



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:50 PM GMT

PDB ID : 4Q4H  
Title : TM287/288 in its apo state  
Authors : Hohl, M.; Gruetter, M.G.; Seeger, M.A.  
Deposited on : 2014-04-14  
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](mailto: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.

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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

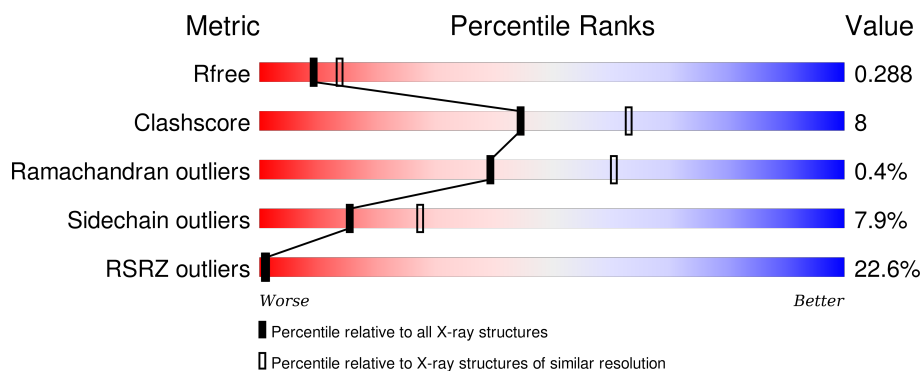
# 1 Overall quality at a glance

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))
$R_{free}$	91344	4241 (2.54-2.50)
Clashscore	102246	4968 (2.54-2.50)
Ramachandran outliers	100387	4873 (2.54-2.50)
Sidechain outliers	100360	4875 (2.54-2.50)
RSRZ outliers	91569	4253 (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  $\geq 3$ , 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>16%</div> <div>73%</div> <div>22%</div> <div>• •</div> </div>
2	B	598	<div> <div>28%</div> <div>73%</div> <div>23%</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			

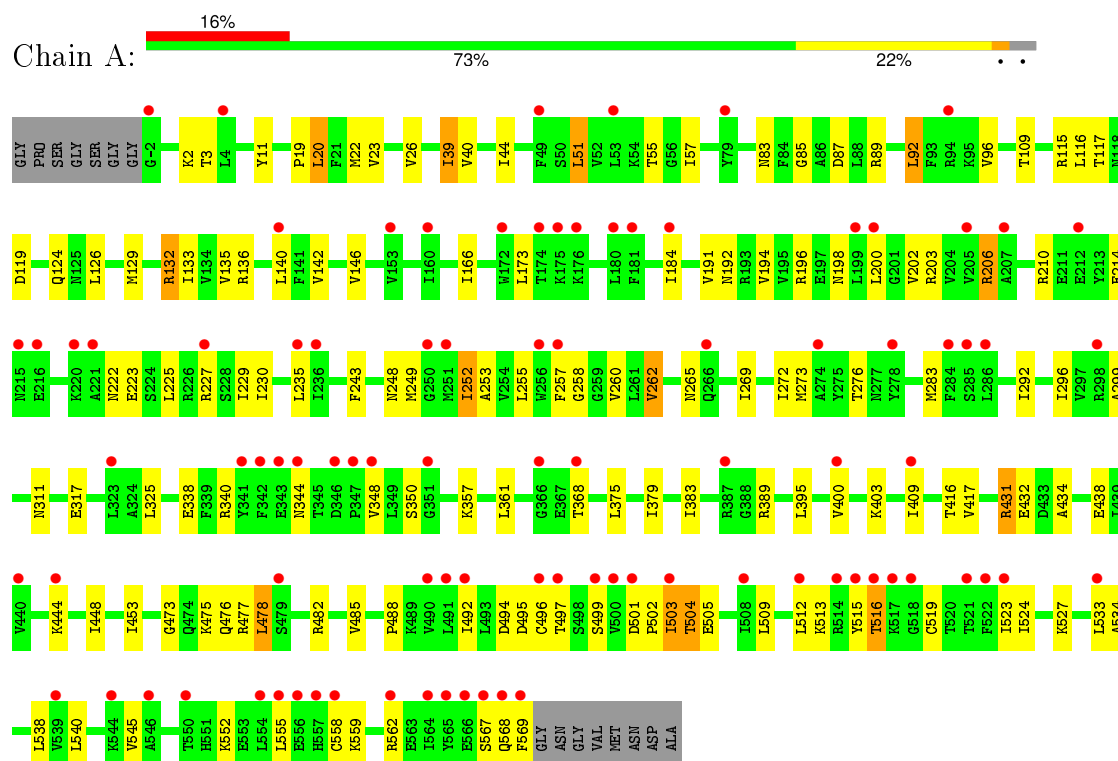
- Molecule 3 is water.

