



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 6, 2023 – 01:33 pm GMT

PDB ID : 8CAR  
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](mailto: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>.

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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, CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

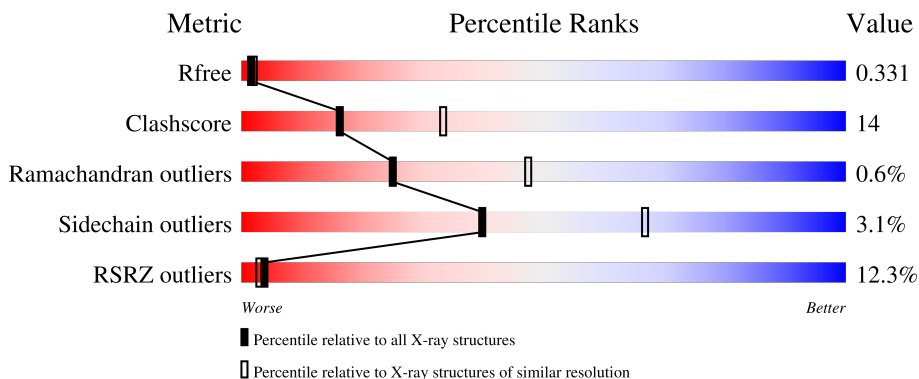
# 1 Overall quality at a glance

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))
$R_{free}$	130704	3863 (2.70-2.66)
Clashscore	141614	4210 (2.70-2.66)
Ramachandran outliers	138981	4141 (2.70-2.66)
Sidechain outliers	138945	4141 (2.70-2.66)
RSRZ outliers	127900	3780 (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  $\geq 3$ , 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	

## 2 Entry composition [i](#)

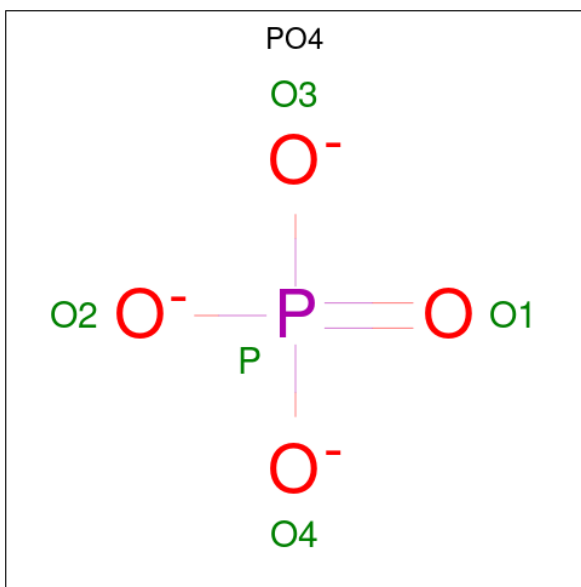
There are 4 unique types of molecules in this entry. The entry contains 12520 atoms, of which 6202 are hydrogens and 0 are deuteriums.

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
			Total	C	H	N	O	S	Se			
1	A	830	12510	3942	6202	1176	1167	13	10	0	3	0

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



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

- Molecule 3 is NITRATE ION (three-letter code: NO3) (formula: NO<sub>3</sub>).



