Full wwPDB X-ray Structure Validation Report (i)

Feb 21, 2024 – 04:47 PM EST

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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (1)) were used in the production of this report:

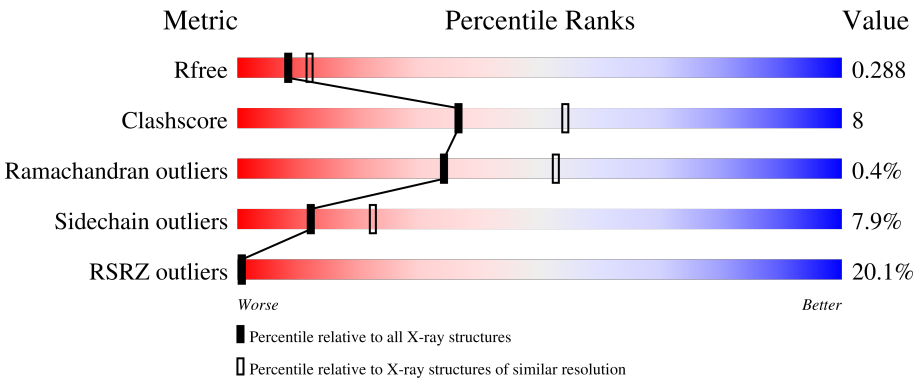
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.53 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}	130704	5743 (2.54-2.50)
Clashscore	141614	6463 (2.54-2.50)
Ramachandran outliers	138981	6335 (2.54-2.50)
Sidechain outliers	138945	6337 (2.54-2.50)
RSRZ outliers	127900	5630 (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 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 <=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	14% 73% 22% • •
2	B	598	25% 73% 23% • •

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
			Total	C	N	O	S			
1	A	572	4485	2889	772	805	19	0	0	0

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
			Total	C	N	O	S			
2	B	583	4641	3000	782	845	14	0	0	0

- Molecule 3 is water.

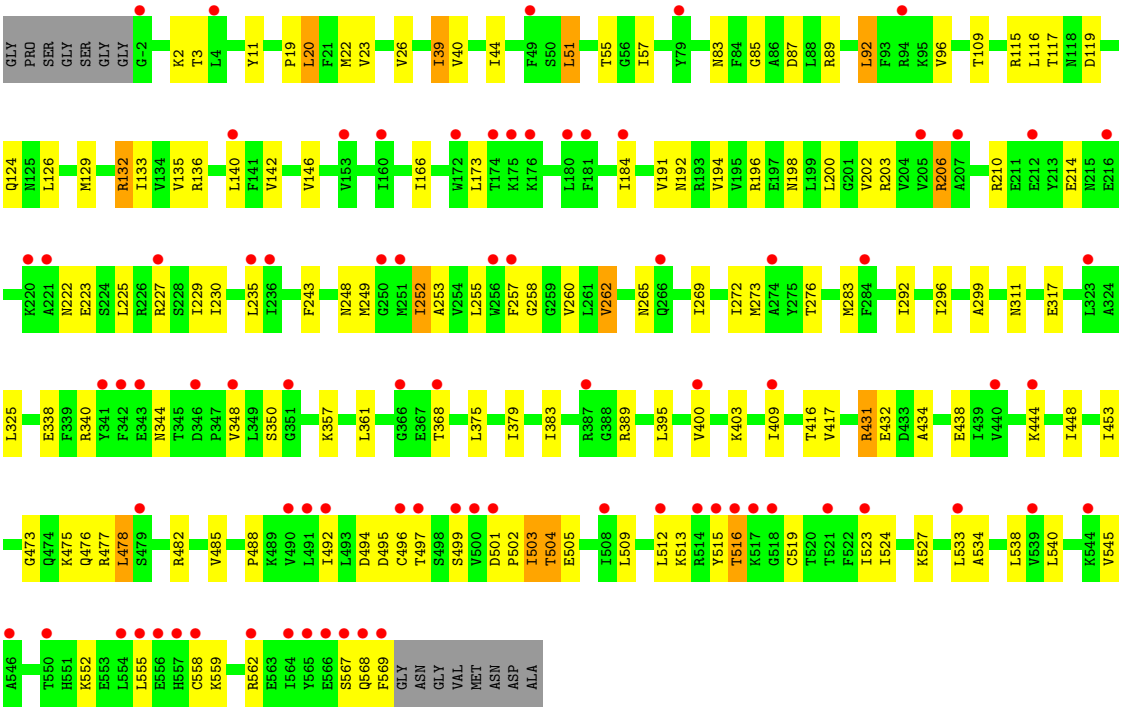
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	8	8	8	0	0
3	B	4	4	4	0	0

