



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 13, 2023 – 08:31 PM JST

PDB ID : 5XVI
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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtrriage (Phenix) : 1.13
EDS : 2.36
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

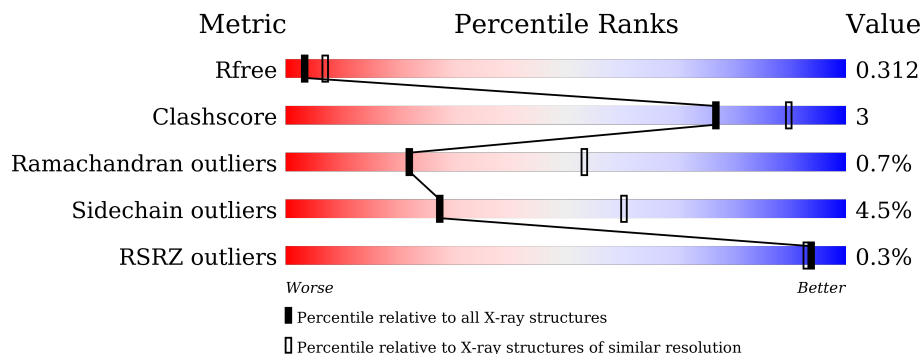
1 Overall quality at a glance

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}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (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	 90% 9% .
1	B	460	 89% 10% .
1	C	460	 88% 11%
1	D	460	 92% 7%
1	E	460	 87% 11% .
1	F	460	 89% 10%

2 Entry composition [i](#)

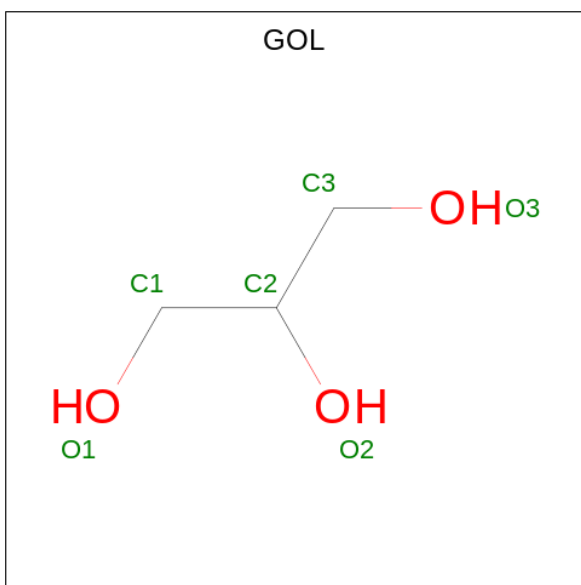
There are 3 unique types of molecules in this entry. The entry contains 21516 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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



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		

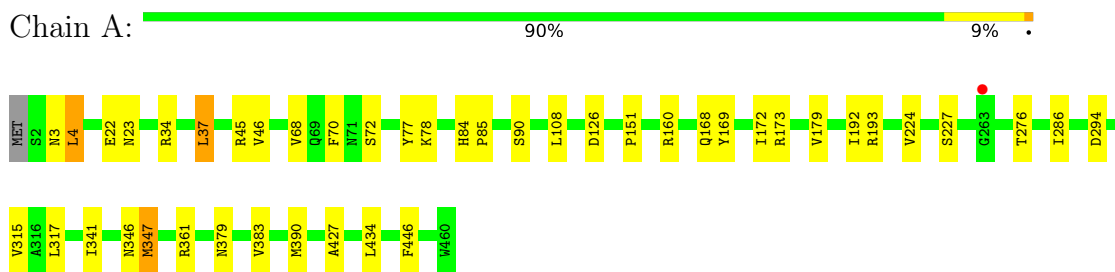
- Molecule 3 is water.