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

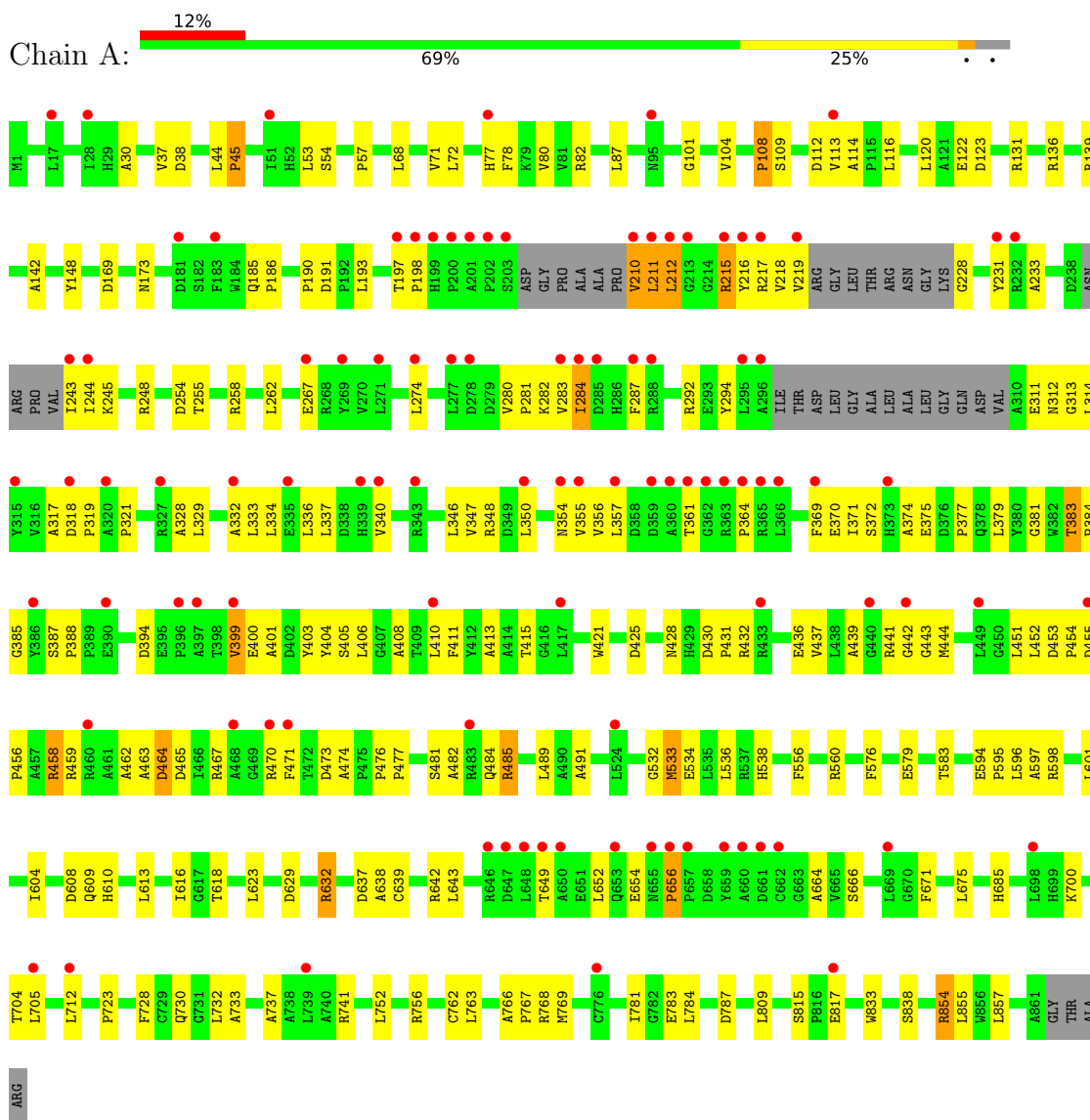
- Molecule 4 is water.

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

### 3 Residue-property plots i

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: Serine/threonine protein kinase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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) 99.8 (48.11-2.68)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.36 (at 2.69Å)	Xtrriage
Refinement program	PHENIX v1.20.1_4487	Depositor
R, $R_{free}$	0.297 , 0.337 0.289 , 0.331	Depositor DCC
$R_{free}$ test set	1130 reflections (2.18%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	87.3	Xtrriage
Anisotropy	0.178	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 84.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	12520	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	134.0	wwPDB-VP

Xtrriage'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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, NO3

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	0.30	0/6462	0.58	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 [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	6308	6202	6199	180	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	180	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 14.

All (180) 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:465:ASP:HB3	1:A:471:PHE:H	1.69	0.56
1:A:243:ILE:HD12	1:A:282:LYS:HZ1	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: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: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:464:ASP:CG	1:A:464:ASP:O	2.49	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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: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:430:ASP:CG	1:A:431:PRO:HD2	2.36	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: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
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:381:GLY:C	1:A:383:THR:N	2.70	0.44
1:A:425:ASP:HB3	1:A:428:ASN:CG	2.38	0.44
1:A:532:GLY:O	1:A:536:LEU:HG	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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: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:217:ARG:C	1:A:218:VAL:HG13	2.39	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:267:GLU:CD	1:A:370:GLU:HG2	2.39	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:456:PRO:C	1:A:458:ARG:H	2.23	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: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: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
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:131:ARG:NH2	1:A:292:ARG:NH2	2.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:401:ALA:C	1:A:403:TYR:N	2.75	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%)	25   47