3 Residue-property plots (i)

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.

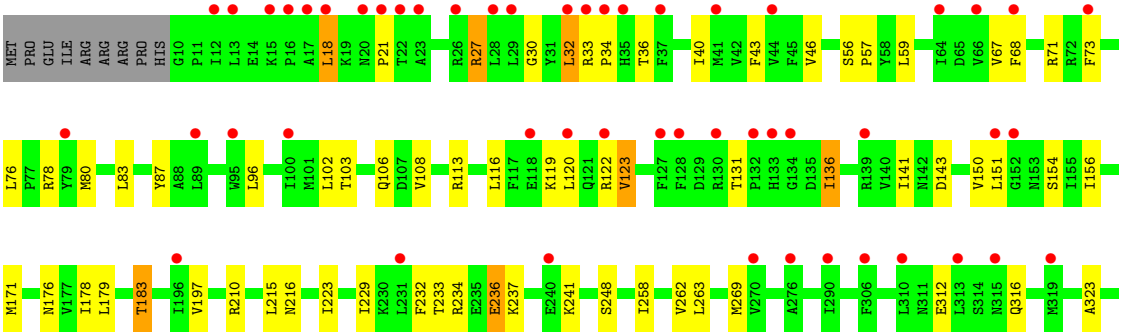
• Molecule 1: ABC transporter

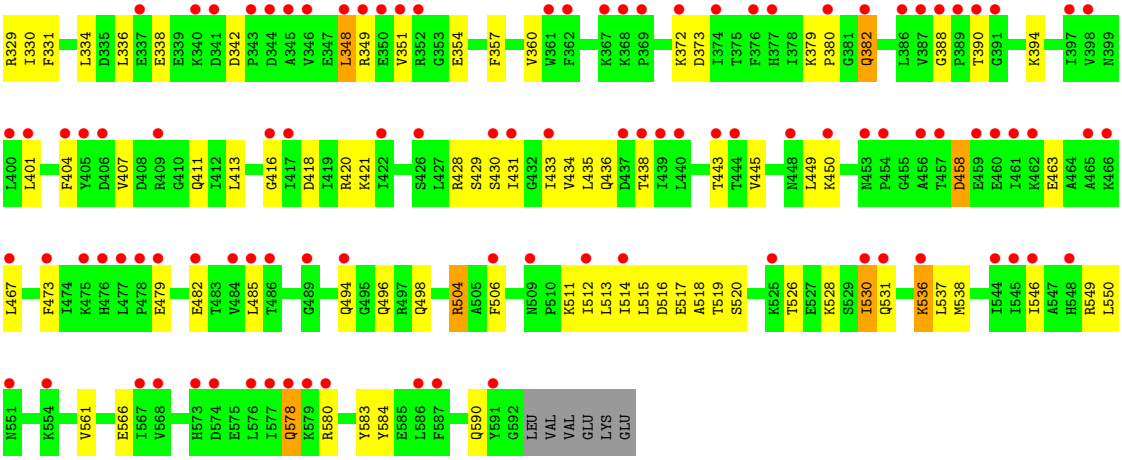
Chain A:



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

Chain B:




R329 I330 F331 L334 D335 L336 E337 E338 E339 K340 D341 D342 P343 D344 A345 V346 E347 L348 R349 E350 V351 R352 G353 E354 F357 V360 W361 F362 K367 K368 P369 K372 D373 I374 T375 F376 H377 I378 K379 P380 G381 Q382 L386 V387 G388 P389 T390 G391 K394 I397 V398 N399
L400 L401 F404 Y405 D406 V407 D408 R409 G410 Q411 I412 L413 G416 I417 D418 I419 R420 K421 I422 S426 L427 R428 S429 S430 I431 G432 I433 V434 L435 Q436 D437 T438 I439 L440 T443 T444 V445 N448 L449 K450 M453 P454 G455 A456 T457 D458 E459 E460 I461 K462 E463 A464 A465 K466
L467 F473 I474 K475 H476 L477 P478 E479 E482 T483 V484 L485 T486 G489 Q494 G495 Q496 R497 Q498 R504 A505 F506 N509 P510 K511 I512 L513 I514 L515 D516 E517 A518 T519 S520 K525 T526 E527 K528 S529 I530 Q531 K536 L537 M538 I544 I545 I546 A547 H548 R549 L550
N551 K554 V561 E566 I567 V568 H573 D574 E575 L576 I577 Q578 K579 R580 Y583 Y584 E585 L586 F587 Q590 Y591 G592 LEU VAL VAL GLU LYS GLU

4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [1]	2.24 (at 2.54Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.237 , 0.290 0.237 , 0.288	Depositor DCC
R_{free} test set	3006 reflections (5.05%)	wwPDB-VP
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]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	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.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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:89:ARG:HD3	2:B:215:LEU:HD11	1.83	0.59
1:A:417:VAL:O	1:A:482:ARG:NH2	2.33	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: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: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:HD22	1:A:51:LEU:HA	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:H	2:B:236:GLU:HG2	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:HD22	2:B:348:LEU:HA	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:119:LYS:NZ	2:B:336:LEU:O	2.34	0.44
2:B:143:ASP:OD1	2:B:329:ARG:NH1	2.50	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:HD12	1:A:252:ILE:HA	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:HA	2:B:210:ARG:HD2	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:2:LYS:HB2	1:A:311:ASN:OD1	2.17	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:117:THR:HG22	2:B:216:ASN:OD1	2.18	0.43
1:A:478:LEU:HD12	1:A:478:LEU:HA	1.84	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: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
2:B:519:THR:HG22	2:B:549:ARG:NH1	2.33	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:HD12	1:A:453:ILE:HA	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: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:HD2	2:B:119:LYS:HA	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: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:56:SER:HB2	2:B:57:PRO:HD3	2.03	0.41
2:B:143:ASP:OD2	2:B:329:ARG:HD2	2.21	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%)	22 37

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	581/598 (97%)	545 (94%)	35 (6%)	1 (0%)	47	67
All	All	1151/1185 (97%)	1086 (94%)	60 (5%)	5 (0%)	34	53

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 (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	496/504 (98%)	456 (92%)	40 (8%)	11	21
2	B	518/533 (97%)	478 (92%)	40 (8%)	13	23
All	All	1014/1037 (98%)	934 (92%)	80 (8%)	12	22

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

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	124	GLN
2	B	316	GLN
2	B	531	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	572/587 (97%)	0.98	80 (13%)	2	2	56, 92, 141, 193	0
2	B	583/598 (97%)	1.43	152 (26%)	0	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	17.3
2	B	351	VAL	12.5
1	A	565	TYR	10.2
2	B	484	VAL	9.6
2	B	478	PRO	8.2
2	B	587	PHE	7.3
1	A	181	PHE	7.2
2	B	352	ARG	7.2
1	A	566	GLU	7.1
2	B	476	HIS	6.6
2	B	453	ASN	6.2
1	A	517	LYS	6.1
2	B	346	VAL	5.9
1	A	515	TYR	5.9
2	B	417	ILE	5.6
1	A	514	ARG	5.4
2	B	343	PRO	5.3
2	B	467	LEU	5.3
2	B	437	ASP	5.2
1	A	497	THR	5.1
1	A	172	TRP	5.0
2	B	349	ARG	5.0
1	A	564	ILE	5.0
2	B	17	ALA	4.9

