



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 05:17 AM UTC

PDB ID : 4R1I / pdb_00004r1i
Title : Structure and Function of Neisseria gonorrhoeae MtrF Illuminates a Class of Antimetabolite Efflux Pumps
Authors : Su, C.-C.; Bolla, J.R.; Yu, E.W.
Deposited on : 2014-08-06
Resolution : 3.96 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

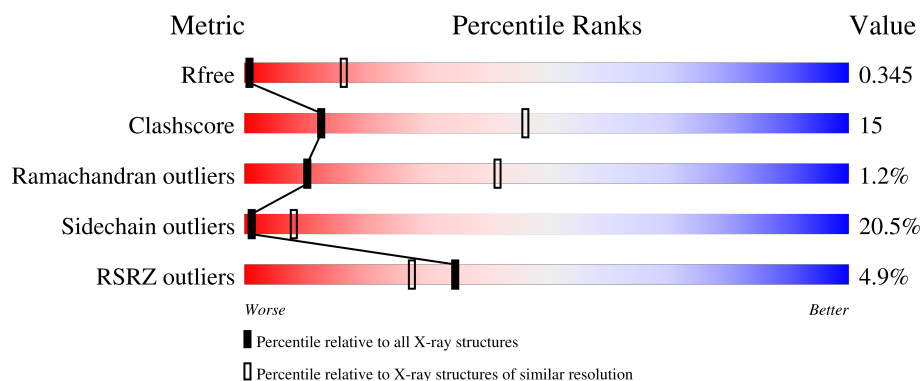
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.96 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	1046 (4.16-3.76)
Clashscore	190562	1019 (4.14-3.78)
Ramachandran outliers	187476	1031 (4.16-3.76)
Sidechain outliers	187428	1024 (4.16-3.76)
RSRZ outliers	180081	1046 (4.16-3.76)

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	522	4% 55% 35% 8% .
1	B	522	5% 54% 37% 6% .

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 7684 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.

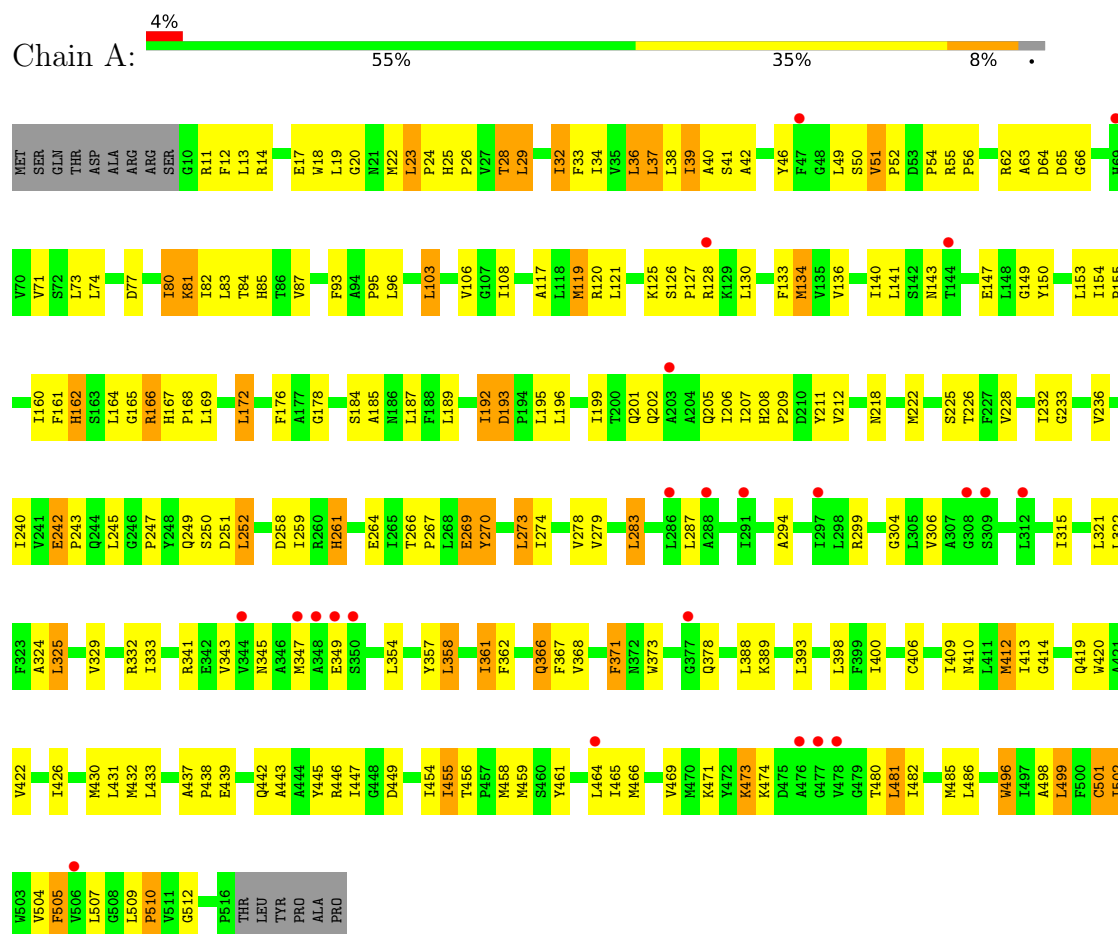
- Molecule 1 is a protein called Aminobenzoyl-glutamate transporter.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	507	Total	C	N	O	S	0	0	0
			3846	2566	609	654	17			
1	B	506	Total	C	N	O	S	0	0	0
			3838	2563	605	653	17			

