



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:49 AM UTC

PDB ID : 8CAR / pdb_00008car
Title : Discovery of the lanthipeptide Curvocidin and structural insights into its tri-functional synthetase CuvL
Authors : Martins, B.M.; Sigurdsson, A.; Duettmann, A.A.; Jasyk, M.; Dimos-Roehl, B.; Schoepf, F.; Gemander, M.; Knittel, C.H.; Schegotzki, R.; Schmid, B.; Kosol, S.; Pommerening, L.; Gonzalez-Viegas, M.; Seidel, M.; Huegelland, M.; Leimkuehler, S.; Dobbek, H.; Mainz, A.; Suessmuth, R.
Deposited on : 2023-01-24
Resolution : 2.68 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
Mogul	:	2022.3.0, CSD as543be (2022)
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)

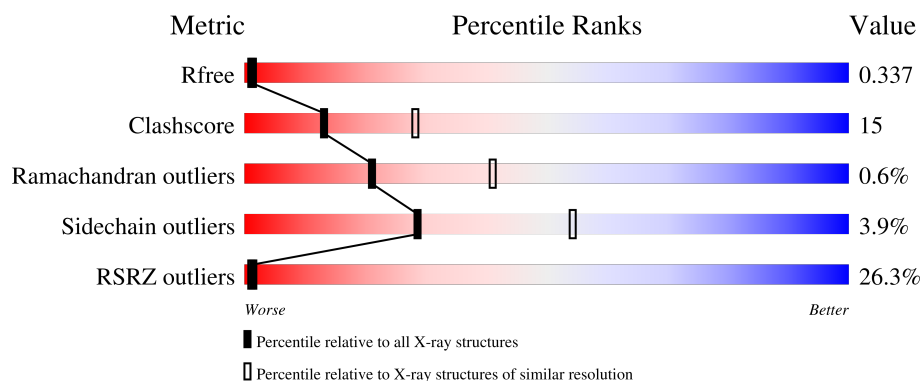
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.68 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	5070 (2.70-2.66)
Clashscore	190562	5409 (2.70-2.66)
Ramachandran outliers	187476	5324 (2.70-2.66)
Sidechain outliers	187428	5324 (2.70-2.66)
RSRZ outliers	180081	5070 (2.70-2.66)

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	865	25% 68% 25% ..

2 Entry composition [i](#)

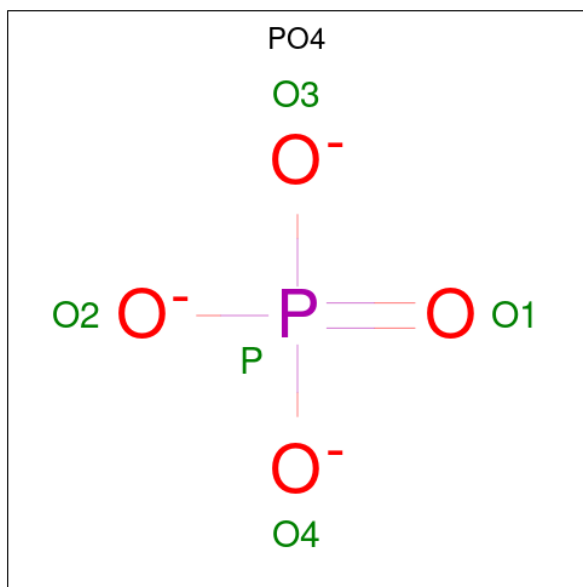
There are 4 unique types of molecules in this entry. The entry contains 12520 atoms, of which 6202 are hydrogens and 0 are deuteriums.

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 Serine/threonine protein kinase.

