



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 10:49 AM UTC

PDB ID : 2NQU / pdb_00002nqu
Title : MoeA E188Q
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Deposited on : 2006-10-31
Resolution : 2.70 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

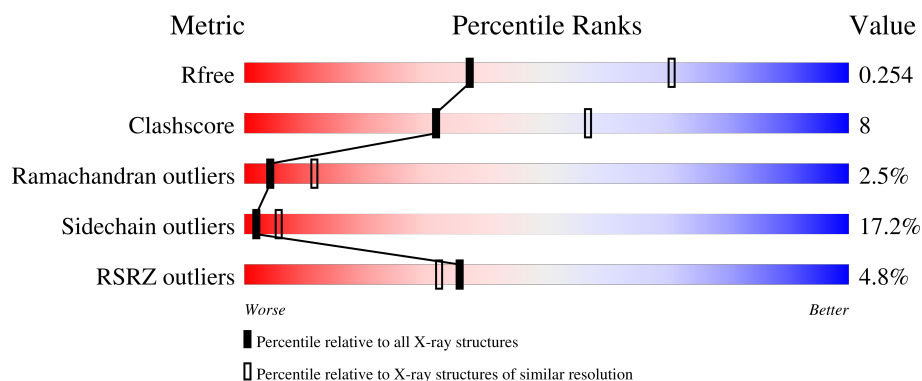
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	411	3% 71% 22% 5% .
1	B	411	7% 72% 20% 5% ..

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 6132 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.

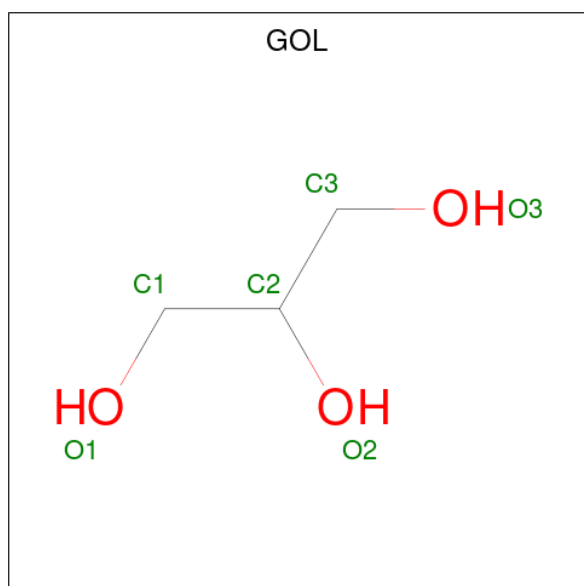
- Molecule 1 is a protein called Molybdopterin biosynthesis protein moeA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	403	Total	C	N	O	S	0	0	0
			3040	1918	532	577	13			
1	B	404	Total	C	N	O	S	0	0	0
			3044	1920	533	578	13			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	188	GLN	GLU	engineered mutation	UNP P12281
B	188	GLN	GLU	engineered mutation	UNP P12281

