



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 8, 2023 – 04:56 PM EDT

PDB ID : 6MBW
Title : Structure of Transcription Factor
Authors : Seo, H.-S.; Dhe-Paganon, S.
Deposited on : 2018-08-30
Resolution : 3.29 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 : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.35.1
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) : 2.35.1

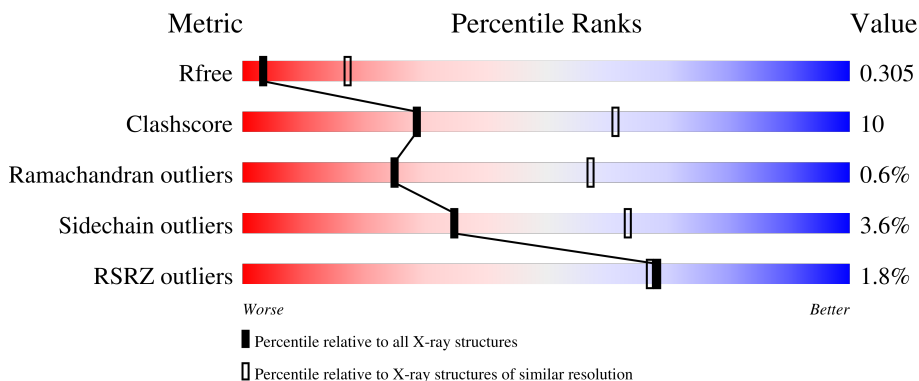
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.29 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	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

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	572	 2% 71% 19% • 8%
1	B	572	 % 72% 19% • 9%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7680 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 Signal transducer and activator of transcription 5B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	524	3789	2409	645	725	10	0	0	0
1	B	523	3888	2495	663	719	11	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	132	SER	-	expression tag	UNP P51692
A	133	THR	-	expression tag	UNP P51692
A	134	GLY	-	expression tag	UNP P51692
A	135	SER	-	expression tag	UNP P51692
B	132	SER	-	expression tag	UNP P51692
B	133	THR	-	expression tag	UNP P51692
B	134	GLY	-	expression tag	UNP P51692
B	135	SER	-	expression tag	UNP P51692

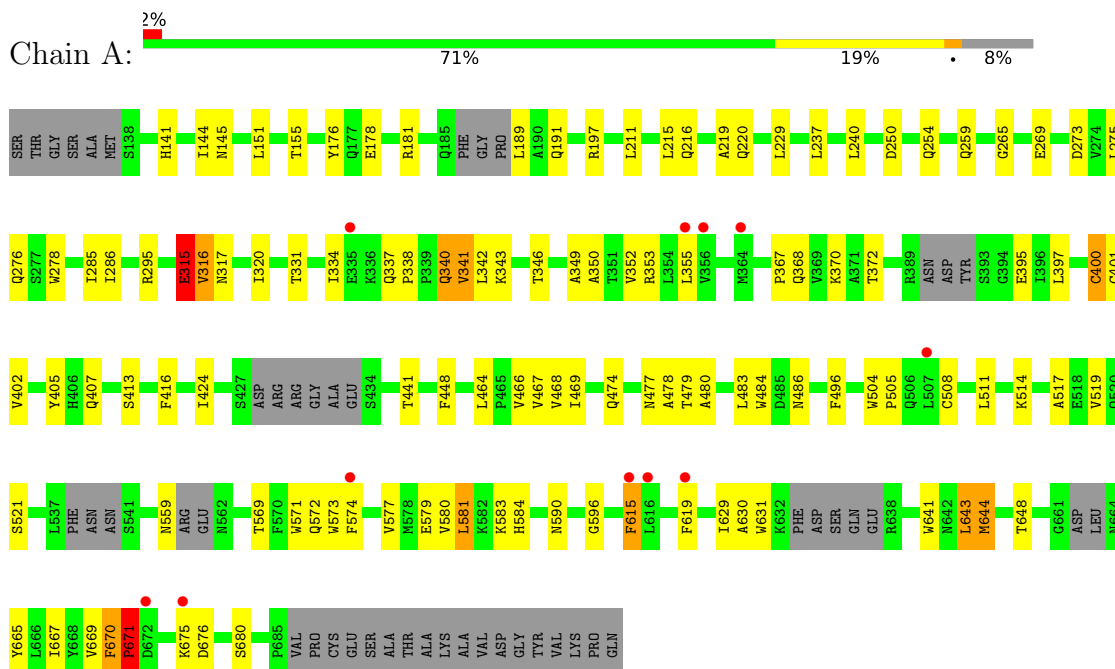
- Molecule 2 is water.