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

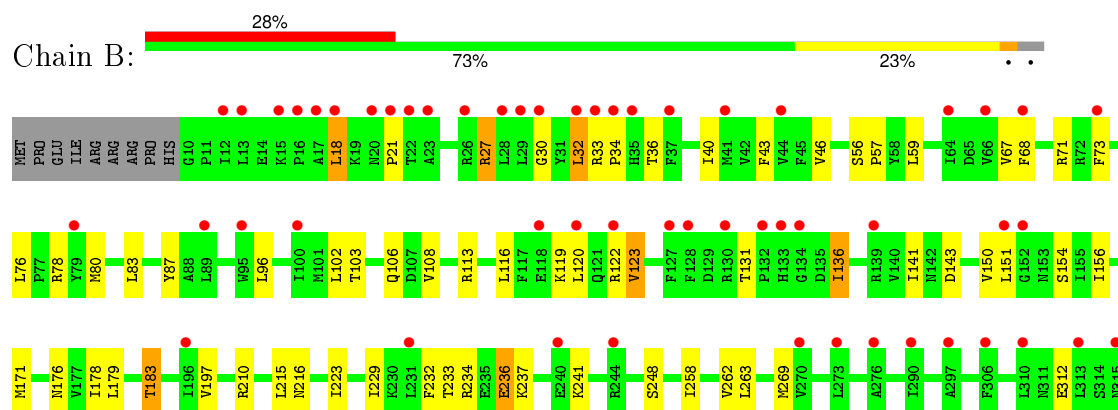
### 3 Residue-property plots

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: 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, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	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 <sup>2</sup> )	39.4	Xtriage
Anisotropy	0.032	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 83.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	1 of 59537 reflections (0.002%)	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	9138	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  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	0.29	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

