



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 29, 2021 – 04:08 pm GMT

PDB ID : 7P9M
Title : Phage resistance protein
Authors : Picton, D.M.; Luyten, Y.; Morgan, R.D.; Nelson, A.; Smith, D.L.; Dryden, D.T.F.; Hinton, J.C.D.; Blower, T.R.
Deposited on : 2021-07-27
Resolution : 2.85 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.4 (270009), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.23.2
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0267
CCP4 : 7.1.010 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.23.2

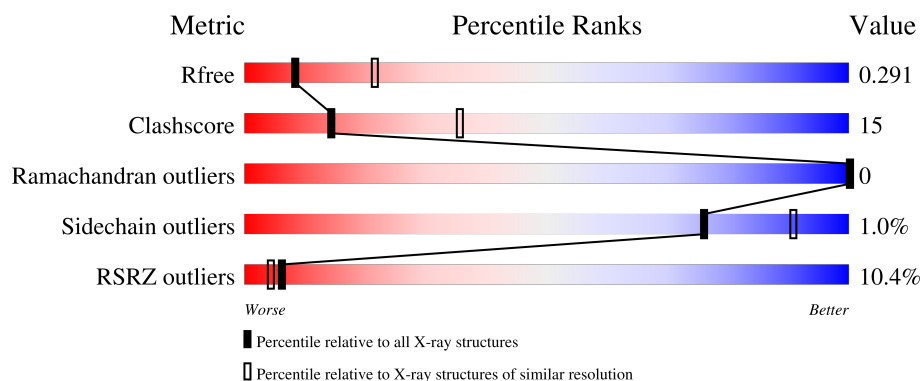
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.85 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	3168 (2.90-2.82)
Clashscore	141614	3438 (2.90-2.82)
Ramachandran outliers	138981	3348 (2.90-2.82)
Sidechain outliers	138945	3351 (2.90-2.82)
RSRZ outliers	127900	3103 (2.90-2.82)

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	<div> <div>9%</div> <div>72%</div> <div>24%</div> <div>.</div> </div>
1	B	587	<div> <div>11%</div> <div>73%</div> <div>21%</div> <div>5%</div> </div>

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 9152 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 DUF262 domain-containing protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	563	Total	C	N	O	S	0	0	0
			4590	2913	804	857	16			
1	B	557	Total	C	N	O	S	0	0	0
			4546	2896	793	842	15			

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		

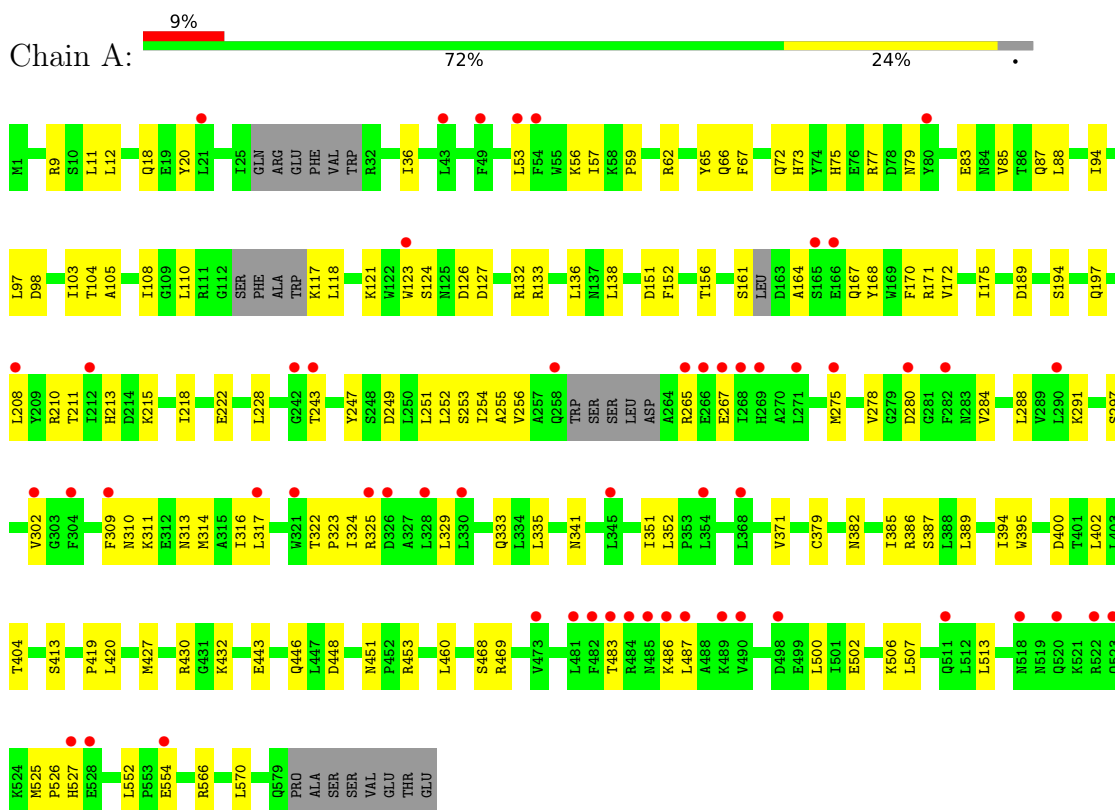
- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Cl	0	0
			1	1		

