



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:59 AM UTC

PDB ID : 4Q4H / pdb_00004q4h
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 ⓘ 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

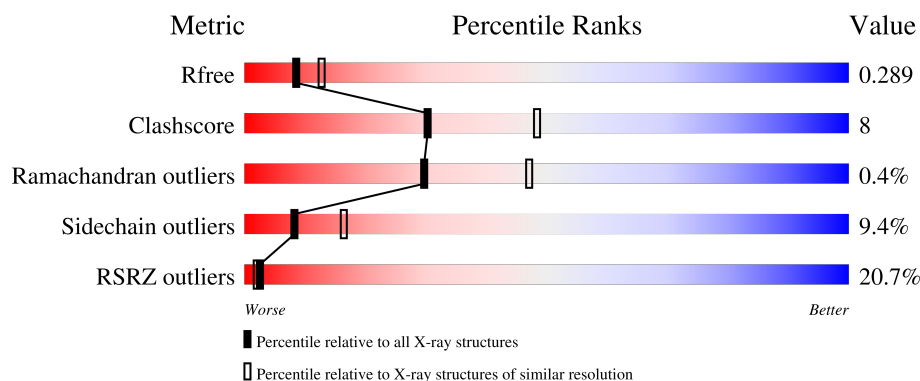
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.53 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}	180053	7383 (2.54-2.50)
Clashscore	190562	8079 (2.54-2.50)
Ramachandran outliers	187476	7944 (2.54-2.50)
Sidechain outliers	187428	7946 (2.54-2.50)
RSRZ outliers	180081	7387 (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 $\leq 5\%$. 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	15% 71% 23% • •
2	B	598	25% 72% 22% • •

2 Entry composition

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			

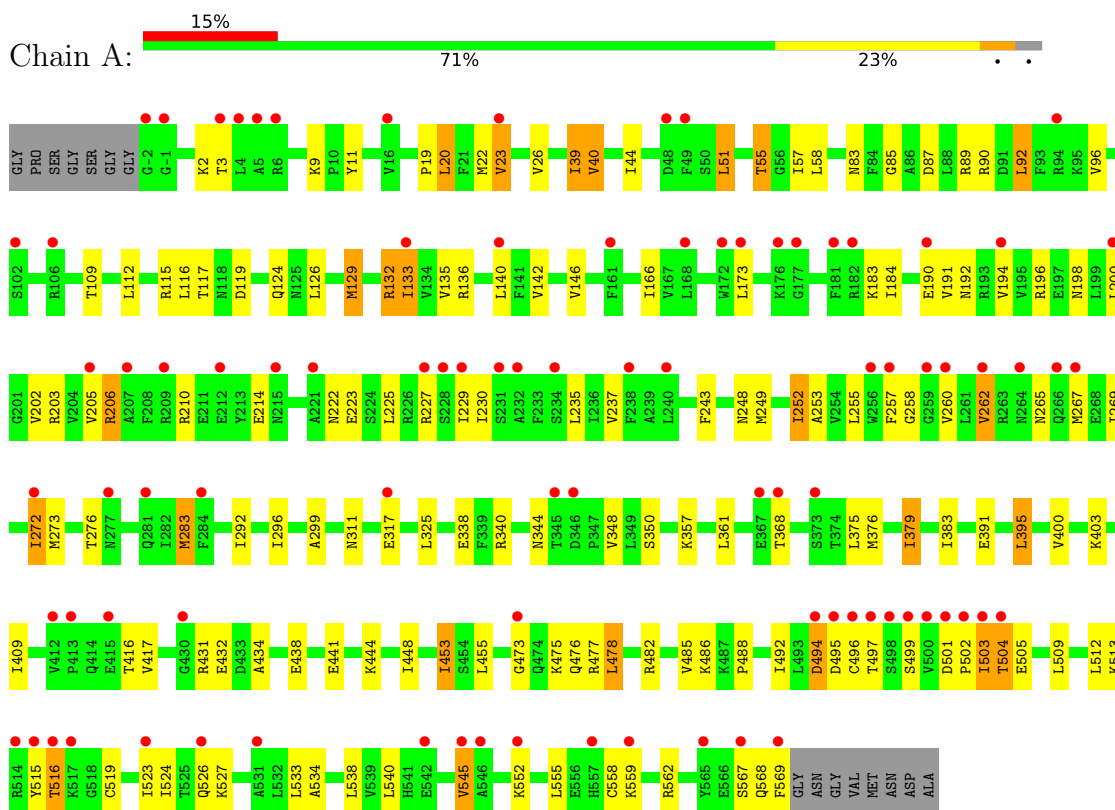
- Molecule 3 is water.

