Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:40 AM GMT

PDB ID	:	2NRS
Title	:	MoeA S371W
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Deposited on	:	2006-11-02
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
http://wwpdb.org/validation/2016/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:

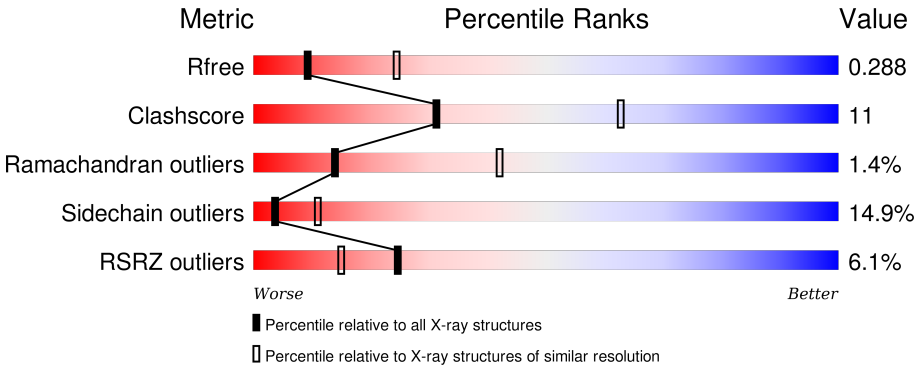
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.80 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}	91344	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (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 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	9% 67% 27%
1	B	411	2% 73% 21%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 6096 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
			3048	1926	532	577	13			
1	B	403	Total	C	N	O	S	0	0	0
			3048	1926	532	577	13			

There are 2 discrepancies between the modelled and reference sequences:

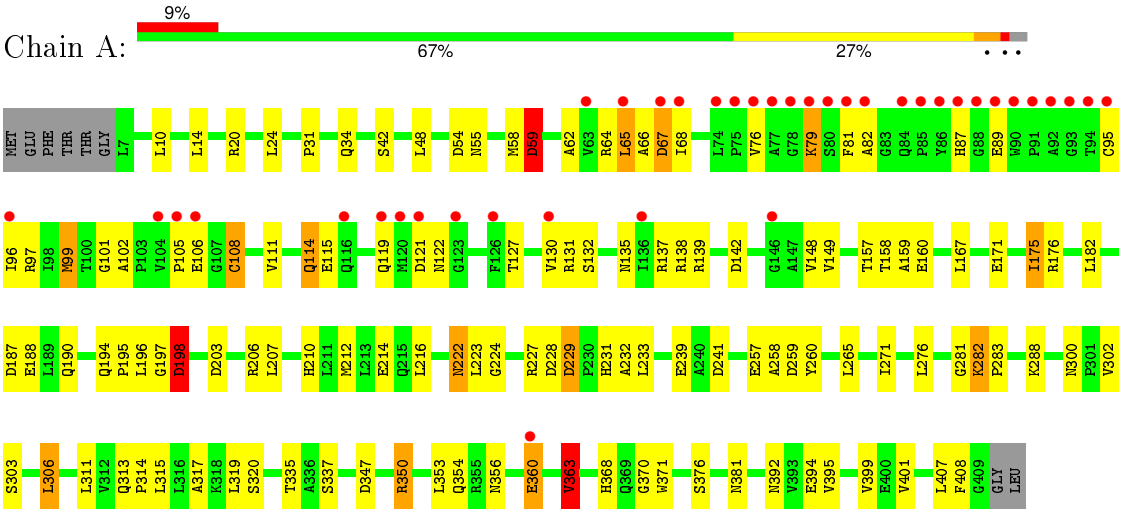
Chain	Residue	Modelled	Actual	Comment	Reference
A	371	TRP	SER	ENGINEERED	UNP P12281
B	371	TRP	SER	ENGINEERED	UNP P12281

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.