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

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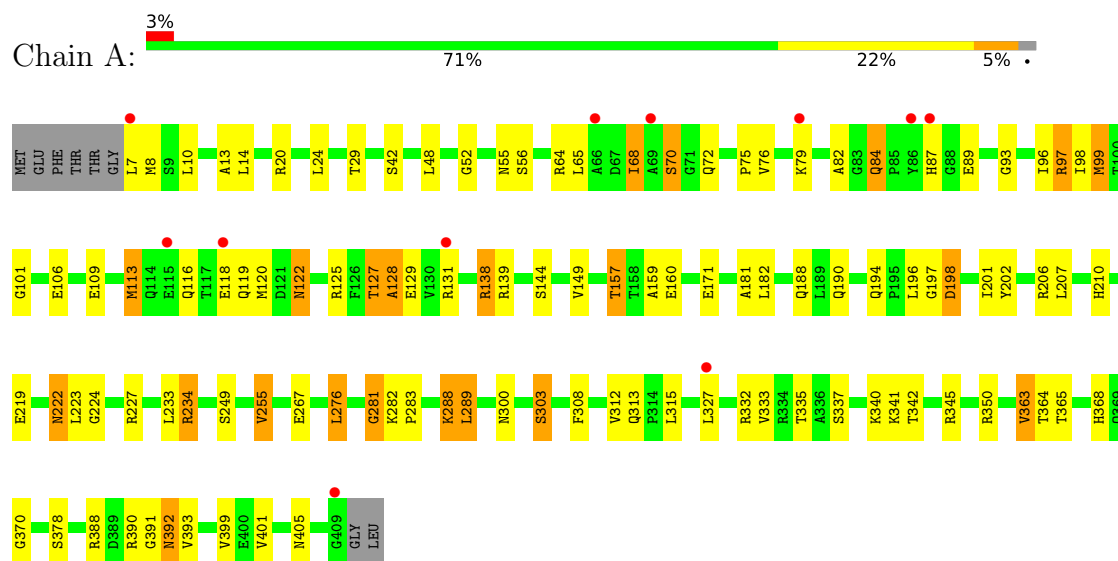
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total 6	C 3	O 3	0	0
2	A	1	Total 6	C 3	O 3	0	0
2	A	1	Total 6	C 3	O 3	0	0
2	B	1	Total 6	C 3	O 3	0	0
2	B	1	Total 6	C 3	O 3	0	0
2	B	1	Total 6	C 3	O 3	0	0
2	B	1	Total 6	C 3	O 3	0	0

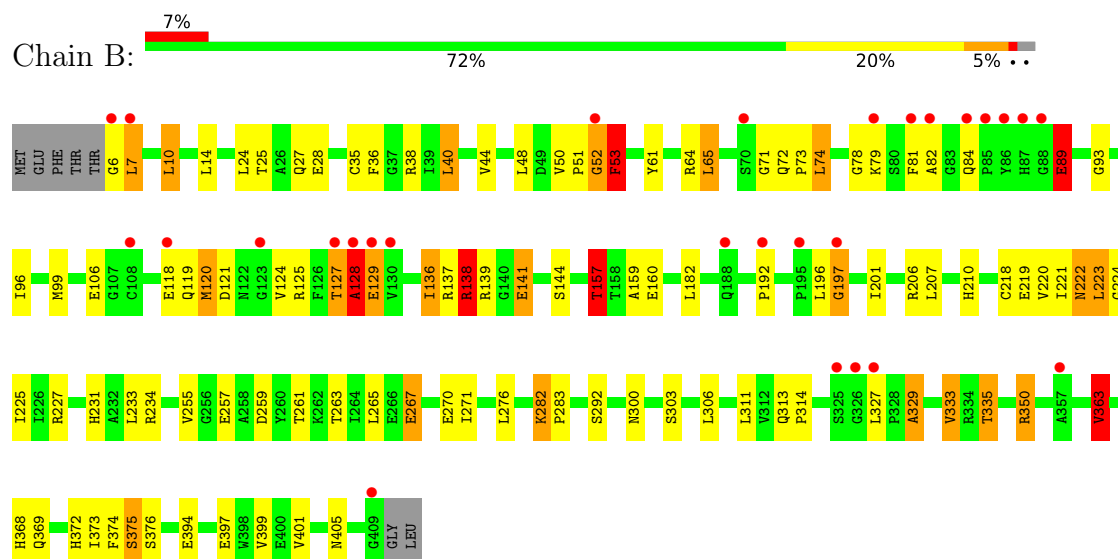
3 Residue-property plots [i](#)

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: Molybdopterin biosynthesis protein moeA



• Molecule 1: Molybdopterin biosynthesis protein moeA



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	69.99Å 98.60Å 157.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.39 – 2.70 49.39 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.39-2.70) 99.9 (49.39-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.82 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.202 , 0.261 0.205 , 0.254	Depositor DCC
R_{free} test set	1557 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	47.8	Xtriage
Anisotropy	0.124	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 37.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6132	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.73% 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	1.13	3/3099 (0.1%)	1.13	5/4212 (0.1%)
1	B	1.16	5/3103 (0.2%)	1.23	15/4217 (0.4%)
All	All	1.14	8/6202 (0.1%)	1.18	20/8429 (0.2%)

