0.56
1:B:290:ALA:N	1:B:291:PRO:CD	2.69	0.55
1:D:107:ASN:HD22	1:D:110:MET:CE	2.19	0.55
1:B:67:ARG:NH1	1:B:79:THR:O	2.39	0.55
1:D:36:GLU:HG2	1:D:200:VAL:HB	1.88	0.54
1:C:11:ARG:NH1	1:C:216:ASP:OD1	2.39	0.54
1:B:289:LEU:C	1:B:291:PRO:HD2	2.33	0.54
1:C:175:MET:HA	1:C:323:MET:HE1	1.90	0.54
1:D:100:ASP:OD1	1:D:277:HIS:HE1	1.91	0.53
1:B:142:HIS:CD2	1:B:146:ASP:OD2	2.62	0.53
1:A:269:LYS:O	1:A:269:LYS:CG	2.56	0.53
1:B:125:LEU:HD23	1:B:128:ALA:HB2	1.92	0.52
1:C:326:MET:HE3	1:C:336:VAL:CG1	2.40	0.52
1:C:52:ILE:O	1:C:112:ALA:HA	2.09	0.51
1:C:326:MET:CE	1:C:336:VAL:HB	2.39	0.51
3:C:564:HOH:O	1:D:103:LYS:HE3	2.10	0.51
1:B:203:THR:HG22	1:B:212:VAL:HG22	1.93	0.51
1:C:96:MET:HE1	1:C:279:THR:CG2	2.41	0.51
1:A:178:TYR:C	1:A:178:TYR:CD1	2.89	0.51
1:B:183:LEU:HD22	1:B:344:ALA:HB2	1.93	0.50
1:C:326:MET:HE3	1:C:336:VAL:HG11	1.93	0.50
1:B:313:GLU:O	1:B:374:ALA:HA	2.11	0.50
1:D:88:CYS:O	1:D:376:LEU:HD11	2.11	0.50
1:C:178:TYR:OH	1:C:322:THR:HG21	2.12	0.50
1:C:36:GLU:HA	1:C:36:GLU:OE1	2.12	0.50
1:C:51:VAL:HG23	1:C:79:THR:CG2	2.42	0.49
1:D:142:HIS:CD2	1:D:146:ASP:HB2	2.46	0.49
1:C:64:GLY:O	1:C:65:PRO:C	2.55	0.49
1:D:102:LEU:CG	1:D:110:MET:HE3	2.34	0.49
1:D:58:PRO:HA	1:D:61:LEU:HD12	1.94	0.49
1:D:277:HIS:HD2	3:D:453:HOH:O	1.94	0.49
1:A:124:VAL:HG12	1:B:124:VAL:HG12	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:311:LEU:O	1:C:372:GLY:HA2	2.14	0.48
1:B:313:GLU:HA	1:B:337:ASN:ND2	2.28	0.48
1:C:163:GLU:OE2	1:C:235:ARG:NH2	2.47	0.47
1:B:118:MET:HE3	1:B:349:VAL:CG2	2.44	0.47
1:D:388:LEU:C	1:D:388:LEU:HD12	2.40	0.47
1:D:70:ALA:O	1:D:73:ALA:HB3	2.15	0.47
1:D:175:MET:HE1	1:D:239:THR:OG1	2.14	0.47
1:A:262:GLU:CD	1:A:265:ARG:HH21	2.22	0.47
1:C:158:GLY:HA3	1:C:234:PHE:CD1	2.50	0.47
1:C:198:GLU:OE1	1:C:359:THR:OG1	2.26	0.47
1:D:310:ASP:O	1:D:335:LYS:HD2	2.15	0.47
1:A:100:ASP:OD2	1:B:101:LEU:HG	2.15	0.47
1:C:296:THR:HG22	1:C:329:HIS:HE1	1.77	0.47
1:D:173:GLU:H	1:D:173:GLU:CD	2.23	0.47
1:D:312:PHE:HB2	1:D:336:VAL:HG22	1.96	0.47
1:B:88:CYS:O	1:B:376:LEU:HD11	2.15	0.46
1:A:78:ALA:HA	1:B:281:SER:O	2.15	0.46
1:A:158:GLY:HA3	1:A:234:PHE:CZ	2.50	0.46
1:A:361:ILE:O	1:A:365:ARG:HG3	2.16	0.46
1:D:237:ASP:OD2	1:D:237:ASP:N	2.48	0.46
1:B:171:THR:OG1	1:B:174:GLU:HG3	2.15	0.46
1:B:162:GLN:HE22	1:B:240:ILE:H	1.64	0.46
1:B:255:LEU:HD21	1:B:358:LEU:HG	1.98	0.46
1:B:266:ARG:HB2	1:B:268:LEU:HD22	1.97	0.46