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		

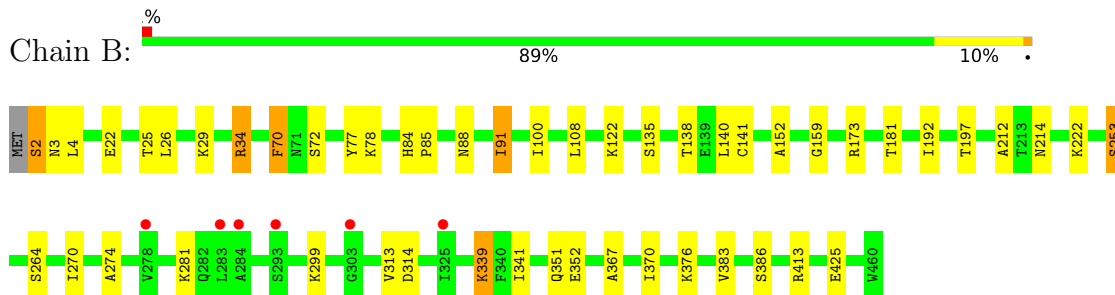
3 Residue-property plots i

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

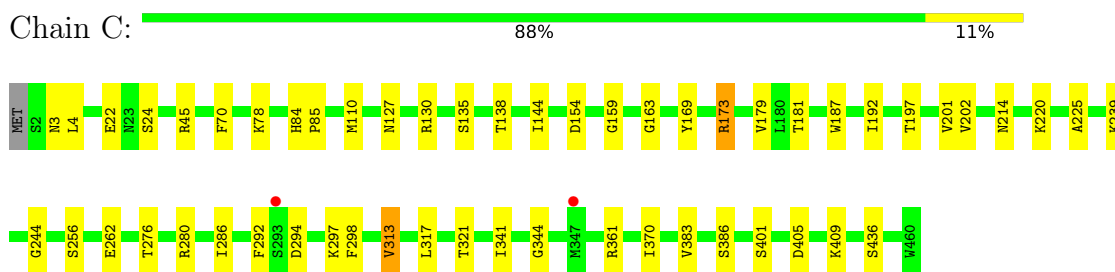
- Molecule 1: Glutamate dehydrogenase



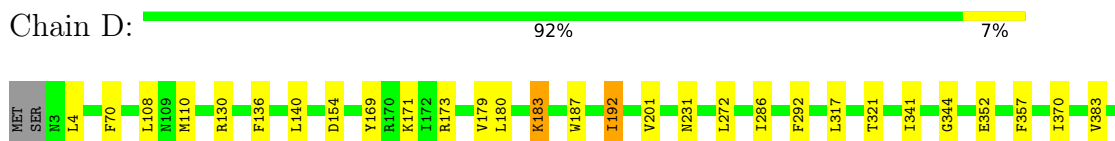
- Molecule 1: Glutamate dehydrogenase



- Molecule 1: Glutamate dehydrogenase



- Molecule 1: Glutamate dehydrogenase





- Molecule 1: Glutamate dehydrogenase

Chain E: 87% 11%



- Molecule 1: Glutamate dehydrogenase

Chain F: 89% 10%



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 34.25 – 2.80	Depositor EDS
% Data completeness (in resolution range)	91.8 (35.00-2.80) 73.0 (34.25-2.80)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.52 (at 2.81Å)	Xtrriage
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	Xtrriage
Anisotropy	0.161	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 8.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.24$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	21516	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtrriage'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	0.55	0/3589	0.74	1/4853 (0.0%)
1	B	0.53	0/3577	0.71	0/4834
1	C	0.52	0/3565	0.72	1/4818 (0.0%)
1	D	0.54	0/3568	0.72	0/4823
1	E	0.55	0/3559	0.71	1/4811 (0.0%)
1	F	0.53	0/3550	0.70	0/4799
All	All	0.54	0/21408	0.72	3/28938 (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 (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	C	45	ARG	NE-CZ-NH2	5.61	123.10	120.30
1	A	45	ARG	NE-CZ-NH2	5.41	123.01	120.30
1	E	252	ASP	CB-CG-OD1	5.10	122.89	118.30

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 [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	3503	0	3445	23	0
1	B	3494	0	3431	22	0
1	C	3485	0	3422	23	0
1	D	3482	0	3420	13	0
1	E	3479	0	3412	33	0
1	F	3476	0	3403	19	0
2	A	6	0	8	0	0
2	D	6	0	8	0	0
3	A	95	0	0	10	0
3	B	95	0	0	6	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	3	0
All	All	21516	0	20549	126	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 (126) 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
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: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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:78:LYS:HD3	1:E:390:MET:HE1	1.89	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:E:150:VAL:HG11	1:E:390:MET:HE3	1.90	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
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: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:E:150:VAL:HG21	1:E:390:MET:HE2	1.92	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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:E:78:LYS:HE2	1:E:390:MET:HE3	1.95	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: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:D:110:MET:HE1	1:D:383:VAL:HG13	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:E:78:LYS:HD3	1:E:390:MET:CE	2.45	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
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: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:D:416:PHE:CZ	1:D:420:LEU:HD22	2.53	0.43
1:E:150:VAL:HG11	1:E:390:MET:CE	2.48	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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: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: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
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:E:301:ILE:HD13	1:E:309:HIS:CG	2.56	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	463/460 (101%)	433 (94%)	26 (6%)	4 (1%)	17	46
1	B	461/460 (100%)	425 (92%)	32 (7%)	4 (1%)	17	46
1	C	460/460 (100%)	426 (93%)	29 (6%)	5 (1%)	14	41
1	D	461/460 (100%)	438 (95%)	21 (5%)	2 (0%)	34	66
1	E	459/460 (100%)	431 (94%)	25 (5%)	3 (1%)	22	53
1	F	458/460 (100%)	433 (94%)	23 (5%)	2 (0%)	34	66
All	All	2762/2760 (100%)	2586 (94%)	156 (6%)	20 (1%)	22	53

