



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 13, 2017 – 12:21 PM EST

PDB ID : 4Q4H
Title : TM287/288 in its apo state
Authors : Hohl, M.; Gruetter, M.G.; Seeger, M.A.
Deposited on : unknown
Resolution : 2.53 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
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030345
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : rb-20030345

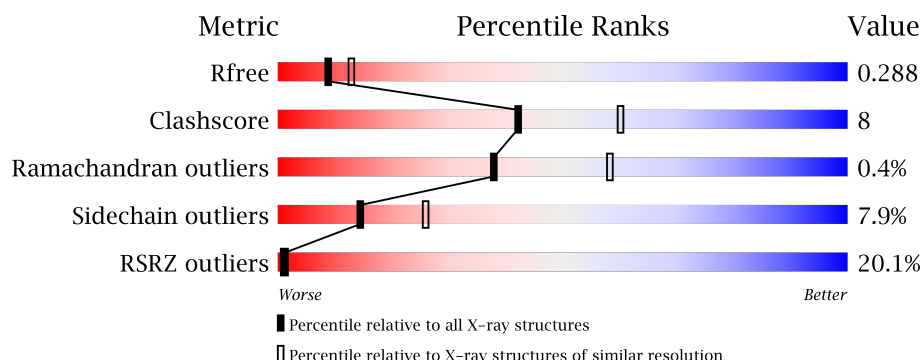
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.53 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}	100719	4636 (2.54-2.50)
Clashscore	112137	5382 (2.54-2.50)
Ramachandran outliers	110173	5282 (2.54-2.50)
Sidechain outliers	110143	5284 (2.54-2.50)
RSRZ outliers	101464	4669 (2.54-2.50)

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 $\leq 5\%$. 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	587	<div> <div>14%</div> <div> <div></div> <div>73%</div> <div>22%</div> <div>• •</div> </div> </div>
2	B	598	<div> <div>25%</div> <div> <div></div> <div>73%</div> <div>23%</div> <div>• •</div> </div> </div>

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 9138 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 ABC transporter.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	572	Total	C	N	O	S	0	0	0
			4485	2889	772	805	19			

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-9	GLY	-	EXPRESSION TAG	UNP Q9WYC3
A	-8	PRO	-	EXPRESSION TAG	UNP Q9WYC3
A	-7	SER	-	EXPRESSION TAG	UNP Q9WYC3
A	-6	GLY	-	EXPRESSION TAG	UNP Q9WYC3
A	-5	SER	-	EXPRESSION TAG	UNP Q9WYC3
A	-4	GLY	-	EXPRESSION TAG	UNP Q9WYC3
A	-3	GLY	-	EXPRESSION TAG	UNP Q9WYC3
A	-2	GLY	-	EXPRESSION TAG	UNP Q9WYC3
A	-1	GLY	-	EXPRESSION TAG	UNP Q9WYC3
A	0	GLY	-	EXPRESSION TAG	UNP Q9WYC3
A	1	SER	-	EXPRESSION TAG	UNP Q9WYC3

- Molecule 2 is a protein called Uncharacterized ABC transporter ATP-binding protein TM_0288.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	583	Total	C	N	O	S	0	0	0
			4641	3000	782	845	14			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	8	Total	O	0	0
			8	8		
3	B	4	Total	O	0	0
			4	4		

