



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:54 PM UTC

PDB ID : 5XVI / pdb_00005xvi
Title : Crystal Structure of Aspergillus niger Apo- Glutamate Dehydrogenase
Authors : Prakash, P.; Puneekar, N.S.; Bhaumik, P.
Deposited on : 2017-06-28
Resolution : 2.80 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

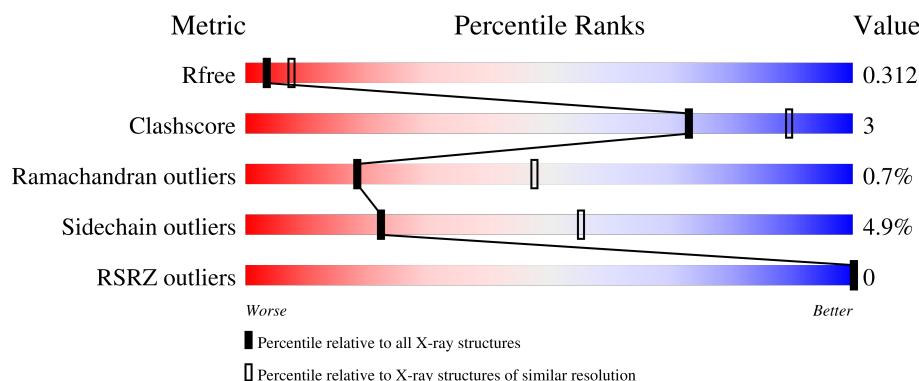
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

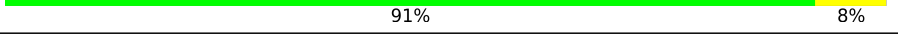
The reported resolution of this entry is 2.80 Å.

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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	460	
1	B	460	
1	C	460	
1	D	460	
1	E	460	

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Mol	Chain	Length	Quality of chain
1	F	460	 88% 11%

2 Entry composition [i](#)

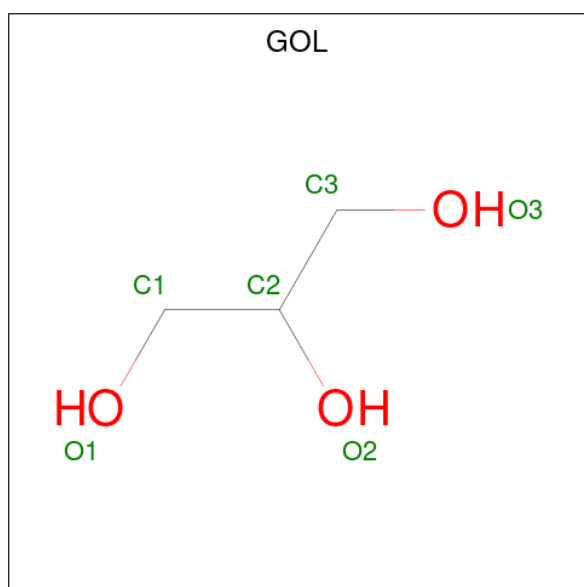
There are 3 unique types of molecules in this entry. The entry contains 21516 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Glutamate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	459	Total	C	N	O	S	0	6	0
			3503	2209	611	670	13			
1	B	459	Total	C	N	O	S	0	4	0
			3494	2203	608	670	13			
1	C	459	Total	C	N	O	S	0	3	0
			3485	2197	607	668	13			
1	D	458	Total	C	N	O	S	0	5	0
			3482	2198	605	665	14			
1	E	458	Total	C	N	O	S	0	3	0
			3479	2193	606	667	13			
1	F	458	Total	C	N	O	S	0	2	0
			3476	2190	606	667	13			

