Full wwPDB X-ray Structure Validation Report

Feb 1, 2016 – 04:39 AM GMT

PDB ID	:	2NQV
Title	:	MoeA D228A
Authors	:	Nciolas, J.; Xiang, S.; Schindelin, H.; Rajagopalan, K.V.
Deposited on	:	2006-10-31
Resolution	:	2.82 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

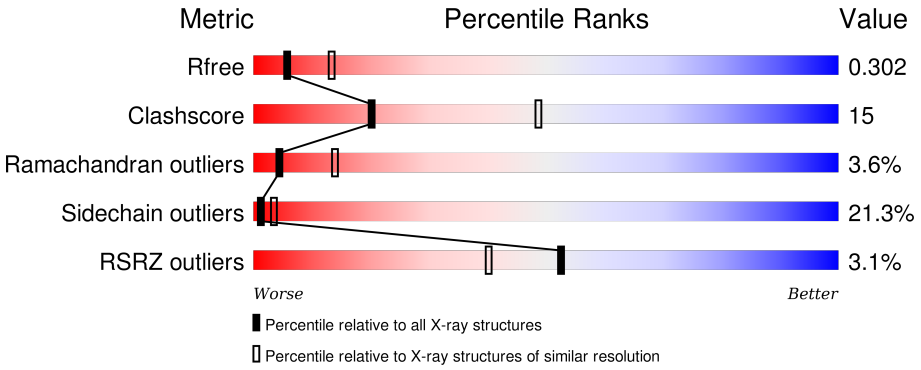
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.82 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}	91344	2676 (2.84-2.80)
Clashscore	102246	3124 (2.84-2.80)
Ramachandran outliers	100387	3072 (2.84-2.80)
Sidechain outliers	100360	3074 (2.84-2.80)
RSRZ outliers	91569	2690 (2.84-2.80)

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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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 <=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	5% 58% 32% 7% ••
1	B	411	% 56% 33% 9% •

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	GOL	A	901	-	-	-	X
2	GOL	A	904	-	-	-	X
2	GOL	A	906	-	-	-	X
2	GOL	B	902	-	-	-	X
2	GOL	B	908	-	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6148 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.

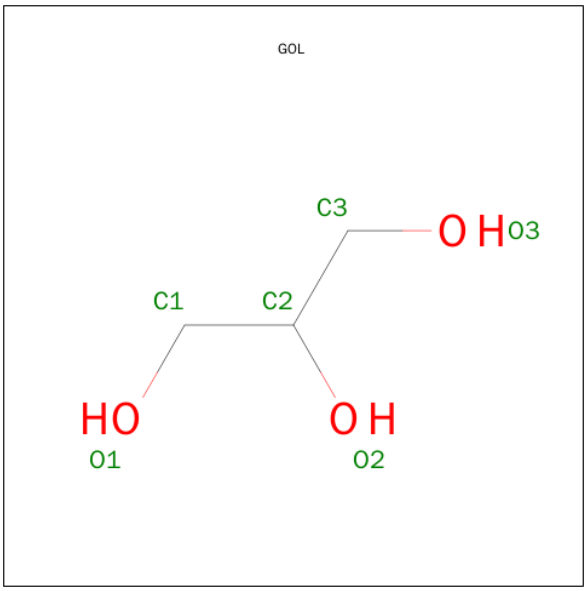
- Molecule 1 is a protein called Molybdopterin biosynthesis protein moeA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	405	Total	C	N	O	S	0	0	0
			3050	1925	533	579	13			
1	B	403	Total	C	N	O	S	0	0	0
			3037	1917	531	576	13			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	228	ALA	ASP	ENGINEERED	UNP P12281
B	228	ALA	ASP	ENGINEERED	UNP P12281

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

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

- Molecule 3 is water.