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:85:GLY:HA3	1:A:124:GLN:HE21	1.67	0.58
1:A:403:LYS:HG3	2:B:233:THR:HG21	1.86	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:482:ARG:HD3	2:B:232:PHE:CZ	2.42	0.55
1:A:252:ILE:HD11	2:B:83:LEU:HB3	1.87	0.55
2:B:67:VAL:HG11	2:B:76:LEU:HD13	1.88	0.54
1:A:497:THR:HB	1:A:505:GLU:HG3	1.89	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:59:LEU:HB3	2:B:83:LEU:HD11	1.92	0.51
2:B:357:PHE:HD2	2:B:360:VAL:HG21	1.75	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
2:B:528:LYS:HA	2:B:531:GLN:HE21	1.79	0.47
1:A:495:ASP:O	1:A:497:THR:N	2.48	0.47
1:A:431:ARG:HD3	1:A:485:VAL:O	2.15	0.47
2:B:580:ARG:HA	2:B:584:TYR:HB2	1.97	0.47
1:A:184:ILE:HD13	1:A:229:ILE:HG12	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
2:B:411:GLN:HA	2:B:420:ARG:HH12	1.79	0.46
1:A:509:LEU:HD13	1:A:533:LEU:HD13	1.96	0.46
2:B:431:ILE:HG12	2:B:512:ILE:HB	1.97	0.46
2:B:236:GLU:HG2	2:B:236:GLU:H	1.48	0.46
2:B:229:ILE:HG23	2:B:234:ARG:HB2	1.97	0.46
2:B:561:VAL:HG21	2:B:583:TYR:HB2	1.97	0.46
1:A:115:ARG:HA	1:A:119:ASP:HB2	1.96	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:516:THR:HA	1:A:519:CYS:HB3	1.98	0.45
1:A:142:VAL:O	1:A:146:VAL:HG23	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:253:ALA:O	1:A:257:PHE:HB2	2.16	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:203:ARG:HG3	2:B:404:PHE:CZ	2.52	0.45
1:A:502:PRO:HB2	1:A:504:THR:HG23	1.99	0.45
1:A:132:ARG:HD2	3:A:607:HOH:O	2.17	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
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:488:PRO:HD2	1:A:515:TYR:OH	2.17	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:33:ARG:N	2:B:34:PRO:HD2	2.33	0.43
2:B:27:ARG:HD2	2:B:331:PHE:CD2	2.53	0.43
1:A:478:LEU:HA	1:A:478:LEU:HD12	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: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
2:B:330:ILE:O	2:B:334:LEU:HG	2.19	0.43
1:A:361:LEU:HD23	1:A:534:ALA:HA	2.01	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
2:B:519:THR:HG22	2:B:549:ARG:NH1	2.33	0.43
1:A:273:MET:O	1:A:276:THR:OG1	2.35	0.43
2:B:96:LEU:HA	2:B:96:LEU:HD23	1.79	0.43
2:B:312:GLU:HB3	2:B:316:GLN:HE22	1.83	0.43
1:A:473:GLY:O	1:A:477:ARG:HG3	2.19	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
1:A:248:ASN:HB3	2:B:87:TYR:CG	2.55	0.42
2:B:526:THR:O	2:B:530:ILE:HG23	2.20	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
1:A:166:ILE:HD13	1:A:243:PHE:CE1	2.54	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:96:VAL:HG11	2:B:223:ILE:HG12	2.02	0.41
1:A:325:LEU:HD11	1:A:400:VAL:HG11	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
2:B:76:LEU:O	2:B:80:MET:HG2	2.20	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: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
2:B:458:ASP:OD1	2:B:458:ASP:N	2.54	0.40
1:A:39:ILE:O	1:A:44:ILE:HG13	2.20	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%)	26 45

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	B	581/598 (97%)	545 (94%)	35 (6%)	1 (0%)	52 74
All	All	1151/1185 (97%)	1086 (94%)	60 (5%)	5 (0%)	39 60

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%)	15 26
2	B	518/533 (97%)	478 (92%)	40 (8%)	16 29
All	All	1014/1037 (98%)	934 (92%)	80 (8%)	15 27

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	572/587 (97%)	1.07	92 (16%) <b>3</b> <b>2</b>	56, 92, 141, 193	0
2	B	583/598 (97%)	1.53	169 (28%) <b>1</b> <b>0</b>	63, 117, 165, 185	0
All	All	1155/1185 (97%)	1.30	261 (22%) <b>1</b> <b>1</b>	56, 104, 161, 193	0

All (261) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	500	VAL	17.9
2	B	351	VAL	12.9
1	A	565	TYR	10.3
2	B	484	VAL	9.8
2	B	478	PRO	8.7
2	B	587	PHE	7.6
2	B	352	ARG	7.5
1	A	566	GLU	7.4
1	A	181	PHE	7.4
2	B	476	HIS	6.8
2	B	453	ASN	6.4
1	A	515	TYR	6.2
2	B	346	VAL	6.2
1	A	517	LYS	6.1
2	B	417	ILE	5.8
2	B	467	LEU	5.7
1	A	514	ARG	5.7
2	B	343	PRO	5.6
2	B	437	ASP	5.4
1	A	497	THR	5.3
1	A	172	TRP	5.2
1	A	564	ILE	5.2
2	B	349	ARG	5.2
2	B	17	ALA	5.0