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	2

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	53	PHE	CA-C	7.06	1.62	1.52
1	A	113	MET	SD-CE	6.99	1.97	1.79
1	B	127	THR	CA-C	6.94	1.59	1.53
1	B	53	PHE	N-CA	5.44	1.53	1.46
1	B	329	ALA	CA-CB	-5.34	1.45	1.53
1	B	25	THR	CA-CB	5.28	1.61	1.54
1	A	99	MET	SD-CE	5.22	1.92	1.79
1	A	181	ALA	CA-C	-5.04	1.46	1.52

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	363	VAL	CB-CA-C	-7.21	99.86	110.81
1	B	192	PRO	N-CA-C	-6.92	99.74	110.95
1	B	255	VAL	N-CA-C	-6.77	104.73	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	363	VAL	N-CA-C	6.67	117.50	108.17
1	A	363	VAL	CB-CA-C	-6.51	101.13	110.83
1	B	53	PHE	N-CA-C	6.48	124.60	110.80
1	B	38	ARG	NE-CZ-NH2	-6.05	113.75	119.20
1	B	218	CYS	N-CA-C	5.86	118.46	110.55
1	B	157	THR	N-CA-CB	-5.84	102.01	111.24
1	B	128	ALA	N-CA-C	5.84	123.23	110.80
1	A	388	ARG	N-CA-C	5.64	117.88	111.11
1	B	335	THR	CB-CA-C	-5.63	100.01	109.53
1	A	289	LEU	N-CA-C	-5.54	101.37	109.63
1	B	65	LEU	N-CA-C	5.52	118.06	111.71
1	B	124	VAL	N-CA-C	5.51	116.16	108.89
1	B	375	SER	N-CA-C	5.22	118.43	111.75
1	B	78	GLY	N-CA-C	5.20	118.16	110.42
1	A	281	GLY	N-CA-C	-5.14	105.69	111.85
1	B	52	GLY	N-CA-C	-5.11	101.06	113.18
1	B	89	GLU	N-CA-C	5.10	121.66	110.80

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	71	GLY	Peptide
1	B	81	PHE	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	3040	0	3039	45	0
1	B	3044	0	3042	54	0
2	A	24	0	32	1	0
2	B	24	0	32	3	0
All	All	6132	0	6145	99	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 8.