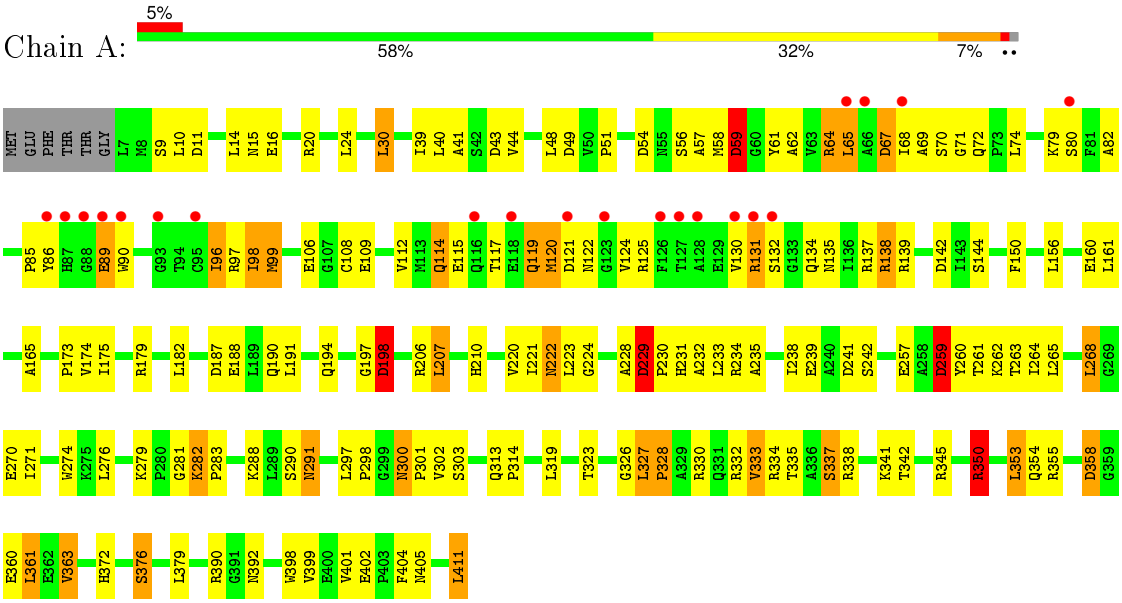
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	7	Total O 7 7	0	0
3	B	6	Total O 6 6	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

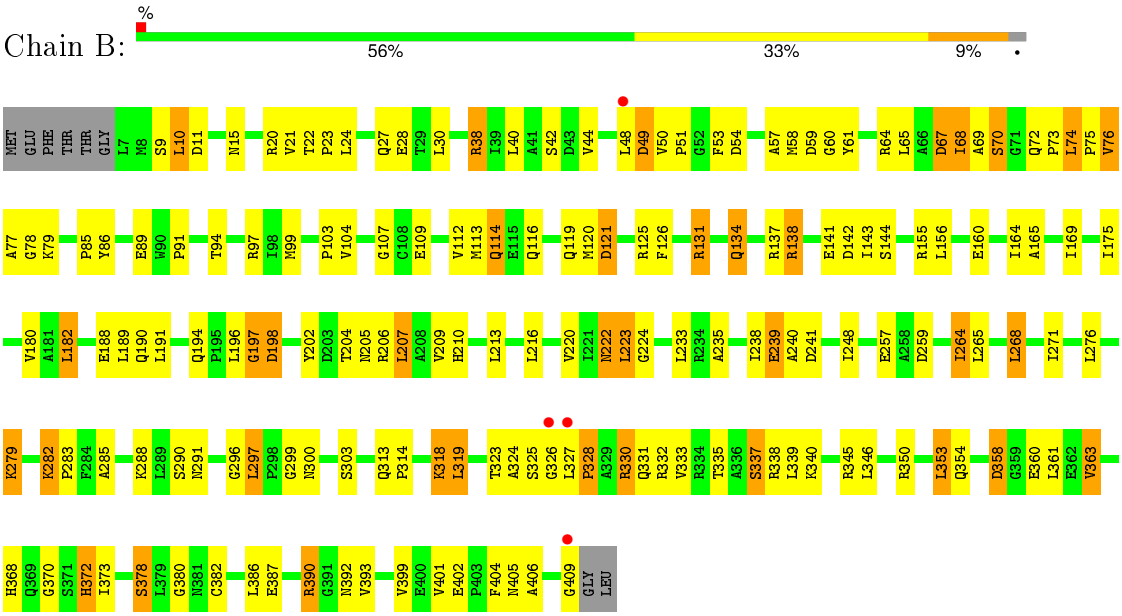
- Molecule 1: Molybdopterin biosynthesis protein moeA

Chain A:



- Molecule 1: Molybdopterin biosynthesis protein moeA

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	67.67Å 98.13Å 160.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.82 47.06 – 2.82	Depositor EDS
% Data completeness (in resolution range)	73.4 (50.00-2.82) 73.4 (47.06-2.82)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.55 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.240 , 0.319 0.237 , 0.302	Depositor DCC
R_{free} test set	992 reflections (5.36%)	DCC
Wilson B-factor (Å^2)	63.6	Xtriage
Anisotropy	0.189	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 43.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	0 of 19535 reflections	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	6148	wwPDB-VP
Average B, all atoms (Å^2)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.62% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	0.71	0/3109	0.93	12/4224 (0.3%)
1	B	0.75	0/3096	0.94	10/4208 (0.2%)
All	All	0.73	0/6205	0.93	22/8432 (0.3%)

There are no bond length outliers.