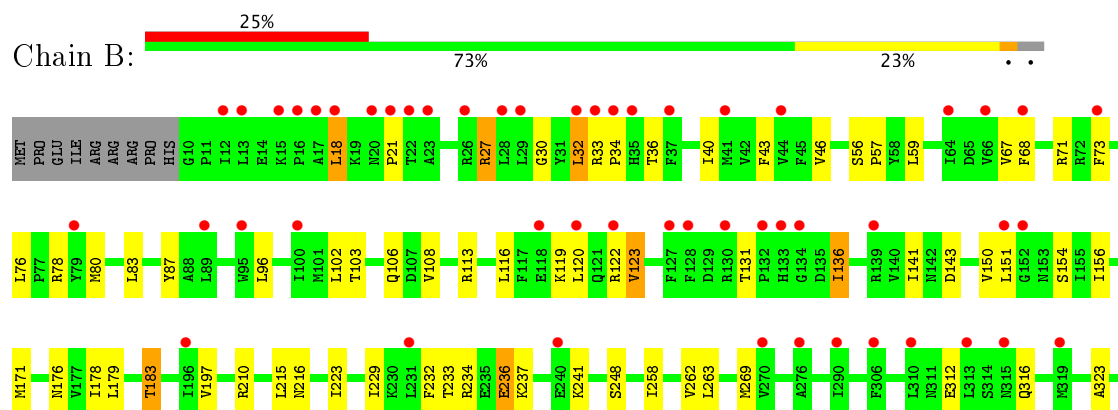
3 Residue-property plots [i](#)

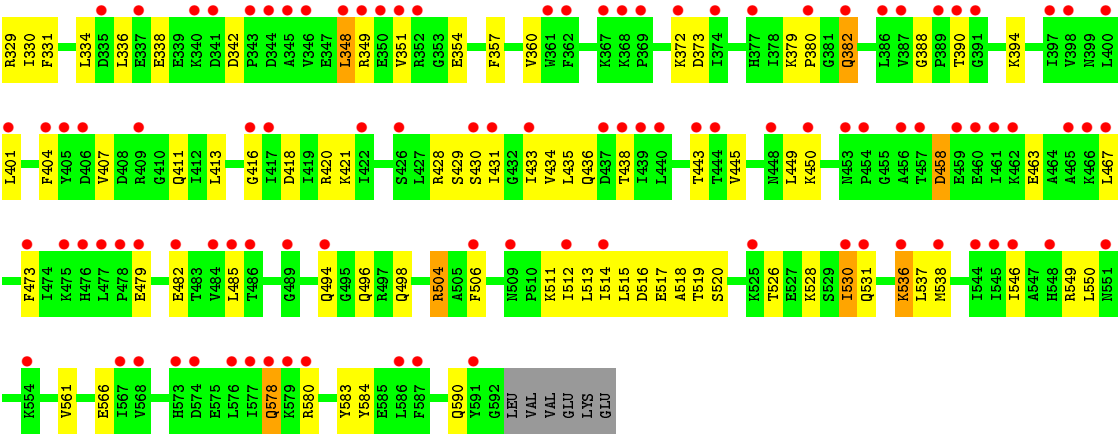
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: ABC transporter



• Molecule 2: Uncharacterized ABC transporter ATP-binding protein TM_0288





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	214.64Å 84.01Å 114.11Å 90.00° 93.27° 90.00°	Depositor
Resolution (Å)	29.51 – 2.53 29.51 – 2.53	Depositor EDS
% Data completeness (in resolution range)	87.3 (29.51-2.53) 87.4 (29.51-2.53)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.24 (at 2.54Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.237 , 0.290 0.232 , 0.288	Depositor DCC
R_{free} test set	3003 reflections (5.05%)	DCC
Wilson B-factor (Å ²)	39.4	Xtriage
Anisotropy	0.032	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 83.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	9138	wwPDB-VP
Average B, all atoms (Å ²)	108.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.60% 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	0.29	0/4560	0.49	0/6166
2	B	0.26	0/4722	0.45	0/6385
All	All	0.28	0/9282	0.47	0/12551

There are no bond length outliers.

There are no bond angle outliers.

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	4485	0	4683	84	0
2	B	4641	0	4829	84	0
3	A	8	0	0	1	0
3	B	4	0	0	0	0
All	All	9138	0	9512	148	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 8.