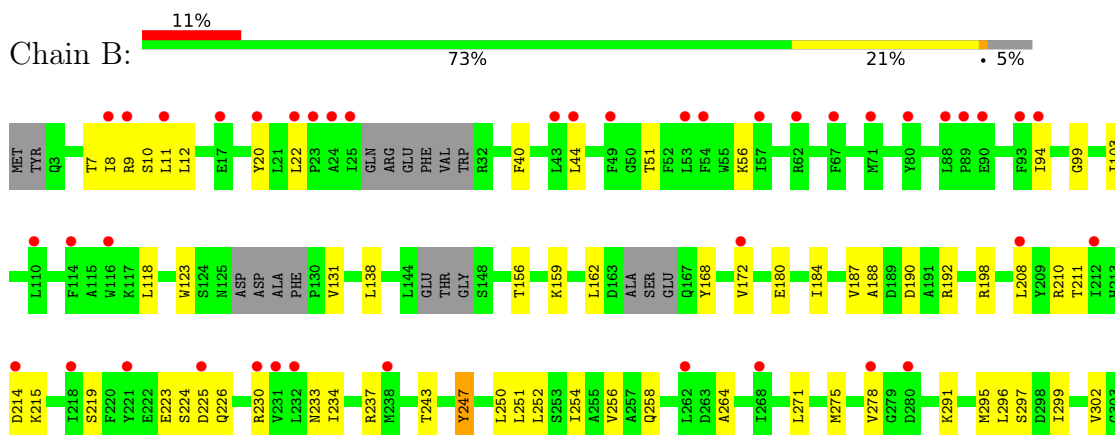
3 Residue-property plots

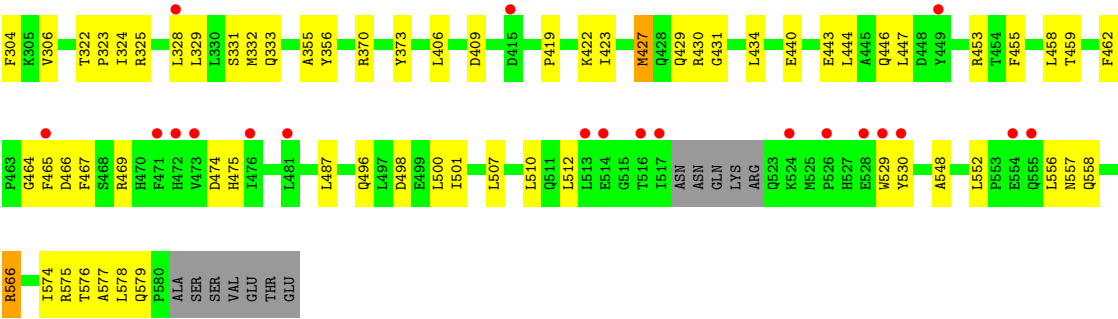
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: DUF262 domain-containing protein



• Molecule 1: DUF262 domain-containing protein





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	196.88Å 68.37Å 129.59Å 90.00° 94.45° 90.00°	Depositor
Resolution (Å)	98.14 – 2.85 98.14 – 2.85	Depositor Estimate
% Data completeness (in resolution range)	93.4 (98.14-2.85) 93.4 (98.14-2.85)	Depositor Estimate
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.96 (at 2.86Å)	Xtriage
Refinement program	REFMAC CCP4 Program Suite v7.1.015, PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.266 , 0.278 0.280 , 0.291	Depositor Depositor
R_{free} test set	1784 reflections (4.70%)	wwPDB
Wilson B-factor (Å ²)	98.1	Xtriage
Anisotropy	0.053	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	(Not available) , (Not available)	Estimate
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	Estimate
Total number of atoms	9152	wwPDB
Average B, all atoms (Å ²)	97.0	wwPDB

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.83% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, CL

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	0.60	0/4684	0.80	0/6323
1	B	0.61	0/4643	0.83	0/6271
All	All	0.60	0/9327	0.82	0/12594