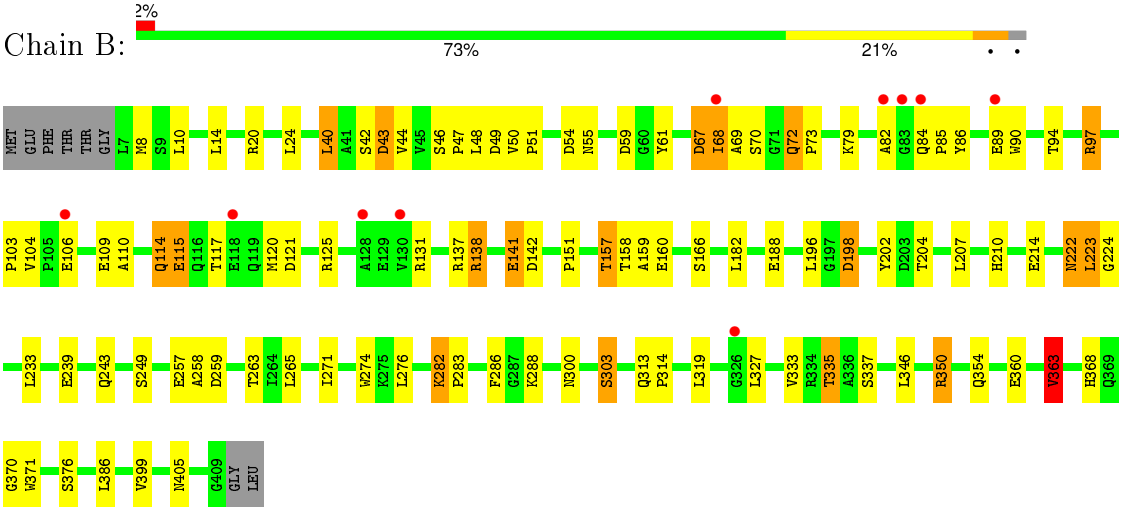
- Molecule 1: Molybdopterin biosynthesis protein moeA

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	68.48Å 98.71Å 159.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.39 – 2.80 46.86 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.7 (49.39-2.80) 98.7 (46.86-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.33 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.247 , 0.303 0.229 , 0.288	Depositor DCC
R_{free} test set	1377 reflections (5.37%)	DCC
Wilson B-factor (Å^2)	55.8	Xtriage
Anisotropy	0.176	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 35.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Outliers	0 of 27021 reflections	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	6096	wwPDB-VP
Average B, all atoms (Å^2)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.85% 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

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	0.81	0/3109	0.95	11/4227 (0.3%)
1	B	0.87	0/3109	0.98	9/4227 (0.2%)
All	All	0.84	0/6218	0.96	20/8454 (0.2%)

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	59	ASP	CB-CG-OD2	7.12	124.71	118.30
1	B	121	ASP	CB-CG-OD2	7.09	124.69	118.30
1	A	198	ASP	CB-CG-OD2	6.57	124.22	118.30
1	A	142	ASP	CB-CG-OD2	6.52	124.17	118.30
1	A	187	ASP	CB-CG-OD2	6.44	124.10	118.30
1	B	198	ASP	CB-CG-OD2	6.15	123.83	118.30
1	B	67	ASP	CB-CG-OD2	6.03	123.72	118.30
1	B	142	ASP	CB-CG-OD2	5.90	123.61	118.30
1	A	67	ASP	CB-CG-OD2	5.77	123.50	118.30
1	B	49	ASP	CB-CG-OD2	5.55	123.29	118.30
1	B	363	VAL	CB-CA-C	-5.51	100.92	111.40
1	A	203	ASP	CB-CG-OD2	5.50	123.25	118.30
1	B	59	ASP	CB-CG-OD2	5.44	123.20	118.30
1	A	241	ASP	CB-CG-OD2	5.44	123.20	118.30
1	A	121	ASP	CB-CG-OD2	5.44	123.19	118.30
1	A	229	ASP	CB-CG-OD2	5.42	123.18	118.30
1	A	363	VAL	CB-CA-C	-5.27	101.38	111.40
1	B	54	ASP	CB-CG-OD2	5.23	123.01	118.30
1	B	137	ARG	NE-CZ-NH1	5.11	122.86	120.30
1	A	347	ASP	CB-CG-OD2	5.04	122.84	118.30

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	3048	0	3042	74	0
1	B	3048	0	3042	58	0
All	All	6096	0	6084	131	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 11.