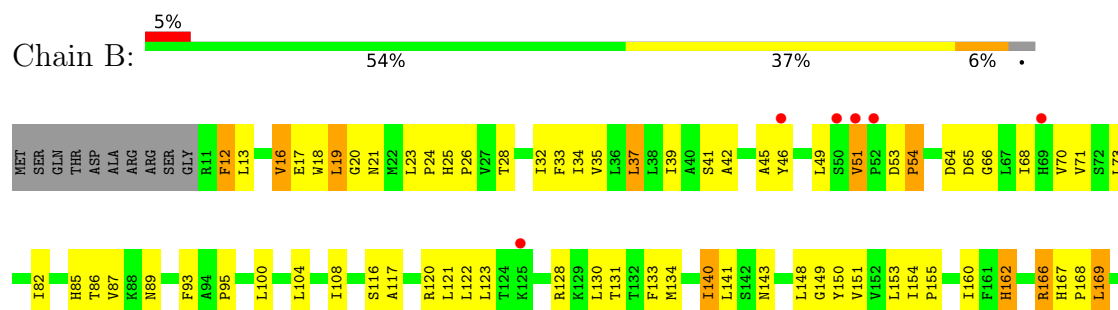
3 Residue-property plots

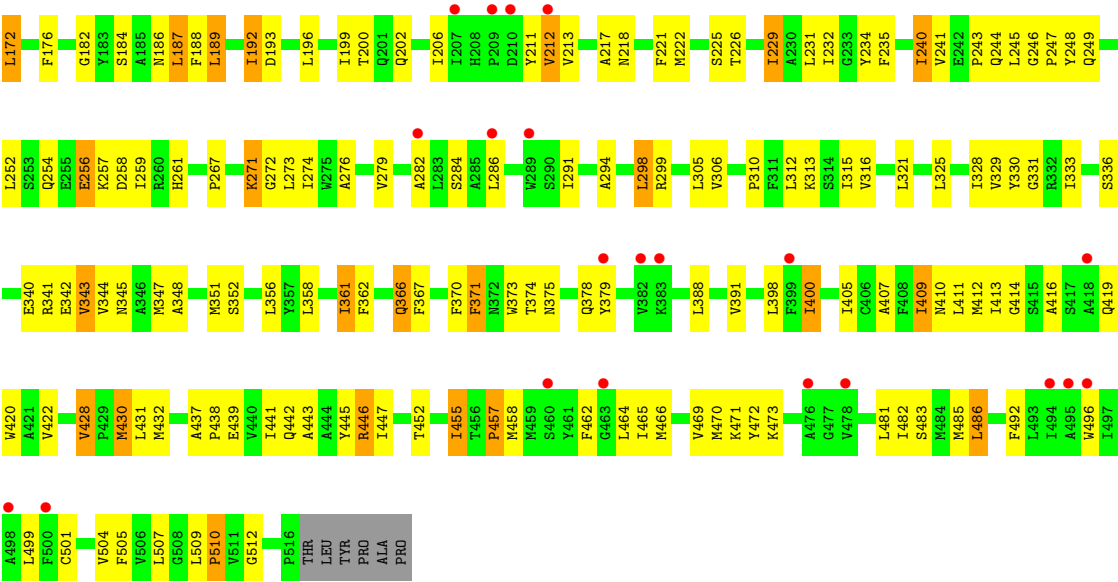
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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



• Molecule 1: Aminobenzoyl-glutamate transporter





4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α , β , γ	120.77Å 120.77Å 233.90Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.74 – 3.96 47.74 – 3.96	Depositor EDS
% Data completeness (in resolution range)	97.4 (47.74-3.96) 97.8 (47.74-3.96)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.82 (at 4.00Å)	Xtriage
Refinement program	PHENIX 1.8.1_1168	Depositor
R, R_{free}	0.311 , 0.338 0.315 , 0.345	Depositor DCC
R_{free} test set	870 reflections (4.56%)	wwPDB-VP
Wilson B-factor (Å ²)	202.7	Xtriage
Anisotropy	0.407	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.21 , 265.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.368 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	7684	wwPDB-VP
Average B, all atoms (Å ²)	163.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.24% 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	0.38	0/3945	0.91	6/5381 (0.1%)
1	B	0.35	0/3938	0.88	10/5374 (0.2%)
All	All	0.36	0/7883	0.89	16/10755 (0.1%)

