Full wwPDB X-ray Structure Validation Report ⓘ

Oct 11, 2021 – 12:54 PM EDT

PDB ID	:	2NQM
Title	:	MoeA T100A mutant
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Deposited on	:	2006-10-31
Resolution	:	3.00 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 following versions of software and data (see references ⓘ) were used in the production of this report:

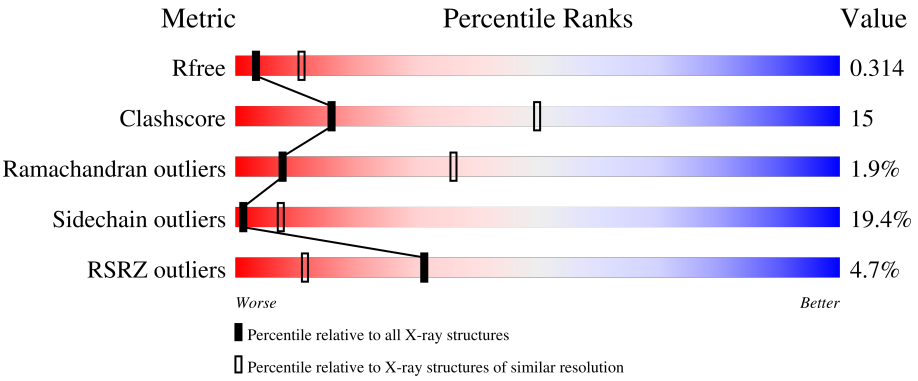
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

1 Overall quality at a glance (i)

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

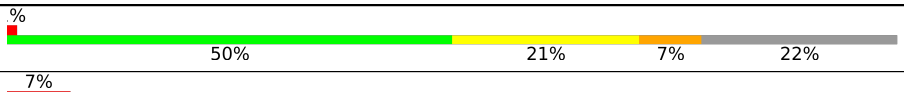
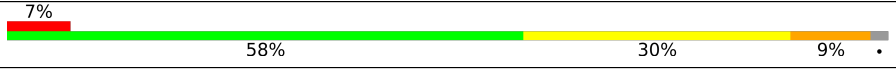
The reported resolution of this entry is 3.00 Å.

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	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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 <=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	
1	B	411	

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 5482 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	322	Total	C	N	O	S	0	0	0
			2444	1550	426	461	7			
1	B	403	Total	C	N	O	S	0	0	0
			3038	1917	531	577	13			

There are 2 discrepancies between the modelled and reference sequences:

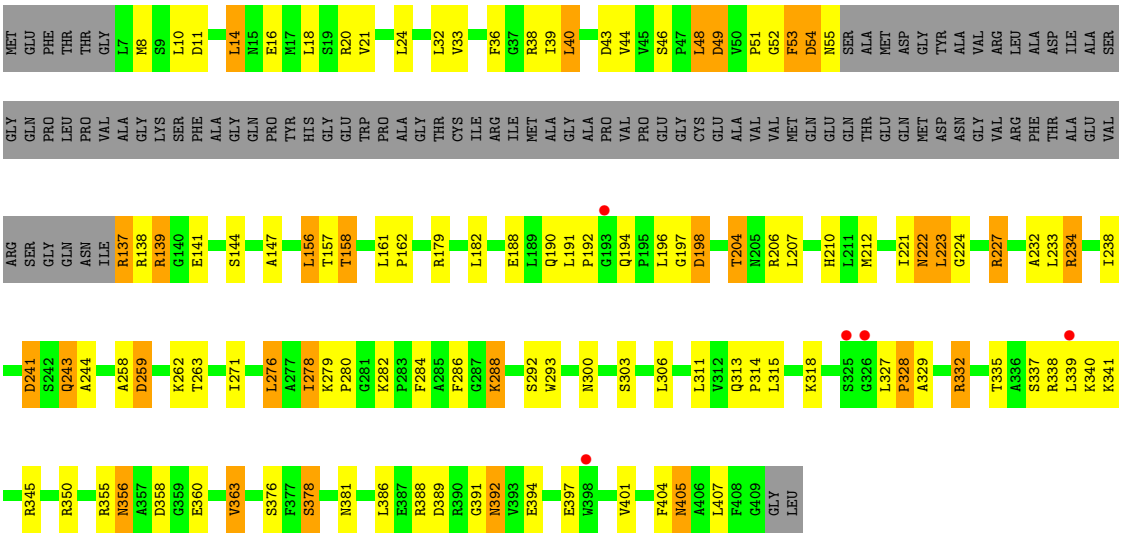
Chain	Residue	Modelled	Actual	Comment	Reference
A	100	ALA	THR	engineered mutation	UNP P12281
B	100	ALA	THR	engineered mutation	UNP P12281