All (148) 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:129:MET:HG3	1:A:133:ILE:HD11	1.65	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:432:GLU:OE2	2:B:237:LYS:NZ	2.20	0.75
1:A:206:ARG:NH2	2:B:123:VAL:O	2.15	0.70
2:B:467:LEU:HB3	2:B:536:LYS:HD3	1.73	0.70
1:A:265:ASN:OD1	2:B:71:ARG:NH2	2.27	0.67
2:B:150:VAL:HA	2:B:154:SER:HB2	1.77	0.66
2:B:18:LEU:HD22	2:B:21:PRO:HB3	1.78	0.66
2:B:71:ARG:HD2	2:B:73:PHE:HE2	1.64	0.62
1:A:448:ILE:HG12	1:A:478:LEU:HD13	1.80	0.62
1:A:567:SER:HB3	2:B:528:LYS:HE3	1.83	0.60
1:A:379:ILE:HG22	1:A:409:ILE:HD13	1.83	0.60
2:B:401:LEU:HD23	2:B:514:ILE:HD11	1.82	0.60
1:A:417:VAL:O	1:A:482:ARG:NH2	2.33	0.59
1:A:89:ARG:HD3	2:B:215:LEU:HD11	1.83	0.59
1:A:92:LEU:HB3	1:A:116:LEU:HG	1.84	0.59
1:A:502:PRO:HG3	2:B:390:THR:H	1.68	0.59
1:A:340:ARG:HA	1:A:348:VAL:HG23	1.83	0.59
1:A:403:LYS:HG3	2:B:233:THR:HG21	1.86	0.58
1:A:85:GLY:HA3	1:A:124:GLN:HE21	1.67	0.58
2:B:436:GLN:HG3	2:B:518:ALA:HB2	1.87	0.56
2:B:517:GLU:HB3	2:B:549:ARG:HH21	1.69	0.56
2:B:179:LEU:O	2:B:183:THR:HG23	2.06	0.56
2:B:122:ARG:HB3	2:B:338:GLU:HB3	1.87	0.56
1:A:19:PRO:HB3	1:A:135:VAL:HG21	1.87	0.56
2:B:32:LEU:HD23	2:B:151:LEU:HD21	1.88	0.56
1:A:192:ASN:HB3	1:A:196:ARG:HH21	1.71	0.55
1:A:527:LYS:HA	1:A:568:GLN:HE22	1.72	0.55
2:B:354:GLU:HB3	2:B:380:PRO:HD3	1.87	0.55
1:A:252:ILE:HD11	2:B:83:LEU:HB3	1.87	0.55
1:A:482:ARG:HD3	2:B:232:PHE:CZ	2.42	0.55
1:A:497:THR:HB	1:A:505:GLU:HG3	1.89	0.54
2:B:67:VAL:HG11	2:B:76:LEU:HD13	1.88	0.54
1:A:51:LEU:O	1:A:55:THR:HG23	2.07	0.54
2:B:434:VAL:HB	2:B:515:LEU:HD23	1.89	0.54
1:A:126:LEU:HD12	1:A:299:ALA:HB1	1.90	0.54
1:A:258:GLY:O	1:A:262:VAL:HG12	2.08	0.53
1:A:191:VAL:HG21	1:A:225:LEU:HD22	1.89	0.53
2:B:116:LEU:HD21	2:B:330:ILE:HG23	1.89	0.53
2:B:30:GLY:HA2	2:B:33:ARG:HD2	1.90	0.53
1:A:416:THR:OG1	1:A:475:LYS:HB3	2.09	0.52
2:B:388:GLY:O	2:B:394:LYS:NZ	2.32	0.52
1:A:222:ASN:OD1	2:B:113:ARG:NH1	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:357:PHE:HD2	2:B:360:VAL:HG21	1.75	0.51
2:B:59:LEU:HB3	2:B:83:LEU:HD11	1.92	0.51
1:A:361:LEU:HD22	1:A:513:LYS:HD3	1.92	0.50
2:B:413:LEU:HB3	2:B:418:ASP:HA	1.93	0.50
1:A:22:MET:SD	1:A:136:ARG:HB2	2.52	0.50
1:A:416:THR:HG21	1:A:476:GLN:HA	1.93	0.50
