



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 29, 2025 – 10:08 AM EDT

PDB ID : 4Q4J / pdb_00004q4j
Title : Structure of crosslinked TM287/288_S498C_S520C mutant
Authors : Hohl, M.; Schoeppe, J.; Gruetter, M.G.; Seeger, M.A.
Deposited on : 2014-04-14
Resolution : 3.20 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 Phenix2.0rc1
Xtriage (Phenix) : 2.0rc1
EDS : 3.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.006 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.43.1

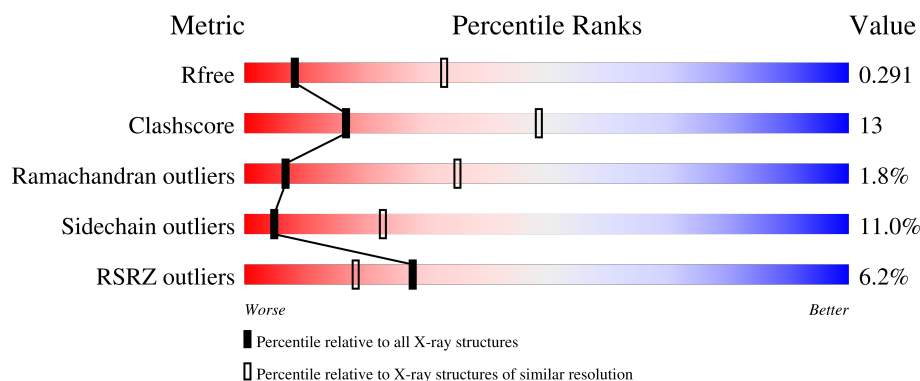
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION



The reported resolution of this entry is 3.20 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}	164625	1370 (3.20-3.20)
Clashscore	180529	1497 (3.20-3.20)
Ramachandran outliers	177936	1479 (3.20-3.20)
Sidechain outliers	177891	1478 (3.20-3.20)
RSRZ outliers	164620	1371 (3.20-3.20)

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	
2	B	598	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9126 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	809	15			

There are 17 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
A	28	SER	CYS	engineered mutation	UNP Q9WYC3
A	73	SER	CYS	engineered mutation	UNP Q9WYC3
A	496	SER	CYS	engineered mutation	UNP Q9WYC3
A	498	CYS	SER	engineered mutation	UNP Q9WYC3
A	519	SER	CYS	engineered mutation	UNP Q9WYC3
A	558	SER	CYS	engineered mutation	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	844	15			

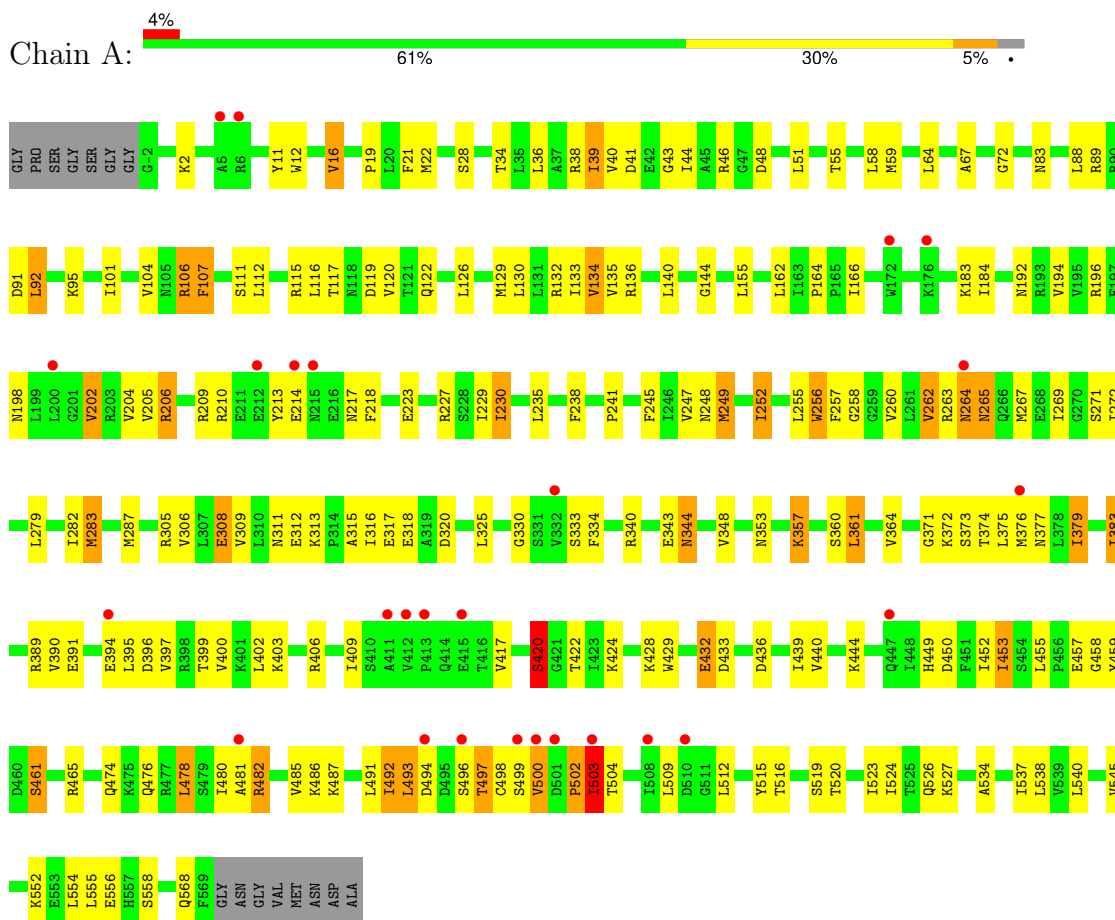
There is a discrepancy between the modelled and reference sequences:

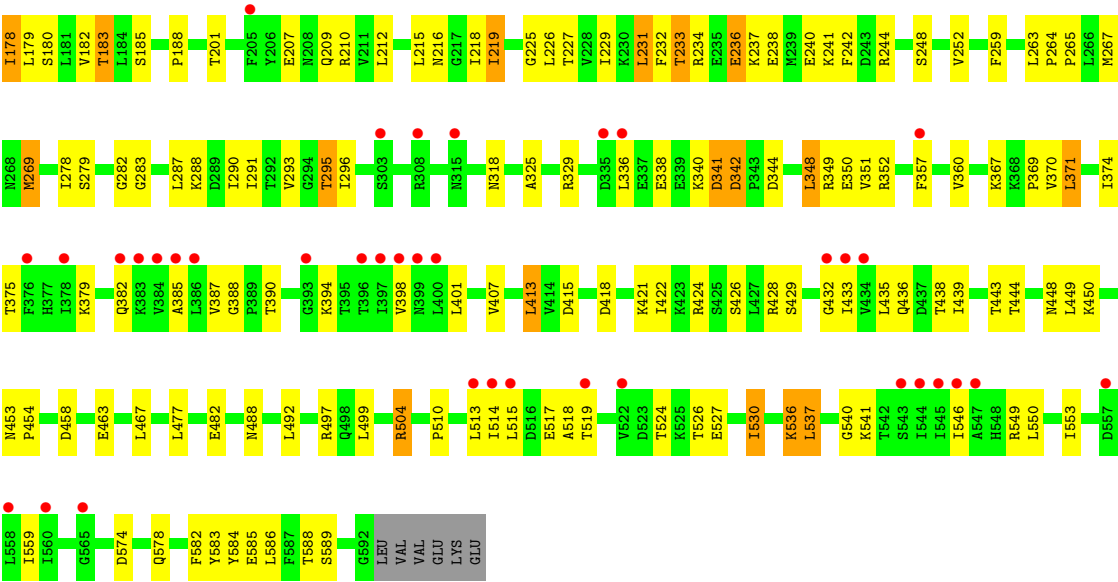
Chain	Residue	Modelled	Actual	Comment	Reference
B	520	CYS	SER	engineered mutation	UNP Q9WYC4

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





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	216.67Å 84.14Å 113.46Å 90.00° 93.32° 90.00°	Depositor
Resolution (Å)	48.46 – 3.20 48.46 – 3.20	Depositor EDS
% Data completeness (in resolution range)	98.3 (48.46-3.20) 98.7 (48.46-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.77 (at 3.19Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.237 , 0.287 0.241 , 0.291	Depositor DCC
R_{free} test set	1675 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	109.0	Xtriage
Anisotropy	0.154	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 49.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	9126	wwPDB-VP
Average B, all atoms (Å ²)	106.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.35% 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	0.58	0/4560	0.96	8/6166 (0.1%)
2	B	0.47	0/4722	0.88	3/6385 (0.0%)
All	All	0.53	0/9282	0.92	11/12551 (0.1%)

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	379	ILE	CA-C-N	-6.66	112.60	120.13
1	A	379	ILE	C-N-CA	-6.66	112.60	120.13
2	B	477	LEU	CA-C-N	5.98	127.31	119.84
2	B	477	LEU	C-N-CA	5.98	127.31	119.84
1	A	134	VAL	N-CA-C	-5.84	106.03	113.22
1	A	164	PRO	N-CA-C	5.79	117.76	110.70
1	A	455	LEU	CA-C-N	5.49	126.70	119.84
1	A	455	LEU	C-N-CA	5.49	126.70	119.84
2	B	81	LEU	N-CA-C	-5.24	106.94	113.55
1	A	325	LEU	CA-C-N	5.11	126.23	119.84
1	A	325	LEU	C-N-CA	5.11	126.23	119.84

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	4682	130	0
2	B	4641	0	4828	130	0
All	All	9126	0	9510	235	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 13.