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.

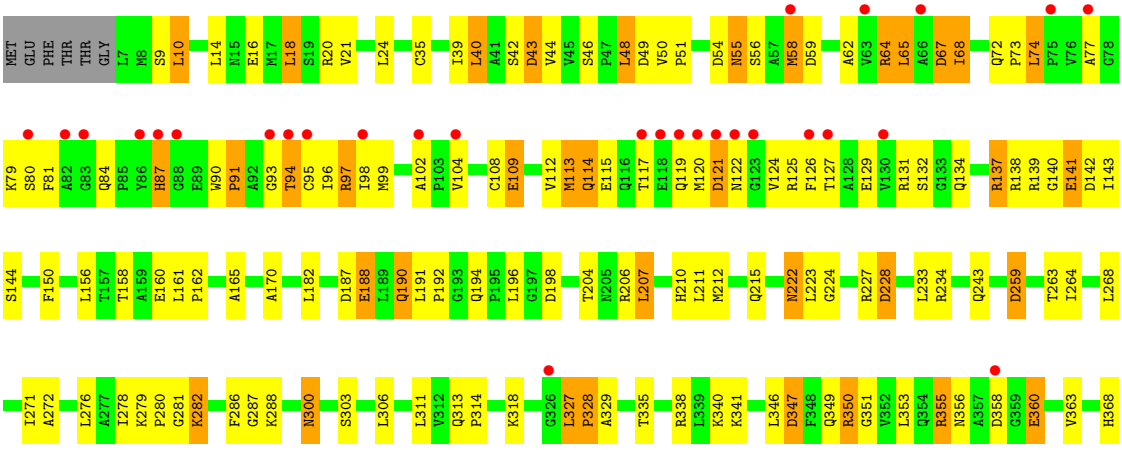
• Molecule 1: Molybdopterin biosynthesis protein moeA

Chain A:



• Molecule 1: Molybdopterin biosynthesis protein moeA

Chain B:




H372
S376
F377
S378
I384
V385
L386
E387
R388
G391
N392
V401
N405
A406
L407
F408
G409
GLY
LEU

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	81.91Å 99.36Å 104.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.39 – 3.00 40.95 – 3.00	Depositor EDS
% Data completeness (in resolution range)	90.2 (49.39-3.00) 90.3 (40.95-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.19 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.268 , 0.345 0.239 , 0.314	Depositor DCC
R_{free} test set	808 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å^2)	79.4	Xtriage
Anisotropy	0.205	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 47.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.033 for -h,l,k	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	5482	wwPDB-VP
Average B, all atoms (Å^2)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.49% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	0.67	0/2489	0.85	7/3381 (0.2%)
1	B	0.66	0/3097	0.82	9/4209 (0.2%)
All	All	0.66	0/5586	0.83	16/7590 (0.2%)