1:A:512:LEU:O	1:A:516:THR:HG23	2.12	0.50
1:A:11:TYR:CZ	1:A:83:ASN:HB3	2.47	0.50
1:A:206:ARG:HG2	2:B:428:ARG:HH12	1.77	0.49
1:A:198:ASN:ND2	1:A:214:GLU:OE1	2.40	0.49
1:A:202:VAL:O	1:A:206:ARG:HB2	2.12	0.49
1:A:569:PHE:HD1	2:B:550:LEU:HD22	1.77	0.49
2:B:176:ASN:HD22	2:B:179:LEU:HB2	1.78	0.49
1:A:223:GLU:HB3	1:A:227:ARG:HH12	1.79	0.48
1:A:51:LEU:HA	1:A:51:LEU:HD22	1.76	0.47
1:A:431:ARG:HD3	1:A:485:VAL:O	2.15	0.47
1:A:495:ASP:O	1:A:497:THR:N	2.48	0.47
2:B:528:LYS:HA	2:B:531:GLN:HE21	1.79	0.47
1:A:184:ILE:HD13	1:A:229:ILE:HG12	1.97	0.47
2:B:580:ARG:HA	2:B:584:TYR:HB2	1.97	0.47
1:A:133:ILE:HD13	1:A:292:ILE:HG12	1.96	0.47
2:B:379:LYS:O	2:B:382:GLN:HB2	2.14	0.47
2:B:150:VAL:HG21	2:B:323:ALA:HB2	1.97	0.46
1:A:509:LEU:HD13	1:A:533:LEU:HD13	1.96	0.46
2:B:411:GLN:HA	2:B:420:ARG:HH12	1.79	0.46
2:B:431:ILE:HG12	2:B:512:ILE:HB	1.97	0.46
1:A:115:ARG:HA	1:A:119:ASP:HB2	1.96	0.46
2:B:229:ILE:HG23	2:B:234:ARG:HB2	1.97	0.46
2:B:236:GLU:HG2	2:B:236:GLU:H	1.48	0.46
2:B:561:VAL:HG21	2:B:583:TYR:HB2	1.97	0.46
1:A:292:ILE:O	1:A:296:ILE:HG12	2.15	0.46
1:A:540:LEU:HD23	1:A:545:VAL:HA	1.97	0.46
1:A:85:GLY:HA3	1:A:124:GLN:NE2	2.30	0.46
2:B:516:ASP:HB2	2:B:546:ILE:HD12	1.98	0.46
1:A:431:ARG:HH22	1:A:438:GLU:CD	2.19	0.46
1:A:223:GLU:HB3	1:A:227:ARG:NH1	2.30	0.46
2:B:348:LEU:HA	2:B:348:LEU:HD22	1.85	0.46
2:B:494:GLN:NE2	2:B:498:GLN:OE1	2.42	0.45
1:A:492:ILE:HG22	1:A:524:ILE:HD11	1.98	0.45
1:A:142:VAL:O	1:A:146:VAL:HG23	2.16	0.45
1:A:253:ALA:O	1:A:257:PHE:HB2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:516:THR:HA	1:A:519:CYS:HB3	1.98	0.45
1:A:203:ARG:HG3	2:B:404:PHE:CZ	2.52	0.45
2:B:413:LEU:HD13	2:B:416:GLY:HA2	1.99	0.45
2:B:433:ILE:HD11	2:B:435:LEU:HD21	1.99	0.45
1:A:132:ARG:HD2	3:A:607:HOH:O	2.17	0.45
1:A:502:PRO:HB2	1:A:504:THR:HG23	1.99	0.45
1:A:89:ARG:HD3	2:B:215:LEU:CD1	2.47	0.45
2:B:513:LEU:HD23	2:B:538:MET:HG2	1.99	0.45
1:A:488:PRO:HD2	1:A:515:TYR:OH	2.17	0.44
2:B:143:ASP:OD1	2:B:329:ARG:NH1	2.50	0.44
2:B:119:LYS:NZ	2:B:336:LEU:O	2.34	0.44
1:A:40:VAL:HG11	1:A:273:MET:CE	2.46	0.44
2:B:430:SER:O	2:B:511:LYS:N	2.49	0.44
1:A:252:ILE:HA	1:A:252:ILE:HD12	1.82	0.44
2:B:578:GLN:O	2:B:580:ARG:HD3	2.18	0.44
1:A:431:ARG:HG3	1:A:434:ALA:HB2	1.99	0.44