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



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

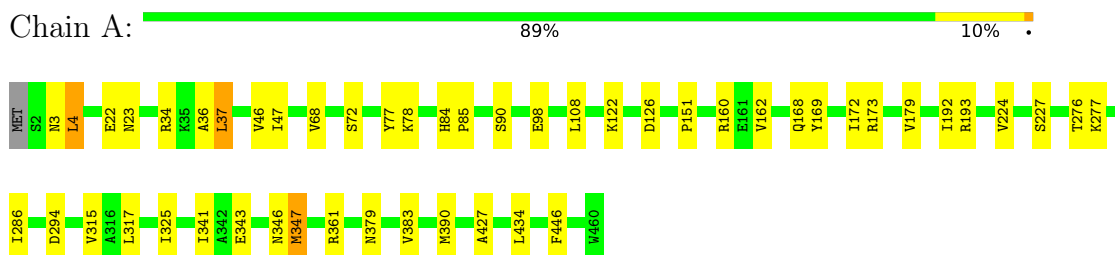
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	95	Total	O	0	0
			95	95		
3	B	95	Total	O	0	0
			95	95		
3	C	84	Total	O	0	0
			84	84		
3	D	104	Total	O	0	0
			104	104		
3	E	99	Total	O	0	0
			99	99		
3	F	108	Total	O	0	0
			108	108		

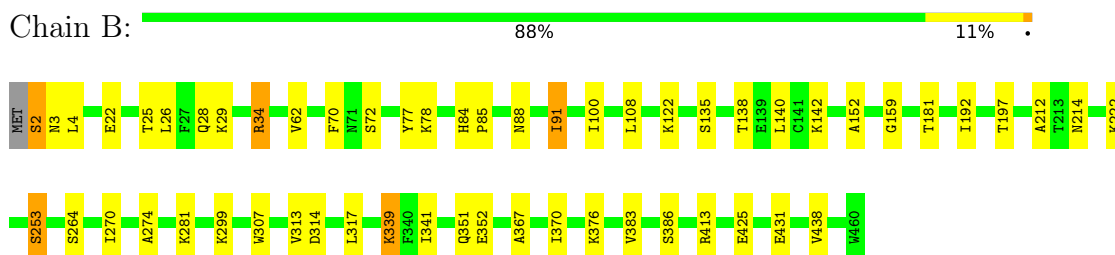
3 Residue-property plots

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.