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	259	ASP	CB-CG-OD2	6.64	124.27	118.30
1	B	59	ASP	CB-CG-OD2	6.54	124.19	118.30
1	B	142	ASP	CB-CG-OD2	6.52	124.17	118.30
1	A	241	ASP	CB-CG-OD2	5.99	123.69	118.30
1	B	358	ASP	CB-CG-OD2	5.91	123.62	118.30
1	A	358	ASP	CB-CG-OD2	5.89	123.60	118.30
1	A	43	ASP	CB-CG-OD2	5.89	123.60	118.30
1	A	389	ASP	CB-CG-OD2	5.81	123.53	118.30
1	B	43	ASP	CB-CG-OD2	5.73	123.46	118.30
1	B	259	ASP	CB-CG-OD2	5.60	123.34	118.30
1	B	228	ASP	CB-CG-OD2	5.57	123.31	118.30
1	B	121	ASP	CB-CG-OD2	5.55	123.29	118.30
1	A	49	ASP	CB-CG-OD2	5.53	123.28	118.30
1	B	67	ASP	CB-CG-OD2	5.40	123.16	118.30
1	A	11	ASP	CB-CG-OD2	5.39	123.15	118.30
1	B	347	ASP	CB-CG-OD2	5.12	122.91	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2444	0	2465	72	0
1	B	3038	0	3035	95	0
All	All	5482	0	5500	160	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 (160) 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:405:ASN:C	1:B:405:ASN:HD22	1.75	0.91
1:A:405:ASN:C	1:A:405:ASN:HD22	1.75	0.90
1:B:405:ASN:ND2	1:B:407:LEU:H	1.71	0.89
1:B:40:LEU:HD11	1:B:44:VAL:HG23	1.56	0.86
1:B:90:TRP:CE3	1:B:96:ILE:HD13	2.15	0.82
1:B:14:LEU:HD22	1:B:18:LEU:HD11	1.64	0.80
1:A:40:LEU:HD11	1:A:44:VAL:HG23	1.65	0.77
1:A:241:ASP:OD2	1:A:292:SER:OG	2.02	0.76
1:A:53:PHE:O	1:A:54:ASP:HB2	1.86	0.75
1:A:210:HIS:HD2	1:A:222:ASN:OD1	1.69	0.75
1:A:300:ASN:HD22	1:A:303:SER:H	1.35	0.75
1:B:14:LEU:O	1:B:18:LEU:HD12	1.87	0.75
1:B:300:ASN:HD22	1:B:303:SER:H	1.33	0.74
1:A:405:ASN:ND2	1:A:407:LEU:H	1.87	0.73
1:A:405:ASN:HD21	1:A:407:LEU:HB2	1.52	0.72
1:B:21:VAL:O	1:B:318:LYS:NZ	2.27	0.68
1:B:210:HIS:HD2	1:B:222:ASN:OD1	1.78	0.67
1:B:77:ALA:HB2	1:B:94:THR:HG21	1.78	0.64
1:A:55:ASN:O	1:A:137:ARG:N	2.31	0.64
1:B:50:VAL:HA	1:B:51:PRO:C	2.17	0.63
1:A:288:LYS:HG3	1:A:293:TRP:CZ3	2.33	0.63
1:B:405:ASN:C	1:B:405:ASN:ND2	2.49	0.62
1:A:405:ASN:C	1:A:405:ASN:ND2	2.49	0.61
1:A:157:THR:HG21	1:B:408:PHE:O	1.99	0.61
1:B:62:ALA:HB1	1:B:108:CYS:SG	2.40	0.61