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	38	ARG	NE-CZ-NH2	-8.56	116.02	120.30
1	A	229	ASP	CB-CG-OD2	7.31	124.88	118.30
1	B	49	ASP	CB-CG-OD2	6.70	124.33	118.30
1	A	142	ASP	CB-CG-OD2	6.67	124.31	118.30
1	A	259	ASP	CB-CG-OD2	6.64	124.28	118.30
1	A	59	ASP	CB-CG-OD2	6.57	124.21	118.30
1	B	11	ASP	CB-CG-OD2	6.11	123.80	118.30
1	A	358	ASP	CB-CG-OD2	6.00	123.70	118.30
1	B	142	ASP	CB-CG-OD2	5.93	123.63	118.30
1	A	350	ARG	NE-CZ-NH1	5.89	123.24	120.30
1	A	11	ASP	CB-CG-OD2	5.87	123.58	118.30
1	A	187	ASP	CB-CG-OD2	5.79	123.51	118.30
1	B	155	ARG	NE-CZ-NH2	-5.57	117.51	120.30
1	B	38	ARG	NE-CZ-NH1	5.35	122.97	120.30
1	A	54	ASP	CB-CG-OD2	5.32	123.09	118.30
1	A	241	ASP	CB-CG-OD2	5.31	123.08	118.30
1	B	121	ASP	CB-CG-OD2	5.29	123.06	118.30
1	A	43	ASP	CB-CG-OD2	5.25	123.02	118.30
1	A	198	ASP	CB-CG-OD2	5.18	122.96	118.30
1	B	358	ASP	CB-CG-OD2	5.13	122.92	118.30
1	B	241	ASP	CB-CG-OD2	5.13	122.92	118.30
1	B	155	ARG	NE-CZ-NH1	5.07	122.83	120.30

There are no chirality outliers.

There are no planarity outliers.

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	3050	0	3052	96	0
1	B	3037	0	3038	90	0
2	A	30	0	40	6	0
2	B	18	0	24	5	0
3	A	7	0	0	0	0
3	B	6	0	0	1	0
All	All	6148	0	6154	181	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 15.