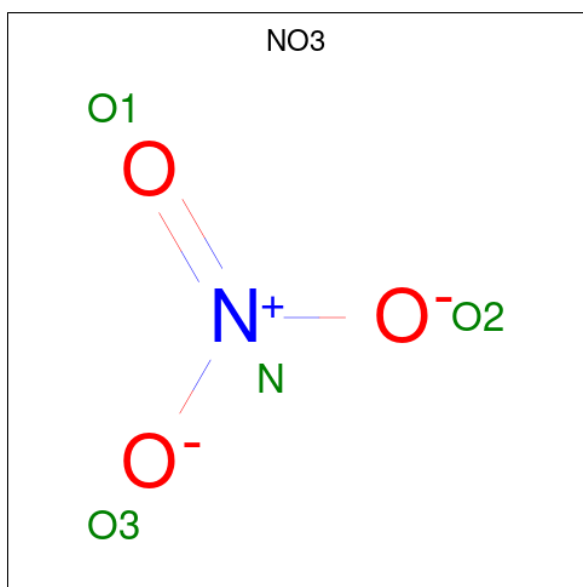
Mol	Chain	Residues	Atoms							ZeroOcc	AltConf	Trace
1	A	830	Total	C	H	N	O	S	Se	0	3	0
			12510	3942	6202	1176	1167	13	10			

- Molecule 2 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



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

- Molecule 3 is NITRATE ION (CCD ID: NO3) (formula: NO_3).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	N	O	0	0
			4	1	3		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	O	0	0
			1	1		

4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	135.65Å 135.65Å 335.44Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.11 – 2.68 48.11 – 2.68	Depositor EDS
% Data completeness (in resolution range)	99.8 (48.11-2.68) 99.7 (48.11-2.68)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.36 (at 2.69Å)	Xtriage
Refinement program	PHENIX v1.20.1_4487	Depositor
R, R_{free}	0.297 , 0.337 0.297 , 0.337	Depositor DCC
R_{free} test set	1130 reflections (2.18%)	wwPDB-VP
Wilson B-factor (Å ²)	87.3	Xtriage
Anisotropy	0.178	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 92.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	12520	wwPDB-VP
Average B, all atoms (Å ²)	134.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.66% 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: NO3, PO4