All (235) 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)
2:B:119:LYS:NZ	2:B:336:LEU:O	2.11	0.81
1:A:206:ARG:NH2	2:B:123:VAL:O	2.15	0.79
1:A:95:LYS:NZ	1:A:312:GLU:O	2.13	0.79
1:A:38:ARG:HE	1:A:55:THR:HG21	1.49	0.76
1:A:92:LEU:HD21	1:A:306:VAL:HG13	1.68	0.73
2:B:122:ARG:HB3	2:B:338:GLU:HB3	1.69	0.73
1:A:526:GLN:NE2	2:B:519:THR:O	2.20	0.73
2:B:467:LEU:HB3	2:B:536:LYS:HD3	1.71	0.71
1:A:432:GLU:OE2	2:B:237:LYS:NZ	2.23	0.71
2:B:585:GLU:O	2:B:589:SER:OG	2.06	0.71
2:B:388:GLY:O	2:B:394:LYS:NZ	2.25	0.70
1:A:198:ASN:OD1	2:B:121:GLN:NE2	2.26	0.69
1:A:428:LYS:HE2	1:A:439:ILE:HD11	1.75	0.69
2:B:517:GLU:HB3	2:B:549:ARG:HH21	1.59	0.66
2:B:559:ILE:HG21	2:B:583:TYR:HE2	1.60	0.66
2:B:67:VAL:HG11	2:B:76:LEU:HD13	1.78	0.66
1:A:424:LYS:HB2	1:A:459:TYR:HB3	1.78	0.66
1:A:458:GLY:O	1:A:461:SER:HB3	1.96	0.65
1:A:361:LEU:HD23	1:A:534:ALA:HA	1.78	0.65
1:A:106:ARG:NH1	1:A:312:GLU:OE1	2.30	0.65
1:A:40:VAL:HG12	1:A:44:ILE:HD12	1.78	0.64
1:A:230:ILE:HD11	2:B:103:THR:HA	1.78	0.64
1:A:527:LYS:HA	1:A:568:GLN:HE22	1.62	0.64
2:B:418:ASP:HB3	2:B:421:LYS:HD2	1.77	0.64
1:A:449:HIS:HD1	1:A:459:TYR:HH	1.44	0.63
1:A:256:TRP:HD1	1:A:257:PHE:HD1	1.47	0.63
1:A:487:LYS:HA	1:A:515:TYR:OH	1.99	0.63
1:A:192:ASN:HB3	1:A:196:ARG:HH21	1.64	0.62
2:B:62:LYS:O	2:B:65:ASP:N	2.32	0.62
2:B:229:ILE:HG23	2:B:234:ARG:HB2	1.82	0.62
2:B:550:LEU:HD12	2:B:553:ILE:HD11	1.81	0.62
1:A:526:GLN:O	1:A:568:GLN:NE2	2.33	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:201:THR:OG1	2:B:259:PHE:O	2.18	0.62
2:B:70:PRO:O	2:B:72:ARG:N	2.32	0.61
2:B:527:GLU:OE2	2:B:549:ARG:NH1	2.33	0.61
1:A:204:VAL:HG21	2:B:439:ILE:HB	1.81	0.61
1:A:372:LYS:HA	1:A:540:LEU:HD12	1.82	0.61
1:A:89:ARG:HB2	1:A:120:VAL:HG11	1.83	0.60
1:A:184:ILE:HD13	1:A:229:ILE:HG12	1.83	0.60
2:B:72:ARG:NH1	2:B:74:ASP:OD2	2.35	0.60
2:B:398:VAL:HG22	2:B:514:ILE:HG21	1.84	0.60
1:A:452:ILE:HG21	1:A:459:TYR:CE1	2.36	0.60
2:B:219:ILE:HD11	2:B:242:PHE:HE2	1.67	0.60
1:A:376:MET:HE1	1:A:494:ASP:HB2	1.84	0.60
1:A:223:GLU:HB3	1:A:227:ARG:HH12	1.67	0.59
1:A:43:GLY:HA2	1:A:48:ASP:OD1	2.03	0.59
2:B:109:VAL:HG11	2:B:148:ASN:HB2	1.83	0.59
2:B:291:ILE:HB	2:B:295:THR:HG21	1.83	0.59
1:A:11:TYR:CZ	1:A:83:ASN:HB3	2.38	0.58
1:A:452:ILE:HG21	1:A:459:TYR:CD1	2.38	0.58
2:B:371:LEU:HD13	2:B:374:ILE:HG13	1.85	0.58
2:B:401:LEU:HD23	2:B:514:ILE:HD11	1.85	0.58
1:A:22:MET:SD	1:A:136:ARG:HB2	2.43	0.58
1:A:474:GLN:O	1:A:478:LEU:HB2	2.04	0.58
2:B:18:LEU:HD22	2:B:21:PRO:HB3	1.85	0.58
1:A:256:TRP:CZ3	2:B:77:PRO:HG3	2.38	0.57
1:A:132:ARG:HD3	1:A:133:ILE:HG23	1.87	0.57
1:A:436:ASP:O	1:A:440:VAL:HG23	2.04	0.57
2:B:143:ASP:OD2	2:B:329:ARG:HD2	2.05	0.56