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4590	0	4527	141	0
1	B	4546	0	4488	148	0
2	A	5	0	0	0	0
2	B	10	0	0	0	0
3	B	1	0	0	0	0
All	All	9152	0	9015	281	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 (281) 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:B:464:GLY:O	1:B:465:PHE:CD1	1.92	1.21
1:B:188:ALA:CA	1:B:198:ARG:HD2	1.72	1.18
1:B:529:TRP:HZ3	1:B:530:TYR:CE1	1.60	1.18
1:B:188:ALA:HA	1:B:198:ARG:CD	1.73	1.16
1:A:57:ILE:HD13	1:A:67:PHE:CZ	1.87	1.10
1:A:9:ARG:HD3	1:A:213:HIS:ND1	1.69	1.08
1:B:529:TRP:CZ3	1:B:530:TYR:CE1	2.45	1.04
1:B:322:THR:OG1	1:B:323:PRO:HD3	1.59	1.03
1:A:117:LYS:HG3	1:A:118:LEU:H	1.28	0.98
1:B:11:LEU:HD21	1:B:103:ILE:HD12	1.42	0.98
1:A:322:THR:OG1	1:A:323:PRO:HD3	1.63	0.98
1:B:464:GLY:O	1:B:465:PHE:HD1	1.47	0.97
1:A:310:ASN:OD1	1:A:313:ASN:HB2	1.66	0.95
1:B:409:ASP:OD2	1:B:422:LYS:HG3	1.64	0.95
1:A:256:VAL:HG11	1:A:311:LYS:HA	1.55	0.88
1:A:97:LEU:HD22	1:B:250:LEU:HD11	1.55	0.88
1:A:400:ASP:O	1:A:404:THR:HG23	1.73	0.88
1:A:448:ASP:OD1	1:A:506:LYS:HD3	1.74	0.87
1:A:85:VAL:CG1	1:A:88:LEU:HD11	2.06	0.85
1:A:123:TRP:CE3	1:A:502:GLU:OE2	2.29	0.85
1:B:11:LEU:HD12	1:B:20:TYR:CD2	2.13	0.84
1:B:8:ILE:O	1:B:12:LEU:HD13	1.78	0.83
1:B:465:PHE:HE2	1:B:512:LEU:HD12	1.43	0.83
1:B:370:ARG:NH2	1:B:373:TYR:HE2	1.77	0.83
1:B:574:ILE:O	1:B:578:LEU:HD13	1.79	0.83
1:B:465:PHE:HE2	1:B:512:LEU:CD1	1.92	0.81
1:B:465:PHE:CE2	1:B:512:LEU:HD13	2.16	0.81
1:B:291:LYS:HE2	1:B:304:PHE:HB2	1.62	0.81
1:B:474:ASP:OD1	1:B:475:HIS:N	2.13	0.81
1:B:507:LEU:HA	1:B:510:LEU:HD12	1.62	0.80
1:B:370:ARG:CZ	1:B:373:TYR:HE2	1.94	0.80
1:B:211:THR:HA	1:B:215:LYS:HG3	1.63	0.79
1:B:230:ARG:NH1	1:B:234:ILE:HD11	1.96	0.79
1:B:465:PHE:CE2	1:B:512:LEU:CD1	2.65	0.79
1:A:9:ARG:HD3	1:A:213:HIS:CE1	2.18	0.78
1:A:210:ARG:O	1:A:215:LYS:HG3	1.84	0.78
1:A:117:LYS:HG3	1:A:118:LEU:N	1.97	0.77
1:A:164:ALA:HB3	1:A:167:GLN:HB2	1.66	0.77
1:B:210:ARG:O	1:B:215:LYS:HE2	1.85	0.77
1:B:223:GLU:HG3	1:B:224:SER:H	1.49	0.76
1:A:12:LEU:HD11	1:A:110:LEU:HD12	1.65	0.76
1:A:123:TRP:HE3	1:A:502:GLU:CD	1.88	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:57:ILE:CD1	1:A:67:PHE:CZ	2.68	0.75
1:A:85:VAL:CG1	1:A:88:LEU:CD1	2.64	0.74
1:A:85:VAL:HG13	1:A:88:LEU:CD1	2.17	0.74
1:B:156:THR:OG1	1:B:159:LYS:HG2	1.87	0.74
1:A:123:TRP:HE3	1:A:502:GLU:OE2	1.69	0.74
1:A:136:LEU:HD12	1:A:151:ASP:O	1.88	0.74
1:B:223:GLU:HG3	1:B:224:SER:N	2.03	0.74
1:A:243:THR:HA	1:B:243:THR:HG23	1.69	0.74
1:B:496:GLN:O	1:B:500:LEU:HD13	1.87	0.74
1:B:11:LEU:HD12	1:B:20:TYR:CE2	2.24	0.73
1:B:271:LEU:HD13	1:B:325:ARG:HG3	1.71	0.73