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	0.21	0/6462	0.42	0/8796

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	6308	6202	6199	187	0
2	A	5	0	0	0	0
3	A	4	0	0	0	0
4	A	1	0	0	0	0
All	All	6318	6202	6199	187	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 (187) 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:346:LEU:HD23	1:A:374:ALA:HB2	1.54	0.90
1:A:656:PRO:HG3	1:A:664:ALA:HB3	1.55	0.86
1:A:317:ALA:HB1	1:A:321:PRO:HD2	1.58	0.84
1:A:357:LEU:HD21	1:A:361:THR:HA	1.65	0.79
1:A:346:LEU:CD1	1:A:399:VAL:HG22	2.13	0.79
1:A:408:ALA:N	1:A:452:LEU:HD21	1.98	0.78
1:A:243:ILE:HD12	1:A:282:LYS:NZ	1.99	0.77
1:A:652:LEU:HD23	1:A:654:GLU:OE2	1.86	0.76
1:A:346:LEU:HD23	1:A:374:ALA:CB	2.17	0.74
1:A:312:ASN:OD1	1:A:313:GLY:N	2.24	0.70
1:A:30:ALA:HB1	1:A:82:ARG:HH12	1.57	0.69
1:A:656:PRO:CG	1:A:664:ALA:HB3	2.23	0.69
1:A:216:TYR:O	1:A:218:VAL:HG22	1.92	0.68
1:A:415:THR:HG22	1:A:436:GLU:HG2	1.75	0.68
1:A:318:ASP:OD1	1:A:768:ARG:NH1	2.27	0.67
1:A:437:VAL:HG21	1:A:477:PRO:HB3	1.74	0.67
1:A:354:ASN:O	1:A:355:VAL:HG13	1.95	0.66
1:A:218:VAL:HB	1:A:233:ALA:HA	1.77	0.66
1:A:439:ALA:HB1	1:A:443:GLY:HA2	1.79	0.65
1:A:245:LYS:NZ	1:A:267:GLU:OE2	2.26	0.64
1:A:37:VAL:HG11	1:A:78:PHE:CZ	2.32	0.64
1:A:533:MSE:HE1	1:A:579:GLU:HB3	1.81	0.62
1:A:556:PHE:O	1:A:560:ARG:NH1	2.29	0.62
1:A:346:LEU:HD12	1:A:399:VAL:HG22	1.81	0.61
1:A:280:VAL:HB	1:A:281:PRO:HD3	1.82	0.61
1:A:675:LEU:HD23	1:A:705:LEU:HG	1.83	0.61
1:A:334:LEU:HA	1:A:337:LEU:HD13	1.82	0.61
1:A:274:LEU:HD11	1:A:281:PRO:HG2	1.83	0.61
1:A:400:GLU:O	1:A:403:TYR:CD1	2.54	0.60
1:A:491:ALA:HB1	1:A:817:GLU:HA	1.83	0.60
1:A:228:GLY:O	1:A:248:ARG:NH2	2.34	0.60
1:A:71:VAL:HG23	1:A:72:LEU:HD12	1.82	0.59
1:A:337:LEU:HD12	1:A:467:ARG:NH1	2.17	0.59
1:A:638:ALA:O	1:A:642:ARG:HG2	2.03	0.59
1:A:210:VAL:HB	1:A:219:VAL:HG13	1.83	0.59
1:A:336:LEU:HD11	1:A:463:ALA:O	2.02	0.58
1:A:333:LEU:HD22	1:A:467:ARG:HA	1.86	0.57
1:A:346:LEU:HD11	1:A:399:VAL:HG22	1.85	0.57
1:A:604:ILE:HD13	1:A:616:ILE:CD1	2.34	0.57
1:A:613:LEU:HB2	1:A:643:LEU:HD21	1.85	0.57
1:A:329:LEU:HA	1:A:444:MSE:HE2	1.87	0.57