All (181) 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:189:LEU:O	2:B:907:GOL:H31	1.47	1.12
1:A:300:ASN:C	1:A:300:ASN:HD22	1.65	0.98
1:B:190:GLN:HG3	1:B:194:GLN:HE21	1.40	0.86
1:B:338:ARG:HH12	1:B:392:ASN:HD22	1.28	0.82
1:B:190:GLN:HG3	1:B:194:GLN:NE2	1.95	0.79
1:A:300:ASN:ND2	1:A:300:ASN:C	2.36	0.79
1:B:330:ARG:HD3	1:B:402:GLU:HB2	1.63	0.79
1:A:206:ARG:HH11	1:A:222:ASN:HD21	1.31	0.78
1:A:190:GLN:HG3	1:A:194:GLN:NE2	1.99	0.77
1:A:228:ALA:O	2:A:903:GOL:H2	1.87	0.74
1:B:300:ASN:HD22	1:B:303:SER:H	1.34	0.72
1:A:179:ARG:NH1	1:A:221:ILE:HD11	2.05	0.71
1:A:56:SER:HB2	1:A:98:ILE:HD13	1.72	0.71
1:B:409:GLY:O	3:B:914:HOH:O	2.08	0.71
1:B:189:LEU:O	2:B:907:GOL:C3	2.35	0.71
1:A:198:ASP:HB2	1:B:85:PRO:HG3	1.72	0.71
1:A:156:LEU:HD13	1:A:161:LEU:HD21	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:378:SER:O	2:B:908:GOL:H2	1.91	0.69
1:A:411:LEU:HD11	2:A:901:GOL:O2	1.92	0.69
1:A:40:LEU:HD21	1:A:44:VAL:HG23	1.76	0.68
1:B:138:ARG:O	1:B:141:GLU:HG2	1.93	0.68
1:A:335:THR:HG22	1:A:337:SER:H	1.60	0.66
1:A:191:LEU:H	1:A:194:GLN:NE2	1.94	0.66
1:A:260:TYR:O	1:A:264:ILE:HD12	1.97	0.65
1:B:346:LEU:HD12	1:B:386:LEU:O	1.97	0.64
1:A:62:ALA:HB3	1:A:96:ILE:HG22	1.81	0.63
1:B:327:LEU:O	1:B:328:PRO:O	2.17	0.62
1:B:265:LEU:HD22	1:B:271:ILE:HG13	1.79	0.62
1:B:368:HIS:HD2	1:B:370:GLY:N	1.97	0.62
1:B:210:HIS:CD2	1:B:220:VAL:HG11	2.33	0.62
1:B:368:HIS:HD2	1:B:370:GLY:H	1.46	0.61
1:B:353:LEU:HD11	1:B:401:VAL:HG11	1.82	0.61
1:A:279:LYS:HG3	1:A:345:ARG:NH2	2.15	0.61
1:B:222:ASN:HD22	1:B:224:GLY:H	1.48	0.61
1:A:41:ALA:HB3	1:A:173:PRO:HB2	1.83	0.60
1:B:206:ARG:HH11	1:B:222:ASN:HD21	1.50	0.60
1:A:350:ARG:HD2	1:A:376:SER:HB2	1.83	0.60
1:B:91:PRO:HG2	1:B:94:THR:HG21	1.82	0.60
1:A:327:LEU:HD12	1:A:328:PRO:HD2	1.84	0.60
1:B:387:GLU:OE1	1:B:390:ARG:HD3	2.01	0.59
1:A:40:LEU:HD13	1:A:156:LEU:HD21	1.84	0.59
1:A:190:GLN:HG3	1:A:194:GLN:HE21	1.67	0.58
1:B:196:LEU:HD13	1:B:202:TYR:CZ	2.39	0.58
1:A:353:LEU:HD11	1:A:401:VAL:HG11	1.86	0.58
1:A:290:SER:HB2	1:A:291:ASN:HD22	1.69	0.56
1:A:39:ILE:O	1:A:174:VAL:HB	2.06	0.56
1:B:327:LEU:HD12	1:B:328:PRO:HD2	1.87	0.56
1:B:196:LEU:O	1:B:197:GLY:O	2.24	0.56
1:B:235:ALA:HA	1:B:238:ILE:HD12	1.87	0.56
1:A:335:THR:CG2	1:A:337:SER:O	2.54	0.56
1:A:330:ARG:HD3	1:A:402:GLU:HB2	1.87	0.56
1:B:282:LYS:N	1:B:283:PRO:CD	2.69	0.55
1:B:239:GLU:HG3	1:B:240:ALA:N	2.22	0.55
1:B:300:ASN:ND2	1:B:303:SER:H	2.05	0.55
1:A:57:ALA:HA	1:A:137:ARG:HD2	1.89	0.55
1:B:189:LEU:O	2:B:907:GOL:H11	2.07	0.54
1:B:180:VAL:HG21	1:B:213:LEU:HD22	1.89	0.54
1:B:76:VAL:O	1:B:78:GLY:N	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:69:ALA:O	1:B:70:SER:C	2.45	0.54
1:B:131:ARG:O	1:B:134:GLN:HB3	2.08	0.54