All (99) 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:378:SER:O	2:A:412:GOL:H2	1.72	0.89
1:A:313:GLN:HE22	1:A:405:ASN:HD21	1.24	0.83
1:B:300:ASN:HD22	1:B:303:SER:H	1.29	0.81
1:A:122:ASN:HD22	1:A:122:ASN:H	1.31	0.79
1:B:157:THR:HG22	1:B:159:ALA:H	1.50	0.76
1:B:329:ALA:HB3	2:B:415:GOL:H2	1.67	0.76
1:B:313:GLN:HE22	1:B:405:ASN:HD21	1.33	0.76
1:B:137:ARG:O	1:B:138:ARG:HB2	1.83	0.76
1:A:190:GLN:HE21	1:A:194:GLN:NE2	1.85	0.74
1:A:157:THR:HG22	1:A:159:ALA:H	1.50	0.74
1:B:259:ASP:OD1	1:B:261:THR:OG1	2.04	0.70
1:B:372:HIS:HD2	1:B:373:ILE:HG23	1.55	0.70
1:A:222:ASN:HD22	1:A:224:GLY:H	1.40	0.68
1:A:391:GLY:O	1:A:392:ASN:O	2.12	0.67
1:B:222:ASN:HD22	1:B:224:GLY:H	1.43	0.66
1:B:206:ARG:HD2	1:B:222:ASN:HD21	1.61	0.66
1:A:281:GLY:HA2	1:A:303:SER:HB3	1.79	0.65
1:B:40:LEU:HD11	1:B:44:VAL:HG23	1.79	0.65
1:A:368:HIS:HD2	1:A:370:GLY:H	1.43	0.64
1:B:300:ASN:ND2	1:B:303:SER:H	1.95	0.64
1:B:350:ARG:HD2	1:B:376:SER:OG	1.97	0.63
1:A:190:GLN:NE2	1:A:194:GLN:NE2	2.47	0.61
1:A:313:GLN:HE22	1:A:405:ASN:ND2	1.98	0.60
1:A:206:ARG:HD2	1:A:222:ASN:HD21	1.67	0.60
1:B:137:ARG:O	1:B:138:ARG:CB	2.52	0.58
1:B:157:THR:HB	1:B:160:GLU:OE2	2.05	0.57
1:A:55:ASN:HD22	1:A:101:GLY:HA2	1.71	0.56
1:B:52:GLY:O	1:B:53:PHE:O	2.23	0.56
1:B:222:ASN:ND2	1:B:224:GLY:H	2.02	0.56
1:B:372:HIS:CD2	1:B:373:ILE:HG23	2.40	0.55
1:A:75:PRO:HD2	1:A:93:GLY:O	2.06	0.55
1:B:265:LEU:HD22	1:B:271:ILE:HG13	1.87	0.55
1:A:222:ASN:ND2	1:A:224:GLY:H	2.05	0.55
1:A:341:LYS:NZ	1:A:345:ARG:O	2.40	0.54
1:A:364:THR:HG22	1:A:365:THR:O	2.07	0.54
1:A:97:ARG:NH2	1:A:99:MET:HE1	2.23	0.54
1:A:13:ALA:HB2	1:A:276:LEU:HD11	1.90	0.54
1:B:394:GLU:O	1:B:397:GLU:HG3	2.08	0.54
1:A:206:ARG:HH11	1:A:222:ASN:HD21	1.55	0.54
1:B:313:GLN:HE22	1:B:405:ASN:ND2	2.03	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:56:SER:HB2	1:A:98:ILE:HD13	1.91	0.53
1:A:300:ASN:HD22	1:A:303:SER:H	1.57	0.53
1:B:137:ARG:C	1:B:141:GLU:OE2	2.52	0.53
1:A:96:ILE:HG22	1:A:97:ARG:O	2.10	0.52
1:B:138:ARG:HH11	1:B:138:ARG:CG	2.23	0.52
1:B:6:GLY:O	1:B:7:LEU:HB2	2.09	0.51
1:A:55:ASN:ND2	1:A:101:GLY:HA2	2.25	0.51
1:A:390:ARG:HE	1:A:393:VAL:HG22	1.75	0.51
1:B:119:GLN:NE2	1:B:120:MET:O	2.43	0.51
1:B:210:HIS:CD2	1:B:220:VAL:HG11	2.46	0.50
1:B:329:ALA:HB3	2:B:415:GOL:C2	2.40	0.50