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	208	HIS	CA-C-N	10.32	132.74	119.84
1	A	208	HIS	C-N-CA	10.32	132.74	119.84
1	B	400	ILE	N-CA-C	-7.66	105.22	111.81
1	B	51	VAL	CA-C-N	7.32	126.85	119.24
1	B	51	VAL	C-N-CA	7.32	126.85	119.24
1	B	428	VAL	CA-C-N	-6.78	112.80	119.64
1	B	428	VAL	C-N-CA	-6.78	112.80	119.64
1	A	242	GLU	CA-C-N	5.89	127.20	119.84
1	A	242	GLU	C-N-CA	5.89	127.20	119.84
1	A	189	LEU	CB-CA-C	-5.73	109.95	116.54
1	A	28	THR	N-CA-C	-5.58	105.73	112.54
1	B	151	VAL	N-CA-C	5.53	115.73	110.53
1	B	246	GLY	CA-C-N	5.22	125.51	119.92
1	B	246	GLY	C-N-CA	5.22	125.51	119.92
1	B	53	ASP	CA-C-N	5.17	126.30	119.84
1	B	53	ASP	C-N-CA	5.17	126.30	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	3846	0	3998	133	0
1	B	3838	0	3990	109	0
All	All	7684	0	7988	238	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 15.