2:B:210:ARG:HD2	2:B:210:ARG:HA	1.77	0.44
1:A:203:ARG:HG3	2:B:404:PHE:CE2	2.53	0.43
2:B:108:VAL:HG11	2:B:151:LEU:HD22	2.00	0.43
2:B:418:ASP:HB3	2:B:421:LYS:HD2	2.00	0.43
2:B:27:ARG:HD2	2:B:331:PHE:CD2	2.53	0.43
2:B:33:ARG:N	2:B:34:PRO:HD2	2.33	0.43
1:A:20:LEU:O	1:A:23:VAL:HG22	2.18	0.43
1:A:26:VAL:HG13	1:A:140:LEU:HD23	2.00	0.43
1:A:2:LYS:HB2	1:A:311:ASN:OD1	2.17	0.43
1:A:478:LEU:HD12	1:A:478:LEU:HA	1.84	0.43
1:A:117:THR:HG22	2:B:216:ASN:OD1	2.18	0.43
2:B:445:VAL:HG22	2:B:485:LEU:HD21	2.00	0.43
1:A:361:LEU:HD23	1:A:534:ALA:HA	2.01	0.43
2:B:330:ILE:O	2:B:334:LEU:HG	2.19	0.43
2:B:136:ILE:HD13	2:B:136:ILE:HA	1.67	0.43
2:B:36:THR:O	2:B:40:ILE:HG12	2.19	0.43
1:A:273:MET:O	1:A:276:THR:OG1	2.35	0.43
1:A:473:GLY:O	1:A:477:ARG:HG3	2.19	0.43
2:B:312:GLU:HB3	2:B:316:GLN:HE22	1.83	0.43
2:B:519:THR:HG22	2:B:549:ARG:NH1	2.33	0.43
2:B:96:LEU:HA	2:B:96:LEU:HD23	1.79	0.43
2:B:258:ILE:O	2:B:262:VAL:HG13	2.19	0.42
2:B:372:LYS:HB2	2:B:566:GLU:HG2	2.01	0.42
1:A:133:ILE:HA	1:A:136:ARG:HB3	2.00	0.42
1:A:206:ARG:HG2	2:B:428:ARG:NH1	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:449:LEU:HA	2:B:504:ARG:HB3	2.01	0.42
1:A:453:ILE:HA	1:A:453:ILE:HD12	1.92	0.42
1:A:559:LYS:HG2	1:A:562:ARG:NH1	2.34	0.42
2:B:349:ARG:O	2:B:351:VAL:HG23	2.19	0.42
2:B:526:THR:O	2:B:530:ILE:HG23	2.20	0.42
1:A:248:ASN:HB3	2:B:87:TYR:CG	2.55	0.42
1:A:166:ILE:HD13	1:A:243:PHE:CE1	2.54	0.42
1:A:194:VAL:O	1:A:198:ASN:HB2	2.19	0.42
2:B:119:LYS:HA	2:B:119:LYS:HD2	1.92	0.42
2:B:102:LEU:O	2:B:106:GLN:HB2	2.20	0.41
2:B:473:PHE:CE1	2:B:496:GLN:HB3	2.55	0.41
1:A:11:TYR:OH	1:A:87:ASP:OD2	2.25	0.41
1:A:325:LEU:HD11	1:A:400:VAL:HG11	2.02	0.41
1:A:96:VAL:HG11	2:B:223:ILE:HG12	2.02	0.41
1:A:338:GLU:HG2	1:A:350:SER:HA	2.03	0.41
2:B:143:ASP:OD2	2:B:329:ARG:HD2	2.21	0.41
2:B:56:SER:HB2	2:B:57:PRO:HD3	2.03	0.41
1:A:257:PHE:O	1:A:260:VAL:HG22	2.21	0.41
1:A:503:ILE:O	1:A:503:ILE:HG12	2.21	0.41
2:B:76:LEU:O	2:B:80:MET:HG2	2.20	0.41
2:B:197:VAL:HG11	2:B:263:LEU:HB2	2.03	0.40
1:A:262:VAL:HG11	2:B:68:PHE:CD2	2.55	0.40
1:A:39:ILE:O	1:A:44:ILE:HG13	2.20	0.40
2:B:458:ASP:OD1	2:B:458:ASP:N	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	570/587 (97%)	541 (95%)	25 (4%)	4 (1%)	25 42