1:B:160:GLU:O	1:B:164:ILE:HG13	2.08	0.53
1:B:313:GLN:N	1:B:314:PRO:HD2	2.23	0.53
1:A:282:LYS:HB3	1:A:283:PRO:HD3	1.90	0.53
1:A:40:LEU:HD21	1:A:44:VAL:CG2	2.38	0.53
1:A:335:THR:HG22	1:A:337:SER:O	2.09	0.53
1:B:335:THR:HA	1:B:363:VAL:HG23	1.91	0.53
1:A:65:LEU:HD22	1:A:109:GLU:HB3	1.91	0.53
1:B:40:LEU:CD1	1:B:156:LEU:HD11	2.39	0.53
1:A:334:ARG:CZ	1:A:398:TRP:CZ2	2.92	0.52
1:A:117:THR:O	1:A:119:GLN:OE1	2.28	0.52
1:B:40:LEU:HD12	1:B:156:LEU:HD11	1.91	0.52
1:A:300:ASN:ND2	1:A:303:SER:H	2.08	0.52
1:A:333:VAL:HG11	1:A:361:LEU:HB3	1.93	0.51
1:A:222:ASN:HD22	1:A:224:GLY:H	1.57	0.51
1:A:353:LEU:CD1	1:A:401:VAL:HG11	2.40	0.51
1:B:57:ALA:HB2	1:B:137:ARG:HG2	1.92	0.51
1:A:300:ASN:ND2	1:A:302:VAL:H	2.07	0.51
1:A:338:ARG:HH12	1:A:392:ASN:HD22	1.58	0.50
1:B:297:LEU:N	1:B:297:LEU:HD23	2.25	0.50
1:A:206:ARG:NH1	1:A:222:ASN:HD21	2.06	0.50
1:A:112:VAL:HG22	1:A:134:GLN:HE22	1.77	0.50
1:B:21:VAL:O	1:B:318:LYS:NZ	2.44	0.50
1:B:372:HIS:O	1:B:373:ILE:HG23	2.12	0.49
1:A:190:GLN:HE21	1:A:194:GLN:CD	2.14	0.49
1:B:205:ASN:ND2	1:B:299:GLY:O	2.44	0.49
1:B:74:LEU:HD11	1:B:126:PHE:HE1	1.77	0.49
1:B:67:ASP:O	1:B:68:ILE:C	2.51	0.49
1:A:165:ALA:HB2	1:B:207:LEU:HD12	1.95	0.49
1:B:380:GLY:O	2:B:908:GOL:C1	2.61	0.49
1:A:120:MET:HG2	1:A:121:ASP:N	2.26	0.48
1:A:235:ALA:HA	1:A:238:ILE:HD12	1.95	0.48
1:B:205:ASN:O	1:B:209:VAL:HG23	2.13	0.48
1:A:279:LYS:CG	1:A:345:ARG:NH2	2.76	0.48
1:A:30:LEU:N	1:A:30:LEU:HD12	2.29	0.47
1:A:291:ASN:O	2:A:905:GOL:O2	2.16	0.47
1:B:216:LEU:HD21	1:B:313:GLN:HE21	1.79	0.47
1:A:119:GLN:HG3	1:A:124:VAL:HG13	1.95	0.47
1:A:230:PRO:O	1:A:234:ARG:HG3	2.13	0.47
1:A:150:PHE:CE2	1:A:160:GLU:HG3	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:179:ARG:HH11	1:A:221:ILE:HD11	1.77	0.46
1:B:40:LEU:HD21	1:B:44:VAL:HG23	1.97	0.46
1:A:59:ASP:HA	1:A:99:MET:HA	1.97	0.46
1:B:50:VAL:HB	1:B:143:ILE:HB	1.96	0.46
1:A:259:ASP:OD1	1:A:261:THR:OG1	2.22	0.46
1:A:41:ALA:HA	1:A:175:ILE:CD1	2.46	0.46
1:A:69:ALA:C	1:A:71:GLY:N	2.68	0.46
1:A:300:ASN:ND2	1:A:302:VAL:N	2.63	0.46
1:A:156:LEU:HD13	1:A:161:LEU:CD2	2.44	0.46
1:B:279:LYS:HG3	1:B:345:ARG:NH2	2.30	0.46
1:A:57:ALA:HB3	1:A:135:ASN:HB3	1.96	0.46
1:B:50:VAL:HA	1:B:51:PRO:C	2.36	0.46
1:B:282:LYS:HB3	1:B:283:PRO:HD3	1.98	0.46
1:A:108:CYS:SG	1:A:109:GLU:N	2.89	0.46
1:B:53:PHE:CE1	1:B:103:PRO:HG3	2.51	0.45
1:A:330:ARG:HA	1:A:401:VAL:O	2.17	0.45
1:A:190:GLN:HE21	1:A:194:GLN:NE2	2.15	0.45
1:B:107:GLY:O	1:B:109:GLU:HG2	2.16	0.45
1:A:229:ASP:OD2	1:A:231:HIS:HB2	2.17	0.45
1:A:61:TYR:CE1	1:A:114:GLN:HB3	2.51	0.45
1:B:335:THR:HG22	1:B:337:SER:H	1.82	0.44
1:A:265:LEU:HD22	1:A:271:ILE:HG13	1.98	0.44
1:B:390:ARG:HH11	1:B:390:ARG:CG	2.30	0.44
1:A:238:ILE:O	1:A:242:SER:HB3	2.17	0.44