1:B:90:TRP:HD1	1:B:91:PRO:O	1.83	0.60
1:B:150:PHE:CE2	1:B:160:GLU:HG3	2.37	0.60
1:B:405:ASN:HD22	1:B:407:LEU:H	1.47	0.60
1:B:137:ARG:HB3	1:B:141:GLU:OE1	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:35:CYS:HB3	1:B:156:LEU:HD12	1.85	0.59
1:B:405:ASN:ND2	1:B:407:LEU:N	2.46	0.59
1:B:368:HIS:CD2	1:B:372:HIS:HE1	2.21	0.59
1:A:204:THR:HG22	1:B:165:ALA:HB3	1.83	0.59
1:B:271:ILE:HA	1:B:287:GLY:HA3	1.85	0.58
1:A:244:ALA:O	1:A:292:SER:HB3	2.03	0.57
1:A:210:HIS:CD2	1:A:222:ASN:OD1	2.55	0.57
1:A:313:GLN:HB3	1:A:314:PRO:HD3	1.86	0.57
1:B:353:LEU:HD13	1:B:401:VAL:HG11	1.87	0.57
1:A:51:PRO:O	1:A:139:ARG:HA	2.04	0.56
1:B:117:THR:OG1	1:B:124:VAL:HG12	2.05	0.56
1:A:137:ARG:HG3	1:A:141:GLU:OE2	2.06	0.56
1:B:117:THR:HA	1:B:127:THR:H	1.71	0.56
1:A:327:LEU:O	1:A:328:PRO:C	2.45	0.55
1:B:405:ASN:HD22	1:B:406:ALA:N	2.05	0.55
1:B:356:ASN:OD1	1:B:360:GLU:HG2	2.07	0.55
1:B:206:ARG:HH11	1:B:206:ARG:HG2	1.72	0.54
1:A:405:ASN:ND2	1:A:407:LEU:N	2.53	0.54
1:A:405:ASN:HD21	1:A:407:LEU:CB	2.17	0.54
1:A:258:ALA:HA	1:A:262:LYS:HD3	1.90	0.54
1:B:279:LYS:HG2	1:B:280:PRO:HA	1.90	0.54
1:A:21:VAL:O	1:A:318:LYS:NZ	2.41	0.54
1:A:191:LEU:HB3	1:A:192:PRO:HD2	1.88	0.53
1:B:347:ASP:OD1	1:B:349:GLN:HG3	2.07	0.53
1:B:46:SER:OG	1:B:48:LEU:O	2.26	0.53
1:B:313:GLN:HB3	1:B:314:PRO:HD3	1.91	0.53
1:B:65:LEU:HA	1:B:68:ILE:HG22	1.91	0.53
1:B:81:PHE:HB2	1:B:84:GLN:HB3	1.92	0.52
1:A:259:ASP:OD1	1:A:259:ASP:C	2.48	0.52
1:B:272:ALA:N	1:B:286:PHE:O	2.42	0.52
1:B:187:ASP:OD2	1:B:188:GLU:N	2.43	0.52
1:A:14:LEU:HD22	1:A:18:LEU:HD11	1.92	0.51
1:B:87:HIS:N	1:B:87:HIS:ND1	2.58	0.51
1:A:300:ASN:ND2	1:A:303:SER:H	2.06	0.51
1:A:341:LYS:O	1:A:391:GLY:HA2	2.11	0.51
1:B:156:LEU:HD13	1:B:161:LEU:HD21	1.93	0.50
1:B:97:ARG:HG3	1:B:98:ILE:N	2.24	0.50
1:A:36:PHE:CZ	1:B:215:GLN:HG3	2.47	0.50
1:A:53:PHE:O	1:A:54:ASP:CB	2.59	0.50
1:B:191:LEU:HB3	1:B:192:PRO:HD2	1.94	0.50
1:A:279:LYS:HG2	1:A:280:PRO:HA	1.92	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:49:ASP:O	1:A:52:GLY:HA2	2.11	0.49
