



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:16 AM UTC

PDB ID : 2NRS / pdb_00002nrs
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

<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
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

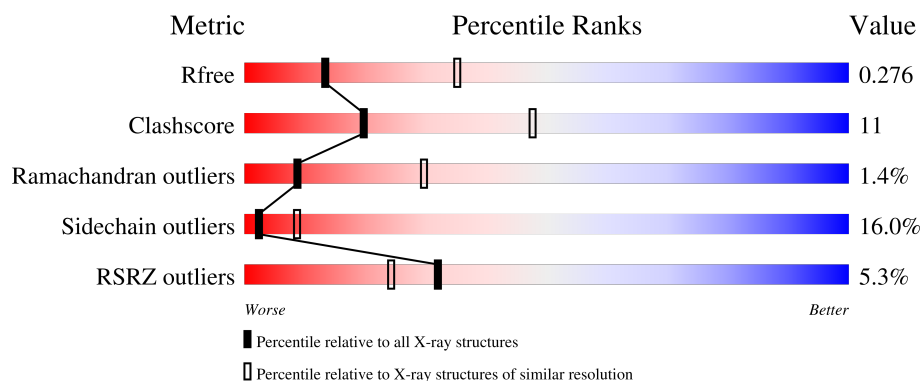
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	411	6% 66% 28% • •
1	B	411	4% 70% 23% • •

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.

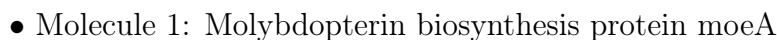
- Molecule 1 is a protein called Molybdopterin biosynthesis protein moeA.

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 mutation	UNP P12281
B	371	TRP	SER	engineered mutation	UNP P12281

- 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	68.48Å 98.71Å 159.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.39 – 2.80 49.39 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.7 (49.39-2.80) 98.6 (49.39-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.33 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.247 , 0.303 (Not available) , 0.276	Depositor DCC
R_{free} test set	1377 reflections (5.03%)	wwPDB-VP
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 , 35.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	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.*

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 [i](#)

5.1 Standard geometry [i](#)

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	1.08	4/3109 (0.1%)	1.10	2/4227 (0.0%)
1	B	1.17	6/3109 (0.2%)	1.14	5/4227 (0.1%)
All	All	1.13	10/6218 (0.2%)	1.12	7/8454 (0.1%)

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	172	VAL	C-O	-6.68	1.19	1.24
1	B	58	MET	SD-CE	6.16	1.95	1.79
1	A	295	CYS	CA-C	-6.11	1.45	1.52
1	B	165	ALA	CA-CB	-5.80	1.43	1.53
1	B	161	LEU	C-O	-5.46	1.17	1.24
1	A	402	GLU	C-O	-5.40	1.19	1.24
1	B	156	LEU	C-O	-5.34	1.17	1.23
1	A	406	ALA	CA-CB	-5.29	1.44	1.53
1	A	402	GLU	CA-C	-5.15	1.46	1.52
1	B	124	VAL	C-O	-5.05	1.19	1.24

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	363	VAL	CB-CA-C	-6.51	100.92	110.62
1	A	363	VAL	CB-CA-C	-6.20	101.38	110.81
1	B	58	MET	N-CA-C	6.19	118.19	108.96
1	B	187	ASP	N-CA-C	5.39	118.64	111.75
1	B	335	THR	CB-CA-C	-5.25	101.19	109.80
1	B	268	LEU	N-CA-C	5.11	119.56	113.23
1	A	27	GLN	N-CA-C	5.04	116.85	109.24