1:A:256:TRP:HD1	1:A:257:PHE:CD1	2.23	0.56
1:A:166:ILE:HD12	1:A:283:MET:HE3	1.87	0.56
2:B:444:THR:O	2:B:448:ASN:ND2	2.37	0.56
1:A:245:PHE:O	1:A:249:MET:N	2.38	0.56
1:A:403:LYS:HG3	2:B:233:THR:HG21	1.87	0.56
2:B:229:ILE:HD13	2:B:238:GLU:HG3	1.86	0.56
2:B:78:ARG:O	2:B:82:ILE:HG13	2.05	0.56
1:A:256:TRP:HZ3	2:B:77:PRO:HG3	1.71	0.56
2:B:76:LEU:HB3	2:B:77:PRO:HD3	1.86	0.56
1:A:2:LYS:HG3	1:A:311:ASN:OD1	2.06	0.56
1:A:313:LYS:HE2	1:A:317:GLU:OE2	2.05	0.56
2:B:179:LEU:O	2:B:183:THR:HG23	2.06	0.55
2:B:176:ASN:OD1	2:B:178:ILE:HG12	2.06	0.55
1:A:258:GLY:O	1:A:262:VAL:HG12	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:509:LEU:HD23	1:A:512:LEU:HD12	1.89	0.54
2:B:59:LEU:HB3	2:B:83:LEU:HD11	1.89	0.54
2:B:584:TYR:CZ	2:B:588:THR:HG21	2.43	0.54
2:B:526:THR:O	2:B:530:ILE:HG23	2.08	0.53
1:A:357:LYS:O	1:A:360:SER:OG	2.25	0.53
1:A:364:VAL:HB	1:A:524:ILE:HG13	1.91	0.53
2:B:349:ARG:O	2:B:351:VAL:HG23	2.08	0.53
1:A:115:ARG:HD3	1:A:305:ARG:HB3	1.90	0.53
1:A:248:ASN:HB3	2:B:87:TYR:CD2	2.44	0.53
1:A:389:ARG:NH2	1:A:391:GLU:OE2	2.37	0.52
2:B:263:LEU:HB3	2:B:264:PRO:HD3	1.91	0.52
2:B:513:LEU:HD22	2:B:537:LEU:HD12	1.91	0.52
1:A:223:GLU:HB3	1:A:227:ARG:NH1	2.24	0.52
1:A:440:VAL:HG12	1:A:444:LYS:HE3	1.91	0.52
1:A:379:ILE:HG22	1:A:409:ILE:HD13	1.92	0.52
1:A:263:ARG:C	1:A:265:ASN:H	2.17	0.52
1:A:491:LEU:HD21	1:A:493:LEU:HD21	1.92	0.51
2:B:96:LEU:C	2:B:98:GLY:H	2.16	0.51
2:B:341:ASP:CG	2:B:424:ARG:H	2.19	0.51
1:A:340:ARG:HA	1:A:348:VAL:HG23	1.93	0.51
1:A:38:ARG:NE	1:A:55:THR:HG21	2.22	0.51
1:A:371:GLY:O	1:A:374:THR:OG1	2.20	0.51
2:B:357:PHE:HD2	2:B:360:VAL:HG21	1.75	0.51
1:A:206:ARG:HG2	2:B:428:ARG:HH12	1.75	0.51
1:A:482:ARG:HD3	2:B:232:PHE:CZ	2.46	0.51
1:A:198:ASN:HB3	2:B:120:LEU:HD21	1.93	0.50
2:B:248:SER:O	2:B:252:VAL:HG23	2.11	0.50
2:B:59:LEU:HD23	2:B:83:LEU:HD12	1.94	0.50
2:B:527:GLU:CD	2:B:549:ARG:HH12	2.20	0.50
1:A:117:THR:HG22	2:B:216:ASN:OD1	2.11	0.49
2:B:379:LYS:O	2:B:382:GLN:HB2	2.12	0.49
1:A:377:ASN:HB3	1:A:383:ILE:HD11	1.94	0.49
1:A:481:ALA:O	1:A:485:VAL:HG23	2.12	0.49
1:A:88:LEU:HD21	1:A:306:VAL:HG11	1.93	0.49
2:B:426:SER:O	2:B:429:SER:OG	2.26	0.49
1:A:238:PHE:O	1:A:241:PRO:HD2	2.13	0.49
2:B:236:GLU:O	2:B:240:GLU:HG3	2.13	0.49
2:B:433:ILE:HD11	2:B:435:LEU:HD21	1.94	0.49
1:A:202:VAL:O	1:A:206:ARG:HB2	2.11	0.49
1:A:420:SER:OG	1:A:465:ARG:HG2	2.12	0.48
2:B:66:VAL:HG11	2:B:79:TYR:CZ	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:476:GLN:O	1:A:480:ILE:HG13	2.14	0.48
1:A:263:ARG:HA	2:B:71:ARG:NH1	2.28	0.48
1:A:344:ASN:OD1	1:A:344:ASN:N	2.46	0.48
2:B:109:VAL:O	2:B:113:ARG:HG3	2.14	0.48