1:B:10:LEU:CD2	1:B:311:LEU:HD21	2.41	0.49
1:B:313:GLN:HB3	1:B:314:PRO:HD3	1.94	0.49
1:B:136:ILE:HG22	1:B:136:ILE:O	2.11	0.49
1:A:288:LYS:HD3	1:A:289:LEU:O	2.13	0.49
1:B:196:LEU:O	1:B:197:GLY:O	2.31	0.49
1:A:255:VAL:HB	1:A:283:PRO:HB2	1.94	0.48
1:B:51:PRO:C	1:B:52:GLY:O	2.55	0.48
1:B:234:ARG:NH1	1:B:267:GLU:OE1	2.46	0.48
1:A:390:ARG:NE	1:A:393:VAL:HG22	2.28	0.47
1:A:122:ASN:H	1:A:122:ASN:ND2	2.08	0.47
1:B:222:ASN:HD22	1:B:222:ASN:C	2.23	0.46
1:A:196:LEU:HD13	1:A:202:TYR:CZ	2.52	0.45
1:A:315:LEU:C	1:A:315:LEU:HD23	2.42	0.45
1:A:138:ARG:O	1:A:139:ARG:C	2.60	0.44
1:A:368:HIS:HD2	1:A:370:GLY:N	2.13	0.44
1:B:221:ILE:HG22	1:B:223:LEU:CD1	2.47	0.44
1:B:128:ALA:O	1:B:129:GLU:O	2.35	0.44
1:B:368:HIS:HD2	1:B:369:GLN:N	2.15	0.43
1:B:74:LEU:HD13	1:B:93:GLY:O	2.18	0.43
1:A:341:LYS:HD2	1:A:342:THR:N	2.33	0.43
1:A:210:HIS:HD2	1:A:222:ASN:OD1	2.01	0.43
1:B:405:ASN:OD1	1:B:405:ASN:C	2.59	0.43
1:A:157:THR:CG2	1:A:159:ALA:H	2.27	0.43
1:B:35:CYS:O	1:B:36:PHE:C	2.60	0.43
1:B:128:ALA:C	1:B:129:GLU:O	2.62	0.43
1:B:137:ARG:O	1:B:141:GLU:OE2	2.37	0.43
1:B:61:TYR:HA	1:B:96:ILE:O	2.18	0.43
1:A:52:GLY:O	1:A:139:ARG:HG3	2.18	0.42
1:A:84:GLN:HE21	1:A:84:GLN:HB3	1.67	0.42
1:B:282:LYS:HB3	1:B:283:PRO:HD3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:311:LEU:C	1:B:314:PRO:HD2	2.43	0.42
1:B:375:SER:O	1:B:376:SER:C	2.60	0.42
1:B:333:VAL:CG1	1:B:363:VAL:HG22	2.49	0.42
1:B:282:LYS:N	1:B:283:PRO:CD	2.82	0.42
1:A:68:ILE:HD12	1:A:68:ILE:HA	1.87	0.42
1:A:308:PHE:CD1	1:A:312:VAL:HB	2.55	0.42
1:B:221:ILE:HG22	1:B:223:LEU:HD13	2.02	0.42
1:B:222:ASN:HD22	1:B:224:GLY:N	2.14	0.42
1:A:127:THR:O	1:A:128:ALA:O	2.38	0.41
1:B:136:ILE:O	1:B:137:ARG:HB2	2.20	0.41
1:A:157:THR:HB	1:A:160:GLU:OE2	2.21	0.41
1:A:234:ARG:HH11	1:A:234:ARG:CG	2.34	0.41
1:A:222:ASN:HD22	1:A:222:ASN:C	2.29	0.41
1:B:374:PHE:H	2:B:414:GOL:H2	1.86	0.40
1:B:50:VAL:HA	1:B:51:PRO:C	2.46	0.40
1:B:136:ILE:O	1:B:138:ARG:N	2.54	0.40
1:A:391:GLY:C	1:A:392:ASN:O	2.65	0.40
1:B:138:ARG:HH11	1:B:138:ARG:HG3	1.87	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	401/411 (98%)	366 (91%)	25 (6%)	10 (2%)	4	11
1	B	402/411 (98%)	373 (93%)	19 (5%)	10 (2%)	4	11
All	All	803/822 (98%)	739 (92%)	44 (6%)	20 (2%)	4	11