1:B:302:VAL:HG12	1:B:302:VAL:O	1.88	0.73
1:A:57:ILE:CD1	1:A:67:PHE:CE1	2.72	0.72
1:B:230:ARG:HH11	1:B:234:ILE:HD11	1.55	0.72
1:A:85:VAL:HG13	1:A:88:LEU:HD11	1.69	0.72
1:B:138:LEU:HD12	1:B:168:TYR:HD2	1.53	0.72
1:A:56:LYS:HE3	1:A:222:GLU:HG2	1.72	0.71
1:A:20:TYR:CE1	1:A:94:ILE:HD13	2.27	0.70
1:B:256:VAL:HG13	1:B:264:ALA:HB3	1.74	0.70
1:B:458:LEU:HD21	1:B:507:LEU:HD11	1.74	0.69
1:B:465:PHE:CD2	1:B:512:LEU:HD13	2.26	0.69
1:B:210:ARG:O	1:B:215:LYS:CE	2.41	0.69
1:B:427:MET:HE1	1:B:434:LEU:HD11	1.74	0.69
1:B:252:LEU:O	1:B:256:VAL:HG23	1.92	0.69
1:B:370:ARG:NH2	1:B:373:TYR:CE2	2.60	0.69
1:A:243:THR:HA	1:B:243:THR:CG2	2.23	0.68
1:A:85:VAL:HG11	1:A:88:LEU:HD11	1.74	0.68
1:B:254:ILE:HD13	1:B:306:VAL:HG21	1.74	0.68
1:A:309:PHE:HA	1:A:314:MET:HE3	1.75	0.68
1:B:11:LEU:HD12	1:B:20:TYR:HD2	1.59	0.67
1:B:247:TYR:HD2	1:B:251:LEU:HD11	1.59	0.67
1:A:322:THR:OG1	1:A:323:PRO:CD	2.41	0.66
1:A:172:VAL:HG13	1:A:208:LEU:HD21	1.78	0.66
1:A:97:LEU:HD22	1:B:250:LEU:CD1	2.24	0.65
1:B:138:LEU:HD12	1:B:168:TYR:CD2	2.32	0.65
1:A:448:ASP:OD1	1:A:506:LYS:CD	2.43	0.65
1:B:51:THR:HA	1:B:219:SER:OG	1.96	0.64
1:B:225:ASP:OD1	1:B:226:GLN:N	2.30	0.64
1:A:59:PRO:HA	1:A:62:ARG:HB3	1.78	0.64
1:B:118:LEU:HD12	1:B:118:LEU:O	1.98	0.64
1:B:427:MET:CE	1:B:434:LEU:HD11	2.28	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:310:ASN:OD1	1:A:313:ASN:CB	2.43	0.63
1:B:230:ARG:NH1	1:B:234:ILE:CD1	2.61	0.63
1:B:322:THR:OG1	1:B:323:PRO:CD	2.44	0.63
1:B:11:LEU:CD1	1:B:20:TYR:CD2	2.82	0.62
1:B:172:VAL:HG13	1:B:208:LEU:HD21	1.82	0.62
1:A:194:SER:HB2	1:A:197:GLN:HG2	1.81	0.62
1:A:527:HIS:HB3	1:A:554:GLU:OE1	2.00	0.61
1:B:271:LEU:HD13	1:B:325:ARG:CG	2.31	0.61
1:A:79:ASN:ND2	1:A:83:GLU:OE2	2.34	0.61
1:A:110:LEU:CD2	1:A:172:VAL:HG12	2.31	0.61
1:B:247:TYR:CD2	1:B:251:LEU:HD11	2.35	0.60
1:B:296:LEU:CD2	1:B:356:TYR:HA	2.31	0.60
1:B:427:MET:HE1	1:B:434:LEU:CD1	2.30	0.60
1:B:529:TRP:HZ3	1:B:530:TYR:HE1	1.40	0.60
1:B:578:LEU:N	1:B:578:LEU:HD12	2.16	0.60
1:A:487:LEU:HD13	1:A:500:LEU:HD23	1.83	0.60
1:A:138:LEU:HD12	1:A:168:TYR:CD1	2.36	0.60
1:A:127:ASP:OD1	1:A:127:ASP:O	2.20	0.60
1:A:123:TRP:CD1	1:A:124:SER:N	2.69	0.60
1:A:256:VAL:HG13	1:A:311:LYS:HG3	1.81	0.60
1:B:254:ILE:HD13	1:B:306:VAL:CG2	2.32	0.60
1:B:577:ALA:C	1:B:578:LEU:HD12	2.21	0.60
1:A:288:LEU:HD12	1:A:352:LEU:HD21	1.83	0.60
1:B:406:LEU:HD22	1:B:423:ILE:HG23	1.83	0.60
1:A:59:PRO:O	1:A:62:ARG:HG2	2.01	0.59
1:A:267:GLU:OE1	1:A:325:ARG:NH1	2.35	0.59
1:A:85:VAL:HG11	1:A:88:LEU:CD1	2.29	0.59
1:A:123:TRP:CZ3	1:A:502:GLU:OE2	2.55	0.59