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

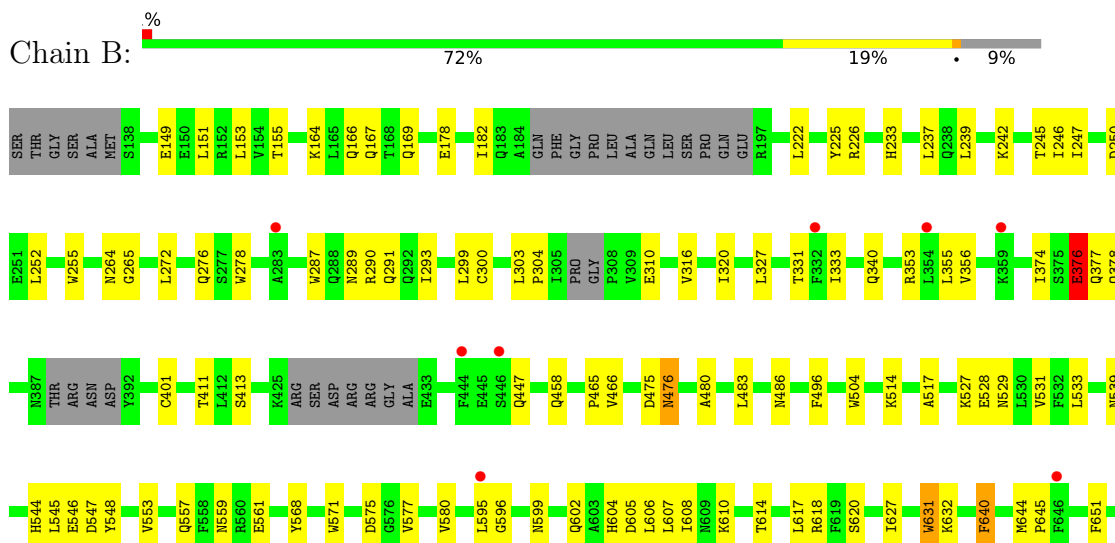
3 Residue-property plots

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: Signal transducer and activator of transcription 5B



- Molecule 1: Signal transducer and activator of transcription 5B



L656		VAL
Y665		PRO
Y668		CYS
V669		GLU
F670		SER
F685		ALA
		THR
		ALA
		LYS
		ALA
		VAL
		ASP
		GLY
		TYR
		VAL
		LYS
		PRO
		GLN

4 Data and refinement statistics i

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	134.60Å 138.62Å 76.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	96.57 – 3.29 96.57 – 3.29	Depositor EDS
% Data completeness (in resolution range)	98.1 (96.57-3.29) 98.2 (96.57-3.29)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.83 (at 3.26Å)	Xtrriage
Refinement program	PHENIX (1.14_3260: ???)	Depositor
R, R_{free}	0.266 , 0.305 0.266 , 0.305	Depositor DCC
R_{free} test set	1150 reflections (5.23%)	wwPDB-VP
Wilson B-factor (Å ²)	113.3	Xtrriage
Anisotropy	0.519	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 84.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.000 for k,h,-l	Xtrriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	7680	wwPDB-VP
Average B, all atoms (Å ²)	109.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.28% 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	0.25	0/3868	0.45	0/5292
1	B	0.25	0/3973	0.44	0/5428
All	All	0.25	0/7841	0.44	0/10720

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	A	0	4
1	B	0	2
All	All	0	6

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	315	GLU	Peptide
1	A	340	GLN	Peptide
1	A	670	PHE	Peptide
1	A	671	PRO	Peptide
1	B	374	ILE	Peptide
1	B	376	GLU	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	3789	0	3337	74	0
1	B	3888	0	3565	68	0
2	A	3	0	0	1	0
All	All	7680	0	6902	142	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 10.