1:B:285:ALA:HB3	1:B:296:GLY:HA3	2.00	0.44
1:A:300:ASN:HD22	1:A:301:PRO:N	2.15	0.44
1:B:60:GLY:HA2	1:B:114:GLN:HG3	1.99	0.44
1:B:164:ILE:HG22	1:B:169:ILE:HB	1.98	0.44
1:B:210:HIS:HD2	1:B:222:ASN:OD1	2.00	0.44
1:B:202:TYR:O	1:B:204:THR:HG23	2.18	0.43
1:B:22:THR:HA	1:B:23:PRO:HD2	1.89	0.43
1:B:21:VAL:CG1	1:B:319:LEU:HG	2.49	0.43
1:B:338:ARG:HH12	1:B:392:ASN:ND2	2.05	0.43
1:A:355:ARG:HH11	1:B:331:GLN:HA	1.84	0.43
1:A:411:LEU:HD13	2:A:901:GOL:H12	2.01	0.43
1:A:335:THR:HG21	1:A:337:SER:O	2.17	0.43
1:A:16:GLU:HG2	1:A:274:TRP:CZ2	2.54	0.43
1:B:119:GLN:O	1:B:120:MET:SD	2.77	0.42
1:A:335:THR:HA	1:A:363:VAL:HG23	2.01	0.42
1:A:341:LYS:NZ	1:A:342:THR:O	2.48	0.42
1:A:67:ASP:O	1:A:74:LEU:HD11	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:222:ASN:HD22	1:A:222:ASN:C	2.23	0.42
1:A:86:TYR:CE2	1:A:96:ILE:HD11	2.54	0.42
1:A:291:ASN:N	1:A:291:ASN:HD22	2.18	0.42
1:B:113:MET:HB2	1:B:116:GLN:HG3	2.01	0.42
1:B:89:GLU:H	1:B:89:GLU:CD	2.22	0.42
1:A:51:PRO:HG2	1:A:138:ARG:O	2.20	0.42
1:A:411:LEU:HD11	2:A:901:GOL:C2	2.49	0.42
1:B:38:ARG:O	1:B:156:LEU:HG	2.20	0.42
1:B:335:THR:HG21	1:B:339:LEU:HG	2.01	0.41
1:B:68:ILE:HD13	1:B:126:PHE:CD1	2.55	0.41
1:A:281:GLY:O	1:A:282:LYS:CB	2.67	0.41
1:A:411:LEU:HB3	1:B:405:ASN:HB2	2.02	0.41
1:A:264:ILE:O	1:A:268:LEU:HB2	2.19	0.41
1:B:386:LEU:HD22	1:B:393:VAL:HG21	2.01	0.41
1:A:207:LEU:HD12	1:B:165:ALA:HB2	2.02	0.41
1:A:210:HIS:CD2	1:A:220:VAL:HG11	2.55	0.41
1:B:330:ARG:HD3	1:B:402:GLU:CB	2.42	0.41
1:A:353:LEU:HD12	1:A:363:VAL:HG13	2.01	0.41
1:B:327:LEU:O	1:B:328:PRO:C	2.58	0.41
1:B:223:LEU:HD21	1:B:239:GLU:HG2	2.01	0.41
1:B:78:GLY:HA3	1:B:86:TYR:CE2	2.56	0.41
1:A:283:PRO:HG2	1:A:298:PRO:HB3	2.02	0.41
1:A:49:ASP:HB2	1:A:139:ARG:HH21	1.85	0.41
1:A:405:ASN:OD1	1:A:405:ASN:C	2.58	0.41
1:A:281:GLY:O	1:A:282:LYS:HB2	2.19	0.41
1:A:231:HIS:O	1:A:232:ALA:C	2.59	0.41
1:B:9:SER:O	1:B:10:LEU:C	2.59	0.41
1:B:264:ILE:O	1:B:268:LEU:HB2	2.21	0.41
1:A:65:LEU:HD21	1:A:132:SER:HA	2.03	0.41
1:B:297:LEU:N	1:B:297:LEU:CD2	2.84	0.41
1:A:150:PHE:CE2	1:A:160:GLU:CG	3.04	0.41
1:A:313:GLN:HB3	1:A:314:PRO:HD3	2.03	0.41
1:A:156:LEU:CD1	1:A:161:LEU:HD21	2.48	0.40
1:B:74:LEU:HD11	1:B:126:PHE:CE1	2.56	0.40
1:A:64:ARG:HD2	1:A:90:TRP:CZ3	2.56	0.40
1:B:182:LEU:HD23	1:B:248:ILE:O	2.21	0.40
1:A:228:ALA:O	2:A:903:GOL:C2	2.65	0.40
1:B:353:LEU:CD1	1:B:401:VAL:HG11	2.48	0.40
1:B:196:LEU:HA	1:B:196:LEU:HD12	1.86	0.40
1:B:372:HIS:O	1:B:373:ILE:CG2	2.69	0.40
1:B:38:ARG:NH1	1:B:175:ILE:O	2.54	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	403/411 (98%)	353 (88%)	37 (9%)	13 (3%)	5	16
1	B	401/411 (98%)	351 (88%)	34 (8%)	16 (4%)	4	11
All	All	804/822 (98%)	704 (88%)	71 (9%)	29 (4%)	4	14