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	3048	0	3042	79	0
1	B	3048	0	3042	62	0
All	All	6096	0	6084	140	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 (140) 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:B:8:MET:HE1	1:B:274:TRP:CD1	2.07	0.89
1:A:157:THR:HB	1:A:160:GLU:OE2	1.76	0.85
1:B:222:ASN:C	1:B:222:ASN:HD22	1.85	0.83
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:138:ARG:O	1:B:141:GLU:HG2	1.96	0.66
1:B:138:ARG:HH11	1:B:138:ARG:HG2	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:B:67:ASP:O	1:B:68:ILE:C	2.44	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:CA	1:B:114:GLN:OE1	2.49	0.59
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:A:381:ASN:OD1	1:A:381:ASN:C	2.44	0.57
1:A:265:LEU:HD22	1:A:271:ILE:HG13	1.86	0.56
1:A:54:ASP:HA	1:A:137:ARG:O	2.06	0.56
1:A:222:ASN:HD22	1:A:222:ASN:C	2.13	0.56
1:A:300:ASN:ND2	1:A:303:SER:N	2.44	0.55
1:B:50:VAL:HA	1:B:51:PRO:C	2.32	0.55
1:B:346:LEU:HD12	1:B:386:LEU:O	2.07	0.54
1:A:282:LYS:HB3	1:A:283:PRO:HD3	1.90	0.53
1:A:55:ASN:HD22	1:A:101:GLY:HA2	1.72	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: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: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:394:GLU:O	1:A:395:VAL:C	2.48	0.52
1:A:76:VAL:HG23	1:A:76:VAL:O	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:212:MET:HG2	1:A:407:LEU:HD13	1.92	0.51
1:B:259:ASP:C	1:B:259:ASP:OD1	2.52	0.51
1:A:157:THR:CG2	1:A:158:THR:H	2.24	0.50
1:B:368:HIS:HD2	1:B:370:GLY:N	2.10	0.49
1:A:311:LEU:O	1:A:314:PRO:HG2	2.12	0.49
1:A:350:ARG:CD	1:A:376:SER:OG	2.59	0.49
1:A:115:GLU:H	1:A:115:GLU:CD	2.20	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:ASP:OD2	1:A:59:ASP:N	2.45	0.49
1:A:31:PRO:HG2	1:A:34:GLN:NE2	2.28	0.48
1:A:148:VAL:O	1:A:148:VAL:HG12	2.12	0.48
1:B:90:TRP:CD1	1:B:94:THR:HG1	2.31	0.48
1:B:282:LYS:N	1:B:283:PRO:HD3	2.27	0.48
1:A:231:HIS:O	1:A:232:ALA:C	2.55	0.48
1:A:17:MET:HE2	1:A:315:LEU:HD12	1.95	0.48
1:B:85:PRO:HB3	1:B:103:PRO:HG2	1.95	0.48
1:A:194:GLN:HB3	1:A:195:PRO:HD2	1.96	0.47
1:A:62:ALA:HB3	1:A:96:ILE:HB	1.95	0.47
1:A:408:PHE:C	1:B:157:THR:HG21	2.39	0.47
1:A:8:MET:HE1	1:A:274:TRP:CD1	2.50	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:286:PHE:CD2	1:B:286:PHE:C	2.93	0.47
1:A:353:LEU:HD13	1:A:363:VAL:HG13	1.97	0.47
1:B:114:GLN:OE1	1:B:114:GLN:HA	2.14	0.47
1:B:210:HIS:HE1	1:B:214:GLU:OE2	1.98	0.47
1:B:114:GLN:OE1	1:B:114:GLN:N	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:A:260:TYR:CD1	1:A:260:TYR:C	2.95	0.45
1:B:69:ALA:O	1:B:70:SER:C	2.58	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:128:ALA:O	1:A:129:GLU:C	2.60	0.44
1:B:222:ASN:C	1:B:222:ASN:ND2	2.57	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:371:TRP:CD1	1:B:371:TRP:C	2.95	0.43
1:B:327:LEU:HD12	1:B:327:LEU:HA	1.83	0.43
1:B:67:ASP:O	1:B:69:ALA:N	2.52	0.43
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:138:ARG:O	1:A:139:ARG:C	2.61	0.43
1:A:335:THR:HA	1:A:363:VAL:HG23	1.99	0.42
1:B:90:TRP:HD1	1:B:94:THR:OG1	2.02	0.42
1:B:279:LYS:HA	1:B:280:PRO:C	2.43	0.42
1:B:46:SER:HA	1:B:47:PRO:HD3	1.88	0.42
1:A:127:THR:O	1:A:128:ALA:C	2.62	0.42
1:B:138:ARG:CG	1:B:138:ARG:NH1	2.71	0.42
1:A:206:ARG:HH11	1:A:222:ASN:ND2	2.16	0.42
1:A:65:LEU:HD11	1:A:130:VAL:O	2.20	0.41
1:B:259:ASP:OD1	1:B:261:THR:OG1	2.35	0.41
1:B:313:GLN:HB3	1:B:314:PRO:CD	2.51	0.41
1:B:258:ALA:O	1:B:259:ASP:HB3	2.19	0.41
1:B:335:THR:HA	1:B:363:VAL:HG23	2.02	0.41
1:A:212:MET:O	1:A:216:LEU:HG	2.21	0.41
1:B:138:ARG:HH11	1:B:138:ARG:HG3	1.83	0.41
1:B:183:PHE:C	1:B:183:PHE:CD1	2.99	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:196:LEU:HD12	1:A:196:LEU:HA	1.91	0.40
1:A:306:LEU:O	1:A:306:LEU:HD22	2.20	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