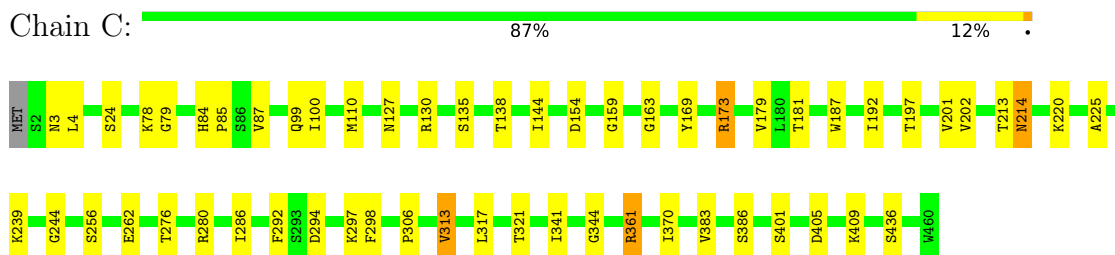
- Molecule 1: Glutamate dehydrogenase



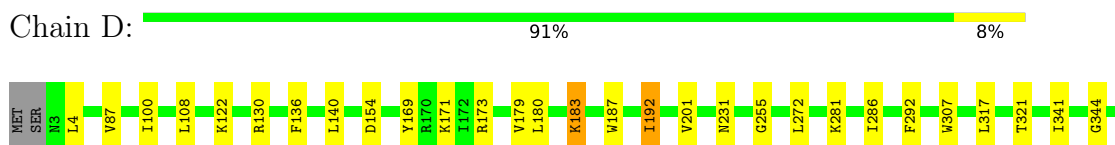
- Molecule 1: Glutamate dehydrogenase



- Molecule 1: Glutamate dehydrogenase



- Molecule 1: Glutamate dehydrogenase





- Molecule 1: Glutamate dehydrogenase

Chain E: 87% 11%



- Molecule 1: Glutamate dehydrogenase

Chain F: 88% 11%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	92.80Å 92.82Å 111.69Å 103.46° 94.17° 120.13°	Depositor
Resolution (Å)	35.00 – 2.80 35.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	91.8 (35.00-2.80) 73.0 (35.00-2.80)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.52 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.226 , 0.310 0.231 , 0.312	Depositor DCC
R_{free} test set	3451 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	27.1	Xtriage
Anisotropy	0.161	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 17.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	21516	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.13% 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: 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	0.77	0/3589	1.02	0/4853
1	B	0.76	0/3577	0.98	2/4834 (0.0%)
1	C	0.74	0/3565	1.02	4/4818 (0.1%)
1	D	0.76	0/3568	1.00	3/4823 (0.1%)
1	E	0.77	0/3559	0.99	3/4811 (0.1%)
1	F	0.73	0/3550	0.97	0/4799
All	All	0.76	0/21408	1.00	12/28938 (0.0%)

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	B	0	1

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	255	GLY	N-CA-C	5.90	119.75	111.19
1	C	79	GLY	N-CA-C	5.65	119.36	111.00
1	B	142	LYS	N-CA-C	5.58	118.13	111.71
1	C	87	VAL	N-CA-C	5.57	116.59	109.30
1	B	307	TRP	N-CA-C	5.35	116.92	111.14
1	E	64	ARG	CA-C-N	5.23	125.21	121.65
1	E	64	ARG	C-N-CA	5.23	125.21	121.65
1	C	306	PRO	N-CA-C	5.20	120.60	113.84
1	E	100	ILE	CB-CA-C	-5.19	105.13	112.14
1	D	100	ILE	CB-CA-C	-5.19	105.33	111.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	100	ILE	CB-CA-C	-5.17	105.35	111.97
1	D	307	TRP	N-CA-C	5.09	116.52	111.07