2:B:264:PRO:HB2	2:B:265:PRO:HD3	1.94	0.48
2:B:499:LEU:HG	2:B:530:ILE:HG22	1.95	0.48
1:A:452:ILE:O	1:A:458:GLY:HA2	2.13	0.48
2:B:449:LEU:HA	2:B:504:ARG:HB3	1.96	0.48
2:B:517:GLU:HB3	2:B:549:ARG:NH2	2.27	0.48
2:B:385:ALA:HB3	2:B:559:ILE:HG12	1.94	0.48
1:A:19:PRO:HB3	1:A:135:VAL:HG21	1.95	0.47
1:A:453:ILE:HD12	1:A:453:ILE:HA	1.67	0.47
2:B:48:VAL:HG23	2:B:93:LEU:HD13	1.96	0.47
2:B:153:ASN:OD1	2:B:157:GLN:HG3	2.13	0.47
1:A:202:VAL:HG11	2:B:128:PHE:HD2	1.80	0.47
1:A:450:ASP:O	1:A:453:ILE:HG22	2.14	0.47
1:A:512:LEU:O	1:A:516:THR:HG23	2.14	0.47
2:B:210:ARG:HD2	2:B:210:ARG:HA	1.60	0.47
1:A:44:ILE:HD11	2:B:283:GLY:HA2	1.95	0.47
2:B:123:VAL:HG22	2:B:124:PRO:HD2	1.96	0.47
1:A:155:LEU:HD23	1:A:267:MET:HE1	1.97	0.47
1:A:433:ASP:OD1	1:A:433:ASP:N	2.43	0.47
1:A:502:PRO:HG2	1:A:504:THR:HG23	1.96	0.47
2:B:67:VAL:HG21	2:B:76:LEU:HA	1.97	0.47
2:B:225:GLY:O	2:B:229:ILE:HG13	2.15	0.47
1:A:390:VAL:O	1:A:397:VAL:HG22	2.15	0.47
1:A:334:PHE:O	1:A:353:ASN:HA	2.15	0.46
1:A:440:VAL:HG13	1:A:449:HIS:CE1	2.49	0.46
2:B:436:GLN:HG3	2:B:518:ALA:HB2	1.97	0.46
1:A:376:MET:HB2	1:A:376:MET:HE3	1.63	0.46
2:B:582:PHE:O	2:B:586:LEU:HB2	2.15	0.46
1:A:252:ILE:HD12	1:A:252:ILE:HA	1.77	0.46
1:A:417:VAL:O	1:A:482:ARG:NH2	2.48	0.46
1:A:133:ILE:HA	1:A:136:ARG:HB3	1.97	0.46
1:A:496:SER:HA	1:A:497:THR:C	2.41	0.46
1:A:104:VAL:HG21	2:B:226:LEU:HD23	1.98	0.46
1:A:397:VAL:O	1:A:400:VAL:HG22	2.16	0.46
1:A:486:LYS:NZ	2:B:231:LEU:O	2.46	0.46
1:A:214:GLU:HA	1:A:217:ASN:HB2	1.98	0.46
1:A:502:PRO:HB3	2:B:390:THR:H	1.81	0.45
2:B:207:GLU:HG2	2:B:252:VAL:HG11	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:21:PHE:CD2	1:A:72:GLY:HA3	2.51	0.45
1:A:129:MET:HB2	1:A:129:MET:HE3	1.65	0.45
1:A:402:LEU:HD22	1:A:406:ARG:NH2	2.30	0.45
2:B:287:LEU:HD23	2:B:287:LEU:HA	1.80	0.45
1:A:449:HIS:ND1	1:A:459:TYR:OH	2.36	0.45
1:A:503:ILE:HD13	1:A:503:ILE:O	2.16	0.45
2:B:183:THR:HG22	2:B:278:ILE:HG12	1.98	0.45
2:B:282:GLY:C	2:B:296:ILE:HD11	2.42	0.45
1:A:16:VAL:C	1:A:19:PRO:HD2	2.42	0.45
1:A:389:ARG:HD2	1:A:396:ASP:OD2	2.17	0.45
2:B:236:GLU:H	2:B:236:GLU:HG2	1.48	0.45
1:A:330:GLY:O	1:A:520:THR:OG1	2.24	0.45
1:A:162:LEU:HB3	1:A:283:MET:HE2	1.98	0.44
1:A:209:ARG:NH1	2:B:429:SER:HA	2.33	0.44
2:B:66:VAL:HG11	2:B:79:TYR:CE1	2.53	0.44
2:B:342:ASP:HB3	2:B:344:ASP:OD1	2.18	0.44
2:B:394:LYS:HD2	2:B:546:ILE:HG23	2.00	0.44
1:A:67:ALA:HB2	2:B:269:MET:HG3	1.98	0.44
1:A:315:ALA:O	1:A:316:ILE:HD13	2.18	0.44
2:B:33:ARG:N	2:B:34:PRO:HD2	2.33	0.44
2:B:36:THR:O	2:B:40:ILE:HG12	2.18	0.44
1:A:111:SER:O	1:A:115:ARG:HG3	2.16	0.44
1:A:21:PHE:HD2	1:A:72:GLY:HA3	1.83	0.43
1:A:39:ILE:HD12	2:B:279:SER:HB3	2.00	0.43