1:A:314:MET:HE2	1:A:317:LEU:HD22	1.83	0.59
1:B:188:ALA:HA	1:B:198:ARG:HD2	0.79	0.59
1:B:214:ASP:O	1:B:215:LYS:HG2	2.03	0.58
1:B:427:MET:CE	1:B:434:LEU:CD1	2.81	0.58
1:A:210:ARG:O	1:A:215:LYS:CG	2.50	0.58
1:B:11:LEU:CD1	1:B:20:TYR:CE2	2.86	0.58
1:A:11:LEU:HD21	1:A:103:ILE:HG12	1.86	0.58
1:B:223:GLU:CG	1:B:224:SER:H	2.16	0.57
1:A:302:VAL:HG12	1:A:302:VAL:O	2.03	0.57
1:B:576:THR:HA	1:B:579:GLN:CD	2.25	0.57
1:A:297:SER:HB3	1:A:316:ILE:HG22	1.87	0.57
1:A:72:GLN:HG3	1:A:73:HIS:ND1	2.20	0.57
1:A:211:THR:HA	1:A:215:LYS:HD2	1.86	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:12:LEU:CD1	1:A:110:LEU:HD12	2.32	0.56
1:A:254:ILE:HG21	1:A:265:ARG:HB2	1.87	0.56
1:A:11:LEU:HD22	1:A:218:ILE:HD13	1.87	0.56
1:B:370:ARG:CZ	1:B:373:TYR:CE2	2.83	0.56
1:A:526:PRO:HB2	1:A:552:LEU:HD13	1.88	0.56
1:A:18:GLN:OE1	1:A:87:GLN:HB3	2.05	0.56
1:B:156:THR:HG1	1:B:159:LYS:HG2	1.71	0.56
1:A:57:ILE:HD11	1:A:67:PHE:CE1	2.40	0.55
1:B:271:LEU:HD22	1:B:325:ARG:HG3	1.87	0.55
1:A:59:PRO:O	1:A:62:ARG:NH2	2.36	0.55
1:A:278:VAL:HG11	1:A:333:GLN:HG2	1.89	0.55
1:A:394:ILE:HA	1:A:432:LYS:HG2	1.88	0.55
1:B:9:ARG:HG3	1:B:10:SER:N	2.22	0.55
1:B:430:ARG:O	1:B:430:ARG:HG3	2.05	0.55
1:A:275:MET:HE2	1:A:284:VAL:HG21	1.89	0.55
1:B:466:ASP:OD2	1:B:469:ARG:CD	2.54	0.55
1:A:56:LYS:HE3	1:A:222:GLU:CG	2.36	0.55
1:A:72:GLN:HG3	1:A:73:HIS:N	2.22	0.55
1:B:302:VAL:O	1:B:302:VAL:CG1	2.55	0.55
1:A:11:LEU:HB2	1:A:218:ILE:HD13	1.88	0.54
1:A:123:TRP:CE3	1:A:502:GLU:CD	2.75	0.54
1:B:498:ASP:HA	1:B:501:ILE:HG12	1.89	0.54
1:B:498:ASP:CG	1:B:498:ASP:O	2.47	0.53
1:A:170:PHE:HE2	1:A:175:ILE:HG12	1.73	0.53
1:B:464:GLY:C	1:B:465:PHE:CD1	2.75	0.53
1:B:156:THR:OG1	1:B:159:LYS:CG	2.54	0.53
1:B:190:ASP:OD2	1:B:192:ARG:HB3	2.08	0.53
1:A:329:LEU:O	1:A:333:GLN:HG3	2.09	0.53
1:B:214:ASP:O	1:B:215:LYS:HD3	2.09	0.53
1:A:210:ARG:O	1:A:215:LYS:CD	2.56	0.53
1:B:458:LEU:HD21	1:B:507:LEU:CD1	2.38	0.53
1:B:131:VAL:HG23	1:B:131:VAL:O	2.09	0.53
1:B:440:GLU:O	1:B:444:LEU:HG	2.09	0.53
1:B:159:LYS:O	1:B:162:LEU:HG	2.10	0.52
1:B:466:ASP:OD2	1:B:469:ARG:HG3	2.09	0.52
1:B:20:TYR:HE1	1:B:94:ILE:HD12	1.73	0.52
1:B:322:THR:HG1	1:B:323:PRO:HD3	1.72	0.52
1:A:161:SER:O	1:A:161:SER:OG	2.22	0.52
1:A:387:SER:HB3	1:A:395:TRP:HE1	1.73	0.51
1:B:223:GLU:CG	1:B:224:SER:N	2.72	0.51
1:A:379:CYS:SG	1:A:420:LEU:HB2	2.50	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:123:TRP:CG	1:A:124:SER:N	2.79	0.51
1:B:214:ASP:O	1:B:215:LYS:CG	2.58	0.51
1:B:278:VAL:HG21	1:B:332:MET:HB2	1.92	0.51
1:A:11:LEU:HB2	1:A:218:ILE:CD1	2.41	0.51
1:A:379:CYS:SG	1:A:420:LEU:HD22	2.51	0.51