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Mol	Chain	Res	Type	RSRZ
2	B	340	LYS	5.0
1	A	49	PHE	4.9
1	A	266	GLN	4.8
2	B	35	HIS	4.8
2	B	22	THR	4.8
1	A	175	LYS	4.8
2	B	362	PHE	4.8
2	B	369	PRO	4.7
2	B	568	VAL	4.7
2	B	398	VAL	4.7
2	B	391	GLY	4.7
1	A	207	ALA	4.7
2	B	310	LEU	4.6
2	B	573	HIS	4.6
1	A	518	GLY	4.6
2	B	345	ALA	4.6
1	A	220	LYS	4.6
2	B	486	THR	4.6
2	B	576	LEU	4.5
1	A	257	PHE	4.5
1	A	153	VAL	4.5
1	A	569	PHE	4.5
1	A	351	GLY	4.4
2	B	151	LEU	4.4
2	B	344	ASP	4.4
2	B	438	THR	4.4
1	A	440	VAL	4.3
2	B	577	ILE	4.3
1	A	501	ASP	4.3
2	B	416	GLY	4.3
2	B	457	THR	4.3
1	A	212	GLU	4.2
2	B	29	LEU	4.2
2	B	28	LEU	4.2
2	B	551	ASN	4.1
2	B	439	ILE	4.1
2	B	430	SER	4.1
2	B	37	PHE	4.1
1	A	400	VAL	4.1
2	B	426	SER	4.1
2	B	444	THR	4.1
2	B	18	LEU	4.0

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Mol	Chain	Res	Type	RSRZ
2	B	68	PHE	3.9
1	A	341	TYR	3.9
2	B	348	LEU	3.9
2	B	34	PRO	3.9
2	B	382	GLN	3.9
2	B	531	GLN	3.8
2	B	460	GLU	3.8
2	B	12	ILE	3.8
2	B	23	ALA	3.8
1	A	490	VAL	3.7
2	B	397	ILE	3.7
1	A	366	GLY	3.7
2	B	139	ARG	3.6
2	B	13	LEU	3.6
2	B	16	PRO	3.6
2	B	20	ASN	3.6
1	A	368	THR	3.6
1	A	205	VAL	3.6
2	B	567	ILE	3.6
1	A	567	SER	3.5
2	B	459	GLU	3.5
1	A	342	PHE	3.4
1	A	496	CYS	3.4
2	B	580	ARG	3.4
2	B	341	ASP	3.4
2	B	21	PRO	3.3
2	B	122	ARG	3.3
1	A	256	TRP	3.3
2	B	485	LEU	3.3
2	B	368	LYS	3.3
2	B	554	LYS	3.3
2	B	374	ILE	3.3
2	B	422	ILE	3.3
2	B	33	ARG	3.3
2	B	26	ARG	3.3
1	A	557	HIS	3.3
1	A	346	ASP	3.2
2	B	133	HIS	3.2
2	B	73	PHE	3.2
1	A	-2	GLY	3.2
2	B	350	GLU	3.1
2	B	506	PHE	3.1

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Mol	Chain	Res	Type	RSRZ
2	B	367	LYS	3.1
2	B	586	LEU	3.1
1	A	387	ARG	3.1
2	B	130	ARG	3.1
2	B	456	ALA	3.1
2	B	433	ILE	3.1
2	B	95	TRP	3.1
1	A	348	VAL	3.1
1	A	176	LYS	3.1
1	A	558	CYS	3.1
2	B	32	LEU	3.0
2	B	591	TYR	3.0
2	B	489	GLY	3.0
1	A	516	THR	3.0
1	A	491	LEU	3.0
2	B	461	ILE	3.0
1	A	556	GLU	3.0
2	B	401	LEU	2.9
1	A	508	ILE	2.9
2	B	544	ILE	2.9
2	B	479	GLU	2.9
2	B	152	GLY	2.9
2	B	386	LEU	2.9
2	B	44	VAL	2.9
2	B	319	MET	2.9
2	B	530	ILE	2.9
2	B	465	ALA	2.9
2	B	574	ASP	2.9
2	B	361	TRP	2.8
1	A	343	GLU	2.8
1	A	499	SER	2.8
1	A	284	PHE	2.8
1	A	555	LEU	2.8
2	B	134	GLY	2.7
2	B	306	PHE	2.7
1	A	512	LEU	2.7
1	A	235	LEU	2.7
2	B	118	GLU	2.7
2	B	372	LYS	2.7
2	B	431	ILE	2.7
2	B	477	LEU	2.7
2	B	380	PRO	2.7

