



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 09:52 pm GMT

PDB ID : 2ZT8  
Title : Crystal structure of human Glycyl-tRNA synthetase (GlyRS) in complex with Gly-AMP analog  
Authors : Guo, R.T.; Yang, X.L.; Schimmel, P.  
Deposited on : 2008-09-19  
Resolution : 3.35 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

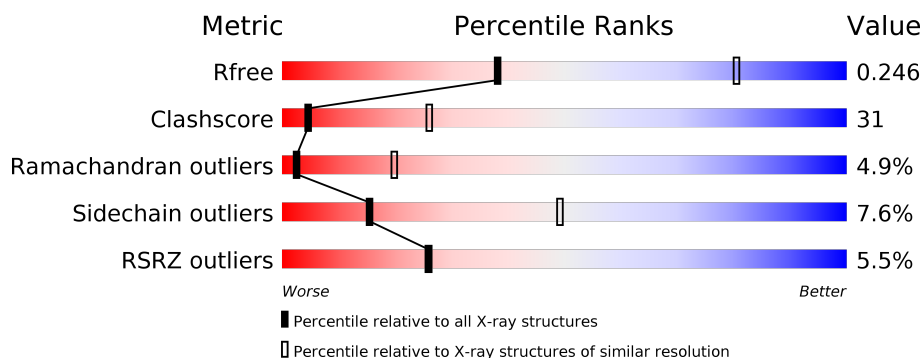
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.35 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))
$R_{free}$	100719	1156 (3.42-3.30)
Clashscore	112137	1231 (3.42-3.30)
Ramachandran outliers	110173	1212 (3.42-3.30)
Sidechain outliers	110143	1211 (3.42-3.30)
RSRZ outliers	101464	1165 (3.42-3.30)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	693	<div> <div>4%</div> <div>35%</div> <div>36%</div> <div>5%</div> <div>24%</div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4317 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.

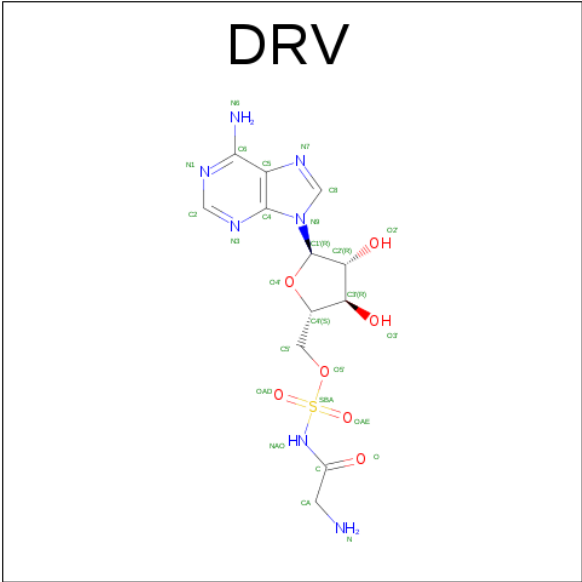
- Molecule 1 is a protein called Glycyl-tRNA synthetase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	530	4228	2689	728	787	24	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	686	LEU	-	EXPRESSION TAG	UNP P41250
A	687	GLU	-	EXPRESSION TAG	UNP P41250
A	688	HIS	-	EXPRESSION TAG	UNP P41250
A	689	HIS	-	EXPRESSION TAG	UNP P41250
A	690	HIS	-	EXPRESSION TAG	UNP P41250
A	691	HIS	-	EXPRESSION TAG	UNP P41250
A	692	HIS	-	EXPRESSION TAG	UNP P41250
A	693	HIS	-	EXPRESSION TAG	UNP P41250

- Molecule 2 is [(2S,3R,4R,5R)-5-(6-AMINO-9H-PURIN-9-YL)-3,4-DIHYDROXYTETRAHYDROFURAN-2-YL]METHYL (AMINOACETYL)SULFAMATE (three-letter code: DRV) (formula: C<sub>12</sub>H<sub>17</sub>N<sub>7</sub>O<sub>7</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			27	12	7	7	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	62	Total	O	0	0
			62	62		



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	119.60Å 138.26Å 132.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.35 47.87 – 3.29	Depositor EDS
% Data completeness (in resolution range)	92.9 (50.00-3.35) 89.5 (47.87-3.29)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.57 (at 3.25Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.221 , 0.246 0.221 , 0.246	Depositor DCC
$R_{free}$ test set	743 reflections (4.95%)	DCC
Wilson B-factor (Å <sup>2</sup> )	97.3	Xtriage
Anisotropy	0.795	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 94.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	4317	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	132.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.30% 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: DRV

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	0.27	0/4326	0.56	0/5847

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	4228	0	4145	261	0
2	A	27	0	17	6	0
3	A	62	0	0	0	1
All	All	4317	0	4162	262	1

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 31.