All (238) 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:437:ALA:H	1:A:512:GLY:H	1.22	0.88
1:A:456:THR:HG23	1:A:482:ILE:HD12	1.60	0.82
1:A:393:LEU:HB3	1:A:398:LEU:HB2	1.65	0.79
1:B:131:THR:HA	1:B:134:MET:HB2	1.67	0.76
1:A:184:SER:HB2	1:A:446:ARG:HG2	1.69	0.75
1:B:414:GLY:HA2	1:B:419:GLN:HB2	1.66	0.75
1:B:16:VAL:HG21	1:B:455:ILE:HD11	1.71	0.72
1:B:430:MET:HG2	1:B:431:LEU:HD12	1.70	0.71
1:A:439:GLU:HG3	1:A:510:PRO:HG2	1.73	0.70
1:B:117:ALA:HA	1:B:120:ARG:HB2	1.74	0.69
1:B:410:ASN:HA	1:B:414:GLY:HA3	1.76	0.67
1:B:218:ASN:ND2	1:B:442:GLN:OE1	2.28	0.67
1:B:437:ALA:H	1:B:512:GLY:H	1.43	0.67
1:A:103:LEU:HD13	1:A:354:LEU:HD11	1.77	0.66
1:B:331:GLY:HA2	1:B:336:SER:HB2	1.77	0.66
1:B:176:PHE:HD1	1:B:485:MET:HE3	1.60	0.64
1:A:36:LEU:O	1:A:40:ALA:N	2.29	0.64
1:B:140:ILE:HG13	1:B:182:GLY:HA3	1.78	0.64
1:B:409:ILE:HG12	1:B:412:MET:HE2	1.79	0.64
1:B:196:LEU:HD13	1:B:446:ARG:HD2	1.81	0.62
1:A:22:MET:HE3	1:A:23:LEU:HG	1.81	0.62
1:A:24:PRO:HA	1:B:341:ARG:HD3	1.82	0.62
1:A:28:THR:O	1:A:32:ILE:HG23	1.98	0.62
1:A:127:PRO:HD2	1:A:130:LEU:HD12	1.81	0.62
1:A:279:VAL:HG21	1:A:329:VAL:HG21	1.82	0.62
1:A:228:VAL:HG21	1:A:499:LEU:HG	1.82	0.61
1:A:225:SER:OG	1:A:496:TRP:NE1	2.34	0.61
1:A:39:ILE:HA	1:A:42:ALA:HB3	1.83	0.61
1:A:117:ALA:HA	1:A:120:ARG:HB3	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:89:ASN:HD21	1:B:373:TRP:HH2	1.49	0.60
1:B:341:ARG:O	1:B:345:ASN:ND2	2.30	0.60
1:A:130:LEU:O	1:A:134:MET:N	2.33	0.60
1:A:466:MET:HA	1:A:469:VAL:HG12	1.82	0.59
1:A:93:PHE:CE1	1:A:202:GLN:HG2	2.37	0.59
1:B:184:SER:OG	1:B:446:ARG:O	2.09	0.59
1:B:21:ASN:ND2	1:B:458:MET:SD	2.76	0.59
1:A:501:CYS:HA	1:A:504:VAL:HG12	1.85	0.59
1:B:108:ILE:HD11	1:B:347:MET:HE2	1.85	0.58
1:A:160:ILE:HG23	1:A:164:LEU:HB2	1.85	0.58
1:A:341:ARG:O	1:A:345:ASN:ND2	2.26	0.58
1:A:56:PRO:HB2	1:A:63:ALA:HA	1.84	0.58
1:A:251:ASP:HB3	1:A:252:LEU:HD22	1.86	0.58
1:B:455:ILE:HD12	1:B:482:ILE:HD11	1.86	0.58
1:A:459:MET:HG2	1:A:461:TYR:H	1.69	0.57
1:B:370:PHE:O	1:B:374:THR:OG1	2.21	0.57
1:B:116:SER:HA	1:B:148:LEU:HD11	1.87	0.57
1:A:211:TYR:HE2	1:A:438:PRO:HD2	1.69	0.57
1:B:247:PRO:HB2	1:B:252:LEU:HD11	1.87	0.57
1:B:416:ALA:O	1:B:445:TYR:OH	2.22	0.57
1:A:266:THR:OG1	1:A:269:GLU:OE1	2.23	0.56
1:A:410:ASN:OD1	1:A:419:GLN:NE2	2.39	0.56
1:A:410:ASN:HA	1:A:414:GLY:HA3	1.86	0.56
1:A:169:LEU:HD22	1:A:473:LYS:HB2	1.88	0.56
1:A:172:LEU:HD11	1:A:481:LEU:HD11	1.86	0.56
1:B:100:LEU:HD22	1:B:351:MET:HE1	1.87	0.56
1:A:32:ILE:HG13	1:A:33:PHE:N	2.21	0.55
1:A:249:GLN:O	1:A:251:ASP:N	2.39	0.55
1:A:167:HIS:HB3	1:A:240:ILE:HD11	1.89	0.55
1:A:245:LEU:HB3	1:A:247:PRO:HD2	1.89	0.55
1:A:388:LEU:HD13	1:A:398:LEU:HD11	1.88	0.55
1:A:119:MET:SD	1:A:119:MET:N	2.79	0.55
1:B:169:LEU:HD23	1:B:472:TYR:HB2	1.90	0.54
1:B:291:ILE:HD11	1:B:306:VAL:HG13	1.90	0.54
1:A:409:ILE:HG13	1:A:412:MET:HE2	1.88	0.54
1:B:186:ASN:ND2	1:B:188:PHE:O	2.41	0.54
1:A:82:ILE:HD13	1:A:373:TRP:HZ2	1.71	0.54
1:A:117:ALA:HA	1:A:120:ARG:HD2	1.89	0.54
1:A:283:LEU:HD11	1:A:325:LEU:HB3	1.89	0.54
1:A:33:PHE:HB3	1:A:367:PHE:CE1	2.43	0.54
1:A:77:ASP:O	1:A:81:LYS:HE3	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:462:PHE:O	1:B:466:MET:N	2.36	0.54
1:A:36:LEU:HD12	1:A:40:ALA:HB2	1.90	0.54
1:A:33:PHE:HE2	1:A:422:VAL:HG13	1.72	0.53
1:B:19:LEU:HD23	1:B:411:LEU:HB2	1.89	0.53
1:B:367:PHE:O	1:B:371:PHE:HB2	2.08	0.53
1:A:120:ARG:NH2	1:A:269:GLU:OE2	2.42	0.53
1:A:420:TRP:HB2	1:A:445:TYR:CZ	2.43	0.53
1:A:247:PRO:HG3	1:A:473:LYS:HD3	1.90	0.52
1:B:256:GLU:HG3	1:B:471:LYS:HD2	1.89	0.52
1:B:252:LEU:HB3	1:B:472:TYR:HA	1.91	0.52