1:B:300:ASN:ND2	1:B:303:SER:H	2.08	0.49
1:B:327:LEU:O	1:B:328:PRO:C	2.51	0.49
1:B:327:LEU:O	1:B:328:PRO:O	2.31	0.49
1:B:405:ASN:HD22	1:B:407:LEU:N	2.07	0.49
1:A:378:SER:OG	1:B:160:GLU:OE1	2.31	0.49
1:B:346:LEU:HD11	1:B:385:VAL:HG12	1.95	0.48
1:B:65:LEU:HA	1:B:68:ILE:CG2	2.43	0.48
1:B:405:ASN:HD21	1:B:407:LEU:CB	2.26	0.48
1:B:341:LYS:NZ	1:B:388:ARG:O	2.47	0.48
1:B:387:GLU:OE1	1:B:387:GLU:N	2.43	0.48
1:A:51:PRO:HG2	1:A:139:ARG:HA	1.95	0.48
1:B:64:ARG:HD3	1:B:90:TRP:CZ2	2.48	0.48
1:A:21:VAL:HG21	1:A:315:LEU:HD12	1.96	0.47
1:A:21:VAL:HG21	1:A:315:LEU:CD1	2.45	0.47
1:A:284:PHE:CE2	1:A:286:PHE:HB2	2.50	0.47
1:B:192:PRO:C	1:B:194:GLN:H	2.17	0.47
1:A:221:ILE:HG22	1:A:223:LEU:HD13	1.97	0.47
1:B:64:ARG:HA	1:B:109:GLU:HG3	1.96	0.46
1:A:332:ARG:HG3	1:B:355:ARG:HH22	1.79	0.46
1:B:405:ASN:HD21	1:B:407:LEU:CG	2.28	0.46
1:A:161:LEU:N	1:A:162:PRO:CD	2.78	0.46
1:A:341:LYS:HB2	1:A:386:LEU:CD1	2.45	0.46
1:B:405:ASN:HD21	1:B:407:LEU:HG	1.80	0.46
1:B:259:ASP:C	1:B:259:ASP:OD1	2.53	0.46
1:B:140:GLY:HA2	1:B:143:ILE:O	2.15	0.46
1:B:222:ASN:C	1:B:222:ASN:HD22	2.19	0.46
1:B:222:ASN:HD22	1:B:224:GLY:H	1.64	0.45
1:B:98:ILE:HG12	1:B:102:ALA:HB3	1.99	0.45
1:B:42:SER:O	1:B:43:ASP:C	2.54	0.45
1:B:190:GLN:OE1	1:B:190:GLN:HA	2.17	0.44
1:B:264:ILE:O	1:B:268:LEU:HG	2.17	0.44
1:A:38:ARG:O	1:A:156:LEU:HG	2.17	0.44
1:A:206:ARG:HH11	1:A:222:ASN:HD21	1.65	0.44
1:B:350:ARG:HD3	1:B:376:SER:HB2	1.99	0.44
1:A:278:ILE:O	1:A:345:ARG:NH1	2.37	0.44
1:A:279:LYS:HA	1:A:280:PRO:C	2.36	0.44
1:B:10:LEU:CD2	1:B:311:LEU:HD21	2.48	0.44
1:A:222:ASN:HD22	1:A:222:ASN:C	2.20	0.44
1:B:39:ILE:N	1:B:39:ILE:HD13	2.33	0.44
1:A:14:LEU:O	1:A:18:LEU:HD12	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:391:GLY:O	1:B:392:ASN:C	2.56	0.44
1:A:197:GLY:O	1:A:198:ASP:O	2.36	0.43
1:B:346:LEU:HD11	1:B:385:VAL:CG1	2.47	0.43
1:A:288:LYS:HG3	1:A:293:TRP:CH2	2.52	0.43
1:B:207:LEU:HD22	1:B:211:LEU:CD1	2.47	0.43
1:B:74:LEU:HD12	1:B:126:PHE:HE1	1.84	0.43
1:B:49:ASP:OD1	1:B:144:SER:HA	2.19	0.43