1:B:459:THR:HG23	1:B:467:PHE:CE1	2.46	0.51
1:A:385:ILE:O	1:A:389:LEU:HG	2.09	0.51
1:A:11:LEU:HD12	1:A:20:TYR:CD2	2.46	0.50
1:A:85:VAL:HG13	1:A:88:LEU:HD12	1.92	0.50
1:A:249:ASP:HA	1:A:252:LEU:HD13	1.93	0.50
1:A:132:ARG:HG2	1:A:156:THR:OG1	2.11	0.50
1:A:121:LYS:HB3	1:A:123:TRP:CZ2	2.47	0.50
1:B:507:LEU:CA	1:B:510:LEU:HD12	2.37	0.50
1:A:20:TYR:HE1	1:A:94:ILE:HD13	1.75	0.50
1:A:280:ASP:HB2	1:A:341:ASN:OD1	2.11	0.50
1:A:314:MET:CE	1:A:317:LEU:HD22	2.41	0.50
1:B:296:LEU:HD23	1:B:356:TYR:HA	1.94	0.50
1:B:578:LEU:N	1:B:578:LEU:CD1	2.74	0.50
1:A:117:LYS:CG	1:A:118:LEU:H	2.03	0.50
1:B:557:ASN:OD1	1:B:558:GLN:HG2	2.12	0.50
1:A:382:ASN:ND2	1:A:386:ARG:NH1	2.59	0.49
1:A:527:HIS:O	1:A:527:HIS:ND1	2.45	0.49
1:B:419:PRO:O	1:B:423:ILE:HG12	2.12	0.49
1:A:385:ILE:HG21	1:A:460:LEU:HB2	1.94	0.49
1:A:194:SER:H	1:A:197:GLN:CG	2.24	0.49
1:B:187:VAL:HG12	1:B:198:ARG:HG3	1.94	0.49
1:A:56:LYS:CE	1:A:222:GLU:HG2	2.41	0.49
1:A:371:VAL:HG12	1:A:371:VAL:O	2.11	0.49
1:A:189:ASP:OD1	1:A:189:ASP:O	2.31	0.49
1:A:251:LEU:HA	1:A:254:ILE:HG12	1.95	0.49
1:A:85:VAL:CG1	1:A:88:LEU:HD12	2.43	0.48
1:B:180:GLU:O	1:B:184:ILE:HG12	2.13	0.48
1:B:8:ILE:O	1:B:12:LEU:CD1	2.56	0.48
1:B:118:LEU:HD12	1:B:118:LEU:C	2.33	0.48
1:B:247:TYR:O	1:B:250:LEU:HB3	2.13	0.48
1:A:66:GLN:OE1	1:B:258:GLN:HA	2.12	0.48
1:A:104:THR:O	1:A:108:ILE:HG12	2.14	0.48
1:B:529:TRP:CZ3	1:B:530:TYR:CD1	2.98	0.48
1:B:576:THR:HA	1:B:579:GLN:HG3	1.94	0.48
1:A:430:ARG:HG3	1:A:430:ARG:O	2.13	0.48
1:B:296:LEU:HD12	1:B:324:ILE:HG23	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:210:ARG:O	1:B:215:LYS:CG	2.62	0.48
1:B:214:ASP:O	1:B:215:LYS:CD	2.62	0.47
1:A:11:LEU:HD22	1:A:218:ILE:CD1	2.44	0.47
1:B:462:PHE:HB3	1:B:465:PHE:CZ	2.50	0.47
1:A:256:VAL:CG1	1:A:311:LYS:HG3	2.45	0.47
1:A:288:LEU:CD1	1:A:352:LEU:HD21	2.45	0.47
1:A:483:THR:OG1	1:A:486:LYS:CB	2.63	0.47
1:A:335:LEU:HD11	1:A:351:ILE:HG12	1.96	0.46
1:B:40:PHE:O	1:B:44:LEU:HD13	2.15	0.46
1:A:56:LYS:CG	1:A:222:GLU:HG2	2.45	0.46
1:A:138:LEU:HD12	1:A:168:TYR:HD1	1.78	0.46
1:B:188:ALA:CB	1:B:198:ARG:HH11	2.29	0.46
1:B:328:LEU:HD23	1:B:355:ALA:HB1	1.96	0.46
1:A:483:THR:OG1	1:A:486:LYS:HB2	2.16	0.46
1:A:59:PRO:HB3	1:A:62:ARG:HD3	1.98	0.46
1:B:211:THR:HA	1:B:215:LYS:CG	2.42	0.46
1:A:468:SER:OG	1:A:469:ARG:N	2.49	0.45
1:B:188:ALA:HB1	1:B:198:ARG:NH1	2.32	0.45
1:B:210:ARG:O	1:B:215:LYS:HG2	2.16	0.45
1:A:451:ASN:HD21	1:A:453:ARG:HH11	1.63	0.45
1:A:36:ILE:HD12	1:A:105:ALA:CB	2.46	0.45
1:B:99:GLY:O	1:B:103:ILE:HG12	2.17	0.45
1:A:253:SER:C	1:A:255:ALA:N	2.69	0.45
1:B:466:ASP:OD2	1:B:469:ARG:NE	2.48	0.45