1:B:230:LEU:CD1	1:B:243:ALA:HB2	2.46	0.46
1:D:142:HIS:CD2	1:D:146:ASP:OD2	2.67	0.46
1:C:355:ARG:HD2	1:C:355:ARG:C	2.41	0.45
1:B:204:VAL:O	1:B:205:THR:HB	2.16	0.45
1:B:157:MET:HE3	1:B:287:PHE:CE2	2.51	0.45
1:B:295:MET:CE	1:B:312:PHE:CE1	3.00	0.44
1:C:304:TRP:CZ2	1:C:371:ARG:HD3	2.52	0.44
1:A:133:ARG:O	1:C:129:ARG:HG3	2.16	0.44
1:C:11:ARG:HD3	1:C:198:GLU:HG3	1.99	0.44
1:C:310:ASP:O	1:C:311:LEU:HD23	2.18	0.44
1:C:6:ILE:HG21	1:C:255:LEU:HD23	1.99	0.44
1:D:125:LEU:HD23	1:D:128:ALA:HB2	1.99	0.44
1:D:195:LEU:HD21	1:D:339:TYR:HB3	1.99	0.44
1:C:281:SER:O	1:D:78:ALA:HA	2.18	0.44
1:A:80:GLY:HA2	1:B:382:GLU:OE2	2.18	0.44
1:C:218:GLN:N	1:C:219:PRO:CD	2.81	0.43
1:C:123:TYR:HB3	1:C:139:ILE:HG12	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:125:LEU:N	1:A:125:LEU:HD12	2.34	0.43
1:A:144:PHE:O	1:A:149:GLU:HG2	2.18	0.43
1:C:261:GLU:OE2	1:C:261:GLU:N	2.49	0.43
1:D:249:SER:OG	1:D:347:HIS:N	2.52	0.43
1:B:316:GLU:O	1:B:317:ALA:C	2.61	0.43
1:A:382:GLU:OE2	1:B:80:GLY:HA2	2.18	0.42
1:D:355:ARG:HD2	1:D:355:ARG:C	2.44	0.42
1:C:296:THR:CG2	1:C:329:HIS:CE1	3.01	0.42
1:A:124:VAL:HG22	1:A:140:LYS:HB2	2.01	0.42
1:B:86:LYS:HD3	1:B:378:ILE:CD1	2.49	0.42
1:C:313:GLU:O	1:C:374:ALA:HA	2.20	0.42
1:C:319:ALA:C	1:C:323:MET:HE3	2.45	0.42
1:C:320:MET:CA	1:C:323:MET:HE3	2.49	0.42
1:A:2:SER:O	1:A:103:LYS:NZ	2.51	0.41
1:B:289:LEU:C	1:B:291:PRO:CD	2.93	0.41
1:A:97:LEU:HD23	1:B:101:LEU:HD11	2.02	0.41
1:C:6:ILE:CG2	1:C:255:LEU:HD23	2.50	0.41
1:D:125:LEU:CD2	1:D:128:ALA:HB2	2.50	0.41
1:B:292:ILE:HD13	1:B:328:GLU:HG3	2.01	0.41
1:D:218:GLN:N	1:D:219:PRO:CD	2.84	0.41
1:D:174:GLU:HB3	1:D:323:MET:HE1	2.03	0.41
1:D:352:THR:O	1:D:356:ILE:HG12	2.21	0.41
1:B:11:ARG:HH11	1:B:11:ARG:HD2	1.76	0.40
1:B:280:GLN:NE2	1:B:297:ASN:HD21	2.19	0.40
1:C:306:LYS:HE3	1:C:330:GLY:O	2.22	0.40
1:C:39:GLN:OE1	1:C:39:GLN:O	2.38	0.40
1:D:46:GLU:HA	1:D:76:PRO:HG3	2.03	0.40
1:A:13:PRO:HD3	1:A:200:VAL:O	2.21	0.40
1:A:162:GLN:NE2	3:A:417:HOH:O	2.54	0.40
1:A:277:HIS:HD2	3:A:471:HOH:O	2.03	0.40
1:A:295:MET:HE1	1:A:314:ILE:HD13	2.03	0.40
1:C:318:PHE:O	1:C:319:ALA:C	2.63	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	388/399 (97%)	374 (96%)	14 (4%)	0	100	100
1	B	383/399 (96%)	371 (97%)	11 (3%)	1 (0%)	36	46
1	C	382/399 (96%)	363 (95%)	18 (5%)	1 (0%)	36	46
1	D	382/399 (96%)	365 (96%)	17 (4%)	0	100	100
All	All	1535/1596 (96%)	1473 (96%)	60 (4%)	2 (0%)	48	60