1:A:107:PHE:HE2	1:A:308:GLU:HB3	1.82	0.43
1:A:396:ASP:HB3	1:A:399:THR:OG1	2.18	0.43
1:A:428:LYS:HE2	1:A:439:ILE:CD1	2.47	0.43
2:B:453:ASN:HA	2:B:454:PRO:HD2	1.89	0.43
2:B:218:ILE:HD13	2:B:241:LYS:HD2	2.00	0.43
2:B:352:ARG:NH1	2:B:540:GLY:O	2.52	0.43
2:B:524:THR:O	2:B:527:GLU:HB3	2.19	0.43
2:B:171:MET:HE3	2:B:171:MET:HB2	1.79	0.43
2:B:71:ARG:O	2:B:73:PHE:N	2.50	0.42
2:B:515:LEU:HD22	2:B:517:GLU:HG2	2.01	0.42
2:B:530:ILE:HD11	2:B:549:ARG:NH2	2.33	0.42
1:A:136:ARG:CZ	1:A:140:LEU:HD11	2.48	0.42
1:A:40:VAL:HG23	1:A:41:ASP:OD1	2.20	0.42
2:B:55:LEU:HD23	2:B:55:LEU:HA	1.86	0.42
2:B:288:LYS:HB3	2:B:290:ILE:HG13	2.00	0.42
1:A:210:ARG:HG3	1:A:213:TYR:HB3	2.01	0.42
1:A:499:SER:HA	1:A:500:VAL:HA	1.39	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:168:ALA:O	2:B:172:MET:HB2	2.19	0.42
2:B:537:LEU:O	2:B:541:LYS:NZ	2.34	0.42
2:B:553:ILE:O	2:B:559:ILE:HD11	2.19	0.42
1:A:112:LEU:HD12	1:A:112:LEU:HA	1.65	0.42
2:B:367:LYS:O	2:B:369:PRO:HD3	2.19	0.42
1:A:92:LEU:HD12	1:A:309:VAL:HG12	2.02	0.42
2:B:158:PHE:O	2:B:162:ILE:HG12	2.19	0.42
1:A:130:LEU:HA	1:A:134:VAL:HB	2.02	0.42
1:A:379:ILE:HD12	1:A:492:ILE:HD13	2.01	0.42
2:B:492:LEU:O	2:B:497:ARG:NH1	2.52	0.42
1:A:194:VAL:HG11	1:A:218:PHE:HA	2.02	0.42
1:A:36:LEU:HD13	2:B:279:SER:OG	2.19	0.42
2:B:267:MET:HE2	2:B:267:MET:HA	2.02	0.42
2:B:458:ASP:OD1	2:B:458:ASP:N	2.53	0.42
1:A:537:ILE:HB	1:A:554:LEU:CD1	2.49	0.41
2:B:185:SER:C	2:B:188:PRO:HD2	2.45	0.41
2:B:16:PRO:HB2	2:B:325:ALA:HB2	2.03	0.41
2:B:348:LEU:HD23	2:B:422:ILE:HG21	2.02	0.41
1:A:64:LEU:HD23	1:A:64:LEU:HA	1.86	0.41
2:B:30:GLY:HA2	2:B:33:ARG:HD2	2.03	0.41
2:B:70:PRO:C	2:B:72:ARG:H	2.28	0.41
2:B:136:ILE:HD13	2:B:136:ILE:HA	1.66	0.41
2:B:413:LEU:HB3	2:B:418:ASP:HA	2.01	0.41
1:A:11:TYR:CE2	1:A:83:ASN:HB3	2.55	0.41
2:B:212:LEU:O	2:B:212:LEU:HG	2.14	0.41
2:B:341:ASP:OD2	2:B:424:ARG:N	2.53	0.41
2:B:574:ASP:O	2:B:578:GLN:HB2	2.21	0.41
1:A:206:ARG:HG2	2:B:428:ARG:NH1	2.36	0.41
2:B:349:ARG:NH2	2:B:415:ASP:O	2.54	0.41
2:B:370:VAL:O	2:B:371:LEU:HD23	2.21	0.41
2:B:559:ILE:HG21	2:B:583:TYR:CE2	2.48	0.41
1:A:144:GLY:C	1:A:282:ILE:HD11	2.46	0.41
1:A:247:VAL:HG22	1:A:283:MET:HG3	2.03	0.41
1:A:12:TRP:O	1:A:16:VAL:HG13	2.20	0.40
1:A:457:GLU:OE2	1:A:457:GLU:N	2.54	0.40
2:B:15:LYS:HE3	2:B:318:ASN:OD1	2.21	0.40
2:B:291:ILE:HD12	2:B:295:THR:HG22	2.03	0.40
2:B:432:GLY:HA3	2:B:510:PRO:HG3	2.04	0.40
1:A:115:ARG:HA	1:A:119:ASP:OD2	2.22	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%)	517 (91%)	41 (7%)	12 (2%)	5	31
2	B	581/598 (97%)	525 (90%)	47 (8%)	9 (2%)	8	38
All	All	1151/1185 (97%)	1042 (90%)	88 (8%)	21 (2%)	7	35