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	B	581/598 (97%)	545 (94%)	35 (6%)	1 (0%)	51 72
All	All	1151/1185 (97%)	1086 (94%)	60 (5%)	5 (0%)	38 58

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	496	CYS
2	B	520	SER
1	A	499	SER
1	A	558	CYS
1	A	516	THR

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	496/504 (98%)	456 (92%)	40 (8%)	14 25
2	B	518/533 (97%)	478 (92%)	40 (8%)	15 27
All	All	1014/1037 (98%)	934 (92%)	80 (8%)	14 26

All (80) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	THR
1	A	20	LEU
1	A	39	ILE
1	A	51	LEU
1	A	57	ILE
1	A	92	LEU
1	A	109	THR
1	A	132	ARG
1	A	173	LEU
1	A	200	LEU
1	A	206	ARG

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Mol	Chain	Res	Type
1	A	210	ARG
1	A	230	ILE
1	A	235	LEU
1	A	249	MET
1	A	252	ILE
1	A	255	LEU
1	A	262	VAL
1	A	269	ILE
1	A	272	ILE
1	A	283	MET
1	A	317	GLU
1	A	344	ASN
1	A	357	LYS
1	A	368	THR
1	A	375	LEU
1	A	383	ILE
1	A	389	ARG
1	A	395	LEU
1	A	431	ARG
1	A	444	LYS
1	A	478	LEU
1	A	494	ASP
1	A	501	ASP
1	A	503	ILE
1	A	504	THR
1	A	523	ILE
1	A	538	LEU
1	A	552	LYS
1	A	555	LEU
2	B	18	LEU
2	B	27	ARG
2	B	32	LEU
2	B	43	PHE
2	B	46	VAL
2	B	78	ARG
2	B	103	THR
2	B	120	LEU
2	B	123	VAL
2	B	131	THR
2	B	136	ILE
2	B	141	ILE
2	B	156	ILE

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Mol	Chain	Res	Type
2	B	171	MET
2	B	178	ILE
2	B	183	THR
2	B	236	GLU
2	B	241	LYS
2	B	248	SER
2	B	269	MET
2	B	342	ASP
2	B	348	LEU
2	B	373	ASP
2	B	382	GLN
2	B	407	VAL
2	B	429	SER
2	B	438	THR
2	B	443	THR
2	B	450	LYS
2	B	458	ASP
2	B	463	GLU
2	B	479	GLU
2	B	482	GLU
2	B	504	ARG
2	B	506	PHE
2	B	530	ILE
2	B	536	LYS
2	B	537	LEU
2	B	578	GLN
2	B	590	GLN

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

Mol	Chain	Res	Type
1	A	124	GLN
2	B	316	GLN
2	B	531	GLN

5.3.3 RNA ⓘ

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 carbohydrates 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	572/587 (97%)	0.99	80 (13%) 3 3	56, 92, 141, 193	0
2	B	583/598 (97%)	1.43	152 (26%) 1 0	63, 117, 165, 185	0
All	All	1155/1185 (97%)	1.21	232 (20%) 1 1	56, 104, 161, 193	0