1:A:302:VAL:O	1:A:302:VAL:CG1	2.65	0.45
1:B:575:ARG:O	1:B:579:GLN:HG3	2.17	0.44
1:B:297:SER:HB2	1:B:299:ILE:HG12	1.99	0.44
1:B:465:PHE:HB2	1:B:467:PHE:CE1	2.53	0.44
1:A:72:GLN:HG3	1:A:73:HIS:H	1.83	0.43
1:B:7:THR:HG22	1:B:215:LYS:O	2.19	0.43
1:A:133:ARG:HE	1:A:171:ARG:HD2	1.83	0.43
1:B:56:LYS:HG2	1:B:94:ILE:HG12	2.01	0.43
1:B:529:TRP:CE3	1:B:530:TYR:CE1	3.03	0.43
1:A:402:LEU:HD11	1:A:427:MET:HG2	2.01	0.43
1:A:278:VAL:CG1	1:A:333:GLN:HG2	2.48	0.43
1:A:324:ILE:O	1:A:325:ARG:C	2.57	0.43
1:B:275:MET:O	1:B:278:VAL:HG23	2.19	0.43
1:A:97:LEU:CD2	1:B:250:LEU:HD11	2.39	0.43
1:B:576:THR:HA	1:B:579:GLN:CG	2.48	0.43
1:A:124:SER:OG	1:A:126:ASP:O	2.35	0.42
1:A:507:LEU:HG	1:A:570:LEU:HD13	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:65:TYR:HB2	1:A:67:PHE:CZ	2.54	0.42
1:B:329:LEU:O	1:B:333:GLN:HG3	2.19	0.42
1:B:459:THR:HG23	1:B:467:PHE:CZ	2.54	0.42
1:B:552:LEU:HD23	1:B:552:LEU:HA	1.92	0.42
1:A:53:LEU:H	1:A:98:ASP:HB3	1.84	0.42
1:B:487:LEU:HD23	1:B:556:LEU:HD23	2.00	0.42
1:B:443:GLU:O	1:B:446:GLN:HG3	2.19	0.42
1:A:136:LEU:HD13	1:A:152:PHE:CE1	2.55	0.42
1:A:513:LEU:HA	1:A:513:LEU:HD12	1.80	0.42
1:A:552:LEU:HD23	1:A:552:LEU:HA	1.87	0.42
1:B:328:LEU:O	1:B:331:SER:HB2	2.20	0.42
1:A:57:ILE:HD13	1:A:67:PHE:HZ	1.67	0.41
1:A:194:SER:H	1:A:197:GLN:HG3	1.84	0.41
1:A:243:THR:HB	1:B:243:THR:OG1	2.20	0.41
1:B:233:ASN:HB3	1:B:237:ARG:HH12	1.84	0.41
1:B:496:GLN:O	1:B:500:LEU:CD1	2.65	0.41
1:A:291:LYS:HE2	1:A:302:VAL:HG12	2.02	0.41
1:A:443:GLU:O	1:A:446:GLN:HG3	2.20	0.41
1:B:529:TRP:CE3	1:B:530:TYR:CD1	3.08	0.41
1:B:444:LEU:O	1:B:447:LEU:HG	2.20	0.41
1:A:75:HIS:CE1	1:A:77:ARG:HB3	2.55	0.41
1:B:328:LEU:HD23	1:B:355:ALA:CB	2.51	0.41
1:B:429:GLN:C	1:B:431:GLY:H	2.23	0.41
1:B:556:LEU:HD12	1:B:556:LEU:HA	1.94	0.41
1:A:243:THR:HG23	1:A:243:THR:O	2.20	0.41
1:A:413:SER:HB3	1:A:419:PRO:HB3	2.03	0.41
1:A:136:LEU:HD13	1:A:152:PHE:CD1	2.55	0.41
1:B:548:ALA:HB3	1:B:566:ARG:NH1	2.36	0.41
1:B:430:ARG:O	1:B:430:ARG:CG	2.69	0.40
1:A:228:LEU:HD21	1:B:250:LEU:HD21	2.03	0.40
1:A:110:LEU:HD23	1:A:172:VAL:HG12	2.04	0.40
1:B:22:LEU:HD23	1:B:22:LEU:HA	1.90	0.40
1:A:251:LEU:C	1:A:253:SER:N	2.75	0.40
1:B:51:THR:HA	1:B:219:SER:HG	1.86	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	553/587 (94%)	518 (94%)	35 (6%)	0	100	100
1	B	545/587 (93%)	522 (96%)	23 (4%)	0	100	100
All	All	1098/1174 (94%)	1040 (95%)	58 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	494/516 (96%)	491 (99%)	3 (1%)	86	95
1	B	490/516 (95%)	483 (99%)	7 (1%)	67	86
All	All	984/1032 (95%)	974 (99%)	10 (1%)	76	91