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Mol	Chain	Res	Type	RSRZ
2	B	482	GLU	2.7
2	B	400	LEU	2.7
1	A	492	ILE	2.7
2	B	313	LEU	2.7
2	B	377	HIS	2.7
2	B	509	ASN	2.7
2	B	466	LYS	2.6
2	B	409	ARG	2.6
1	A	250	GLY	2.6
1	A	140	LEU	2.6
2	B	404	PHE	2.6
1	A	409	ILE	2.6
2	B	443	THR	2.6
2	B	290	ILE	2.6
2	B	66	VAL	2.5
1	A	323	LEU	2.5
2	B	546	ILE	2.5
1	A	274	ALA	2.5
1	A	236	ILE	2.5
1	A	184	ILE	2.5
2	B	514	ILE	2.5
2	B	15	LYS	2.5
2	B	462	LYS	2.5
2	B	337	GLU	2.5
2	B	231	LEU	2.4
2	B	545	ILE	2.4
1	A	79	TYR	2.4
2	B	41	MET	2.4
2	B	525	LYS	2.4
1	A	4	LEU	2.4
1	A	523	ILE	2.4
2	B	79	TYR	2.4
1	A	251	MET	2.4
1	A	94	ARG	2.4
1	A	227	ARG	2.4
2	B	270	VAL	2.4
2	B	390	THR	2.4
1	A	444	LYS	2.4
1	A	568	GLN	2.4
2	B	406	ASP	2.4
1	A	221	ALA	2.4
2	B	548	HIS	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	216	GLU	2.4
1	A	479	SER	2.4
1	A	550	THR	2.3
2	B	64	ILE	2.3
2	B	450	LYS	2.3
1	A	533	LEU	2.3
2	B	473	PHE	2.3
1	A	180	LEU	2.3
2	B	120	LEU	2.3
2	B	440	LEU	2.3
2	B	132	PRO	2.3
2	B	196	ILE	2.3
2	B	276	ALA	2.3
2	B	387	VAL	2.3
2	B	127	PHE	2.3
1	A	174	THR	2.3
1	A	554	LEU	2.3
2	B	315	ASN	2.3
2	B	579	LYS	2.3
1	A	521	THR	2.3
2	B	512	ILE	2.2
2	B	475	LYS	2.2
2	B	494	GLN	2.2
2	B	578	GLN	2.2
1	A	562	ARG	2.2
2	B	389	PRO	2.2
2	B	536	LYS	2.2
1	A	160	ILE	2.2
2	B	100	ILE	2.2
1	A	539	VAL	2.2
2	B	335	ASP	2.2
1	A	544	LYS	2.2
2	B	538	MET	2.2
2	B	89	LEU	2.2
2	B	448	ASN	2.2
1	A	546	ALA	2.1
2	B	405	TYR	2.1
2	B	454	PRO	2.1
2	B	240	GLU	2.1
2	B	388	GLY	2.1
2	B	128	PHE	2.1
1	A	503	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	344	ASN	2.1
1	A	53	LEU	2.1
1	A	286	LEU	2.1
2	B	30	GLY	2.1
1	A	298	ARG	2.1
2	B	376	PHE	2.1
2	B	297	ALA	2.1
2	B	445	VAL	2.1
1	A	278	TYR	2.1
2	B	244	ARG	2.1
2	B	497	ARG	2.1
2	B	384	VAL	2.0
1	A	347	PRO	2.0
1	A	522	PHE	2.0
2	B	550	LEU	2.0
2	B	412	ILE	2.0
2	B	273	LEU	2.0
1	A	285	SER	2.0
2	B	375	THR	2.0
2	B	428	ARG	2.0
2	B	359	ASN	2.0
2	B	381	GLY	2.0
1	A	199	LEU	2.0
1	A	200	LEU	2.0
2	B	493	SER	2.0
1	A	215	ASN	2.0
2	B	555	ASN	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.