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

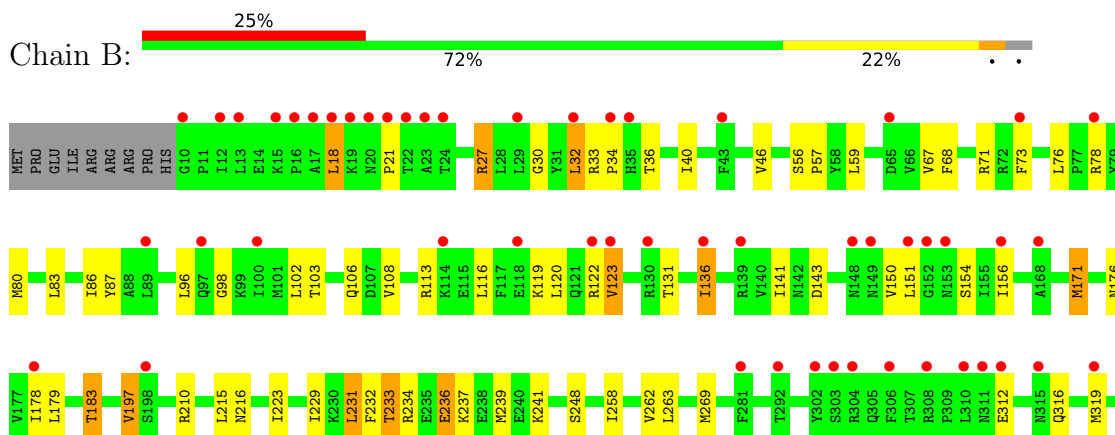
3 Residue-property plots

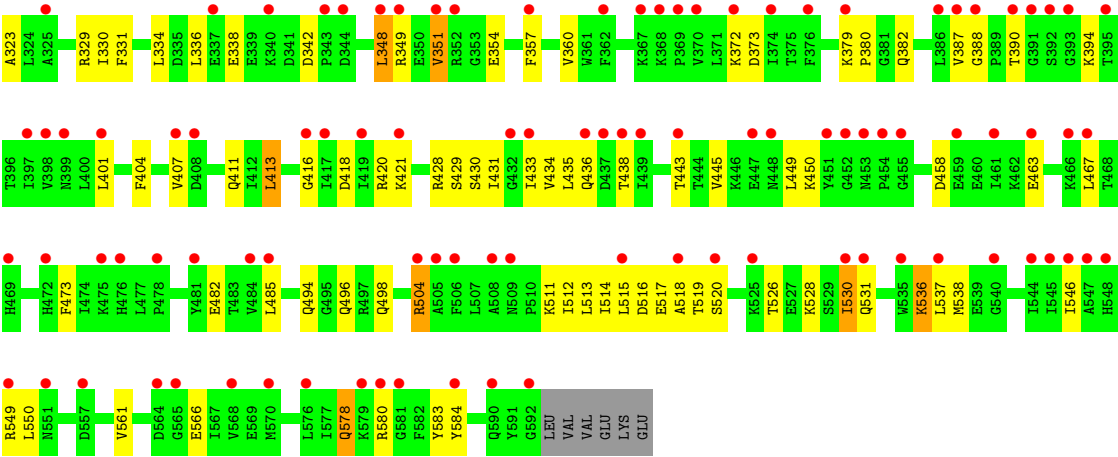
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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



• 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) 87.3 (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 0.237 , 0.289	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)	0.29 , 76.4	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	0.91	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	0.40	0/4560	0.82	4/6166 (0.1%)
2	B	0.35	0/4722	0.78	0/6385
All	All	0.37	0/9282	0.80	4/12551 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	379	ILE	CA-C-N	-7.05	112.67	120.14
1	A	379	ILE	C-N-CA	-7.05	112.67	120.14
1	A	455	LEU	CA-C-N	5.96	126.11	119.32
1	A	455	LEU	C-N-CA	5.96	126.11	119.32