All (131) 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:190:GLN:NE2	1:A:194:GLN:HE21	1.40	1.18
1:B:157:THR:HG22	1:B:159:ALA:H	1.27	0.99
1:A:300:ASN:ND2	1:A:303:SER:H	1.61	0.99
1:A:190:GLN:NE2	1:A:194:GLN:NE2	2.15	0.94
1:A:368:HIS:HD2	1:A:370:GLY:H	1.15	0.93
1:A:190:GLN:HE21	1:A:194:GLN:HE21	1.14	0.92
1:A:300:ASN:HD22	1:A:303:SER:H	0.95	0.89
1:A:157:THR:HB	1:A:160:GLU:OE2	1.76	0.85
1:B:300:ASN:HD22	1:B:303:SER:H	1.25	0.82
1:A:157:THR:HG22	1:A:158:THR:N	1.95	0.82
1:B:222:ASN:HD22	1:B:222:ASN:C	1.85	0.79
1:B:40:LEU:HD11	1:B:44:VAL:HG23	1.67	0.77
1:B:114:GLN:O	1:B:117:THR:HG22	1.85	0.75
1:B:138:ARG:HH11	1:B:138:ARG:CG	2.00	0.75
1:A:368:HIS:CD2	1:A:370:GLY:H	2.03	0.72
1:B:70:SER:OG	1:B:72:GLN:NE2	2.19	0.72
1:A:190:GLN:HE22	1:A:194:GLN:NE2	1.88	0.70
1:A:300:ASN:HD22	1:A:303:SER:N	1.81	0.69
1:B:115:GLU:N	1:B:115:GLU:OE2	2.26	0.68
1:B:350:ARG:HD2	1:B:376:SER:OG	1.93	0.68
1:B:222:ASN:ND2	1:B:224:GLY:H	1.91	0.67
1:A:157:THR:CG2	1:A:158:THR:N	2.58	0.67
1:B:300:ASN:ND2	1:B:303:SER:H	1.93	0.67
1:A:206:ARG:HH11	1:A:222:ASN:HD21	1.44	0.66
1:B:138:ARG:O	1:B:141:GLU:HG2	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:138:ARG:HG2	1:B:138:ARG:HH11	1.61	0.64
1:B:79:LYS:O	1:B:86:TYR:HB2	1.98	0.64
1:B:157:THR:HB	1:B:160:GLU:OE2	1.98	0.64
1:A:190:GLN:HE21	1:A:194:GLN:CB	2.12	0.62
1:A:315:LEU:HD23	1:A:319:LEU:HD12	1.82	0.62
1:A:350:ARG:HD2	1:A:376:SER:OG	2.01	0.61
1:A:157:THR:HG22	1:A:159:ALA:H	1.67	0.60
1:A:190:GLN:HE21	1:A:194:GLN:NE2	1.89	0.60
1:B:114:GLN:OE1	1:B:114:GLN:CA	2.49	0.60
1:B:196:LEU:HD13	1:B:202:TYR:CZ	2.39	0.58
1:B:157:THR:CG2	1:B:158:THR:N	2.67	0.58
1:A:368:HIS:HD2	1:A:370:GLY:N	1.96	0.57
1:B:8:MET:HE1	1:B:274:TRP:CD1	2.40	0.57
1:A:265:LEU:HD22	1:A:271:ILE:HG13	1.86	0.56
1:B:67:ASP:O	1:B:68:ILE:C	2.44	0.56
1:A:54:ASP:HA	1:A:137:ARG:O	2.06	0.56
1:A:300:ASN:ND2	1:A:303:SER:N	2.44	0.55
1:B:346:LEU:HD12	1:B:386:LEU:O	2.07	0.54