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Mol	Chain	Res	Type	RSRZ
2	B	340	LYS	4.8
1	A	49	PHE	4.7
1	A	266	GLN	4.7
2	B	362	PHE	4.6
2	B	35	HIS	4.6
2	B	22	THR	4.6
1	A	175	LYS	4.6
2	B	391	GLY	4.6
2	B	398	VAL	4.5
2	B	568	VAL	4.5
2	B	310	LEU	4.5
1	A	207	ALA	4.4
2	B	369	PRO	4.4
2	B	345	ALA	4.4
2	B	486	THR	4.4
2	B	573	HIS	4.4
1	A	220	LYS	4.4
2	B	576	LEU	4.3
1	A	518	GLY	4.3
1	A	257	PHE	4.3
1	A	153	VAL	4.3
2	B	577	ILE	4.2
1	A	569	PHE	4.2
2	B	344	ASP	4.2
2	B	151	LEU	4.2
1	A	351	GLY	4.2
2	B	438	THR	4.2
1	A	501	ASP	4.2
2	B	457	THR	4.1
2	B	29	LEU	4.1
1	A	440	VAL	4.1
2	B	416	GLY	4.0
1	A	212	GLU	4.0
2	B	430	SER	4.0
2	B	28	LEU	4.0
2	B	37	PHE	4.0
2	B	551	ASN	3.9
2	B	18	LEU	3.9
2	B	426	SER	3.9
2	B	439	ILE	3.8
1	A	400	VAL	3.8
1	A	341	TYR	3.8

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Mol	Chain	Res	Type	RSRZ
2	B	68	PHE	3.8
2	B	444	THR	3.8
2	B	348	LEU	3.8
2	B	382	GLN	3.7
2	B	23	ALA	3.7
2	B	531	GLN	3.7
2	B	460	GLU	3.6
2	B	34	PRO	3.6
2	B	12	ILE	3.6
2	B	397	ILE	3.6
1	A	490	VAL	3.6
2	B	139	ARG	3.5
2	B	13	LEU	3.4
1	A	366	GLY	3.4
1	A	368	THR	3.4
1	A	205	VAL	3.4
2	B	20	ASN	3.4
1	A	342	PHE	3.3
2	B	16	PRO	3.3
2	B	567	ILE	3.3
2	B	459	GLU	3.3
1	A	567	SER	3.3
2	B	368	LYS	3.2
1	A	557	HIS	3.2
2	B	21	PRO	3.2
1	A	256	TRP	3.2
2	B	33	ARG	3.2
2	B	122	ARG	3.2
2	B	580	ARG	3.2
2	B	26	ARG	3.2
2	B	341	ASP	3.2
2	B	485	LEU	3.2
2	B	374	ILE	3.1
2	B	422	ILE	3.1
1	A	496	CYS	3.1
2	B	554	LYS	3.1
1	A	-2	GLY	3.1
2	B	73	PHE	3.0
2	B	367	LYS	3.0
2	B	133	HIS	3.0
2	B	506	PHE	3.0
2	B	95	TRP	3.0