All (262) 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:265:LEU:HD21	1:A:518:PRO:HG3	1.49	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:381:ASN:H	1:A:381:ASN:HD22	1.15	0.92
1:A:132:GLU:HB3	1:A:133:PRO:HD3	1.50	0.91
1:A:126:CYS:H	1:A:271:GLN:NE2	1.68	0.89
1:A:148:MET:HB2	1:A:280:ILE:HD13	1.53	0.88
1:A:194:ASN:HD21	1:A:379:MET:CB	1.87	0.87
1:A:617:THR:HB	1:A:631:THR:HB	1.57	0.86
1:A:194:ASN:HD21	1:A:379:MET:HB3	1.40	0.86
1:A:213:ILE:HD12	1:A:214:THR:HG22	1.59	0.85
1:A:567:LEU:HD13	1:A:619:ASP:HA	1.59	0.84
1:A:194:ASN:HD22	1:A:381:ASN:ND2	1.74	0.84
1:A:645:ILE:HA	1:A:648:LEU:HD12	1.58	0.84
1:A:194:ASN:HD22	1:A:381:ASN:HD21	1.22	0.82
1:A:258:LEU:HG	1:A:263:GLY:HA2	1.58	0.82
1:A:153:LYS:HG3	1:A:216:ASN:ND2	1.95	0.81
1:A:91:SER:HB2	1:A:282:PRO:HG2	1.63	0.80
1:A:664:ASP:HB3	1:A:668:ARG:NH1	1.98	0.79
1:A:607:THR:HG23	1:A:612:VAL:HB	1.64	0.79
1:A:410:ARG:HD3	1:A:414:ASP:OD2	1.85	0.76
1:A:214:THR:HG23	1:A:216:ASN:OD1	1.86	0.75
1:A:411:SER:O	1:A:413:TYR:N	2.19	0.75
1:A:565:LEU:HD12	1:A:565:LEU:O	1.86	0.74
1:A:145:ALA:HB2	1:A:225:ASN:HA	1.70	0.73
1:A:526:GLY:HA3	2:A:699:DRV:O2'	1.91	0.71
1:A:306:LYS:HD3	1:A:349:ASN:ND2	2.06	0.70
1:A:381:ASN:ND2	1:A:381:ASN:H	1.88	0.70
1:A:230:THR:HG23	1:A:231:PHE:N	2.08	0.69
1:A:229:LYS:HD3	1:A:230:THR:N	2.06	0.69
1:A:194:ASN:ND2	1:A:381:ASN:ND2	2.41	0.68
1:A:574:MET:HB2	1:A:575:PRO:HD3	1.77	0.67
1:A:641:ILE:HD13	1:A:671:LEU:HA	1.77	0.66
1:A:668:ARG:HG3	1:A:668:ARG:HH11	1.60	0.66
1:A:211:SER:H	1:A:218:LEU:HD13	1.61	0.65
1:A:322:TYR:CE2	1:A:327:GLN:HG2	2.31	0.65
1:A:648:LEU:O	1:A:652:VAL:HG23	1.96	0.65
1:A:67:ARG:O	1:A:71:GLU:HG3	1.96	0.65
1:A:147:PHE:HA	1:A:222:VAL:O	1.97	0.64
1:A:337:ARG:NH1	1:A:339:GLY:HA3	2.12	0.64
1:A:633:ARG:HB2	1:A:640:GLN:HG2	1.80	0.64
1:A:119:GLU:HB2	1:A:121:ILE:HG13	1.79	0.64
1:A:287:ILE:HD11	1:A:532:TYR:CD2	2.33	0.63
1:A:165:LYS:O	1:A:169:GLN:HG3	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:194:ASN:HD21	1:A:379:MET:HB2	1.64	0.62
1:A:206:ASN:N	1:A:206:ASN:HD22	1.98	0.62
1:A:262:GLN:O	1:A:264:LYS:HD3	2.00	0.62
1:A:404:ILE:HG13	1:A:405:VAL:HG23	1.81	0.62
1:A:411:SER:C	1:A:413:TYR:H	2.02	0.62
1:A:293:THR:HG22	1:A:527:LEU:HD12	1.81	0.61
1:A:381:ASN:N	1:A:381:ASN:HD22	1.83	0.61
1:A:230:THR:CG2	1:A:231:PHE:N	2.62	0.61
1:A:284:SER:HB2	1:A:288:ARG:HB2	1.82	0.61