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	2	SER	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	3503	0	3445	25	0
1	B	3494	0	3431	23	0
1	C	3485	0	3422	24	0
1	D	3482	0	3420	13	0
1	E	3479	0	3412	34	0
1	F	3476	0	3403	23	0
2	A	6	0	8	0	0
2	D	6	0	8	0	0
3	A	95	0	0	11	0
3	B	95	0	0	7	0
3	C	84	0	0	0	0
3	D	104	0	0	1	0
3	E	99	0	0	2	0
3	F	108	0	0	4	0
All	All	21516	0	20549	134	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 (134) 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:B:351:GLN:NE2	3:B:501:HOH:O	2.05	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:270:ILE:HG22	3:B:517:HOH:O	1.79	0.80
1:F:47:ILE:O	3:F:501:HOH:O	2.03	0.76
1:F:67:ARG:O	3:F:501:HOH:O	2.05	0.75
1:C:138:THR:HG21	1:E:171:LYS:HD3	1.69	0.72
1:A:37:LEU:HA	3:A:601:HOH:O	1.92	0.70
1:E:78:LYS:HD3	1:E:390:MET:HE1	1.75	0.68
1:E:22:GLU:OE2	1:E:34:ARG:NH1	2.26	0.67
1:B:22:GLU:HG3	3:B:539:HOH:O	1.94	0.67
1:A:446:PHE:HE1	3:A:601:HOH:O	1.77	0.67
1:E:150:VAL:HG11	1:E:390:MET:HE3	1.77	0.66
1:A:37:LEU:N	3:A:601:HOH:O	2.30	0.64
1:A:446:PHE:CE1	3:A:601:HOH:O	2.50	0.64
1:C:297:LYS:HG2	1:C:298:PHE:CD2	2.33	0.64
1:E:16:GLU:O	1:E:20:THR:HG23	1.99	0.62
1:B:138:THR:HG21	1:D:171:LYS:HE3	1.82	0.62
1:B:339:LYS:HA	1:B:370:ILE:HA	1.82	0.61
1:C:138:THR:CG2	1:E:171:LYS:HD3	2.31	0.61
1:F:94:PHE:O	1:F:98:GLU:HG3	2.01	0.60
1:C:280:ARG:O	1:C:280:ARG:HG3	2.01	0.59
1:F:192:ILE:HG22	1:F:192:ILE:O	2.03	0.59
1:A:37:LEU:CA	3:A:601:HOH:O	2.49	0.59
1:D:183:LYS:HG2	1:D:187:TRP:CZ3	2.38	0.58
1:C:276:THR:HG21	1:C:286:ILE:HG21	1.87	0.56
1:A:276:THR:HG21	1:A:286:ILE:HG21	1.86	0.56
1:E:11:GLU:O	1:E:15:LYS:HG3	2.07	0.55
1:E:72:SER:HB3	1:E:77:TYR:CE1	2.42	0.55
1:A:224:VAL:HG13	1:A:315:VAL:HB	1.89	0.54
1:D:169:TYR:CE1	1:D:179:VAL:HG21	2.42	0.54
1:A:72:SER:HB3	1:A:77:TYR:CE1	2.42	0.54
1:B:72:SER:HB3	1:B:77:TYR:CE1	2.44	0.53
1:B:152:ALA:HB2	1:B:181:THR:OG1	2.08	0.53
1:C:84:HIS:CD2	1:C:85:PRO:HD2	2.42	0.53
1:B:274:ALA:HB2	3:B:517:HOH:O	2.09	0.53
1:A:347:MET:SD	3:A:668:HOH:O	2.58	0.53
1:B:25:THR:O	1:B:29:LYS:HG3	2.09	0.53
1:C:127:ASN:OD1	1:C:130:ARG:NH1	2.39	0.53
1:B:88:ASN:OD1	1:B:91:ILE:HG13	2.09	0.52
1:C:201:VAL:HG21	1:C:344:GLY:HA2	1.90	0.52
1:E:280:ARG:HG2	3:E:542:HOH:O	2.09	0.52
1:C:169:TYR:CE1	1:C:179:VAL:HG21	2.45	0.52
1:A:169:TYR:CE1	1:A:179:VAL:HG21	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:216[B]:GLN:HA	1:E:216[B]:GLN:OE1	2.08	0.52
1:C:144:ILE:O	1:C:173:ARG:NH2	2.43	0.52
1:E:458:ASP:OD2	1:F:170:ARG:NH2	2.43	0.51
1:E:192:ILE:O	1:E:192:ILE:HG22	2.10	0.51
1:F:227:SER:OG	1:F:324:GLU:OE2	2.24	0.51
1:B:413:ARG:HD3	3:B:524:HOH:O	2.11	0.51
1:E:70:PHE:HB3	1:E:100:ILE:HD11	1.93	0.51
1:D:201:VAL:HG21	1:D:344:GLY:HA2	1.93	0.50
1:A:78:LYS:HE2	1:A:390:MET:SD	2.51	0.50
1:B:222:LYS:HD3	1:B:314:ASP:HB3	1.93	0.50
1:E:150:VAL:CG1	1:E:390:MET:HE3	2.41	0.50
1:E:283:LEU:O	1:E:287:VAL:HG23	2.12	0.49
1:F:276:THR:HG21	1:F:286:ILE:HG21	1.93	0.49
1:C:225:ALA:HB2	1:C:313:VAL:HG21	1.94	0.49
1:D:180:LEU:O	1:D:183:LYS:HD3	2.12	0.49
1:F:44:GLU:OE1	1:F:77:TYR:OH	2.28	0.49
1:E:11:GLU:O	1:E:15:LYS:CG	2.61	0.48
1:E:374:PRO:HG3	1:E:438:VAL:HA	1.95	0.48
1:C:197:THR:O	1:C:201:VAL:HG23	2.13	0.48
1:B:22:GLU:OE1	1:B:34:ARG:NH1	2.47	0.48
1:E:183:LYS:HG2	1:E:187:TRP:CE3	2.48	0.48
1:A:84:HIS:CG	1:A:85:PRO:HD2	2.49	0.47
1:E:51:VAL:HG11	1:E:132:PHE:CE1	2.49	0.47