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	116	GLN
1	A	127	THR
1	A	128	ALA
1	A	198	ASP
1	A	282	LYS
1	A	392	ASN
1	B	53	PHE
1	B	89	GLU
1	B	128	ALA
1	B	129	GLU
1	B	138	ARG
1	B	282	LYS
1	A	197	GLY
1	B	7	LEU
1	B	197	GLY
1	A	82	ALA
1	B	82	ALA
1	A	8	MET
1	A	70	SER
1	B	73	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	325/331 (98%)	264 (81%)	61 (19%)	1	4
1	B	325/331 (98%)	274 (84%)	51 (16%)	2	7
All	All	650/662 (98%)	538 (83%)	112 (17%)	2	6

All (112) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	LEU
1	A	10	LEU
1	A	14	LEU
1	A	20	ARG

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Mol	Chain	Res	Type
1	A	24	LEU
1	A	29	THR
1	A	42	SER
1	A	48	LEU
1	A	64	ARG
1	A	65	LEU
1	A	68	ILE
1	A	70	SER
1	A	72	GLN
1	A	76	VAL
1	A	79	LYS
1	A	84	GLN
1	A	87	HIS
1	A	89	GLU
1	A	97	ARG
1	A	106	GLU
1	A	109	GLU
1	A	113	MET
1	A	118	GLU
1	A	119	GLN
1	A	120	MET
1	A	122	ASN
1	A	125	ARG
1	A	129	GLU
1	A	131	ARG
1	A	138	ARG
1	A	144	SER
1	A	149	VAL
1	A	157	THR
1	A	171	GLU
1	A	182	LEU
1	A	188	GLN
1	A	198	ASP
1	A	201	ILE
1	A	207	LEU
1	A	219	GLU
1	A	222	ASN
1	A	223	LEU
1	A	227	ARG
1	A	233	LEU
1	A	234	ARG
1	A	249	SER

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Mol	Chain	Res	Type
1	A	255	VAL
1	A	267	GLU
1	A	276	LEU
1	A	288	LYS
1	A	303	SER
1	A	327	LEU
1	A	332	ARG
1	A	333	VAL
1	A	335	THR
1	A	337	SER
1	A	340	LYS
1	A	350	ARG
1	A	363	VAL
1	A	399	VAL
1	A	401	VAL
1	B	10	LEU
1	B	14	LEU
1	B	24	LEU
1	B	27	GLN
1	B	28	GLU
1	B	40	LEU
1	B	48	LEU
1	B	64	ARG
1	B	65	LEU
1	B	72	GLN
1	B	74	LEU
1	B	79	LYS
1	B	84	GLN
1	B	89	GLU
1	B	99	MET
1	B	106	GLU
1	B	118	GLU
1	B	120	MET
1	B	121	ASP
1	B	125	ARG
1	B	127	THR
1	B	136	ILE
1	B	138	ARG
1	B	139	ARG
1	B	141	GLU
1	B	144	SER
1	B	157	THR

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Mol	Chain	Res	Type
1	B	182	LEU
1	B	201	ILE
1	B	207	LEU
1	B	219	GLU
1	B	222	ASN
1	B	223	LEU
1	B	225	ILE
1	B	227	ARG
1	B	231	HIS
1	B	233	LEU
1	B	257	GLU
1	B	263	THR
1	B	267	GLU
1	B	270	GLU
1	B	276	LEU
1	B	292	SER
1	B	306	LEU
1	B	327	LEU
1	B	333	VAL
1	B	335	THR
1	B	350	ARG
1	B	363	VAL
1	B	399	VAL
1	B	401	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	ASN
1	A	55	ASN
1	A	84	GLN
1	A	119	GLN
1	A	122	ASN
1	A	188	GLN
1	A	190	GLN
1	A	194	GLN
1	A	210	HIS
1	A	215	GLN
1	A	222	ASN
1	A	243	GLN
1	A	300	ASN
1	A	313	GLN

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Mol	Chain	Res	Type
1	A	354	GLN
1	A	368	HIS
1	B	27	GLN
1	B	114	GLN
1	B	134	GLN
1	B	210	HIS
1	B	222	ASN
1	B	300	ASN
1	B	313	GLN
1	B	331	GLN
1	B	368	HIS
1	B	372	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