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
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 [i](#)

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%)	352 (97%)	10 (3%)	43	77
1	B	360/357 (101%)	339 (94%)	21 (6%)	20	50
1	C	359/357 (101%)	345 (96%)	14 (4%)	32	66
1	D	358/357 (100%)	344 (96%)	14 (4%)	32	66
1	E	358/357 (100%)	338 (94%)	20 (6%)	21	51
1	F	357/357 (100%)	337 (94%)	20 (6%)	21	51
All	All	2154/2142 (101%)	2055 (95%)	99 (5%)	27	60

All (99) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LEU
1	A	37	LEU
1	A	70	PHE
1	A	90	SER
1	A	108	LEU
1	A	227	SER
1	A	317	LEU
1	A	341	ILE
1	A	347	MET
1	A	383	VAL
1	B	26	LEU
1	B	34	ARG
1	B	70	PHE
1	B	91	ILE
1	B	108	LEU
1	B	122	LYS
1	B	135	SER
1	B	141[A]	CYS
1	B	141[B]	CYS
1	B	173	ARG
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	339	LYS
1	B	341	ILE
1	B	352	GLU
1	B	376	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	383	VAL
1	C	3	ASN
1	C	4	LEU
1	C	22	GLU
1	C	24	SER
1	C	70	PHE
1	C	135	SER
1	C	173	ARG
1	C	256	SER
1	C	262	GLU
1	C	313	VAL
1	C	317	LEU
1	C	321	THR
1	C	383	VAL
1	C	401	SER
1	D	4	LEU
1	D	70	PHE
1	D	108	LEU
1	D	130	ARG
1	D	173	ARG
1	D	183	LYS
1	D	231	ASN
1	D	317	LEU
1	D	321	THR
1	D	341	ILE
1	D	352	GLU
1	D	386	SER
1	D	394	SER
1	D	401	SER
1	E	20	THR
1	E	24	SER
1	E	35	LYS
1	E	69	GLN
1	E	70	PHE
1	E	94	PHE
1	E	105	LEU
1	E	108	LEU
1	E	141[A]	CYS
1	E	141[B]	CYS
1	E	183	LYS
1	E	231	ASN
1	E	280	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	317	LEU
1	E	328	GLU
1	E	341	ILE
1	E	402	GLU
1	E	409	LYS
1	E	428	THR
1	E	438	VAL
1	F	4	LEU
1	F	19	SER
1	F	70	PHE
1	F	94	PHE
1	F	102	LYS
1	F	108	LEU
1	F	171	LYS
1	F	173	ARG
1	F	229	SER
1	F	262	GLU
1	F	277	LYS
1	F	279	GLU
1	F	317	LEU
1	F	386[A]	SER
1	F	386[B]	SER
1	F	402	GLU
1	F	410	ASP
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 (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	109	ASN
1	A	168	GLN
1	B	30	ASN
1	B	442	ASN
1	C	30	ASN
1	C	335	ASN
1	D	254	GLN
1	D	379	ASN
1	F	23	ASN
1	F	99	GLN
1	F	424	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	0.50	0	5,5,5	0.37	0
2	GOL	D	501	-	5,5,5	0.53	0	5,5,5	0.26	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%)	-0.40	1 (0%) 95 94	12, 24, 48, 53	0
1	B	459/460 (99%)	-0.17	6 (1%) 77 72	14, 32, 62, 87	0
1	C	459/460 (99%)	-0.32	2 (0%) 92 91	14, 27, 52, 69	0
1	D	458/460 (99%)	-0.44	0 100 100	12, 24, 42, 61	0
1	E	458/460 (99%)	-0.41	0 100 100	12, 24, 41, 53	0
1	F	458/460 (99%)	-0.40	0 100 100	12, 26, 40, 54	0
All	All	2751/2760 (99%)	-0.36	9 (0%) 94 93	12, 25, 49, 87	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	284	ALA	3.5
1	B	325	ILE	3.3
1	B	303	GLY	3.2
1	B	283	LEU	2.5
1	C	293	SER	2.3
1	B	278	VAL	2.2
1	A	263	GLY	2.2
1	B	293	SER	2.1
1	C	347	MET	2.0

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 monosaccharides 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	0.78	0.27	28,30,31,31	0
2	GOL	D	501	6/6	0.89	0.11	27,28,28,29	0

6.5 Other polymers [i](#)

There are no such residues in this entry.