1:B:222:ASN:C	1:B:222:ASN:ND2	2.57	0.54
1:A:282:LYS:HB3	1:A:283:PRO:HD3	1.90	0.53
1:A:210:HIS:HE1	1:A:214:GLU:OE2	1.91	0.53
1:A:335:THR:HG22	1:A:337:SER:H	1.73	0.53
1:A:55:ASN:HD22	1:A:101:GLY:HA2	1.72	0.53
1:A:300:ASN:HD21	1:A:302:VAL:HB	1.74	0.53
1:A:111:VAL:HB	1:A:135:ASN:HB2	1.91	0.53
1:B:313:GLN:HE22	1:B:405:ASN:HD21	1.57	0.53
1:A:381:ASN:C	1:A:381:ASN:OD1	2.44	0.52
1:B:222:ASN:HD22	1:B:224:GLY:H	1.53	0.52
1:A:190:GLN:HE21	1:A:194:GLN:HB2	1.73	0.52
1:A:76:VAL:O	1:A:76:VAL:HG23	2.09	0.52
1:A:149:VAL:HG21	1:A:167:LEU:HD11	1.92	0.52
1:B:222:ASN:HD22	1:B:223:LEU:N	2.08	0.51
1:A:222:ASN:C	1:A:222:ASN:HD22	2.13	0.51
1:A:212:MET:HG2	1:A:407:LEU:HD13	1.92	0.51
1:B:8:MET:CE	1:B:274:TRP:CD1	2.94	0.50
1:A:157:THR:CG2	1:A:158:THR:H	2.24	0.50
1:B:50:VAL:HA	1:B:51:PRO:C	2.32	0.50
1:B:368:HIS:HD2	1:B:370:GLY:N	2.10	0.49
1:A:350:ARG:CD	1:A:376:SER:OG	2.59	0.49
1:A:311:LEU:O	1:A:314:PRO:HG2	2.12	0.49
1:A:59:ASP:OD2	1:A:59:ASP:N	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:PRO:HG2	1:A:34:GLN:NE2	2.28	0.48
1:A:148:VAL:HG12	1:A:148:VAL:O	2.12	0.48
1:B:282:LYS:N	1:B:283:PRO:HD3	2.27	0.48
1:B:85:PRO:HB3	1:B:103:PRO:HG2	1.95	0.48
1:B:259:ASP:C	1:B:259:ASP:OD1	2.52	0.48
1:A:194:GLN:HB3	1:A:195:PRO:HD2	1.96	0.47
1:A:394:GLU:O	1:A:395:VAL:C	2.48	0.47
1:A:62:ALA:HB3	1:A:96:ILE:HB	1.95	0.47
1:A:281:GLY:HA2	1:A:303:SER:OG	2.14	0.47
1:B:97:ARG:NH2	1:B:114:GLN:HE22	2.13	0.47
1:A:313:GLN:HB3	1:A:314:PRO:CD	2.44	0.47
1:B:43:ASP:OD1	1:B:151:PRO:HA	2.15	0.47
1:B:114:GLN:HA	1:B:114:GLN:OE1	2.14	0.47
1:A:353:LEU:HD13	1:A:363:VAL:HG13	1.97	0.47
1:B:210:HIS:HE1	1:B:214:GLU:OE2	1.98	0.47
1:B:114:GLN:N	1:B:114:GLN:OE1	2.48	0.47
1:A:105:PRO:HD2	1:A:108:CYS:HB2	1.96	0.46
1:A:210:HIS:HD2	1:A:222:ASN:OD1	1.98	0.46
1:B:265:LEU:HD22	1:B:271:ILE:HG13	1.97	0.46
1:A:105:PRO:HD2	1:A:108:CYS:CB	2.45	0.46
1:A:222:ASN:HD22	1:A:224:GLY:H	1.62	0.46
1:A:212:MET:CG	1:A:407:LEU:HD13	2.46	0.46