All (232) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	500	VAL	17.2
2	B	351	VAL	12.4
1	A	565	TYR	10.0
2	B	484	VAL	9.4
2	B	478	PRO	8.3
2	B	587	PHE	7.3
2	B	352	ARG	7.2
1	A	566	GLU	7.2
1	A	181	PHE	7.2
2	B	476	HIS	6.5
2	B	453	ASN	6.2
1	A	515	TYR	6.0
1	A	517	LYS	5.9
2	B	346	VAL	5.9
2	B	417	ILE	5.6
2	B	467	LEU	5.5
1	A	514	ARG	5.5
2	B	343	PRO	5.3
2	B	437	ASP	5.2
1	A	497	THR	5.0
1	A	172	TRP	5.0
2	B	349	ARG	5.0
1	A	564	ILE	5.0
2	B	340	LYS	4.8

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Mol	Chain	Res	Type	RSRZ
2	B	17	ALA	4.8
1	A	49	PHE	4.8
1	A	266	GLN	4.7
2	B	35	HIS	4.6
1	A	175	LYS	4.6
2	B	362	PHE	4.6
2	B	22	THR	4.6
2	B	568	VAL	4.5
2	B	369	PRO	4.5
2	B	398	VAL	4.5
2	B	391	GLY	4.5
1	A	207	ALA	4.5
2	B	310	LEU	4.5
2	B	573	HIS	4.4
1	A	220	LYS	4.4
1	A	518	GLY	4.4
1	A	257	PHE	4.4
2	B	486	THR	4.4
2	B	345	ALA	4.3
2	B	576	LEU	4.3
1	A	569	PHE	4.3
1	A	153	VAL	4.3
2	B	151	LEU	4.2
1	A	351	GLY	4.2
2	B	438	THR	4.2
2	B	344	ASP	4.2
2	B	577	ILE	4.1
1	A	440	VAL	4.1
1	A	501	ASP	4.1
1	A	212	GLU	4.1
2	B	416	GLY	4.1
2	B	457	THR	4.1
2	B	29	LEU	4.0
2	B	28	LEU	4.0
2	B	551	ASN	4.0
2	B	430	SER	4.0
2	B	37	PHE	3.9
2	B	439	ILE	3.9
2	B	426	SER	3.9
2	B	444	THR	3.9
1	A	400	VAL	3.9
2	B	18	LEU	3.8