8 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	413	-	5,5,5	0.35	0	5,5,5	0.41	0
2	GOL	A	414	-	5,5,5	0.49	0	5,5,5	0.31	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	GOL	A	415	-	5,5,5	0.26	0	5,5,5	1.19	0
2	GOL	A	412	-	5,5,5	0.66	0	5,5,5	0.70	0
2	GOL	B	413	-	5,5,5	0.45	0	5,5,5	0.56	0
2	GOL	B	412	-	5,5,5	0.64	0	5,5,5	0.93	0
2	GOL	B	414	-	5,5,5	0.63	0	5,5,5	0.94	0
2	GOL	B	415	-	5,5,5	0.88	0	5,5,5	1.06	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	413	-	-	2/4/4/4	-
2	GOL	A	414	-	-	4/4/4/4	-
2	GOL	A	415	-	-	0/4/4/4	-
2	GOL	A	412	-	-	1/4/4/4	-
2	GOL	B	413	-	-	2/4/4/4	-
2	GOL	B	412	-	-	1/4/4/4	-
2	GOL	B	414	-	-	2/4/4/4	-
2	GOL	B	415	-	-	0/4/4/4	-

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	413	GOL	C1-C2-C3-O3
2	A	414	GOL	O1-C1-C2-O2
2	A	414	GOL	O1-C1-C2-C3
2	A	414	GOL	C1-C2-C3-O3
2	B	414	GOL	O1-C1-C2-C3
2	B	413	GOL	O2-C2-C3-O3
2	A	414	GOL	O2-C2-C3-O3
2	B	414	GOL	O1-C1-C2-O2
2	A	413	GOL	O2-C2-C3-O3
2	B	412	GOL	O2-C2-C3-O3
2	A	413	GOL	O1-C1-C2-O2
2	A	412	GOL	O1-C1-C2-O2

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	412	GOL	1	0
2	B	414	GOL	1	0
2	B	415	GOL	2	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	403/411 (98%)	0.13	11 (2%) 56 53	22, 48, 78, 104	0
1	B	404/411 (98%)	0.20	28 (6%) 23 20	20, 44, 84, 111	0
All	All	807/822 (98%)	0.16	39 (4%) 35 32	20, 45, 82, 111	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	7	LEU	5.7
1	B	87	HIS	4.8
1	B	82	ALA	4.4
1	B	128	ALA	4.2
1	B	127	THR	3.8
1	B	129	GLU	3.3
1	A	115	GLU	3.3
1	A	69	ALA	3.3
1	B	79	LYS	3.3
1	B	81	PHE	3.2
1	A	409	GLY	3.0
1	B	118	GLU	2.9
1	B	188	GLN	2.8
1	A	118	GLU	2.6
1	B	192	PRO	2.6
1	A	87	HIS	2.5
1	B	86	TYR	2.5
1	B	88	GLY	2.5
1	B	7	LEU	2.5
1	B	123	GLY	2.4
1	B	6	GLY	2.4
1	A	131	ARG	2.4
1	A	86	TYR	2.3
1	B	52	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	327	LEU	2.3
1	B	70	SER	2.3
1	A	79	LYS	2.2
1	B	357	ALA	2.2
1	B	84	GLN	2.2
1	B	409	GLY	2.2
1	B	325	SER	2.1
1	A	66	ALA	2.1
1	B	85	PRO	2.1
1	B	108	CYS	2.1
1	B	197	GLY	2.1
1	B	326	GLY	2.1
1	B	327	LEU	2.1
1	B	195	PRO	2.0
1	B	130	VAL	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 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	414	6/6	0.55	0.23	97,98,98,99	0
2	GOL	B	413	6/6	0.73	0.22	71,72,73,73	0
2	GOL	A	412	6/6	0.79	0.14	60,61,62,62	0
2	GOL	B	415	6/6	0.80	0.31	72,74,75,75	0
2	GOL	A	415	6/6	0.81	0.17	51,56,59,60	0
2	GOL	B	412	6/6	0.83	0.22	61,64,66,67	0
2	GOL	A	413	6/6	0.84	0.18	62,65,66,69	0
2	GOL	B	414	6/6	0.86	0.17	55,56,57,58	0

6.5 Other polymers [i](#)

There are no such residues in this entry.