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	247	TYR
1	A	525	MET
1	A	566	ARG
1	B	123	TRP
1	B	247	TYR
1	B	295	MET
1	B	427	MET
1	B	453	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	455	PHE
1	B	566	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 1 is monoatomic - leaving 3 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	563/587 (95%)	0.58	55 (9%) 7 5	69, 97, 129, 146	0
1	B	557/587 (94%)	0.61	62 (11%) 5 3	64, 92, 123, 141	0
All	All	1120/1174 (95%)	0.60	117 (10%) 6 4	64, 95, 126, 146	0

All (117) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	24	ALA	4.8
1	A	520	GLN	4.6
1	B	53	LEU	4.6
1	A	489	LYS	4.4
1	A	269	HIS	4.2
1	A	490	VAL	4.1
1	A	212	ILE	4.1
1	A	268	ILE	4.0
1	A	528	GLU	4.0
1	B	473	VAL	4.0
1	A	522	ARG	3.9
1	B	9	ARG	3.9
1	B	54	PHE	3.9
1	B	20	TYR	3.8
1	A	554	GLU	3.8
1	A	123	TRP	3.7
1	A	481	LEU	3.7
1	B	528	GLU	3.6
1	A	267	GLU	3.6
1	B	44	LEU	3.5
1	B	93	PHE	3.4
1	B	262	LEU	3.4
1	B	110	LEU	3.3
1	A	265	ARG	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	481	LEU	3.3
1	A	242	GLY	3.2
1	B	529	TRP	3.2
1	A	330	LEU	3.2
1	A	486	LYS	3.2
1	A	321	TRP	3.2
1	A	325	ARG	3.2
1	B	57	ILE	3.2
1	B	90	GLU	3.2
1	B	80	TYR	3.2
1	A	304	PHE	3.1
1	A	518	ASN	3.1
1	A	473	VAL	3.1
1	B	25	ILE	3.1
1	A	290	LEU	3.0
1	B	554	GLU	3.0
1	B	526	PRO	3.0
1	A	165	SER	3.0
1	B	114	PHE	3.0
1	A	166	GLU	2.9
1	B	94	ILE	2.9
1	B	516	THR	2.9
1	A	485	ASN	2.9
1	B	471	PHE	2.8
1	A	527	HIS	2.8
1	A	271	LEU	2.7
1	A	317	LEU	2.7
1	B	476	ILE	2.7
1	A	487	LEU	2.7
1	B	88	LEU	2.7
1	B	67	PHE	2.7
1	B	268	ILE	2.7
1	B	221	TYR	2.7
1	B	517	ILE	2.6
1	A	208	LEU	2.6
1	B	212	ILE	2.6
1	B	62	ARG	2.6
1	B	524	LYS	2.6
1	A	282	PHE	2.6
1	A	80	TYR	2.6
1	B	208	LEU	2.5
1	B	231	VAL	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	280	ASP	2.5
1	A	266	GLU	2.5
1	B	278	VAL	2.5
1	B	232	LEU	2.5
1	A	302	VAL	2.5
1	A	326	ASP	2.5
1	B	530	TYR	2.5
1	B	238	MET	2.5
1	A	484	ARG	2.5
1	B	465	PHE	2.5
1	A	243	THR	2.5
1	A	345	LEU	2.5
1	B	449	TYR	2.5
1	B	23	PRO	2.4
1	B	22	LEU	2.4
1	B	89	PRO	2.4
1	A	275	MET	2.4
1	B	225	ASP	2.4
1	B	230	ARG	2.4
1	A	54	PHE	2.3
1	A	49	PHE	2.3
1	B	472	HIS	2.3
1	B	49	PHE	2.3
1	B	328	LEU	2.3
1	B	280	ASP	2.3
1	B	11	LEU	2.3
1	B	116	TRP	2.2
1	A	498	ASP	2.2
1	A	354	LEU	2.2
1	A	21	LEU	2.2
1	A	53	LEU	2.2
1	A	309	PHE	2.2
1	A	483	THR	2.2
1	B	172	VAL	2.2
1	B	8	ILE	2.2
1	A	511	GLN	2.2
1	B	71	MET	2.2
1	A	482	PHE	2.1
1	B	218	ILE	2.1
1	A	43	LEU	2.1
1	B	43	LEU	2.1
1	B	17	GLU	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	328	LEU	2.1
1	B	514	GLU	2.1
1	B	214	ASP	2.1
1	A	523	GLN	2.1
1	B	513	LEU	2.1
1	A	258	GLN	2.1
1	B	555	GLN	2.0
1	B	415	ASP	2.0
1	A	368	LEU	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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	SO4	A	601	5/5	0.91	0.14	90,103,109,114	0
2	SO4	B	602	5/5	0.91	0.18	120,123,133,143	0
3	CL	B	603	1/1	0.91	0.31	107,107,107,107	0
2	SO4	B	601	5/5	0.94	0.17	90,99,108,118	0

6.5 Other polymers [i](#)

There are no such residues in this entry.