All (29) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	82	ALA
1	A	89	GLU
1	A	282	LYS
1	A	404	PHE
1	B	68	ILE
1	B	70	SER
1	B	77	ALA
1	B	197	GLY
1	B	282	LYS
1	B	326	GLY
1	B	404	PHE
1	A	197	GLY
1	A	326	GLY
1	B	73	PRO
1	B	75	PRO
1	B	99	MET
1	B	324	ALA
1	B	328	PRO
1	B	406	ALA
1	A	130	VAL
1	A	131	ARG
1	A	259	ASP

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Mol	Chain	Res	Type
1	B	198	ASP
1	A	70	SER
1	A	328	PRO
1	B	67	ASP
1	B	259	ASP
1	A	68	ILE
1	A	85	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	325/330 (98%)	256 (79%)	69 (21%)	1	3
1	B	324/330 (98%)	255 (79%)	69 (21%)	1	3
All	All	649/660 (98%)	511 (79%)	138 (21%)	1	3

All (138) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	SER
1	A	10	LEU
1	A	14	LEU
1	A	15	ASN
1	A	20	ARG
1	A	24	LEU
1	A	30	LEU
1	A	48	LEU
1	A	58	MET
1	A	59	ASP
1	A	64	ARG
1	A	65	LEU
1	A	67	ASP
1	A	72	GLN
1	A	79	LYS
1	A	80	SER

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Mol	Chain	Res	Type
1	A	89	GLU
1	A	96	ILE
1	A	97	ARG
1	A	98	ILE
1	A	99	MET
1	A	106	GLU
1	A	114	GLN
1	A	115	GLU
1	A	119	GLN
1	A	120	MET
1	A	122	ASN
1	A	125	ARG
1	A	131	ARG
1	A	138	ARG
1	A	144	SER
1	A	182	LEU
1	A	188	GLU
1	A	198	ASP
1	A	207	LEU
1	A	222	ASN
1	A	223	LEU
1	A	229	ASP
1	A	233	LEU
1	A	239	GLU
1	A	257	GLU
1	A	262	LYS
1	A	263	THR
1	A	268	LEU
1	A	270	GLU
1	A	276	LEU
1	A	288	LYS
1	A	291	ASN
1	A	297	LEU
1	A	300	ASN
1	A	319	LEU
1	A	323	THR
1	A	327	LEU
1	A	332	ARG
1	A	333	VAL
1	A	337	SER
1	A	350	ARG
1	A	353	LEU

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Mol	Chain	Res	Type
1	A	354	GLN
1	A	358	ASP
1	A	360	GLU
1	A	361	LEU
1	A	363	VAL
1	A	372	HIS
1	A	376	SER
1	A	379	LEU
1	A	390	ARG
1	A	399	VAL
1	A	411	LEU
1	B	10	LEU
1	B	15	ASN
1	B	20	ARG
1	B	24	LEU
1	B	27	GLN
1	B	28	GLU
1	B	30	LEU
1	B	42	SER
1	B	48	LEU
1	B	49	ASP
1	B	54	ASP
1	B	58	MET
1	B	59	ASP
1	B	61	TYR
1	B	64	ARG
1	B	65	LEU
1	B	72	GLN
1	B	74	LEU
1	B	76	VAL
1	B	79	LYS
1	B	97	ARG
1	B	104	VAL
1	B	112	VAL
1	B	114	GLN
1	B	121	ASP
1	B	125	ARG
1	B	131	ARG
1	B	134	GLN
1	B	138	ARG
1	B	144	SER
1	B	182	LEU