1:F:64:ARG:O	1:F:117:SER:OG	2.25	0.47
1:E:193:ARG:HB3	1:E:194:PRO:HD3	1.97	0.47
1:D:192:ILE:HG22	1:D:192:ILE:O	2.14	0.47
1:D:286:ILE:HD12	1:D:292:PHE:CE2	2.49	0.47
1:E:228:GLY:CA	1:E:320:ALA:HB2	2.45	0.47
1:E:150:VAL:HG21	1:E:390:MET:HE2	1.96	0.47
1:F:328:GLU:O	1:F:332:VAL:HG23	2.14	0.46
1:F:74:LEU:O	1:F:109:ASN:HA	2.15	0.46
1:E:108:LEU:HB2	1:E:110:MET:HE2	1.97	0.46
1:B:84:HIS:CG	1:B:85:PRO:HD2	2.52	0.45
1:A:46:VAL:HG22	1:A:68:VAL:HG13	1.98	0.45
1:C:138:THR:HG22	1:E:171:LYS:HE2	1.98	0.45
1:A:22:GLU:OE2	1:A:34:ARG:NH1	2.31	0.45
1:E:163:GLY:HA2	1:E:187:TRP:CH2	2.52	0.45
1:F:343:GLU:OE2	1:F:348:GLY:N	2.49	0.45
1:C:405:ASP:O	1:C:409:LYS:HG3	2.16	0.45
1:D:183:LYS:HG2	1:D:187:TRP:CE3	2.52	0.45
1:A:168:GLN:HE21	1:A:172:ILE:HD11	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:272:LEU:HD22	3:D:658:HOH:O	2.15	0.44
1:A:427:ALA:HB1	3:A:660:HOH:O	2.17	0.44
1:B:2:SER:OG	1:B:3:ASN:N	2.50	0.44
1:E:78:LYS:HD3	1:E:390:MET:CE	2.45	0.44
1:E:273:ILE:O	1:E:277:LYS:HB2	2.18	0.43
1:E:366:GLY:N	1:E:432:GLY:O	2.52	0.43
1:F:47:ILE:N	3:F:501:HOH:O	2.38	0.43
1:C:341:ILE:HD12	1:C:370:ILE:HD11	1.99	0.43
1:C:213:THR:O	1:C:214:ASN:C	2.62	0.43
1:D:416:PHE:CZ	1:D:420:LEU:HD22	2.53	0.43
1:C:286:ILE:HD12	1:C:292:PHE:CE2	2.54	0.43
1:C:163:GLY:HA2	1:C:187:TRP:CH2	2.54	0.43
1:C:181:THR:HG21	1:C:386:SER:HB3	2.01	0.42
1:C:361:ARG:NH2	1:C:436:SER:HB2	2.34	0.42
1:F:144:ILE:HA	1:F:149:ASP:HB3	2.01	0.42
1:B:212:ALA:O	1:B:367:ALA:HB2	2.19	0.42
1:F:67:ARG:C	3:F:501:HOH:O	2.59	0.42
1:F:247:VAL:N	1:F:264:SER:OG	2.51	0.42
1:C:220:LYS:HA	1:C:244:GLY:O	2.19	0.42
1:E:383:VAL:HG23	3:E:507:HOH:O	2.17	0.42
1:D:390:MET:HE3	1:E:396:ARG:NH1	2.35	0.42
1:A:379:ASN:HA	3:A:616:HOH:O	2.19	0.42
1:B:70:PHE:HB3	1:B:100:ILE:HD11	2.01	0.42
1:C:138:THR:CG2	1:E:171:LYS:HE2	2.50	0.42
1:B:78:LYS:HE3	1:B:386:SER:HB3	2.02	0.42
1:A:361:ARG:NH1	1:A:434:LEU:O	2.43	0.41
1:F:313:VAL:HG13	1:F:338:CYS:HB2	2.01	0.41
1:A:98:GLU:HG2	1:A:347:MET:HE1	2.02	0.41
1:B:2:SER:HB3	1:B:4:LEU:CD2	2.50	0.41
1:F:22:GLU:OE1	1:F:34:ARG:NH1	2.53	0.41
1:A:36:ALA:C	3:A:601:HOH:O	2.61	0.41
3:B:504:HOH:O	1:F:453:MET:HE3	2.21	0.41
1:E:201:VAL:HG21	1:E:344:GLY:HA2	2.03	0.41
1:A:346:ASN:ND2	3:A:603:HOH:O	2.53	0.41
1:C:78:LYS:HG2	1:C:110:MET:SD	2.61	0.41
1:B:2:SER:HB3	1:B:4:LEU:HD23	2.03	0.41
1:D:136:PHE:CE2	1:D:140:LEU:HD22	2.56	0.41
1:F:341:ILE:HD13	1:F:357:PHE:CZ	2.56	0.41
1:A:3:ASN:O	1:A:4:LEU:HD13	2.20	0.40
1:C:202:VAL:HG11	1:C:239:LYS:HG3	2.02	0.40
1:D:357:PHE:CE1	1:D:370:ILE:HD13	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:179:VAL:HG13	1:F:180:LEU:HG	2.03	0.40
1:F:192:ILE:O	1:F:192:ILE:CG2	2.69	0.40
1:A:193[A]:ARG:NH1	3:A:605:HOH:O	2.54	0.40
1:B:425:GLU:OE1	3:B:502:HOH:O	2.22	0.40
1:E:72:SER:OG	1:F:170:ARG:NH1	2.53	0.40
1:A:126:ASP:OD1	1:A:160:ARG:NH1	2.54	0.40
1:B:88:ASN:OD1	1:B:88:ASN:C	2.65	0.40
1:E:301:ILE:HD13	1:E:309:HIS:CG	2.56	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	463/460 (101%)	433 (94%)	26 (6%)	4 (1%)	14	41
1	B	461/460 (100%)	425 (92%)	32 (7%)	4 (1%)	14	41
1	C	460/460 (100%)	426 (93%)	29 (6%)	5 (1%)	11	36
1	D	461/460 (100%)	438 (95%)	21 (5%)	2 (0%)	30	60
1	E	459/460 (100%)	431 (94%)	25 (5%)	3 (1%)	18	47
1	F	458/460 (100%)	433 (94%)	23 (5%)	2 (0%)	30	60
All	All	2762/2760 (100%)	2586 (94%)	156 (6%)	20 (1%)	18	47