1:A:93:PHE:HE2	1:A:361:ILE:HG12	1.75	0.52
1:A:393:LEU:HD13	1:A:398:LEU:HD13	1.92	0.52
1:A:136:VAL:HG21	1:A:233:GLY:HA3	1.90	0.52
1:A:161:PHE:HA	1:A:165:GLY:HA3	1.91	0.51
1:A:432:MET:HG3	1:A:438:PRO:HD3	1.91	0.51
1:A:26:PRO:HA	1:A:29:LEU:HB2	1.91	0.51
1:A:367:PHE:O	1:A:371:PHE:HB2	2.10	0.51
1:A:93:PHE:CE2	1:A:361:ILE:HG12	2.45	0.51
1:B:388:LEU:HD13	1:B:398:LEU:HD11	1.92	0.51
1:A:357:TYR:CZ	1:A:361:ILE:HD12	2.46	0.50
1:A:406:CYS:HA	1:A:409:ILE:HG22	1.93	0.50
1:B:20:GLY:HA2	1:B:412:MET:HA	1.93	0.50
1:B:172:LEU:HD11	1:B:465:ILE:HG23	1.92	0.50
1:A:136:VAL:O	1:A:140:ILE:HG12	2.11	0.50
1:B:45:ALA:HB2	1:B:70:VAL:HG23	1.94	0.50
1:B:33:PHE:HE2	1:B:422:VAL:HG13	1.76	0.50
1:B:184:SER:HB2	1:B:446:ARG:HG2	1.94	0.49
1:B:272:GLY:O	1:B:276:ALA:N	2.45	0.49
1:A:176:PHE:CD2	1:A:485:MET:HE3	2.46	0.49
1:B:420:TRP:HB2	1:B:445:TYR:CZ	2.47	0.49
1:A:458:MET:HA	1:A:458:MET:HE3	1.94	0.49
1:B:501:CYS:HA	1:B:504:VAL:HG12	1.95	0.49
1:A:108:ILE:HD11	1:A:347:MET:HE2	1.95	0.49
1:A:267:PRO:HA	1:A:270:TYR:HB2	1.94	0.49
1:B:254:GLN:HA	1:B:257:LYS:HE2	1.94	0.49
1:B:348:ALA:O	1:B:352:SER:OG	2.27	0.49
1:A:95:PRO:HG2	1:A:361:ILE:HD11	1.96	0.48
1:A:283:LEU:HB3	1:A:322:LEU:HD23	1.95	0.48
1:A:23:LEU:HD13	1:A:413:ILE:HD13	1.94	0.48
1:A:37:LEU:HA	1:A:40:ALA:HB3	1.94	0.48
1:A:108:ILE:HD12	1:A:324:ALA:HB1	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:140:ILE:HG22	1:B:141:LEU:HD12	1.96	0.48
1:A:167:HIS:CD2	1:A:168:PRO:HD2	2.49	0.48
1:B:240:ILE:HG23	1:B:241:VAL:HG23	1.96	0.48
1:A:455:ILE:HG13	1:A:482:ILE:HD11	1.95	0.48
1:B:331:GLY:O	1:B:336:SER:N	2.47	0.48
1:B:375:ASN:ND2	1:B:378:GLN:OE1	2.47	0.48
1:B:42:ALA:HB2	1:B:73:LEU:HG	1.96	0.48
1:A:162:HIS:CE1	1:A:168:PRO:HG3	2.49	0.48
1:B:85:HIS:O	1:B:89:ASN:ND2	2.47	0.47
1:B:150:TYR:HB3	1:B:464:LEU:HD23	1.96	0.47
1:B:189:LEU:HD22	1:B:189:LEU:H	1.78	0.47
1:B:93:PHE:CE1	1:B:202:GLN:HG2	2.49	0.47
1:A:22:MET:HE2	1:A:22:MET:HB3	1.76	0.47
1:B:167:HIS:ND1	1:B:168:PRO:HD2	2.28	0.47
1:B:37:LEU:HD11	1:B:371:PHE:CD1	2.49	0.47
1:B:192:ILE:HD13	1:B:446:ARG:HH22	1.80	0.47
1:B:466:MET:O	1:B:470:MET:HG2	2.14	0.47
1:A:196:LEU:HD13	1:A:446:ARG:HG3	1.97	0.46
1:B:122:LEU:HD12	1:B:123:LEU:N	2.30	0.46
1:A:33:PHE:CE2	1:A:422:VAL:HG13	2.51	0.46
1:A:343:VAL:O	1:A:347:MET:HG3	2.15	0.46
1:B:162:HIS:CE1	1:B:249:GLN:HA	2.51	0.46
1:A:54:PRO:O	1:A:56:PRO:HD3	2.15	0.46
1:B:222:MET:HE3	1:B:446:ARG:HB3	1.98	0.46
1:B:343:VAL:O	1:B:347:MET:HG3	2.16	0.46
1:A:185:ALA:HA	1:A:222:MET:HB3	1.97	0.46
1:A:443:ALA:O	1:A:447:ILE:HG12	2.16	0.46
1:B:298:LEU:HD21	1:B:310:PRO:HB2	1.97	0.46
1:A:160:ILE:O	1:A:164:LEU:N	2.44	0.46
1:A:154:ILE:HB	1:A:155:PRO:HD3	1.98	0.46
1:A:258:ASP:O	1:A:261:HIS:ND1	2.42	0.46
1:B:12:PHE:HZ	1:B:486:LEU:HD21	1.81	0.46
1:B:33:PHE:HB3	1:B:367:PHE:CE1	2.51	0.46
1:B:362:PHE:O	1:B:366:GLN:HB2	2.16	0.46
1:A:13:LEU:HD21	1:A:482:ILE:HD13	1.98	0.46
1:A:37:LEU:HA	1:A:37:LEU:HD23	1.72	0.46
1:A:498:ALA:O	1:A:502:ILE:HD12	2.15	0.46
1:A:150:TYR:HE1	1:A:461:TYR:HB3	1.81	0.45
1:A:166:ARG:N	1:A:166:ARG:HD2	2.31	0.45
1:A:358:LEU:O	1:A:362:PHE:N	2.49	0.45
1:B:82:ILE:O	1:B:86:THR:OG1	2.35	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:154:ILE:HB	1:B:155:PRO:HD3	1.98	0.45
1:A:64:ASP:C	1:A:66:GLY:H	2.25	0.45
1:A:192:ILE:HA	1:A:195:LEU:HB3	1.98	0.45
1:B:54:PRO:HD3	1:B:66:GLY:HA2	1.99	0.45
1:A:140:ILE:HG21	1:A:226:THR:HG23	1.99	0.45
1:B:28:THR:O	1:B:32:ILE:HG23	2.17	0.45
1:B:247:PRO:HG3	1:B:473:LYS:HG2	1.98	0.45
1:B:294:ALA:HA	1:B:299:ARG:NH2	2.31	0.45
1:A:25:HIS:HD2	1:B:344:VAL:HG11	1.83	0.44