All (142) 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:237:LEU:HD22	1:A:316:VAL:HG13	1.49	0.92
1:B:289:ASN:O	1:B:293:ILE:HD13	1.75	0.86
1:A:341:VAL:HG12	1:A:467:VAL:HB	1.61	0.81
1:A:315:GLU:O	1:A:317:ASN:N	2.15	0.80
1:B:237:LEU:HD21	1:B:320:ILE:HG12	1.64	0.77
1:A:483:LEU:HD12	1:A:514:LYS:HD2	1.65	0.76
1:A:237:LEU:HD21	1:A:320:ILE:HG23	1.67	0.74
1:B:644:MET:HG2	1:B:645:PRO:HD2	1.69	0.74
1:B:376:GLU:O	1:B:378:GLN:N	2.21	0.73
1:A:644:MET:N	1:A:644:MET:SD	2.61	0.73
1:B:447:GLN:HG3	1:B:458:GLN:HG2	1.69	0.73
1:B:596:GLY:HA2	1:B:618:ARG:HA	1.69	0.72
1:A:370:LYS:HA	1:A:400:CYS:HB2	1.70	0.72
1:B:151:LEU:HD21	1:B:239:LEU:HD22	1.73	0.70
1:B:327:LEU:O	1:B:331:THR:OG1	2.08	0.70
1:B:529:ASN:O	1:B:533:LEU:HD12	1.92	0.69
1:B:226:ARG:NH1	1:B:300:CYS:SG	2.67	0.68
1:A:259:GLN:HG3	1:A:269:GLU:HG2	1.78	0.66
1:A:191:GLN:HA	1:A:197:ARG:HD2	1.77	0.66
1:B:149:GLU:O	1:B:153:LEU:HD22	1.97	0.65
1:B:504:TRP:HE3	1:B:553:VAL:HG11	1.62	0.64
1:A:334:ILE:HG22	1:A:352:VAL:HG12	1.81	0.63
1:A:441:THR:HB	1:A:496:PHE:HZ	1.63	0.63
1:A:276:GLN:NE2	1:A:355:LEU:O	2.31	0.62
1:B:651:PHE:HE1	1:B:656:LEU:HB2	1.64	0.62
1:A:667:ILE:O	1:A:675:LYS:N	2.33	0.62
1:B:265:GLY:HA3	1:B:517:ALA:HB2	1.84	0.60
1:A:340:GLN:OE1	1:A:486:ASN:ND2	2.30	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:216:GLN:HA	1:A:219:ALA:HB3	1.84	0.59
1:A:615:PHE:HB2	1:A:669:VAL:HG12	1.85	0.59
1:B:353:ARG:HH21	1:B:411:THR:HG21	1.68	0.59
1:B:272:LEU:HD23	1:B:353:ARG:HH11	1.67	0.58
1:B:544:HIS:NE2	1:B:546:GLU:OE1	2.36	0.58
1:A:178:GLU:HA	1:A:181:ARG:HB3	1.84	0.58
1:B:299:LEU:O	1:B:304:PRO:HD3	2.04	0.56
1:B:559:ASN:O	1:B:559:ASN:ND2	2.38	0.56
1:A:579:GLU:HG3	1:A:583:LYS:HE2	1.86	0.56
1:A:265:GLY:HA3	1:A:517:ALA:HB2	1.87	0.56
1:A:584:HIS:HE1	1:A:648:THR:HG23	1.70	0.56
1:A:229:LEU:C	1:A:229:LEU:HD13	2.25	0.56
1:A:577:VAL:HA	1:A:580:VAL:HG12	1.88	0.56
1:B:290:ARG:HG3	1:B:320:ILE:HG21	1.89	0.54
1:B:331:THR:HG21	1:B:356:VAL:HG12	1.89	0.54
1:B:447:GLN:OE1	1:B:458:GLN:NE2	2.34	0.54
1:A:596:GLY:HA2	1:A:619:PHE:CE2	2.43	0.54
1:A:350:ALA:O	1:A:416:PHE:HB2	2.08	0.53
1:A:368:GLN:HA	1:A:402:VAL:HA	1.90	0.53
1:A:480:ALA:HB2	1:A:571:TRP:NE1	2.22	0.53
1:B:632:LYS:HA	1:B:640:PHE:HB3	1.90	0.53
1:A:584:HIS:CE1	1:A:648:THR:HG23	2.44	0.53
1:B:544:HIS:CE1	1:B:546:GLU:HB2	2.44	0.52
1:B:169:GLN:HE21	1:B:303:LEU:HD22	1.74	0.52
1:B:617:LEU:HD23	1:B:617:LEU:H	1.75	0.52
1:A:469:ILE:HG23	1:A:474:GLN:HB2	1.92	0.52
1:B:557:GLN:HA	1:B:561:GLU:HB2	1.90	0.52
1:A:480:ALA:HB2	1:A:571:TRP:CD1	2.46	0.51
1:A:569:THR:O	1:A:572:GLN:N	2.43	0.51
1:B:544:HIS:ND1	1:B:547:ASP:OD2	2.31	0.51
1:B:607:LEU:HA	1:B:610:LYS:HD3	1.94	0.50
1:B:539:ASN:N	1:B:539:ASN:OD1	2.44	0.50
1:A:343:LYS:O	1:A:346:THR:OG1	2.29	0.50
1:B:480:ALA:HB2	1:B:571:TRP:CD1	2.46	0.50
1:A:340:GLN:HA	1:A:466:VAL:HG23	1.94	0.49
1:B:333:ILE:HG12	1:B:355:LEU:HD21	1.94	0.49
1:A:477:ASN:OD1	1:A:559:ASN:ND2	2.40	0.48
1:A:215:LEU:O	1:A:216:GLN:HB3	2.13	0.48
1:A:342:LEU:HD23	1:A:466:VAL:HG21	1.96	0.48
1:B:340:GLN:HA	1:B:466:VAL:HG12	1.96	0.48
1:A:629:ILE:HG13	1:A:643:LEU:HD22	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:476:ASN:ND2	1:B:575:ASP:OD2	2.26	0.48
1:A:372:THR:HA	1:A:397:LEU:HD23	1.96	0.47
1:B:483:LEU:HD12	1:B:514:LYS:HG3	1.95	0.47