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Mol	Chain	Res	Type	RSRZ
2	B	130	ARG	3.0
1	A	346	ASP	3.0
2	B	433	ILE	3.0
2	B	350	GLU	3.0
1	A	387	ARG	3.0
2	B	456	ALA	2.9
2	B	586	LEU	2.9
1	A	348	VAL	2.9
1	A	176	LYS	2.9
1	A	556	GLU	2.9
2	B	591	TYR	2.9
2	B	479	GLU	2.8
1	A	558	CYS	2.8
1	A	516	THR	2.8
2	B	489	GLY	2.8
1	A	491	LEU	2.8
2	B	32	LEU	2.8
2	B	544	ILE	2.8
2	B	461	ILE	2.8
2	B	44	VAL	2.8
1	A	343	GLU	2.8
2	B	401	LEU	2.8
2	B	152	GLY	2.7
1	A	508	ILE	2.7
1	A	499	SER	2.7
2	B	319	MET	2.7
2	B	361	TRP	2.7
1	A	284	PHE	2.7
2	B	386	LEU	2.7
2	B	530	ILE	2.7
2	B	465	ALA	2.7
2	B	118	GLU	2.6
2	B	574	ASP	2.6
2	B	482	GLU	2.6
2	B	313	LEU	2.6
2	B	372	LYS	2.6
2	B	306	PHE	2.6
2	B	431	ILE	2.6
2	B	380	PRO	2.5
2	B	466	LYS	2.5
2	B	509	ASN	2.5
1	A	555	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	235	LEU	2.5
1	A	512	LEU	2.5
1	A	492	ILE	2.5
2	B	377	HIS	2.5
2	B	134	GLY	2.5
2	B	443	THR	2.5
2	B	400	LEU	2.5
2	B	477	LEU	2.5
2	B	409	ARG	2.5
1	A	250	GLY	2.5
2	B	290	ILE	2.5
2	B	404	PHE	2.5
1	A	140	LEU	2.4
1	A	184	ILE	2.4
1	A	409	ILE	2.4
2	B	66	VAL	2.4
2	B	15	LYS	2.4
2	B	546	ILE	2.4
1	A	274	ALA	2.4
2	B	548	HIS	2.4
2	B	337	GLU	2.4
1	A	236	ILE	2.3
1	A	79	TYR	2.3
2	B	231	LEU	2.3
1	A	568	GLN	2.3
2	B	462	LYS	2.3
2	B	545	ILE	2.3
1	A	323	LEU	2.3
2	B	514	ILE	2.3
1	A	94	ARG	2.3
1	A	216	GLU	2.3
1	A	227	ARG	2.3
2	B	79	TYR	2.3
1	A	4	LEU	2.3
2	B	270	VAL	2.3
2	B	41	MET	2.3
2	B	450	LYS	2.3
2	B	525	LYS	2.3
1	A	523	ILE	2.2
2	B	120	LEU	2.2
1	A	444	LYS	2.2
2	B	473	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	494	GLN	2.2
2	B	276	ALA	2.2
1	A	533	LEU	2.2
1	A	554	LEU	2.2
1	A	479	SER	2.2
1	A	251	MET	2.2
1	A	221	ALA	2.2
2	B	64	ILE	2.2
2	B	406	ASP	2.2
2	B	440	LEU	2.2
1	A	550	THR	2.2
2	B	132	PRO	2.2
2	B	578	GLN	2.1
2	B	579	LYS	2.1
1	A	174	THR	2.1
2	B	196	ILE	2.1
1	A	180	LEU	2.1
2	B	315	ASN	2.1
1	A	521	THR	2.1
1	A	160	ILE	2.1
2	B	100	ILE	2.1
2	B	389	PRO	2.1
2	B	512	ILE	2.1
2	B	536	LYS	2.1
2	B	387	VAL	2.1
2	B	390	THR	2.1
1	A	562	ARG	2.1
2	B	89	LEU	2.1
2	B	127	PHE	2.1
2	B	475	LYS	2.1
2	B	405	TYR	2.1
2	B	128	PHE	2.1
2	B	240	GLU	2.0
1	A	546	ALA	2.0
1	A	544	LYS	2.0
2	B	448	ASN	2.0
1	A	539	VAL	2.0
2	B	388	GLY	2.0
2	B	376	PHE	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 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.