1:A:193:ASP:OD1	1:A:446:ARG:NH1	2.48	0.44
1:A:150:TYR:CE1	1:A:461:TYR:HB3	2.53	0.44
1:A:357:TYR:O	1:A:361:ILE:HB	2.17	0.44
1:B:432:MET:HE2	1:B:432:MET:HB3	1.91	0.44
1:B:457:PRO:HB2	1:B:458:MET:H	1.46	0.44
1:A:41:SER:HB3	1:A:71:VAL:O	2.18	0.44
1:A:149:GLY:O	1:A:154:ILE:HG12	2.18	0.44
1:B:149:GLY:O	1:B:154:ILE:HG12	2.17	0.44
1:B:221:PHE:CZ	1:B:447:ILE:HD11	2.53	0.44
1:A:77:ASP:OD1	1:A:77:ASP:N	2.51	0.44
1:B:229:ILE:HG23	1:B:492:PHE:CE2	2.53	0.44
1:A:341:ARG:HD3	1:B:24:PRO:HA	1.99	0.44
1:B:509:LEU:HB2	1:B:510:PRO:HD3	2.00	0.44
1:A:206:ILE:HG22	1:A:378:GLN:HG2	2.00	0.44
1:B:211:TYR:HD1	1:B:212:VAL:H	1.66	0.44
1:A:176:PHE:CE1	1:A:465:ILE:HG13	2.52	0.43
1:B:33:PHE:O	1:B:37:LEU:HB2	2.18	0.43
1:B:34:ILE:HB	1:B:370:PHE:CD2	2.53	0.43
1:B:93:PHE:CD1	1:B:202:GLN:HG2	2.53	0.43
1:A:126:SER:HA	1:A:127:PRO:HD3	1.87	0.43
1:A:358:LEU:HA	1:A:358:LEU:HD12	1.75	0.43
1:B:432:MET:HG2	1:B:438:PRO:HD3	2.00	0.43
1:A:471:LYS:HE3	1:A:471:LYS:HB3	1.81	0.43
1:A:49:LEU:HD22	1:A:50:SER:H	1.84	0.43
1:A:362:PHE:O	1:A:366:GLN:HB2	2.18	0.43
1:A:505:PHE:HD1	1:A:505:PHE:HA	1.67	0.43
1:B:361:ILE:HD13	1:B:361:ILE:HA	1.86	0.43
1:A:140:ILE:HD13	1:A:178:GLY:O	2.19	0.43
1:B:26:PRO:HD3	1:B:413:ILE:HD11	2.00	0.43
1:B:93:PHE:CD2	1:B:95:PRO:HD2	2.54	0.43
1:A:207:ILE:HG21	1:A:433:LEU:HD21	2.00	0.43
1:A:406:CYS:O	1:A:410:ASN:HB2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:141:LEU:HD11	1:B:187:LEU:HD13	2.01	0.43
1:A:51:VAL:HA	1:A:52:PRO:HD3	1.73	0.42
1:B:23:LEU:HA	1:B:24:PRO:HD3	1.90	0.42
1:A:81:LYS:O	1:A:85:HIS:HB2	2.19	0.42
1:A:400:ILE:HD11	1:A:501:CYS:SG	2.59	0.42
1:A:287:LEU:HD12	1:A:322:LEU:HD11	2.02	0.42
1:B:130:LEU:HD12	1:B:130:LEU:HA	1.87	0.42
1:B:25:HIS:CG	1:B:26:PRO:HD2	2.54	0.42
1:B:187:LEU:HD12	1:B:226:THR:HG21	2.01	0.42
1:B:407:ALA:O	1:B:452:THR:HG21	2.20	0.42
1:A:201:GLN:O	1:A:205:GLN:HG2	2.20	0.42
1:A:269:GLU:O	1:A:273:LEU:HB2	2.20	0.42
1:A:413:ILE:HD12	1:A:413:ILE:HA	1.93	0.42
1:A:34:ILE:O	1:A:38:LEU:HG	2.19	0.42
1:B:166:ARG:HE	1:B:166:ARG:N	2.18	0.42
1:B:282:ALA:O	1:B:286:LEU:HG	2.19	0.42
1:B:41:SER:HB3	1:B:71:VAL:O	2.20	0.41
1:B:267:PRO:O	1:B:271:LYS:HB2	2.20	0.41
1:A:25:HIS:HB2	1:B:341:ARG:HG2	2.01	0.41
1:A:393:LEU:HD22	1:A:398:LEU:HA	2.03	0.41
1:B:276:ALA:HB2	1:B:330:TYR:HB2	2.02	0.41
1:A:202:GLN:O	1:A:368:VAL:HG21	2.20	0.41
1:A:228:VAL:O	1:A:232:ILE:HG13	2.20	0.41
1:A:454:ILE:HG22	1:A:485:MET:HB3	2.02	0.41
1:B:49:LEU:HD11	1:B:379:TYR:CE1	2.55	0.41
1:B:206:ILE:HG22	1:B:378:GLN:HG2	2.00	0.41
1:A:430:MET:HG3	1:A:431:LEU:HD12	2.02	0.41
1:A:20:GLY:HA2	1:A:412:MET:HA	2.02	0.41
1:A:141:LEU:HD21	1:A:187:LEU:HD12	2.01	0.41
1:A:166:ARG:HD2	1:A:166:ARG:H	1.86	0.41
1:B:221:PHE:HD2	1:B:443:ALA:HB1	1.85	0.41
1:A:420:TRP:HB2	1:A:445:TYR:OH	2.21	0.41
1:B:225:SER:OG	1:B:496:TRP:NE1	2.54	0.41
1:B:232:ILE:HB	1:B:492:PHE:CE2	2.56	0.41
1:A:80:ILE:O	1:A:84:THR:HG23	2.21	0.41
1:B:413:ILE:HD12	1:B:413:ILE:HA	1.88	0.41
1:A:245:LEU:HD12	1:A:245:LEU:HA	1.89	0.40
1:A:169:LEU:HD12	1:A:169:LEU:HA	1.85	0.40
1:B:93:PHE:HD2	1:B:361:ILE:HG23	1.87	0.40
1:B:420:TRP:HA	1:B:420:TRP:CE3	2.56	0.40
1:A:55:ARG:HH11	1:A:389:LYS:NZ	2.19	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:200:THR:HG22	1:B:213:VAL:HG21	2.03	0.40
1:A:64:ASP:HB3	1:A:65:ASP:H	1.56	0.40
1:A:294:ALA:HA	1:A:299:ARG:CZ	2.52	0.40
1:B:143:ASN:OD1	1:B:186:ASN:HB3	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	505/522 (97%)	453 (90%)	46 (9%)	6 (1%)	10	42
1	B	504/522 (97%)	447 (89%)	51 (10%)	6 (1%)	10	42
All	All	1009/1044 (97%)	900 (89%)	97 (10%)	12 (1%)	10	42