1:A:577:VAL:O	1:A:581:LEU:HG	2.15	0.47
1:A:629:ILE:HG22	1:A:630:ALA:H	1.79	0.47
1:B:164:LYS:HD2	1:B:225:TYR:HE2	1.79	0.47
1:B:237:LEU:HD22	1:B:316:VAL:HG13	1.97	0.47
1:A:508:CYS:HA	1:A:511:LEU:HD12	1.95	0.46
1:B:602:GLN:N	1:B:602:GLN:OE1	2.47	0.46
1:A:334:ILE:HD12	1:A:334:ILE:O	2.16	0.46
1:A:337:GLN:HG3	1:A:338:PRO:HD2	1.98	0.46
1:B:287:TRP:O	1:B:291:GLN:HG2	2.15	0.46
1:B:252:LEU:HD11	1:B:333:ILE:HG21	1.97	0.45
1:A:353:ARG:HG2	1:A:413:SER:HB3	1.97	0.45
1:A:334:ILE:HD13	1:A:337:GLN:OE1	2.17	0.45
1:A:441:THR:HB	1:A:496:PHE:CZ	2.49	0.45
1:B:247:ILE:HD13	1:B:278:TRP:HB3	1.98	0.45
1:A:574:PHE:O	1:A:577:VAL:HG22	2.16	0.45
1:A:144:ILE:HD11	1:A:278:TRP:CZ2	2.52	0.45
1:B:151:LEU:O	1:B:155:THR:HG23	2.17	0.45
1:A:151:LEU:O	1:A:155:THR:HG23	2.16	0.45
1:A:141:HIS:O	1:A:145:ASN:ND2	2.44	0.45
1:B:226:ARG:HH12	1:B:300:CYS:HA	1.82	0.45
1:A:331:THR:HB	1:A:355:LEU:HB2	1.97	0.44
1:B:618:ARG:O	1:B:627:ILE:HG13	2.18	0.44
1:A:504:TRP:N	1:A:505:PRO:HD2	2.32	0.44
1:B:531:VAL:HG23	1:B:548:TYR:CE2	2.53	0.44
1:B:255:TRP:CE2	1:B:272:LEU:HD13	2.53	0.44
1:B:604:HIS:O	1:B:608:ILE:HG23	2.17	0.44
1:A:265:GLY:HA3	1:A:517:ALA:CB	2.48	0.43
1:B:504:TRP:CE3	1:B:553:VAL:HG11	2.48	0.43
1:A:469:ILE:HD11	1:A:478:ALA:HB2	1.99	0.43
1:A:573:TRP:O	1:A:577:VAL:HG13	2.18	0.43
1:A:211:LEU:HD23	1:A:211:LEU:HA	1.81	0.43
1:A:337:GLN:NE2	1:A:464:LEU:H	2.15	0.43
1:A:615:PHE:HB2	1:A:669:VAL:HA	2.00	0.43
1:B:608:ILE:HG22	1:B:640:PHE:HE2	1.84	0.42
1:A:367:PRO:HG3	1:A:448:PHE:HB3	2.01	0.42
1:A:643:LEU:HG	1:A:644:MET:O	2.19	0.42
1:B:651:PHE:CE1	1:B:656:LEU:HB2	2.49	0.42
1:B:631:TRP:CD1	1:B:631:TRP:N	2.88	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:155:THR:HG21	1:A:285:ILE:HG23	2.00	0.42
1:B:528:GLU:HA	1:B:531:VAL:HG12	2.02	0.42
1:A:395:GLU:CB	1:A:424:ILE:HA	2.50	0.42
1:A:676:ASP:O	1:A:680:SER:N	2.52	0.42
1:B:606:LEU:HG	1:B:670:PHE:CE1	2.55	0.42
1:A:250:ASP:O	1:A:254:GLN:HG3	2.19	0.42
1:B:527:LYS:HD3	1:B:545:LEU:HD23	2.02	0.42
1:B:246:ILE:O	1:B:250:ASP:HB3	2.20	0.42
1:A:424:ILE:HD13	1:A:468:VAL:HG11	2.01	0.41
1:A:349:ALA:HA	1:A:416:PHE:O	2.19	0.41
1:B:614:THR:HG22	1:B:668:TYR:HB2	2.02	0.41
1:B:599:ASN:HB3	1:B:602:GLN:OE1	2.20	0.41
1:A:176:TYR:HA	1:A:215:LEU:HD21	2.02	0.41
1:A:341:VAL:HG21	1:A:479:THR:HG22	2.02	0.41
1:A:275:LEU:HD12	1:A:275:LEU:H	1.85	0.41
1:A:240:LEU:HD21	1:A:286:ILE:HG22	2.02	0.41
1:B:178:GLU:O	1:B:182:ILE:HG12	2.21	0.41
1:B:222:LEU:HD23	1:B:222:LEU:HA	1.93	0.41
1:B:465:PRO:HG3	1:B:496:PHE:CD1	2.55	0.41
1:B:166:GLN:HG2	1:B:299:LEU:HD11	2.02	0.41
1:B:620:SER:OG	1:B:645:PRO:HB3	2.21	0.41
1:B:353:ARG:HG3	1:B:413:SER:HB3	2.03	0.41
1:B:577:VAL:HA	1:B:580:VAL:HG12	2.03	0.41
1:A:189:LEU:N	2:A:803:HOH:O	2.54	0.40
1:A:405:TYR:HE2	1:A:407:GLN:HA	1.85	0.40
1:A:670:PHE:O	1:A:671:PRO:O	2.40	0.40
1:B:233:HIS:CE1	1:B:293:ILE:HD12	2.56	0.40
1:B:340:GLN:OE1	1:B:486:ASN:ND2	2.47	0.40
1:B:595:LEU:HD12	1:B:595:LEU:O	2.22	0.40
1:A:240:LEU:HD12	1:A:240:LEU:HA	1.87	0.40
1:A:519:VAL:HG23	1:A:521:SER:HB3	2.04	0.40
1:B:242:LYS:O	1:B:245:THR:OG1	2.34	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	508/572 (89%)	472 (93%)	32 (6%)	4 (1%)	19	51
1	B	513/572 (90%)	472 (92%)	39 (8%)	2 (0%)	34	66
All	All	1021/1144 (89%)	944 (92%)	71 (7%)	6 (1%)	25	57