1:A:489:LEU:HD23	1:A:809:LEU:HD11	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:243:ILE:HD12	1:A:282:LYS:HZ1	1.69	0.56
1:A:465:ASP:HB3	1:A:471:PHE:H	1.69	0.56
1:A:348:ARG:HE	1:A:371:ILE:HG22	1.71	0.56
1:A:80:VAL:HG22	1:A:104:VAL:HG22	1.88	0.55
1:A:254:ASP:OD1	1:A:255:THR:N	2.39	0.55
1:A:464:ASP:CG	1:A:464:ASP:O	2.49	0.55
1:A:579:GLU:O	1:A:583:THR:HG22	2.07	0.55
1:A:139:ARG:HE	1:A:142:ALA:HB2	1.69	0.55
1:A:347:VAL:HG11	1:A:350:LEU:HD23	1.88	0.54
1:A:597:ALA:O	1:A:632:ARG:NH2	2.41	0.54
1:A:408:ALA:H	1:A:452:LEU:HD21	1.73	0.54
1:A:57:PRO:HD3	1:A:87:LEU:HD22	1.89	0.53
1:A:371:ILE:HG23	1:A:379:LEU:HB2	1.89	0.53
1:A:210:VAL:N	1:A:219:VAL:HG22	2.23	0.53
1:A:334:LEU:O	1:A:337:LEU:HB2	2.09	0.53
1:A:533:MSE:HG2	1:A:855:LEU:HD23	1.90	0.53
1:A:737:ALA:HB1	1:A:741:ARG:HH21	1.72	0.53
1:A:355:VAL:O	1:A:356:VAL:HG23	2.09	0.52
1:A:406:LEU:HD22	1:A:451:LEU:HD21	1.92	0.52
1:A:415:THR:HG22	1:A:436:GLU:CG	2.40	0.52
1:A:700:LYS:O	1:A:704:THR:HG23	2.09	0.52
1:A:136:ARG:HH22	1:A:198:PRO:HG2	1.74	0.52
1:A:430:ASP:CG	1:A:431:PRO:HD2	2.36	0.51
1:A:190:PRO:HA	1:A:197:THR:HG22	1.91	0.51
1:A:37:VAL:HG11	1:A:78:PHE:CE1	2.46	0.51
1:A:258:ARG:HA	1:A:262:LEU:HD22	1.93	0.51
1:A:274:LEU:CD1	1:A:281:PRO:HG2	2.40	0.51
1:A:54:SER:HA	1:A:101:GLY:O	2.11	0.50
1:A:109:SER:OG	1:A:112:ASP:OD2	2.29	0.50
1:A:437:VAL:HG21	1:A:477:PRO:CB	2.40	0.50
1:A:210:VAL:N	1:A:219:VAL:HA	2.27	0.50
1:A:68:LEU:HA	1:A:71:VAL:HG22	1.93	0.50
1:A:244:ILE:O	1:A:244:ILE:HG13	2.12	0.50
1:A:44:LEU:HD12	1:A:45:PRO:HD2	1.93	0.50
1:A:762:CYS:HB3	1:A:781:ILE:HG23	1.93	0.50
1:A:333:LEU:HD22	1:A:467:ARG:CA	2.42	0.50
1:A:411:PHE:CZ	1:A:415:THR:HG21	2.46	0.50
1:A:533:MSE:HE3	1:A:576:PHE:HD1	1.76	0.49
1:A:465:ASP:HB3	1:A:470:ARG:HB2	1.93	0.49
1:A:533:MSE:HE2	1:A:536:LEU:HD12	1.94	0.49
1:A:425:ASP:HB3	1:A:428:ASN:CG	2.38	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:318:ASP:HB2	1:A:319:PRO:HD3	1.94	0.49
1:A:215:ARG:HG2	1:A:287:PHE:CE2	2.48	0.49
1:A:609:GLN:HG2	1:A:671:PHE:CE2	2.48	0.48
1:A:400:GLU:O	1:A:403:TYR:HB3	2.13	0.48
1:A:215:ARG:HG2	1:A:287:PHE:CZ	2.49	0.48
1:A:319:PRO:O	1:A:441:ARG:NH2	2.47	0.48
1:A:384:PRO:O	1:A:388:PRO:HD3	2.14	0.48