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	209	PRO
1	A	243	PRO
1	B	217	ALA
1	A	250	SER
1	A	510	PRO
1	B	187	LEU
1	B	457	PRO
1	B	510	PRO
1	A	264	GLU
1	B	54	PRO
1	B	243	PRO
1	A	304	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	403/418 (96%)	322 (80%)	81 (20%)	1	9
1	B	403/418 (96%)	319 (79%)	84 (21%)	1	7
All	All	806/836 (96%)	641 (80%)	165 (20%)	1	8

All (165) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	ARG
1	A	12	PHE
1	A	14	ARG
1	A	17	GLU
1	A	18	TRP
1	A	19	LEU
1	A	23	LEU
1	A	29	LEU
1	A	32	ILE
1	A	36	LEU
1	A	37	LEU
1	A	39	ILE
1	A	46	TYR
1	A	51	VAL
1	A	62	ARG
1	A	73	LEU
1	A	74	LEU
1	A	80	ILE
1	A	81	LYS
1	A	83	LEU
1	A	87	VAL
1	A	96	LEU
1	A	103	LEU
1	A	106	VAL
1	A	119	MET
1	A	121	LEU
1	A	125	LYS

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Mol	Chain	Res	Type
1	A	128	ARG
1	A	133	PHE
1	A	134	MET
1	A	143	ASN
1	A	147	GLU
1	A	153	LEU
1	A	162	HIS
1	A	166	ARG
1	A	172	LEU
1	A	192	ILE
1	A	193	ASP
1	A	199	ILE
1	A	212	VAL
1	A	218	ASN
1	A	236	VAL
1	A	242	GLU
1	A	252	LEU
1	A	259	ILE
1	A	261	HIS
1	A	269	GLU
1	A	270	TYR
1	A	273	LEU
1	A	274	ILE
1	A	278	VAL
1	A	283	LEU
1	A	306	VAL
1	A	315	ILE
1	A	321	LEU
1	A	325	LEU
1	A	332	ARG
1	A	333	ILE
1	A	349	GLU
1	A	358	LEU
1	A	361	ILE
1	A	366	GLN
1	A	371	PHE
1	A	412	MET
1	A	426	ILE
1	A	442	GLN
1	A	449	ASP
1	A	455	ILE
1	A	464	LEU