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Mol	Chain	Res	Type	RSRZ
2	B	68	PHE	3.8
1	A	341	TYR	3.8
2	B	348	LEU	3.7
2	B	382	GLN	3.7
2	B	531	GLN	3.7
2	B	460	GLU	3.7
2	B	34	PRO	3.7
2	B	12	ILE	3.6
2	B	23	ALA	3.6
2	B	397	ILE	3.6
1	A	490	VAL	3.6
2	B	139	ARG	3.5
1	A	366	GLY	3.5
2	B	13	LEU	3.5
2	B	20	ASN	3.4
2	B	567	ILE	3.4
1	A	368	THR	3.4
1	A	567	SER	3.4
2	B	16	PRO	3.4
1	A	205	VAL	3.4
2	B	459	GLU	3.3
1	A	342	PHE	3.3
2	B	580	ARG	3.2
1	A	496	CYS	3.2
1	A	256	TRP	3.2
2	B	122	ARG	3.2
2	B	368	LYS	3.2
2	B	554	LYS	3.2
2	B	341	ASP	3.2
2	B	485	LEU	3.2
2	B	33	ARG	3.2
2	B	374	ILE	3.1
2	B	422	ILE	3.1
2	B	21	PRO	3.1
2	B	26	ARG	3.1
1	A	557	HIS	3.1
2	B	133	HIS	3.1
2	B	73	PHE	3.1
1	A	346	ASP	3.0
2	B	506	PHE	3.0
2	B	367	LYS	3.0
2	B	350	GLU	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	-2	GLY	3.0
1	A	387	ARG	3.0
2	B	130	ARG	3.0
1	A	176	LYS	3.0
2	B	586	LEU	3.0
2	B	95	TRP	3.0
2	B	433	ILE	2.9
2	B	456	ALA	2.9
1	A	348	VAL	2.9
1	A	558	CYS	2.9
2	B	591	TYR	2.9
2	B	32	LEU	2.9
1	A	491	LEU	2.8
1	A	516	THR	2.8
1	A	556	GLU	2.8
2	B	489	GLY	2.8
2	B	461	ILE	2.8
2	B	401	LEU	2.8
1	A	508	ILE	2.8
2	B	544	ILE	2.8
2	B	479	GLU	2.8
2	B	386	LEU	2.8
2	B	152	GLY	2.7
2	B	361	TRP	2.7
2	B	530	ILE	2.7
2	B	44	VAL	2.7
1	A	343	GLU	2.7
1	A	499	SER	2.7
2	B	319	MET	2.7
2	B	465	ALA	2.7
2	B	574	ASP	2.7
1	A	284	PHE	2.7
1	A	555	LEU	2.6
2	B	306	PHE	2.6
1	A	512	LEU	2.6
2	B	372	LYS	2.6
2	B	118	GLU	2.6
2	B	134	GLY	2.6
1	A	235	LEU	2.6
2	B	477	LEU	2.6
2	B	482	GLU	2.6
2	B	431	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
2	B	400	LEU	2.5
2	B	377	HIS	2.5
2	B	466	LYS	2.5
2	B	380	PRO	2.5
2	B	313	LEU	2.5
1	A	492	ILE	2.5
2	B	509	ASN	2.5
2	B	409	ARG	2.5
2	B	404	PHE	2.5
1	A	140	LEU	2.5
1	A	250	GLY	2.5
1	A	409	ILE	2.4
2	B	443	THR	2.4
2	B	290	ILE	2.4
1	A	323	LEU	2.4
2	B	546	ILE	2.4
2	B	66	VAL	2.4
1	A	274	ALA	2.4
2	B	15	LYS	2.4
2	B	462	LYS	2.4
1	A	236	ILE	2.4
1	A	184	ILE	2.3
2	B	514	ILE	2.3
2	B	337	GLU	2.3
2	B	525	LYS	2.3
1	A	79	TYR	2.3
2	B	231	LEU	2.3
2	B	545	ILE	2.3
2	B	79	TYR	2.3
1	A	4	LEU	2.3
1	A	523	ILE	2.3
1	A	94	ARG	2.3
1	A	227	ARG	2.3
1	A	444	LYS	2.3
2	B	41	MET	2.3
1	A	568	GLN	2.3
2	B	390	THR	2.3
2	B	548	HIS	2.3
1	A	216	GLU	2.3
2	B	270	VAL	2.2
1	A	251	MET	2.2
1	A	479	SER	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	450	LYS	2.2
2	B	406	ASP	2.2
1	A	221	ALA	2.2
2	B	64	ILE	2.2
1	A	550	THR	2.2
2	B	473	PHE	2.2
1	A	533	LEU	2.2
1	A	180	LEU	2.2
2	B	120	LEU	2.2
2	B	440	LEU	2.2
2	B	196	ILE	2.2
2	B	127	PHE	2.2
2	B	579	LYS	2.2
2	B	276	ALA	2.2
2	B	132	PRO	2.2
2	B	475	LYS	2.1
2	B	387	VAL	2.1
2	B	315	ASN	2.1
1	A	174	THR	2.1
1	A	554	LEU	2.1
2	B	494	GLN	2.1
2	B	578	GLN	2.1
1	A	521	THR	2.1
2	B	512	ILE	2.1
1	A	562	ARG	2.1
2	B	536	LYS	2.1
1	A	544	LYS	2.1
2	B	389	PRO	2.1
1	A	160	ILE	2.1
2	B	100	ILE	2.1
2	B	89	LEU	2.1
2	B	448	ASN	2.1
2	B	335	ASP	2.0
1	A	539	VAL	2.0
2	B	405	TYR	2.0
2	B	538	MET	2.0
2	B	240	GLU	2.0
2	B	128	PHE	2.0
1	A	546	ALA	2.0
2	B	454	PRO	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.