1:B:368:HIS:HD2	1:B:370:GLY:H	1.63	0.46
1:A:314:PRO:O	1:A:317:ALA:HB3	2.16	0.46
1:A:190:GLN:NE2	1:A:194:GLN:CB	2.78	0.46
1:A:59:ASP:HB3	1:A:99:MET:SD	2.57	0.45
1:B:114:GLN:HB3	1:B:115:GLU:OE2	2.16	0.45
1:A:175:ILE:HG22	1:A:176:ARG:O	2.16	0.45
1:B:202:TYR:O	1:B:204:THR:HG23	2.17	0.44
1:A:115:GLU:H	1:A:115:GLU:CD	2.20	0.44
1:A:76:VAL:HA	1:A:95:CYS:O	2.16	0.44
1:A:79:LYS:HD2	1:A:81:PHE:HD1	1.83	0.44
1:A:97:ARG:HH22	1:A:114:GLN:HE22	1.65	0.44
1:B:109:GLU:O	1:B:110:ALA:HB2	2.18	0.44
1:B:335:THR:HG22	1:B:337:SER:H	1.83	0.44
1:B:282:LYS:N	1:B:283:PRO:CD	2.80	0.44
1:A:157:THR:HG22	1:A:158:THR:H	1.78	0.43
1:A:356:ASN:HD21	1:A:360:GLU:HG3	1.82	0.43
1:A:231:HIS:O	1:A:232:ALA:C	2.55	0.43
1:B:327:LEU:HA	1:B:327:LEU:HD12	1.83	0.43
1:B:67:ASP:O	1:B:69:ALA:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:72:GLN:HB2	1:B:73:PRO:HD2	2.01	0.43
1:B:313:GLN:HE22	1:B:405:ASN:ND2	2.17	0.43
1:A:222:ASN:ND2	1:A:224:GLY:H	2.16	0.43
1:A:258:ALA:O	1:A:259:ASP:HB3	2.19	0.43
1:A:408:PHE:C	1:B:157:THR:HG21	2.39	0.43
1:A:335:THR:HA	1:A:363:VAL:HG23	1.99	0.42
1:B:258:ALA:O	1:B:259:ASP:HB3	2.19	0.42
1:B:90:TRP:HD1	1:B:94:THR:OG1	2.02	0.42
1:B:286:PHE:C	1:B:286:PHE:CD2	2.93	0.42
1:B:46:SER:HA	1:B:47:PRO:HD3	1.88	0.42
1:B:138:ARG:NH1	1:B:138:ARG:CG	2.71	0.42
1:A:206:ARG:HH11	1:A:222:ASN:ND2	2.16	0.42
1:B:69:ALA:O	1:B:70:SER:C	2.58	0.42
1:B:313:GLN:HB3	1:B:314:PRO:CD	2.51	0.41
1:A:65:LEU:HD11	1:A:130:VAL:O	2.20	0.41
1:B:335:THR:HA	1:B:363:VAL:HG23	2.02	0.41
1:B:138:ARG:HH11	1:B:138:ARG:HG3	1.83	0.41
1:A:212:MET:O	1:A:216:LEU:HG	2.21	0.41
1:A:317:ALA:O	1:A:320:SER:OG	2.28	0.41
1:A:99:MET:O	1:A:102:ALA:CB	2.68	0.41
1:A:260:TYR:CD1	1:A:260:TYR:C	2.95	0.40
1:A:306:LEU:HD22	1:A:306:LEU:O	2.20	0.40
1:A:196:LEU:HD12	1:A:196:LEU:HA	1.91	0.40
1:B:282:LYS:HB3	1:B:283:PRO:HD3	2.04	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%)	369 (92%)	25 (6%)	7 (2%)	11 36