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	498	CYS
1	A	503	ILE
1	A	558	SER
2	B	71	ARG
1	A	46	ARG
1	A	106	ARG
1	A	420	SER
2	B	63	THR
2	B	72	ARG
1	A	394	GLU
1	A	502	PRO
2	B	62	LYS
2	B	84	GLY
2	B	153	ASN
2	B	350	GLU
1	A	264	ASN
1	A	556	GLU
1	A	343	GLU
2	B	97	GLN
1	A	256	TRP
2	B	98	GLY

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%)	433 (87%)	63 (13%)	3	17
2	B	518/533 (97%)	469 (90%)	49 (10%)	7	28
All	All	1014/1037 (98%)	902 (89%)	112 (11%)	5	23

All (112) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	VAL
1	A	28	SER
1	A	34	THR
1	A	39	ILE
1	A	51	LEU
1	A	58	LEU
1	A	59	MET
1	A	91	ASP
1	A	92	LEU
1	A	101	ILE
1	A	107	PHE
1	A	116	LEU
1	A	122	GLN
1	A	126	LEU
1	A	183	LYS
1	A	202	VAL
1	A	205	VAL
1	A	206	ARG
1	A	230	ILE
1	A	235	LEU
1	A	249	MET
1	A	252	ILE
1	A	255	LEU
1	A	260	VAL
1	A	262	VAL
1	A	264	ASN
1	A	265	ASN