1:A:391:GLY:O	1:A:392:ASN:C	2.57	0.43
1:B:113:MET:O	1:B:115:GLU:N	2.52	0.43
1:A:381:ASN:HA	1:A:404:PHE:CD2	2.54	0.43
1:B:58:MET:SD	1:B:113:MET:HG2	2.59	0.42
1:A:46:SER:OG	1:A:48:LEU:O	2.32	0.42
1:A:222:ASN:HD22	1:A:224:GLY:H	1.66	0.42
1:A:227:ARG:HG3	1:A:232:ALA:HB2	2.01	0.42
1:B:64:ARG:HG3	1:B:109:GLU:HG2	2.01	0.42
1:A:278:ILE:O	1:A:345:ARG:HD2	2.20	0.42
1:A:144:SER:O	1:A:147:ALA:HB3	2.20	0.42
1:B:95:CYS:SG	1:B:95:CYS:O	2.78	0.42
1:A:158:THR:HG21	1:B:212:MET:HG3	2.01	0.41
1:A:234:ARG:O	1:A:238:ILE:HG13	2.20	0.41
1:A:356:ASN:OD1	1:A:360:GLU:HG2	2.20	0.41
1:B:73:PRO:HG3	1:B:125:ARG:HG3	2.02	0.41
1:B:127:THR:O	1:B:127:THR:HG22	2.20	0.41
1:B:286:PHE:CG	1:B:287:GLY:N	2.88	0.41
1:A:8:MET:HB3	1:A:276:LEU:HD12	2.02	0.41
1:A:279:LYS:CG	1:A:280:PRO:HA	2.50	0.41
1:B:280:PRO:O	1:B:306:LEU:HD12	2.20	0.41
1:B:281:GLY:O	1:B:282:LYS:HB2	2.21	0.41
1:B:328:PRO:O	1:B:329:ALA:C	2.58	0.41
1:A:179:ARG:NH1	1:A:243:GLN:O	2.53	0.41
1:A:341:LYS:HG3	1:A:391:GLY:HA2	2.01	0.41
1:A:192:PRO:HB2	1:B:170:ALA:HB2	2.01	0.41
1:A:271:ILE:HD12	1:A:271:ILE:N	2.35	0.41
1:A:341:LYS:NZ	1:A:388:ARG:O	2.53	0.41
1:B:350:ARG:CD	1:B:376:SER:HB2	2.50	0.41
1:A:363:VAL:HG11	1:A:401:VAL:HG21	2.02	0.41
1:A:394:GLU:N	1:A:397:GLU:OE2	2.46	0.41
1:B:50:VAL:CA	1:B:51:PRO:C	2.86	0.41
1:A:288:LYS:CG	1:A:293:TRP:CZ3	3.02	0.41
1:B:98:ILE:HD11	1:B:102:ALA:O	2.20	0.41
1:B:161:LEU:HB2	1:B:162:PRO:HD3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:405:ASN:HD21	1:B:407:LEU:HB2	1.86	0.41
1:A:212:MET:HG2	1:A:407:LEU:HD13	2.03	0.41
1:B:18:LEU:O	1:B:318:LYS:NZ	2.49	0.40
1:B:40:LEU:HD11	1:B:44:VAL:CG2	2.37	0.40
1:A:39:ILE:N	1:A:39:ILE:HD13	2.36	0.40
1:B:55:ASN:HD22	1:B:56:SER:N	2.19	0.40
1:B:351:GLY:HA3	1:B:384:ILE:HD11	2.03	0.40
1:A:311:LEU:O	1:A:314:PRO:HD2	2.21	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	318/411 (77%)	291 (92%)	20 (6%)	7 (2%)	6	31
1	B	401/411 (98%)	349 (87%)	45 (11%)	7 (2%)	9	39
All	All	719/822 (88%)	640 (89%)	65 (9%)	14 (2%)	8	36