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	91	0
2	B	4641	0	4829	88	0
3	A	8	0	0	1	0
3	B	4	0	0	0	0
All	All	9138	0	9512	156	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 (156) 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
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
1:A:166:ILE:HD12	1:A:283:MET:HE3	1.77	0.66
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:388:GLY:O	2:B:394:LYS:NZ	2.32	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:376:MET:HE1	1:A:494:ASP:HB2	1.91	0.53
2:B:30:GLY:HA2	2:B:33:ARG:HD2	1.90	0.53
2:B:119:LYS:NZ	2:B:336:LEU:O	2.34	0.53
1:A:416:THR:OG1	1:A:475:LYS:HB3	2.09	0.52
1:A:222:ASN:OD1	2:B:113:ARG:NH1	2.42	0.52
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:431:ARG:HH22	1:A:438:GLU:CD	2.19	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:486:LYS:NZ	2:B:231:LEU:O	2.44	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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
1:A:90:ARG:NH2	2:B:239:MET:HE2	2.31	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
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:391:GLU:HG2	1:A:395:LEU:C	2.43	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:237:VAL:HG21	2:B:98:GLY:C	2.44	0.42
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
2:B:171:MET:HB2	2:B:171:MET:HE3	1.80	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:267:MET:HE2	1:A:272:ILE:HD12	2.02	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

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	570/587 (97%)	541 (95%)	25 (4%)	4 (1%)	18	32
2	B	581/598 (97%)	545 (94%)	35 (6%)	1 (0%)	43	62
All	All	1151/1185 (97%)	1086 (94%)	60 (5%)	5 (0%)	30	47

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%)	443 (89%)	53 (11%)	6	12
2	B	518/533 (97%)	476 (92%)	42 (8%)	11	22
All	All	1014/1037 (98%)	919 (91%)	95 (9%)	8	16

All (95) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	THR

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Mol	Chain	Res	Type
1	A	9	LYS
1	A	20	LEU
1	A	23	VAL
1	A	39	ILE
1	A	40	VAL
1	A	51	LEU
1	A	55	THR
1	A	57	ILE
1	A	58	LEU
1	A	92	LEU
1	A	109	THR
1	A	112	LEU
1	A	129	MET
1	A	132	ARG
1	A	133	ILE
1	A	173	LEU
1	A	183	LYS
1	A	190	GLU
1	A	200	LEU
1	A	205	VAL
1	A	206	ARG
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	395	LEU
1	A	441	GLU
1	A	444	LYS
1	A	453	ILE
1	A	478	LEU

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Mol	Chain	Res	Type
1	A	494	ASP
1	A	501	ASP
1	A	503	ILE
1	A	504	THR
1	A	523	ILE
1	A	526	GLN
1	A	538	LEU
1	A	545	VAL
1	A	552	LYS
1	A	555	LEU
2	B	18	LEU
2	B	27	ARG
2	B	32	LEU
2	B	46	VAL
2	B	78	ARG
2	B	86	ILE
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
2	B	171	MET
2	B	178	ILE
2	B	183	THR
2	B	197	VAL
2	B	231	LEU
2	B	233	THR
2	B	236	GLU
2	B	241	LYS
2	B	248	SER
2	B	269	MET
2	B	319	MET
2	B	342	ASP
2	B	348	LEU
2	B	351	VAL
2	B	373	ASP
2	B	387	VAL
2	B	407	VAL
2	B	413	LEU
2	B	429	SER

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Mol	Chain	Res	Type
2	B	438	THR
2	B	443	THR
2	B	450	LYS
2	B	463	GLU
2	B	482	GLU
2	B	504	ARG
2	B	530	ILE
2	B	536	LYS
2	B	537	LEU
2	B	578	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	124	GLN
2	B	149	ASN
2	B	316	GLN
2	B	321	GLN
2	B	411	GLN
2	B	488	ASN
2	B	494	GLN
2	B	498	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 ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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%)	1.09	90 (15%) 5 4	56, 92, 141, 193	0
2	B	583/598 (97%)	1.48	149 (25%) 1 1	63, 117, 165, 185	0
All	All	1155/1185 (97%)	1.29	239 (20%) 2 2	56, 104, 161, 193	0