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	133	ARG
1	C	133	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	286/295 (97%)	275 (96%)	11 (4%)	29	44
1	B	283/295 (96%)	273 (96%)	10 (4%)	32	48
1	C	282/295 (96%)	272 (96%)	10 (4%)	32	48
1	D	282/295 (96%)	266 (94%)	16 (6%)	18	27
All	All	1133/1180 (96%)	1086 (96%)	47 (4%)	27	41

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	SER
1	A	124	VAL
1	A	148	LEU
1	A	194	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	206	SER
1	A	224	LEU
1	A	236	LYS
1	A	240	ILE
1	A	257	LEU
1	A	261	GLU
1	A	301	ARG
1	B	39	GLN
1	B	86	LYS
1	B	139	ILE
1	B	163	GLU
1	B	183	LEU
1	B	204	VAL
1	B	268	LEU
1	B	301	ARG
1	B	349	VAL
1	B	370	LYS
1	C	2	SER
1	C	39	GLN
1	C	133	ARG
1	C	143	MET
1	C	183	LEU
1	C	203	THR
1	C	210	GLU
1	C	226	LYS
1	C	231	ARG
1	C	284	PRO
1	D	2	SER
1	D	58	PRO
1	D	87	LEU
1	D	88	CYS
1	D	127	LYS
1	D	139	ILE
1	D	173	GLU
1	D	182	SER
1	D	184	LYS
1	D	220	LEU
1	D	229	SER
1	D	261	GLU
1	D	264	GLN
1	D	281	SER
1	D	306	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	389	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	108	GLN
1	A	162	GLN
1	A	277	HIS
1	A	280	GLN
1	A	347	HIS
1	A	362	ASN
1	A	366	GLN
1	B	68	GLN
1	B	107	ASN
1	B	142	HIS
1	B	162	GLN
1	B	277	HIS
1	B	280	GLN
1	B	337	ASN
1	B	345	GLN
1	B	366	GLN
1	C	68	GLN
1	C	223	ASN
1	C	264	GLN
1	C	280	GLN
1	C	282	GLN
1	C	333	HIS
1	C	366	GLN
1	D	68	GLN
1	D	99	HIS
1	D	107	ASN
1	D	108	GLN
1	D	142	HIS
1	D	218	GLN
1	D	277	HIS
1	D	280	GLN
1	D	282	GLN
1	D	315	ASN
1	D	362	ASN
1	D	366	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

1 ligand is 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	$\# Z > 2$
2	GOL	C	401	-	5,5,5	0.21	0	5,5,5	0.47	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	C	401	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	401	GOL	O1-C1-C2-C3
2	C	401	GOL	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	401	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	390/399 (97%)	-0.12	1 (0%) 90 90	16, 26, 40, 69	0
1	B	387/399 (96%)	0.06	5 (1%) 75 76	18, 28, 47, 73	0
1	C	386/399 (96%)	0.04	1 (0%) 90 90	19, 30, 45, 72	0
1	D	386/399 (96%)	0.05	1 (0%) 90 90	19, 30, 47, 69	0
All	All	1549/1596 (97%)	0.01	8 (0%) 87 87	16, 28, 46, 73	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	209	GLY	5.1
1	B	237	ASP	2.7
1	B	391	LEU	2.5
1	D	209	GLY	2.5
1	C	209	GLY	2.4
1	B	224	LEU	2.1
1	B	269	LYS	2.1
1	A	237	ASP	2.1

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	GOL	C	401	6/6	0.88	0.12	30,34,35,36	0

6.5 Other polymers [i](#)

There are no such residues in this entry.