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	54	ASP
1	A	198	ASP
1	A	282	LYS
1	A	392	ASN
1	B	91	PRO
1	B	114	GLN
1	B	198	ASP
1	B	282	LYS
1	A	328	PRO
1	B	328	PRO

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Mol	Chain	Res	Type
1	B	93	GLY
1	A	329	ALA
1	B	68	ILE
1	A	32	LEU

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	264/330 (80%)	219 (83%)	45 (17%)	2 10
1	B	324/330 (98%)	255 (79%)	69 (21%)	1 5
All	All	588/660 (89%)	474 (81%)	114 (19%)	1 7

All (114) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	LEU
1	A	14	LEU
1	A	16	GLU
1	A	20	ARG
1	A	24	LEU
1	A	33	VAL
1	A	40	LEU
1	A	48	LEU
1	A	53	PHE
1	A	137	ARG
1	A	138	ARG
1	A	139	ARG
1	A	156	LEU
1	A	158	THR
1	A	182	LEU
1	A	188	GLU
1	A	190	GLN
1	A	194	GLN
1	A	196	LEU

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Mol	Chain	Res	Type
1	A	204	THR
1	A	207	LEU
1	A	222	ASN
1	A	223	LEU
1	A	227	ARG
1	A	233	LEU
1	A	234	ARG
1	A	243	GLN
1	A	263	THR
1	A	276	LEU
1	A	278	ILE
1	A	288	LYS
1	A	306	LEU
1	A	332	ARG
1	A	335	THR
1	A	337	SER
1	A	338	ARG
1	A	339	LEU
1	A	340	LYS
1	A	350	ARG
1	A	355	ARG
1	A	356	ASN
1	A	363	VAL
1	A	376	SER
1	A	378	SER
1	A	405	ASN
1	B	9	SER
1	B	10	LEU
1	B	16	GLU
1	B	18	LEU
1	B	20	ARG
1	B	24	LEU
1	B	40	LEU
1	B	48	LEU
1	B	54	ASP
1	B	55	ASN
1	B	58	MET
1	B	64	ARG
1	B	65	LEU
1	B	67	ASP
1	B	72	GLN
1	B	74	LEU

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Mol	Chain	Res	Type
1	B	79	LYS
1	B	80	SER
1	B	87	HIS
1	B	94	THR
1	B	97	ARG
1	B	99	MET
1	B	104	VAL
1	B	109	GLU
1	B	112	VAL
1	B	113	MET
1	B	114	GLN
1	B	119	GLN
1	B	120	MET
1	B	121	ASP
1	B	122	ASN
1	B	129	GLU
1	B	131	ARG
1	B	132	SER
1	B	134	GLN
1	B	137	ARG
1	B	138	ARG
1	B	139	ARG
1	B	141	GLU
1	B	158	THR
1	B	182	LEU
1	B	188	GLU
1	B	190	GLN
1	B	196	LEU
1	B	204	THR
1	B	207	LEU
1	B	222	ASN
1	B	223	LEU
1	B	227	ARG
1	B	228	ASP
1	B	233	LEU
1	B	234	ARG
1	B	243	GLN
1	B	263	THR
1	B	276	LEU
1	B	278	ILE
1	B	288	LYS
1	B	300	ASN

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Mol	Chain	Res	Type
1	B	327	LEU
1	B	335	THR
1	B	338	ARG
1	B	340	LYS
1	B	350	ARG
1	B	355	ARG
1	B	360	GLU
1	B	363	VAL
1	B	376	SER
1	B	378	SER
1	B	405	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	210	HIS
1	A	222	ASN
1	A	300	ASN
1	A	313	GLN
1	A	368	HIS
1	A	405	ASN
1	B	15	ASN
1	B	55	ASN
1	B	122	ASN
1	B	190	GLN
1	B	210	HIS
1	B	222	ASN
1	B	300	ASN
1	B	349	GLN
1	B	368	HIS
1	B	372	HIS
1	B	405	ASN

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)

There are no ligands in this entry.

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	322/411 (78%)	-0.16	5 (1%) 72 44	30, 55, 76, 86	0
1	B	403/411 (98%)	0.19	29 (7%) 15 4	31, 59, 113, 141	0
All	All	725/822 (88%)	0.03	34 (4%) 31 11	30, 57, 103, 141	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	326	GLY	7.2
1	B	75	PRO	5.4
1	B	87	HIS	4.9
1	B	82	ALA	4.3
1	B	122	ASN	4.2
1	B	95	CYS	4.1
1	B	94	THR	4.0
1	B	83	GLY	3.8
1	B	88	GLY	3.8
1	B	119	GLN	3.6
1	A	325	SER	3.6
1	B	121	ASP	3.4
1	B	77	ALA	3.4
1	B	66	ALA	3.4
1	B	80	SER	3.2
1	B	86	TYR	3.2
1	B	126	PHE	3.2
1	B	117	THR	3.2
1	B	58	MET	3.0
1	B	63	VAL	2.6
1	B	120	MET	2.5
1	A	398	TRP	2.4
1	B	130	VAL	2.4
1	A	326	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	339	LEU	2.4
1	B	123	GLY	2.3
1	B	98	ILE	2.3
1	B	104	VAL	2.3
1	B	358	ASP	2.2
1	B	93	GLY	2.2
1	A	193	GLY	2.2
1	B	102	ALA	2.1
1	B	127	THR	2.1
1	B	118	GLU	2.1

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.