All (239) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	500	VAL	6.9
2	B	467	LEU	5.7
1	A	212	GLU	5.5
1	A	503	ILE	5.5
2	B	416	GLY	5.1
1	A	502	PRO	4.9
2	B	352	ARG	4.9
1	A	515	TYR	4.8
2	B	438	THR	4.6
1	A	516	THR	4.5
2	B	17	ALA	4.5
1	A	-2	GLY	4.3
2	B	592	GLY	4.3
2	B	546	ILE	4.2
2	B	351	VAL	4.2
2	B	535	TRP	4.2
2	B	525	LYS	4.2
1	A	499	SER	4.1
2	B	369	PRO	4.1
1	A	565	TYR	4.1
2	B	475	LYS	3.9
2	B	303	SER	3.9
1	A	517	LYS	3.9
1	A	257	PHE	3.8

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Mol	Chain	Res	Type	RSRZ
2	B	29	LEU	3.8
2	B	443	THR	3.8
2	B	580	ARG	3.8
2	B	136	ILE	3.8
1	A	514	ARG	3.8
1	A	557	HIS	3.8
1	A	172	TRP	3.7
1	A	221	ALA	3.6
2	B	18	LEU	3.6
2	B	151	LEU	3.6
2	B	390	THR	3.6
2	B	152	GLY	3.6
2	B	139	ARG	3.5
2	B	506	PHE	3.5
2	B	472	HIS	3.5
2	B	178	ILE	3.5
1	A	415	GLU	3.5
2	B	306	PHE	3.5
1	A	215	ASN	3.5
2	B	398	VAL	3.5
2	B	433	ILE	3.5
2	B	357	PHE	3.4
1	A	569	PHE	3.4
2	B	32	LEU	3.4
2	B	466	LYS	3.4
1	A	497	THR	3.3
2	B	439	ILE	3.3
1	A	49	PHE	3.3
2	B	417	ILE	3.3
2	B	518	ALA	3.3
1	A	501	ASP	3.3
2	B	304	ARG	3.3
2	B	564	ASP	3.2
2	B	584	TYR	3.2
2	B	35	HIS	3.2
2	B	437	ASP	3.2
2	B	565	GLY	3.2
2	B	12	ILE	3.2
2	B	557	ASP	3.2
1	A	496	CYS	3.2
1	A	523	ILE	3.2
1	A	181	PHE	3.1

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Mol	Chain	Res	Type	RSRZ
2	B	308	ARG	3.1
1	A	545	VAL	3.1
1	A	367	GLU	3.0
2	B	520	SER	3.0
2	B	156	ILE	3.0
2	B	484	VAL	3.0
2	B	547	ALA	3.0
2	B	343	PRO	3.0
1	A	542	GLU	3.0
2	B	408	ASP	3.0
2	B	20	ASN	3.0
2	B	531	GLN	3.0
1	A	345	THR	2.9
2	B	100	ILE	2.9
1	A	504	THR	2.9
1	A	4	LEU	2.9
1	A	494	ASP	2.9
2	B	509	ASN	2.9
2	B	387	VAL	2.9
2	B	312	GLU	2.9
2	B	549	ARG	2.8
2	B	368	LYS	2.8
2	B	123	VAL	2.8
1	A	531	ALA	2.8
2	B	344	ASP	2.8
1	A	106	ARG	2.8
2	B	568	VAL	2.8
2	B	118	GLU	2.8
1	A	176	LYS	2.8
2	B	19	LYS	2.8
2	B	548	HIS	2.8
2	B	399	ASN	2.8
1	A	413	PRO	2.8
2	B	21	PRO	2.8
1	A	281	GLN	2.8
2	B	349	ARG	2.8
1	A	256	TRP	2.8
2	B	545	ILE	2.8
1	A	173	LEU	2.8
2	B	505	ALA	2.8
2	B	340	LYS	2.8
2	B	65	ASP	2.8