1:A:287:PHE:CE2	1:A:294:TYR:CD1	3.02	0.48
1:A:87:LEU:HD23	1:A:87:LEU:O	2.14	0.48
1:A:217:ARG:C	1:A:218:VAL:HG13	2.39	0.48
1:A:608:ASP:OD1	1:A:609:GLN:N	2.46	0.48
1:A:210:VAL:O	1:A:211:LEU:HD22	2.14	0.48
1:A:410:LEU:HD12	1:A:451:LEU:HD23	1.96	0.47
1:A:267:GLU:CD	1:A:370:GLU:HG2	2.39	0.47
1:A:384:PRO:HB2	1:A:388:PRO:HD3	1.96	0.47
1:A:333:LEU:HD13	1:A:467:ARG:HB3	1.96	0.47
1:A:456:PRO:C	1:A:458:ARG:H	2.23	0.47
1:A:312:ASN:HB3	1:A:355:VAL:O	2.15	0.47
1:A:637:ASP:HA	1:A:685:HIS:HE2	1.80	0.47
1:A:38:ASP:OD1	1:A:77[B]:HIS:NE2	2.48	0.47
1:A:712:LEU:CD1	1:A:732:LEU:HD21	2.45	0.47
1:A:108:PRO:HG2	1:A:113:VAL:HG22	1.97	0.46
1:A:411:PHE:CE1	1:A:415:THR:HG21	2.50	0.46
1:A:328:ALA:H	1:A:442:GLY:HA2	1.79	0.46
1:A:639:CYS:O	1:A:643:LEU:HG	2.14	0.46
1:A:437:VAL:HG22	1:A:437:VAL:O	2.16	0.46
1:A:169:ASP:OD1	1:A:173:ASN:N	2.48	0.46
1:A:346:LEU:O	1:A:372:SER:HA	2.15	0.46
1:A:350:LEU:HD12	1:A:405:SER:OG	2.15	0.46
1:A:410:LEU:O	1:A:413:ALA:HB3	2.16	0.46
1:A:53:LEU:HB2	1:A:104:VAL:HB	1.98	0.46
1:A:403:TYR:CD1	1:A:404:TYR:N	2.84	0.46
1:A:609:GLN:OE1	1:A:618:THR:HG21	2.15	0.46
1:A:387:SER:N	1:A:388:PRO:CD	2.79	0.46
1:A:623:LEU:HB3	1:A:632:ARG:HD3	1.96	0.46
1:A:381:GLY:C	1:A:383:THR:N	2.70	0.46
1:A:357:LEU:HD13	1:A:364:PRO:HA	1.98	0.45
1:A:637:ASP:OD1	1:A:685:HIS:NE2	2.48	0.45
1:A:122:GLU:O	1:A:123:ASP:CB	2.64	0.45
1:A:280:VAL:HA	1:A:364:PRO:O	2.17	0.45
1:A:319:PRO:O	1:A:441:ARG:NE	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:231:TYR:HB2	1:A:244:ILE:HG13	1.98	0.45
1:A:68:LEU:O	1:A:72:LEU:HD13	2.17	0.44
1:A:532:GLY:O	1:A:536:LEU:HG	2.17	0.44
1:A:219:VAL:O	1:A:219:VAL:HG12	2.16	0.44
1:A:369:PHE:HB3	1:A:372:SER:OG	2.18	0.44
1:A:401:ALA:C	1:A:403:TYR:H	2.24	0.44
1:A:455:ASP:N	1:A:456:PRO:CD	2.81	0.44
1:A:649:THR:O	1:A:652:LEU:HD11	2.17	0.44
1:A:384:PRO:HB2	1:A:387:SER:H	1.82	0.44
1:A:384:PRO:CB	1:A:387:SER:HB2	2.47	0.44
1:A:741:ARG:NH2	1:A:787:ASP:OD2	2.37	0.44
1:A:455:ASP:O	1:A:456:PRO:C	2.60	0.44
1:A:274:LEU:HD21	1:A:281:PRO:HB2	2.00	0.43
1:A:403:TYR:HB2	1:A:451:LEU:HD12	2.00	0.43
1:A:473:ASP:OD1	1:A:474:ALA:N	2.49	0.43
1:A:601:LEU:HD23	1:A:604:ILE:HD12	1.99	0.43