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Mol	Chain	Res	Type
1	A	269	ILE
1	A	271	SER
1	A	272	ILE
1	A	279	LEU
1	A	283	MET
1	A	287	MET
1	A	308	GLU
1	A	318	GLU
1	A	320	ASP
1	A	333	SER
1	A	344	ASN
1	A	357	LYS
1	A	361	LEU
1	A	373	SER
1	A	375	LEU
1	A	383	ILE
1	A	395	LEU
1	A	420	SER
1	A	422	THR
1	A	429	TRP
1	A	432	GLU
1	A	453	ILE
1	A	461	SER
1	A	478	LEU
1	A	482	ARG
1	A	492	ILE
1	A	493	LEU
1	A	497	THR
1	A	500	VAL
1	A	503	ILE
1	A	519	SER
1	A	523	ILE
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	54	VAL
2	B	71	ARG

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Mol	Chain	Res	Type
2	B	111	ARG
2	B	123	VAL
2	B	125	VAL
2	B	131	THR
2	B	136	ILE
2	B	141	ILE
2	B	156	ILE
2	B	171	MET
2	B	172	MET
2	B	178	ILE
2	B	180	SER
2	B	182	VAL
2	B	183	THR
2	B	209	GLN
2	B	215	LEU
2	B	219	ILE
2	B	227	THR
2	B	231	LEU
2	B	233	THR
2	B	236	GLU
2	B	244	ARG
2	B	269	MET
2	B	293	VAL
2	B	295	THR
2	B	340	LYS
2	B	341	ASP
2	B	342	ASP
2	B	348	LEU
2	B	371	LEU
2	B	375	THR
2	B	387	VAL
2	B	407	VAL
2	B	413	LEU
2	B	438	THR
2	B	443	THR
2	B	450	LYS
2	B	463	GLU
2	B	482	GLU
2	B	488	ASN
2	B	504	ARG
2	B	530	ILE
2	B	536	LYS

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Mol	Chain	Res	Type
2	B	537	LEU

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	82	GLN
1	A	277	ASN
1	A	336	ASN
1	A	541	HIS
2	B	148	ASN
2	B	382	GLN
2	B	476	HIS
2	B	494	GLN
2	B	498	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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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%)	-0.12	26 (4%) 39 26	55, 87, 136, 166	0
2	B	583/598 (97%)	0.22	46 (7%) 20 14	54, 123, 160, 174	0
All	All	1155/1185 (97%)	0.05	72 (6%) 28 18	54, 101, 153, 174	0

All (72) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	545	ILE	7.7
2	B	546	ILE	7.1
2	B	384	VAL	6.9
2	B	544	ILE	6.9
1	A	412	VAL	6.2
2	B	515	LEU	6.2
2	B	386	LEU	6.0
2	B	398	VAL	5.3
2	B	151	LEU	5.3
2	B	336	LEU	5.3
2	B	382	GLN	5.2
2	B	385	ALA	5.1
1	A	411	ALA	5.0
2	B	433	ILE	4.9
2	B	32	LEU	4.8
2	B	383	LYS	4.7
2	B	399	ASN	4.5
2	B	65	ASP	4.5
1	A	499	SER	4.4
1	A	494	ASP	4.3
2	B	432	GLY	4.1
1	A	5	ALA	4.1
1	A	500	VAL	4.0
1	A	415	GLU	3.8

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Mol	Chain	Res	Type	RSRZ
2	B	376	PHE	3.8
2	B	397	ILE	3.8
1	A	508	ILE	3.7
1	A	413	PRO	3.5
2	B	308	ARG	3.5
1	A	394	GLU	3.5
2	B	357	PHE	3.5
1	A	510	ASP	3.4
1	A	376	MET	3.3
1	A	503	ILE	3.2
2	B	557	ASP	3.2
1	A	501	ASP	3.2
2	B	514	ILE	3.1
2	B	335	ASP	3.1
2	B	303	SER	3.0
1	A	332	VAL	2.9
2	B	152	GLY	2.9
2	B	434	VAL	2.9
2	B	105	SER	2.9
2	B	400	LEU	2.8
1	A	200	LEU	2.7
2	B	547	ALA	2.7
2	B	378	ILE	2.7
1	A	264	ASN	2.7
2	B	11	PRO	2.6
2	B	513	LEU	2.6
1	A	212	GLU	2.6
2	B	205	PHE	2.6
2	B	393	GLY	2.6
1	A	447	GLN	2.5
1	A	214	GLU	2.5
2	B	115	GLU	2.5
1	A	481	ALA	2.5
1	A	6	ARG	2.4
2	B	560	ILE	2.4
2	B	543	SER	2.4
2	B	558	LEU	2.3
1	A	176	LYS	2.3
2	B	519	THR	2.3
2	B	10	GLY	2.3
2	B	396	THR	2.2
2	B	315	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	18	LEU	2.2
1	A	172	TRP	2.1
1	A	215	ASN	2.1
2	B	565	GLY	2.1
2	B	522	VAL	2.1
1	A	496	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 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.