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%)	619 (97%)	20 (3%)	40 67

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	210	VAL
1	A	211	LEU
1	A	212	LEU
1	A	215	ARG
1	A	284	ILE
1	A	383	THR
1	A	394	ASP
1	A	399	VAL
1	A	453	ASP
1	A	458	ARG
1	A	459	ARG
1	A	464	ASP
1	A	485	ARG
1	A	533	MSE
1	A	598	ARG
1	A	610	HIS
1	A	632	ARG
1	A	783	GLU
1	A	784	LEU
1	A	854	ARG

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

### 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 monosaccharides 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	0.90	0	6,6,6	0.56	0
3	NO3	A	1001	-	1,3,3	0.67	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	820/865 (94%)	0.90	101 (12%) <b>4</b> <b>3</b>	60, 111, 204, 294	0

All (101) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	361	THR	10.0
1	A	661	ASP	9.1
1	A	201	ALA	8.4
1	A	202	PRO	8.2
1	A	373	HIS	8.1
1	A	243	ILE	7.9
1	A	200	PRO	7.7
1	A	360	ALA	7.5
1	A	212	LEU	7.5
1	A	340	VAL	7.4
1	A	660	ALA	7.3
1	A	199	HIS	7.2
1	A	662	CYS	6.8
1	A	386	TYR	6.7
1	A	231	TYR	6.5
1	A	318	ASP	6.4
1	A	647	ASP	6.2
1	A	646	ARG	6.0
1	A	471	PHE	5.9
1	A	364	PRO	5.7
1	A	433	ARG	5.3
1	A	357	LEU	5.3
1	A	277	LEU	4.9
1	A	657	PRO	4.8
1	A	350	LEU	4.8
1	A	211	LEU	4.6
1	A	295	LEU	4.6

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	271	LEU	4.5
1	A	365	ARG	4.5
1	A	339	HIS	4.4
1	A	213	GLY	4.3
1	A	363	ARG	4.2
1	A	468	ALA	4.2
1	A	217	ARG	4.2
1	A	366	LEU	4.0
1	A	267	GLU	4.0
1	A	712	LEU	3.9
1	A	656	PRO	3.8
1	A	355	VAL	3.8
1	A	327	ARG	3.6
1	A	285	ASP	3.6
1	A	354	ASN	3.5
1	A	335	GLU	3.5
1	A	648	LEU	3.5
1	A	776	CYS	3.4
1	A	287	PHE	3.4
1	A	653	GLN	3.4
1	A	669	LEU	3.4
1	A	244	ILE	3.4
1	A	397	ALA	3.3
1	A	203	SER	3.3
1	A	362	GLY	3.3
1	A	817	GLU	3.3
1	A	216	TYR	3.2
1	A	650	ALA	3.2
1	A	198	PRO	3.1
1	A	417	LEU	3.1
1	A	296	ALA	3.1
1	A	705	LEU	3.1
1	A	232	ARG	3.1
1	A	278	ASP	3.1
1	A	659	TYR	3.0
1	A	283	VAL	3.0
1	A	369	PHE	3.0
1	A	215	ARG	2.9
1	A	442	GLY	2.8
1	A	483	ARG	2.8
1	A	460	ARG	2.8
1	A	219	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	181	ASP	2.7
1	A	210	VAL	2.7
1	A	655	ASN	2.7
1	A	410	LEU	2.6
1	A	649	THR	2.5
1	A	269	TYR	2.5
1	A	28	ILE	2.5
1	A	274	LEU	2.5
1	A	332	ALA	2.5
1	A	390	GLU	2.5
1	A	17	LEU	2.5
1	A	399	VAL	2.5
1	A	449	LEU	2.4
1	A	183	PHE	2.4
1	A	455	ASP	2.4
1	A	470	ARG	2.4
1	A	284	ILE	2.4
1	A	440	GLY	2.4
1	A	315	TYR	2.3
1	A	698	LEU	2.3
1	A	95	ASN	2.3
1	A	288	ARG	2.3
1	A	77[A]	HIS	2.2
1	A	359	ASP	2.2
1	A	739	LEU	2.2
1	A	113	VAL	2.1
1	A	51	ILE	2.1
1	A	197	THR	2.1
1	A	320	ALA	2.1
1	A	343	ARG	2.0
1	A	396	PRO	2.0
1	A	524	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, 95<sup>th</sup> 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	0.30	102,107,111,119	0
2	PO4	A	1000	5/5	0.91	0.17	73,84,96,103	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.