5.3.1 Protein backbone

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%)	7	25
1	B	401/411 (98%)	376 (94%)	21 (5%)	4 (1%)	12	38
All	All	802/822 (98%)	745 (93%)	46 (6%)	11 (1%)	9	30

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

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%)	274 (84%)	51 (16%)	2	9
1	B	325/331 (98%)	272 (84%)	53 (16%)	2	8

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	650/662 (98%)	546 (84%)	104 (16%)	2 9

All (104) 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	22	THR
1	A	24	LEU
1	A	42	SER
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	87	HIS
1	A	89	GLU
1	A	99	MET
1	A	106	GLU
1	A	114	GLN
1	A	115	GLU
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	148	VAL
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	221	ILE
1	A	223	LEU
1	A	227	ARG
1	A	228	ASP
1	A	233	LEU

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Mol	Chain	Res	Type
1	A	239	GLU
1	A	257	GLU
1	A	276	LEU
1	A	288	LYS
1	A	306	LEU
1	A	319	LEU
1	A	327	LEU
1	A	350	ARG
1	A	354	GLN
1	A	360	GLU
1	A	361	LEU
1	A	363	VAL
1	A	399	VAL
1	A	401	VAL
1	B	10	LEU
1	B	14	LEU
1	B	15	ASN
1	B	20	ARG
1	B	24	LEU
1	B	30	LEU
1	B	40	LEU
1	B	42	SER
1	B	48	LEU
1	B	55	ASN
1	B	58	MET
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	112	VAL
1	B	114	GLN
1	B	115	GLU
1	B	117	THR
1	B	120	MET
1	B	125	ARG
1	B	131	ARG
1	B	138	ARG
1	B	141	GLU
1	B	144	SER
1	B	157	THR

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Mol	Chain	Res	Type
1	B	166	SER
1	B	175	ILE
1	B	182	LEU
1	B	188	GLU
1	B	196	LEU
1	B	198	ASP
1	B	207	LEU
1	B	223	LEU
1	B	233	LEU
1	B	239	GLU
1	B	243	GLN
1	B	257	GLU
1	B	263	THR
1	B	276	LEU
1	B	288	LYS
1	B	300	ASN
1	B	303	SER
1	B	319	LEU
1	B	333	VAL
1	B	335	THR
1	B	354	GLN
1	B	360	GLU
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	27	GLN
1	A	34	GLN
1	A	55	ASN
1	A	84	GLN
1	A	114	GLN
1	A	134	GLN
1	A	190	GLN
1	A	210	HIS
1	A	215	GLN
1	A	222	ASN
1	A	300	ASN
1	A	313	GLN
1	A	331	GLN

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Mol	Chain	Res	Type
1	A	368	HIS
1	A	392	ASN
1	B	27	GLN
1	B	55	ASN
1	B	72	GLN
1	B	119	GLN
1	B	190	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 [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](#)

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, 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%)	0.27	26 (6%) 25 18	19, 45, 97, 123	0
1	B	403/411 (98%)	0.17	17 (4%) 40 32	18, 41, 72, 90	0
All	All	806/822 (98%)	0.22	43 (5%) 32 24	18, 43, 87, 123	0

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	7	LEU	5.2
1	B	7	LEU	4.2
1	B	326	GLY	4.1
1	A	129	GLU	3.6
1	B	82	ALA	3.6
1	A	69	ALA	3.2
1	A	77	ALA	3.1
1	A	81	PHE	3.1
1	A	125	ARG	3.0
1	A	93	GLY	3.0
1	A	120	MET	2.9
1	A	76	VAL	2.9
1	B	328	PRO	2.8
1	B	89	GLU	2.8
1	B	83	GLY	2.8
1	B	106	GLU	2.7
1	A	92	ALA	2.7
1	B	239	GLU	2.7
1	A	86	TYR	2.6
1	A	127	THR	2.6
1	A	361	LEU	2.5
1	A	87	HIS	2.5
1	A	73	PRO	2.5
1	A	119	GLN	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	334	ARG	2.4
1	A	326	GLY	2.3
1	B	79	LYS	2.3
1	A	122	ASN	2.3
1	A	89	GLU	2.3
1	A	130	VAL	2.3
1	A	79	LYS	2.3
1	B	197	GLY	2.3
1	B	11	ASP	2.3
1	B	192	PRO	2.3
1	A	84	GLN	2.2
1	B	115	GLU	2.2
1	A	78	GLY	2.1
1	B	193	GLY	2.1
1	A	121	ASP	2.1
1	A	66	ALA	2.1
1	B	81	PHE	2.1
1	A	88	GLY	2.0
1	B	257	GLU	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.