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Mol	Chain	Res	Type
1	B	188	GLU
1	B	191	LEU
1	B	198	ASP
1	B	207	LEU
1	B	222	ASN
1	B	223	LEU
1	B	233	LEU
1	B	239	GLU
1	B	257	GLU
1	B	264	ILE
1	B	268	LEU
1	B	276	LEU
1	B	279	LYS
1	B	288	LYS
1	B	290	SER
1	B	291	ASN
1	B	297	LEU
1	B	318	LYS
1	B	319	LEU
1	B	323	THR
1	B	325	SER
1	B	330	ARG
1	B	332	ARG
1	B	333	VAL
1	B	337	SER
1	B	340	LYS
1	B	350	ARG
1	B	353	LEU
1	B	354	GLN
1	B	358	ASP
1	B	360	GLU
1	B	361	LEU
1	B	363	VAL
1	B	372	HIS
1	B	378	SER
1	B	382	CYS
1	B	390	ARG
1	B	399	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	55	ASN
1	A	114	GLN
1	A	134	GLN
1	A	190	GLN
1	A	194	GLN
1	A	210	HIS
1	A	222	ASN
1	A	291	ASN
1	A	300	ASN
1	A	354	GLN
1	A	368	HIS
1	A	392	ASN
1	B	27	GLN
1	B	55	ASN
1	B	194	GLN
1	B	210	HIS
1	B	222	ASN
1	B	291	ASN
1	B	300	ASN
1	B	313	GLN
1	B	368	HIS
1	B	392	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

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	901	-	5,5,5	0.61	0	5,5,5	0.75	0
2	GOL	A	903	-	5,5,5	0.36	0	5,5,5	0.55	0
2	GOL	A	904	-	5,5,5	0.57	0	5,5,5	1.04	0
2	GOL	A	905	-	5,5,5	0.44	0	5,5,5	0.41	0
2	GOL	A	906	-	5,5,5	0.44	0	5,5,5	0.66	0
2	GOL	B	902	-	5,5,5	0.33	0	5,5,5	0.30	0
2	GOL	B	907	-	5,5,5	0.50	0	5,5,5	1.19	0
2	GOL	B	908	-	5,5,5	0.14	0	5,5,5	0.44	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	901	-	-	0/4/4/4	0/0/0/0
2	GOL	A	903	-	-	0/4/4/4	0/0/0/0
2	GOL	A	904	-	-	0/4/4/4	0/0/0/0
2	GOL	A	905	-	-	0/4/4/4	0/0/0/0
2	GOL	A	906	-	-	0/4/4/4	0/0/0/0
2	GOL	B	902	-	-	0/4/4/4	0/0/0/0
2	GOL	B	907	-	-	0/4/4/4	0/0/0/0
2	GOL	B	908	-	-	0/4/4/4	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	901	GOL	3	0
2	A	903	GOL	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	905	GOL	1	0
2	B	907	GOL	3	0
2	B	908	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

6.1 Protein, DNA and RNA chains

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, 95^{th} 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	405/411 (98%)	0.16	21 (5%) 31 20	28, 62, 122, 159	0
1	B	403/411 (98%)	-0.12	4 (0%) 84 77	30, 56, 95, 118	0
All	All	808/822 (98%)	0.02	25 (3%) 52 40	28, 59, 111, 159	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	88	GLY	6.3
1	A	87	HIS	4.3
1	A	65	LEU	3.6
1	A	121	ASP	3.5
1	A	89	GLU	3.5
1	A	68	ILE	3.4
1	A	131	ARG	3.4
1	A	86	TYR	3.2
1	A	132	SER	3.2
1	A	128	ALA	3.2
1	A	127	THR	3.0
1	A	130	VAL	3.0
1	A	90	TRP	2.9
1	A	126	PHE	2.9
1	B	327	LEU	2.7
1	B	326	GLY	2.6
1	A	116	GLN	2.6
1	A	93	GLY	2.6
1	A	80	SER	2.4
1	A	118	GLU	2.1
1	A	95	CYS	2.1
1	B	48	LEU	2.0
1	A	66	ALA	2.0
1	A	123	GLY	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	409	GLY	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} 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	LLDF	B-factors(Å^2)	Q<0.9
2	GOL	A	904	6/6	0.66	0.47	10.30	71,73,75,75	0
2	GOL	A	906	6/6	0.88	0.37	8.84	75,75,76,76	0
2	GOL	B	908	6/6	0.90	0.34	4.45	60,62,62,63	0
2	GOL	B	902	6/6	0.90	0.30	4.24	73,77,78,78	0
2	GOL	A	901	6/6	0.94	0.40	3.63	46,50,52,54	0
2	GOL	A	905	6/6	0.90	0.16	-0.09	73,74,74,74	0
2	GOL	B	907	6/6	0.96	0.14	-1.40	31,34,36,37	0
2	GOL	A	903	6/6	0.94	0.15	-	64,66,66,67	0

6.5 Other polymers (i)

There are no such residues in this entry.