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Mol	Chain	Res	Type
1	A	473	LYS
1	A	474	LYS
1	A	480	THR
1	A	481	LEU
1	A	486	LEU
1	A	496	TRP
1	A	499	LEU
1	A	501	CYS
1	A	502	ILE
1	A	505	PHE
1	A	507	LEU
1	A	509	LEU
1	B	12	PHE
1	B	13	LEU
1	B	16	VAL
1	B	17	GLU
1	B	18	TRP
1	B	19	LEU
1	B	35	VAL
1	B	37	LEU
1	B	39	ILE
1	B	46	TYR
1	B	51	VAL
1	B	64	ASP
1	B	65	ASP
1	B	68	ILE
1	B	87	VAL
1	B	104	LEU
1	B	121	LEU
1	B	128	ARG
1	B	133	PHE
1	B	140	ILE
1	B	153	LEU
1	B	160	ILE
1	B	162	HIS
1	B	166	ARG
1	B	169	LEU
1	B	172	LEU
1	B	189	LEU
1	B	192	ILE
1	B	193	ASP
1	B	199	ILE

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Mol	Chain	Res	Type
1	B	212	VAL
1	B	229	ILE
1	B	231	LEU
1	B	234	TYR
1	B	235	PHE
1	B	240	ILE
1	B	244	GLN
1	B	245	LEU
1	B	248	TYR
1	B	256	GLU
1	B	258	ASP
1	B	259	ILE
1	B	261	HIS
1	B	271	LYS
1	B	273	LEU
1	B	274	ILE
1	B	279	VAL
1	B	284	SER
1	B	298	LEU
1	B	305	LEU
1	B	312	LEU
1	B	313	LYS
1	B	315	ILE
1	B	316	VAL
1	B	321	LEU
1	B	325	LEU
1	B	328	ILE
1	B	329	VAL
1	B	333	ILE
1	B	340	GLU
1	B	342	GLU
1	B	343	VAL
1	B	356	LEU
1	B	358	LEU
1	B	361	ILE
1	B	366	GLN
1	B	371	PHE
1	B	391	VAL
1	B	400	ILE
1	B	405	ILE
1	B	409	ILE
1	B	428	VAL

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Mol	Chain	Res	Type
1	B	430	MET
1	B	439	GLU
1	B	441	ILE
1	B	446	ARG
1	B	455	ILE
1	B	469	VAL
1	B	481	LEU
1	B	483	SER
1	B	486	LEU
1	B	499	LEU
1	B	505	PHE
1	B	507	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	25	HIS
1	A	162	HIS
1	A	167	HIS
1	A	410	ASN
1	A	419	GLN
1	B	89	ASN
1	B	375	ASN

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	507/522 (97%)	-0.11	23 (4%) 38 29	54, 157, 245, 345	0
1	B	506/522 (96%)	-0.15	27 (5%) 32 26	44, 153, 257, 321	0
All	All	1013/1044 (97%)	-0.13	50 (4%) 35 28	44, 155, 254, 345	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	349	GLU	5.0
1	A	477	GLY	4.7
1	A	288	ALA	4.6
1	B	383	LYS	4.5
1	B	210	ASP	4.3
1	A	476	ALA	4.1
1	B	476	ALA	4.1
1	A	348	ALA	4.0
1	A	347	MET	4.0
1	B	50	SER	3.8
1	B	379	TYR	3.6
1	A	128	ARG	3.6
1	B	69	HIS	3.5
1	B	463	GLY	3.5
1	A	297	ILE	3.4
1	A	291	ILE	3.3
1	A	464	LEU	3.1
1	B	286	LEU	3.1
1	B	51	VAL	2.9
1	A	350	SER	2.9
1	B	494	ILE	2.8
1	B	498	ALA	2.8
1	B	399	PHE	2.8
1	A	69	HIS	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	460	SER	2.7
1	A	309	SER	2.6
1	A	308	GLY	2.6
1	A	478	VAL	2.5
1	B	478	VAL	2.5
1	B	382	VAL	2.5
1	B	282	ALA	2.5
1	A	312	LEU	2.4
1	A	286	LEU	2.4
1	A	377	GLY	2.4
1	B	52	PRO	2.4
1	A	144	THR	2.4
1	B	496	TRP	2.4
1	B	500	PHE	2.3
1	B	207	ILE	2.3
1	B	212	VAL	2.3
1	B	289	TRP	2.2
1	B	418	ALA	2.2
1	A	47	PHE	2.2
1	B	125	LYS	2.2
1	B	46	TYR	2.2
1	B	495	ALA	2.1
1	B	209	PRO	2.1
1	A	344	VAL	2.0
1	A	506	VAL	2.0
1	A	203	ALA	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.