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Mol	Chain	Res	Type	RSRZ
2	B	540	GLY	2.7
1	A	205	VAL	2.7
2	B	24	THR	2.7
2	B	386	LEU	2.7
2	B	337	GLU	2.7
2	B	419	ILE	2.7
2	B	407	VAL	2.7
1	A	240	LEU	2.7
2	B	310	LEU	2.7
1	A	94	ARG	2.7
1	A	284	PHE	2.7
2	B	281	PHE	2.7
2	B	372	LYS	2.7
1	A	373	SER	2.7
2	B	395	THR	2.7
1	A	229	ILE	2.6
2	B	453	ASN	2.6
1	A	259	GLY	2.6
2	B	34	PRO	2.6
1	A	567	SER	2.6
2	B	393	GLY	2.6
2	B	478	PRO	2.6
2	B	485	LEU	2.6
2	B	311	ASN	2.6
2	B	97	GLN	2.6
2	B	78	ARG	2.6
2	B	581	GLY	2.6
2	B	367	LYS	2.6
2	B	530	ILE	2.5
2	B	459	GLU	2.5
1	A	260	VAL	2.5
1	A	546	ALA	2.5
1	A	3	THR	2.5
2	B	392	SER	2.5
2	B	122	ARG	2.5
1	A	-1	GLY	2.5
1	A	140	LEU	2.5
2	B	448	ASN	2.5
1	A	231	SER	2.5
2	B	454	PRO	2.5
1	A	526	GLN	2.5
2	B	362	PHE	2.5

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Mol	Chain	Res	Type	RSRZ
2	B	15	LYS	2.4
2	B	590	GLN	2.4
1	A	182	ARG	2.4
2	B	570	MET	2.4
2	B	292	THR	2.4
2	B	391	GLY	2.4
2	B	13	LEU	2.4
1	A	16	VAL	2.4
2	B	508	ALA	2.4
2	B	16	PRO	2.4
2	B	421	LYS	2.4
2	B	348	LEU	2.4
2	B	436	GLN	2.4
2	B	452	GLY	2.4
1	A	133	ILE	2.4
2	B	397	ILE	2.4
1	A	48	ASP	2.4
2	B	401	LEU	2.4
1	A	238	PHE	2.4
2	B	315	ASN	2.4
2	B	10	GLY	2.3
1	A	209	ARG	2.3
2	B	89	LEU	2.3
2	B	374	ILE	2.3
2	B	43	PHE	2.3
2	B	481	TYR	2.3
2	B	149	ASN	2.3
1	A	368	THR	2.3
2	B	22	THR	2.3
2	B	515	LEU	2.3
2	B	148	ASN	2.3
1	A	234	SER	2.3
1	A	266	GLN	2.3
2	B	469	HIS	2.3
1	A	346	ASP	2.3
1	A	430	GLY	2.3
1	A	161	PHE	2.3
2	B	447	GLU	2.3
2	B	153	ASN	2.2
2	B	168	ALA	2.2
2	B	114	LYS	2.2
1	A	495	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	194	VAL	2.2
2	B	576	LEU	2.2
1	A	23	VAL	2.2
2	B	455	GLY	2.2
2	B	537	LEU	2.2
1	A	412	VAL	2.2
1	A	207	ALA	2.2
1	A	559	LYS	2.2
2	B	379	LYS	2.2
2	B	476	HIS	2.2
2	B	302	TYR	2.2
2	B	451	TYR	2.2
2	B	544	ILE	2.2
2	B	579	LYS	2.2
1	A	102	SER	2.1
2	B	325	ALA	2.1
1	A	264	ASN	2.1
1	A	277	ASN	2.1
1	A	168	LEU	2.1
1	A	190	GLU	2.1
2	B	504	ARG	2.1
1	A	552	LYS	2.1
2	B	319	MET	2.1
1	A	5	ALA	2.1
2	B	551	ASN	2.1
1	A	177	GLY	2.1
1	A	200	LEU	2.1
2	B	198	SER	2.1
1	A	267	MET	2.1
2	B	376	PHE	2.1
1	A	232	ALA	2.1
1	A	473	GLY	2.1
2	B	73	PHE	2.0
2	B	370	VAL	2.0
1	A	6	ARG	2.0
1	A	227	ARG	2.0
2	B	130	ARG	2.0
2	B	388	GLY	2.0
1	A	272	ILE	2.0
1	A	498	SER	2.0
1	A	262	VAL	2.0
2	B	23	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	317	GLU	2.0
2	B	463	GLU	2.0
2	B	432	GLY	2.0
2	B	461	ILE	2.0
1	A	228	SER	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.