1:A:391:GLN:C	1:A:393:ARG:H	2.27	0.43
1:A:594:GLU:HB3	1:A:595:PRO:HD3	2.01	0.43
1:A:763:LEU:O	1:A:763:LEU:HD13	2.19	0.43
1:A:114:ALA:HA	1:A:193:LEU:HD21	1.99	0.43
1:A:385:GLY:O	1:A:421:TRP:CD2	2.71	0.43
1:A:136:ARG:NH1	1:A:191:ASP:OD2	2.49	0.43
1:A:384:PRO:O	1:A:388:PRO:CD	2.67	0.43
1:A:116:LEU:O	1:A:120:LEU:N	2.47	0.42
1:A:283:VAL:HG22	1:A:284:ILE:H	1.84	0.42
1:A:311:GLU:HG2	1:A:314:LEU:HD13	2.01	0.42
1:A:218:VAL:HG11	1:A:233:ALA:HB1	2.02	0.42
1:A:401:ALA:C	1:A:403:TYR:N	2.75	0.42
1:A:728:PHE:HA	1:A:733:ALA:HB3	2.02	0.42
1:A:287:PHE:CE1	1:A:294:TYR:HB2	2.54	0.42
1:A:148:TYR:CD2	1:A:186:PRO:HG3	2.55	0.42
1:A:800:TRP:CD1	1:A:803:ARG:HH21	2.37	0.42
1:A:384:PRO:C	1:A:386:TYR:N	2.78	0.42
1:A:470:ARG:HB3	1:A:471:PHE:CD1	2.55	0.42
1:A:333:LEU:N	1:A:333:LEU:HD23	2.35	0.42
1:A:629:ASP:HB3	1:A:632:ARG:HG3	2.02	0.42
1:A:833:TRP:HA	1:A:838:SER:OG	2.20	0.41
1:A:462:ALA:HB3	1:A:465:ASP:OD1	2.19	0.41
1:A:37:VAL:O	1:A:37:VAL:HG13	2.19	0.41
1:A:481:SER:HB2	1:A:484:GLN:HB2	2.02	0.41
1:A:212:LEU:HA	1:A:217:ARG:HD3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:465:ASP:HB3	1:A:471:PHE:N	2.35	0.41
1:A:666:SER:HB3	1:A:730:GLN:HB3	2.01	0.41
1:A:185:GLN:HG3	1:A:198:PRO:HD2	2.02	0.41
1:A:332:ALA:HB2	1:A:444:MSE:CE	2.50	0.41
1:A:384:PRO:HB2	1:A:387:SER:HB2	2.02	0.41
1:A:384:PRO:C	1:A:386:TYR:H	2.28	0.41
1:A:415:THR:HG22	1:A:436:GLU:CD	2.46	0.41
1:A:131:ARG:NH2	1:A:292:ARG:NH2	2.68	0.41
1:A:723:PRO:HB3	1:A:769:MSE:SE	2.71	0.41
1:A:766:ALA:N	1:A:767:PRO:HD2	2.35	0.41
1:A:337:LEU:O	1:A:340:VAL:HG22	2.20	0.41
1:A:482:ALA:O	1:A:485:ARG:HB3	2.21	0.41
1:A:752:LEU:O	1:A:756:ARG:HG3	2.20	0.41
1:A:375:GLU:HG3	1:A:377:PRO:HD2	2.03	0.40
1:A:403:TYR:CG	1:A:404:TYR:N	2.89	0.40
1:A:854:ARG:HD2	1:A:857:LEU:HB2	2.03	0.40
1:A:649:THR:O	1:A:652:LEU:CD1	2.70	0.40
1:A:762:CYS:HB3	1:A:781:ILE:HD12	2.04	0.40
1:A:596:LEU:HD12	1:A:596:LEU:HA	1.96	0.40
1:A:432:ARG:HH21	1:A:815:SER:HA	1.87	0.40
1:A:534:GLU:O	1:A:538:HIS:HD2	2.05	0.40
1:A:649:THR:O	1:A:649:THR:HG22	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	823/865 (95%)	749 (91%)	69 (8%)	5 (1%)	21	41