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	401/411 (98%)	376 (94%)	21 (5%)	4 (1%)	19 52
All	All	802/822 (98%)	745 (93%)	46 (6%)	11 (1%)	14 42

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	82	ALA
1	A	282	LYS
1	B	282	LYS
1	A	392	ASN
1	A	198	ASP
1	A	127	THR
1	A	197	GLY
1	B	68	ILE
1	A	66	ALA
1	B	82	ALA
1	B	43	ASP

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	325/331 (98%)	276 (85%)	49 (15%)	3 10
1	B	325/331 (98%)	277 (85%)	48 (15%)	4 11
All	All	650/662 (98%)	553 (85%)	97 (15%)	4 11

All (97) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	LEU
1	A	14	LEU
1	A	20	ARG
1	A	24	LEU
1	A	42	SER

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Mol	Chain	Res	Type
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	68	ILE
1	A	79	LYS
1	A	87	HIS
1	A	89	GLU
1	A	99	MET
1	A	106	GLU
1	A	108	CYS
1	A	114	GLN
1	A	119	GLN
1	A	122	ASN
1	A	131	ARG
1	A	132	SER
1	A	138	ARG
1	A	139	ARG
1	A	171	GLU
1	A	175	ILE
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	227	ARG
1	A	228	ASP
1	A	229	ASP
1	A	233	LEU
1	A	239	GLU
1	A	257	GLU
1	A	276	LEU
1	A	288	LYS
1	A	306	LEU
1	A	350	ARG
1	A	354	GLN
1	A	360	GLU
1	A	363	VAL
1	A	371	TRP

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Mol	Chain	Res	Type
1	A	399	VAL
1	A	401	VAL
1	B	10	LEU
1	B	14	LEU
1	B	20	ARG
1	B	24	LEU
1	B	40	LEU
1	B	42	SER
1	B	48	LEU
1	B	55	ASN
1	B	61	TYR
1	B	72	GLN
1	B	84	GLN
1	B	89	GLU
1	B	97	ARG
1	B	104	VAL
1	B	106	GLU
1	B	114	GLN
1	B	115	GLU
1	B	120	MET
1	B	125	ARG
1	B	131	ARG
1	B	138	ARG
1	B	141	GLU
1	B	157	THR
1	B	166	SER
1	B	182	LEU
1	B	188	GLU
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	243	GLN
1	B	249	SER
1	B	257	GLU
1	B	263	THR
1	B	276	LEU
1	B	288	LYS
1	B	303	SER
1	B	319	LEU

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Mol	Chain	Res	Type
1	B	333	VAL
1	B	335	THR
1	B	350	ARG
1	B	354	GLN
1	B	360	GLU
1	B	363	VAL
1	B	371	TRP
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	27	GLN
1	A	34	GLN
1	A	55	ASN
1	A	84	GLN
1	A	114	GLN
1	A	190	GLN
1	A	210	HIS
1	A	215	GLN
1	A	222	ASN
1	A	300	ASN
1	A	368	HIS
1	B	55	ASN
1	B	72	GLN
1	B	119	GLN
1	B	190	GLN
1	B	194	GLN
1	B	210	HIS
1	B	222	ASN
1	B	243	GLN
1	B	300	ASN
1	B	313	GLN
1	B	368	HIS

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

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	403/411 (98%)	0.44	39 (9%) 10 5	19, 45, 97, 123	0
1	B	403/411 (98%)	0.18	10 (2%) 61 48	18, 41, 72, 90	0
All	All	806/822 (98%)	0.31	49 (6%) 25 15	18, 43, 87, 123	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	87	HIS	6.8
1	A	86	TYR	6.4
1	A	93	GLY	5.2
1	A	78	GLY	4.5
1	A	130	VAL	4.1
1	A	120	MET	3.9
1	A	90	TRP	3.7
1	A	89	GLU	3.6
1	A	119	GLN	3.6
1	A	81	PHE	3.3
1	A	94	THR	3.3
1	B	89	GLU	3.3
1	A	116	GLN	3.3
1	A	77	ALA	3.2
1	A	88	GLY	3.2
1	A	95	CYS	3.2
1	A	92	ALA	3.2
1	A	91	PRO	3.1
1	B	106	GLU	3.1
1	A	121	ASP	3.0
1	A	80	SER	3.0
1	A	123	GLY	3.0
1	B	128	ALA	2.9
1	A	76	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	118	GLU	2.9
1	A	68	ILE	2.8
1	A	74	LEU	2.7
1	A	63	VAL	2.7
1	B	130	VAL	2.7
1	A	104	VAL	2.6
1	A	79	LYS	2.6
1	B	82	ALA	2.5
1	A	360	GLU	2.5
1	A	65	LEU	2.5
1	B	83	GLY	2.5
1	A	75	PRO	2.4
1	A	105	PRO	2.4
1	B	84	GLN	2.4
1	A	67	ASP	2.3
1	A	84	GLN	2.3
1	A	146	GLY	2.3
1	A	136	ILE	2.2
1	A	96	ILE	2.2
1	B	326	GLY	2.2
1	A	126	PHE	2.2
1	A	85	PRO	2.2
1	A	82	ALA	2.1
1	A	106	GLU	2.1
1	B	68	ILE	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)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.