1:A:311:PHE:HE1	1:A:353:GLY:HA3	1.64	0.61
1:A:348:ASN:HD22	1:A:348:ASN:C	2.04	0.61
1:A:169:GLN:HA	1:A:172:MET:HE2	1.82	0.61
1:A:396:LYS:HG2	1:A:401:TRP:CE2	2.35	0.61
1:A:598:GLY:HA3	1:A:602:ARG:HD3	1.82	0.61
1:A:381:ASN:N	1:A:381:ASN:ND2	2.45	0.61
1:A:513:VAL:HG23	1:A:513:VAL:O	2.02	0.60
1:A:124:ILE:O	1:A:271:GLN:HG2	2.01	0.60
1:A:154:ASN:HD22	1:A:154:ASN:N	1.99	0.60
1:A:134:VAL:HG13	1:A:252:LEU:HD11	1.84	0.59
1:A:546:GLU:O	1:A:547:GLN:HB2	2.00	0.59
1:A:637:SER:HB2	1:A:639:ARG:HG3	1.83	0.59
1:A:544:GLY:O	1:A:546:GLU:N	2.35	0.59
1:A:279:GLU:HG2	1:A:288:ARG:HD3	1.84	0.59
1:A:148:MET:HB2	1:A:280:ILE:CD1	2.30	0.59
1:A:323:SER:O	1:A:327:GLN:HG3	2.02	0.59
1:A:348:ASN:C	1:A:348:ASN:ND2	2.56	0.58
1:A:211:SER:HB3	1:A:216:ASN:H	1.67	0.58
1:A:338:LEU:O	1:A:342:VAL:HG23	2.03	0.58
1:A:65:VAL:HG22	1:A:66:ASP:H	1.69	0.58
1:A:308:HIS:HB2	1:A:351:VAL:HA	1.86	0.58
1:A:148:MET:O	1:A:222:VAL:HG22	2.04	0.57
1:A:219:SER:HB2	1:A:220:PRO:HD2	1.84	0.57
1:A:631:THR:HG21	1:A:640:GLN:NE2	2.19	0.57
1:A:552:SER:HA	1:A:635:ARG:NH2	2.19	0.57
1:A:165:LYS:HG3	1:A:189:LEU:HD22	1.86	0.57
1:A:134:VAL:CG1	1:A:252:LEU:HD11	2.35	0.57
1:A:552:SER:HA	1:A:635:ARG:CZ	2.35	0.57
1:A:64:ILE:HD12	1:A:64:ILE:N	2.19	0.57
1:A:132:GLU:HB3	1:A:133:PRO:CD	2.30	0.57
1:A:540:HIS:HB2	1:A:550:PHE:CE1	2.40	0.56
1:A:287:ILE:HD12	1:A:402:ILE:HD12	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:620:PHE:HB3	1:A:624:ASN:ND2	2.20	0.56
1:A:86:ILE:HG13	1:A:87:TYR:CD1	2.40	0.56
1:A:364:THR:HG22	1:A:365:LYS:N	2.21	0.56
1:A:578:LYS:HE2	1:A:582:GLU:OE1	2.06	0.56
1:A:213:ILE:O	1:A:213:ILE:HD12	2.06	0.56
1:A:208:ASN:HD21	1:A:210:LYS:HD2	1.70	0.56
1:A:306:LYS:HD3	1:A:349:ASN:HD22	1.70	0.55
1:A:410:ARG:HG3	1:A:520:VAL:HG13	1.88	0.55
1:A:154:ASN:HD22	1:A:154:ASN:H	1.54	0.55
1:A:83:ALA:HA	1:A:95:ASP:OD2	2.06	0.55
1:A:243:ARG:HG3	1:A:243:ARG:O	2.07	0.55
1:A:152:VAL:HG23	1:A:217:ASP:O	2.07	0.54
1:A:104:LYS:O	1:A:108:ILE:HG13	2.08	0.54
1:A:616:VAL:HA	1:A:631:THR:O	2.07	0.54
1:A:522:GLU:OE2	2:A:699:DRV:HA	2.08	0.54
1:A:169:GLN:HA	1:A:172:MET:CE	2.38	0.54
1:A:230:THR:HG23	1:A:231:PHE:H	1.72	0.54
1:A:348:ASN:ND2	1:A:349:ASN:N	2.56	0.54
1:A:659:ASN:O	1:A:660:ILE:HD12	2.08	0.54
1:A:343:GLU:C	1:A:345:GLY:H	2.11	0.54
1:A:206:ASN:H	1:A:206:ASN:ND2	2.06	0.54
1:A:526:GLY:O	1:A:530:ILE:HG13	2.07	0.54