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	476	PRO
1	A	656	PRO
1	A	454	PRO
1	A	108	PRO
1	A	45	PRO

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	639/651 (98%)	614 (96%)	25 (4%)	28 54

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	61	GLN
1	A	210	VAL
1	A	211	LEU
1	A	212	LEU
1	A	215	ARG
1	A	284	ILE
1	A	333	LEU
1	A	383	THR
1	A	394	ASP
1	A	399	VAL
1	A	406	LEU
1	A	453	ASP
1	A	458	ARG
1	A	464	ASP
1	A	485	ARG
1	A	497	LEU
1	A	533	MSE
1	A	596	LEU
1	A	598	ARG
1	A	610	HIS
1	A	632	ARG
1	A	665	VAL

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Mol	Chain	Res	Type
1	A	783	GLU
1	A	784	LEU
1	A	854	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	339	HIS
1	A	354	ASN
1	A	751	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	PO4	A	1000	-	4,4,4	0.95	0	6,6,6	0.59	0
3	NO3	A	1001	-	1,3,3	0.57	0	0,3,3	-	-

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 [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	820/865 (94%)	1.39	216 (26%) 1 1	57, 123, 221, 317	2 (0%)

All (216) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	386	TYR	12.9
1	A	335	GLU	7.4
1	A	361	THR	6.9
1	A	360	ALA	6.6
1	A	433	ARG	6.5
1	A	320	ALA	6.3
1	A	382	TRP	6.1
1	A	282	LYS	5.9
1	A	312	ASN	5.8
1	A	657	PRO	5.8
1	A	318	ASP	5.7
1	A	373	HIS	5.7
1	A	340	VAL	5.6
1	A	364	PRO	5.6
1	A	277	LEU	5.5
1	A	296	ALA	5.4
1	A	397	ALA	5.4
1	A	861	ALA	5.3
1	A	663	GLY	5.2
1	A	315	TYR	5.1
1	A	387	SER	5.1
1	A	399	VAL	5.1
1	A	355	VAL	5.1
1	A	350	LEU	5.0
1	A	326	LEU	4.9
1	A	331	THR	4.8
1	A	283	VAL	4.8