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	315	GLU
1	A	316	VAL
1	A	671	PRO
1	B	376	GLU
1	B	377	GLN
1	A	341	VAL

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	350/510 (69%)	336 (96%)	14 (4%)	31	61
1	B	374/510 (73%)	362 (97%)	12 (3%)	39	67
All	All	724/1020 (71%)	698 (96%)	26 (4%)	35	63

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	220	GLN
1	A	273	ASP
1	A	295	ARG
1	A	400	CYS
1	A	401	CYS
1	A	484	TRP

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Mol	Chain	Res	Type
1	A	581	LEU
1	A	590	ASN
1	A	615	PHE
1	A	631	TRP
1	A	641	TRP
1	A	643	LEU
1	A	644	MET
1	A	665	TYR
1	B	167	GLN
1	B	264	ASN
1	B	276	GLN
1	B	310	GLU
1	B	401	CYS
1	B	475	ASP
1	B	476	ASN
1	B	568	TYR
1	B	605	ASP
1	B	631	TRP
1	B	640	PHE
1	B	665	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	276	GLN
1	A	584	HIS
1	B	169	GLN

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 [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	524/572 (91%)	-0.03	11 (2%) 63 62	73, 109, 145, 189	0
1	B	523/572 (91%)	0.10	8 (1%) 73 72	73, 106, 138, 164	0
All	All	1047/1144 (91%)	0.04	19 (1%) 68 67	73, 108, 142, 189	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	446	SER	3.6
1	B	444	PHE	3.6
1	A	356	VAL	3.6
1	B	359	LYS	3.2
1	A	672	ASP	3.1
1	A	335	GLU	3.0
1	A	619	PHE	3.0
1	A	355	LEU	2.8
1	A	675	LYS	2.5
1	B	646	PHE	2.5
1	B	283	ALA	2.3
1	B	595	LEU	2.3
1	B	354	LEU	2.3
1	B	332	PHE	2.3
1	A	364	MET	2.2
1	A	574	PHE	2.1
1	A	507	LEU	2.1
1	A	616	LEU	2.0
1	A	615	PHE	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 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.