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	192	ILE
1	A	294	ASP
1	C	192	ILE
1	E	214	ASN

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Mol	Chain	Res	Type
1	B	253	SER
1	C	214	ASN
1	D	192	ILE
1	B	264	SER
1	C	159	GLY
1	C	294	ASP
1	B	159	GLY
1	B	192	ILE
1	E	294	ASP
1	D	154	ASP
1	F	159	GLY
1	F	192	ILE
1	A	23	ASN
1	C	154	ASP
1	E	192	ILE
1	A	151	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	362/357 (101%)	347 (96%)	15 (4%)	27	62
1	B	360/357 (101%)	338 (94%)	22 (6%)	17	46
1	C	359/357 (101%)	345 (96%)	14 (4%)	28	64
1	D	358/357 (100%)	340 (95%)	18 (5%)	22	54
1	E	358/357 (100%)	340 (95%)	18 (5%)	22	54
1	F	357/357 (100%)	337 (94%)	20 (6%)	19	50
All	All	2154/2142 (101%)	2047 (95%)	107 (5%)	22	54

All (107) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LEU
1	A	37	LEU

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Mol	Chain	Res	Type
1	A	47	ILE
1	A	90	SER
1	A	108	LEU
1	A	122	LYS
1	A	162	VAL
1	A	227	SER
1	A	277	LYS
1	A	317	LEU
1	A	325	ILE
1	A	341	ILE
1	A	343	GLU
1	A	347	MET
1	A	383	VAL
1	B	26	LEU
1	B	28	GLN
1	B	34	ARG
1	B	62	VAL
1	B	91	ILE
1	B	108	LEU
1	B	122	LYS
1	B	135	SER
1	B	197	THR
1	B	214	ASN
1	B	253	SER
1	B	281	LYS
1	B	299	LYS
1	B	313	VAL
1	B	317	LEU
1	B	339	LYS
1	B	341	ILE
1	B	352	GLU
1	B	376	LYS
1	B	383	VAL
1	B	431	GLU
1	B	438	VAL
1	C	3	ASN
1	C	4	LEU
1	C	24	SER
1	C	99	GLN
1	C	135	SER
1	C	173	ARG
1	C	256	SER