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Mol	Chain	Res	Type	RSRZ
1	A	178	ALA	4.8
1	A	210	VAL	4.8
1	A	243	ILE	4.7
1	A	357	LEU	4.7
1	A	417	LEU	4.7
1	A	362	GLY	4.6
1	A	438	LEU	4.6
1	A	474	ALA	4.6
1	A	607	THR	4.5
1	A	650	ALA	4.5
1	A	367	VAL	4.5
1	A	647	ASP	4.5
1	A	328	ALA	4.4
1	A	659	TYR	4.4
1	A	366	LEU	4.4
1	A	213	GLY	4.4
1	A	322	PRO	4.3
1	A	466	ILE	4.3
1	A	437	VAL	4.3
1	A	648	LEU	4.2
1	A	284	ILE	4.2
1	A	603	ARG	4.1
1	A	390	GLU	4.1
1	A	374	ALA	4.1
1	A	339	HIS	4.1
1	A	756	ARG	4.0
1	A	420	THR	3.9
1	A	31	ARG	3.9
1	A	316	VAL	3.9
1	A	319	PRO	3.9
1	A	436	GLU	3.9
1	A	200	PRO	3.8
1	A	177	GLY	3.8
1	A	440	GLY	3.8
1	A	460	ARG	3.8
1	A	212	LEU	3.7
1	A	203	SER	3.7
1	A	273	LEU	3.7
1	A	181	ASP	3.6
1	A	202	PRO	3.6
1	A	219	VAL	3.6
1	A	646	ARG	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	410	LEU	3.6
1	A	776	CYS	3.5
1	A	408	ALA	3.5
1	A	730	GLN	3.5
1	A	29	HIS	3.5
1	A	77[A]	HIS	3.5
1	A	154[A]	CYS	3.4
1	A	310	ALA	3.4
1	A	123	ASP	3.4
1	A	141	ASP	3.4
1	A	435	ALA	3.4
1	A	183	PHE	3.3
1	A	851	ALA	3.3
1	A	712	LEU	3.3
1	A	455	ASP	3.3
1	A	139	ARG	3.2
1	A	267	GLU	3.2
1	A	332	ALA	3.2
1	A	468	ALA	3.2
1	A	344	GLY	3.2
1	A	343	ARG	3.1
1	A	479	PRO	3.1
1	A	463	ALA	3.1
1	A	476	PRO	3.1
1	A	369	PHE	3.1
1	A	95	ASN	3.0
1	A	234	ILE	3.0
1	A	406	LEU	3.0
1	A	354	ASN	3.0
1	A	480	PRO	3.0
1	A	32	GLY	3.0
1	A	313	GLY	3.0
1	A	475	PRO	3.0
1	A	393	ARG	2.9
1	A	330	ALA	2.9
1	A	211	LEU	2.9
1	A	432	ARG	2.9
1	A	276	ASP	2.9
1	A	414	ALA	2.9
1	A	352	PRO	2.9
1	A	184	TRP	2.9
1	A	363	ARG	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	403	TYR	2.9
1	A	471	PHE	2.9
1	A	281	PRO	2.9
1	A	381	GLY	2.9
1	A	230	VAL	2.9
1	A	280	VAL	2.9
1	A	15	ALA	2.8
1	A	274	LEU	2.8
1	A	698	LEU	2.8
1	A	238	ASP	2.8
1	A	338	ASP	2.8
1	A	317	ALA	2.8
1	A	449	LEU	2.8
1	A	472	THR	2.8
1	A	482	ALA	2.8
1	A	826	LEU	2.7
1	A	675	LEU	2.7
1	A	323	GLY	2.7
1	A	692	THR	2.7
1	A	795	ARG	2.7
1	A	216	TYR	2.6
1	A	662	CYS	2.6
1	A	385	GLY	2.6
1	A	665	VAL	2.6
1	A	464	ASP	2.6
1	A	28	ILE	2.6
1	A	478	PRO	2.6
1	A	411	PHE	2.6
1	A	38	ASP	2.5
1	A	669	LEU	2.5
1	A	269	TYR	2.5
1	A	34	TRP	2.5
1	A	557	ARG	2.5
1	A	816	PRO	2.5
1	A	228	GLY	2.5
1	A	377	PRO	2.5
1	A	345	VAL	2.5
1	A	434	ALA	2.5
1	A	383	THR	2.5
1	A	441	ARG	2.5
1	A	272	HIS	2.5
1	A	98	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	46	ARG	2.4
1	A	342	ARG	2.4
1	A	245	LYS	2.4
1	A	179	ALA	2.4
1	A	372	SER	2.4
1	A	817	GLU	2.4
1	A	803	ARG	2.4
1	A	749	ASP	2.4
1	A	833	TRP	2.4
1	A	656	PRO	2.4
1	A	356	VAL	2.4
1	A	415	THR	2.3
1	A	346	LEU	2.3
1	A	400	GLU	2.3
1	A	456	PRO	2.3
1	A	860	PRO	2.3
1	A	17	LEU	2.3
1	A	329	LEU	2.3
1	A	337	LEU	2.3
1	A	514	THR	2.3
1	A	384	PRO	2.3
1	A	291	ASP	2.3
1	A	396	PRO	2.3
1	A	643	LEU	2.3
1	A	462	ALA	2.2
1	A	96	HIS	2.2
1	A	416	GLY	2.2
1	A	125	ALA	2.2
1	A	199	HIS	2.2
1	A	477	PRO	2.2
1	A	262	LEU	2.2
1	A	668	THR	2.2
1	A	655	ASN	2.2
1	A	271	LEU	2.2
1	A	244	ILE	2.2
1	A	439	ALA	2.2
1	A	171	GLN	2.2
1	A	427	GLY	2.2
1	A	353	THR	2.1
1	A	765	LEU	2.1
1	A	341	HIS	2.1
1	A	128	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	380	TYR	2.1
1	A	3	HIS	2.1
1	A	679	VAL	2.1
1	A	201	ALA	2.1
1	A	621	LEU	2.1
1	A	51	ILE	2.1
1	A	371	ILE	2.1
1	A	180	ASP	2.1
1	A	336	LEU	2.1
1	A	705	LEU	2.1
1	A	263	ARG	2.0
1	A	358	ASP	2.0
1	A	30	ALA	2.0
1	A	375	GLU	2.0
1	A	97	PRO	2.0
1	A	388	PRO	2.0
1	A	853	PRO	2.0
1	A	58	ALA	2.0
1	A	25	GLY	2.0
1	A	522	ILE	2.0
1	A	459	ARG	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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($\text{\AA}^2$)	Q<0.9
3	NO3	A	1001	4/4	0.84	0.17	102,107,111,119	0
2	PO4	A	1000	5/5	0.91	0.15	73,84,96,103	0

6.5 Other polymers [i](#)

There are no such residues in this entry.