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Mol	Chain	Res	Type
1	C	262	GLU
1	C	313	VAL
1	C	317	LEU
1	C	321	THR
1	C	361	ARG
1	C	383	VAL
1	C	401	SER
1	D	4	LEU
1	D	87	VAL
1	D	108	LEU
1	D	122	LYS
1	D	130	ARG
1	D	173	ARG
1	D	183	LYS
1	D	231	ASN
1	D	281	LYS
1	D	317	LEU
1	D	321	THR
1	D	341	ILE
1	D	352	GLU
1	D	385	VAL
1	D	386	SER
1	D	394	SER
1	D	401	SER
1	D	447	THR
1	E	20	THR
1	E	24	SER
1	E	35	LYS
1	E	60	VAL
1	E	69	GLN
1	E	105	LEU
1	E	108	LEU
1	E	141[A]	CYS
1	E	141[B]	CYS
1	E	183	LYS
1	E	280	ARG
1	E	317	LEU
1	E	328	GLU
1	E	341	ILE
1	E	402	GLU
1	E	409	LYS
1	E	428	THR

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Mol	Chain	Res	Type
1	E	438	VAL
1	F	4	LEU
1	F	19	SER
1	F	22	GLU
1	F	62	VAL
1	F	70	PHE
1	F	108	LEU
1	F	171	LYS
1	F	173	ARG
1	F	229	SER
1	F	232	VAL
1	F	262	GLU
1	F	279	GLU
1	F	315	VAL
1	F	317	LEU
1	F	386[A]	SER
1	F	386[B]	SER
1	F	402	GLU
1	F	413	ARG
1	F	417	LYS
1	F	438	VAL

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	3	ASN
1	A	168	GLN
1	A	175	GLN
1	A	214	ASN
1	B	12	GLN
1	B	28	GLN
1	B	30	ASN
1	B	331	GLN
1	B	442	ASN
1	C	231	ASN
1	C	275	GLN
1	C	335	ASN
1	C	351	GLN
1	C	424	GLN
1	D	6	HIS
1	D	48	GLN
1	D	99	GLN

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Mol	Chain	Res	Type
1	D	351	GLN
1	E	48	GLN
1	E	309	HIS
1	E	424	GLN
1	F	23	ASN
1	F	99	GLN
1	F	424	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 ⓘ

2 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	$\# Z > 2$
2	GOL	A	501	-	5,5,5	0.52	0	5,5,5	0.38	0
2	GOL	D	501	-	5,5,5	0.55	0	5,5,5	0.25	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	501	-	-	2/4/4/4	-
2	GOL	D	501	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	GOL	C1-C2-C3-O3
2	D	501	GOL	O1-C1-C2-C3
2	A	501	GOL	O2-C2-C3-O3
2	D	501	GOL	O1-C1-C2-O2

There are no ring outliers.

No monomer is involved in short contacts.

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	459/460 (99%)	-1.68	0 100 100	9, 24, 48, 53	6 (1%)
1	B	459/460 (99%)	-1.57	0 100 100	12, 32, 62, 87	4 (0%)
1	C	459/460 (99%)	-1.64	0 100 100	11, 27, 52, 69	3 (0%)
1	D	458/460 (99%)	-1.69	0 100 100	9, 24, 42, 61	5 (1%)
1	E	458/460 (99%)	-1.68	0 100 100	10, 24, 41, 53	3 (0%)
1	F	458/460 (99%)	-1.67	0 100 100	10, 26, 40, 54	2 (0%)
All	All	2751/2760 (99%)	-1.65	0 100 100	9, 25, 49, 87	23 (0%)

There are no RSRZ outliers to report.

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
2	GOL	A	501	6/6	0.99	0.04	28,30,31,31	0
2	GOL	D	501	6/6	0.99	0.06	27,28,28,29	0

6.5 Other polymers [i](#)

There are no such residues in this entry.