1:A:153:LYS:HG3	1:A:216:ASN:HD22	1.71	0.53
1:A:311:PHE:CE1	1:A:353:GLY:HA3	2.43	0.53
1:A:547:GLN:HA	1:A:547:GLN:OE1	2.07	0.53
1:A:116:ILE:HA	1:A:121:ILE:HB	1.89	0.53
1:A:308:HIS:CE1	1:A:310:LYS:HB2	2.43	0.53
1:A:337:ARG:HH12	1:A:339:GLY:HA3	1.71	0.53
1:A:164:LEU:O	1:A:164:LEU:HD22	2.08	0.53
1:A:321:LEU:HD23	1:A:375:PHE:HB2	1.90	0.53
1:A:314:VAL:O	1:A:338:LEU:HD12	2.08	0.53
1:A:194:ASN:ND2	1:A:379:MET:HB2	2.23	0.52
1:A:114:HIS:CD2	1:A:362:TYR:HB2	2.44	0.52
1:A:65:VAL:HG22	1:A:66:ASP:N	2.24	0.52
1:A:206:ASN:N	1:A:206:ASN:ND2	2.55	0.52
1:A:152:VAL:HG12	1:A:152:VAL:O	2.09	0.52
1:A:360:TYR:O	1:A:364:THR:HB	2.08	0.52
1:A:159:ARG:HD3	1:A:162:HIS:CE1	2.44	0.52
1:A:211:SER:N	1:A:218:LEU:HD13	2.25	0.52
1:A:661:THR:HG22	1:A:663:ALA:H	1.74	0.52
1:A:126:CYS:H	1:A:271:GLN:HE21	1.53	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:261:ASN:O	1:A:262:GLN:HB2	2.10	0.52
1:A:322:TYR:HD2	1:A:376:ARG:HG3	1.73	0.52
1:A:151:ASP:HB2	1:A:216:ASN:HB2	1.92	0.51
1:A:340:ASP:HA	1:A:343:GLU:HG3	1.92	0.51
1:A:633:ARG:NH2	1:A:638:MET:HG2	2.26	0.51
1:A:119:GLU:HB2	1:A:121:ILE:CG1	2.41	0.51
1:A:154:ASN:H	1:A:154:ASN:ND2	2.07	0.51
1:A:314:VAL:HG21	1:A:354:TYR:HA	1.92	0.51
1:A:583:ALA:HA	1:A:586:ARG:CZ	2.41	0.51
1:A:602:ARG:O	1:A:605:ALA:HB3	2.11	0.50
1:A:211:SER:O	1:A:215:GLY:HA2	2.11	0.50
1:A:318:HIS:HA	1:A:336:MET:O	2.12	0.50
1:A:69:LYS:HE3	1:A:549:THR:CG2	2.41	0.50
1:A:429:GLU:HA	1:A:514:GLU:O	2.12	0.50
1:A:637:SER:O	1:A:638:MET:HB2	2.11	0.50
1:A:145:ALA:CB	1:A:225:ASN:HA	2.41	0.50
1:A:348:ASN:OD1	1:A:349:ASN:ND2	2.45	0.49
1:A:651:ILE:HG22	1:A:655:LEU:HD12	1.94	0.49
1:A:297:ILE:HB	1:A:523:PRO:HD2	1.94	0.49
1:A:318:HIS:CE1	1:A:337:ARG:HB2	2.47	0.49
1:A:514:GLU:HG2	1:A:515:GLU:N	2.28	0.49
1:A:366:VAL:HG12	1:A:534:VAL:HG21	1.93	0.49
1:A:396:LYS:HG2	1:A:401:TRP:CD2	2.47	0.49
1:A:661:THR:HG22	1:A:662:TRP:N	2.28	0.49
1:A:265:LEU:HD21	1:A:518:PRO:CG	2.32	0.48
1:A:105:ASN:O	1:A:109:GLN:HB2	2.13	0.48
1:A:544:GLY:O	1:A:545:ASP:C	2.51	0.48
1:A:596:SER:HB2	1:A:606:ARG:NH1	2.29	0.48
1:A:86:ILE:HG13	1:A:87:TYR:HD1	1.78	0.48
1:A:626:THR:HA	1:A:627:PRO:C	2.34	0.48
1:A:631:THR:HG23	1:A:640:GLN:HB3	1.95	0.48
1:A:305:GLU:O	1:A:307:ASP:N	2.41	0.47
1:A:348:ASN:CG	1:A:349:ASN:N	2.65	0.47
1:A:213:ILE:CD1	1:A:214:THR:HG22	2.35	0.47
1:A:368:ILE:HG23	1:A:537:HIS:ND1	2.29	0.47
1:A:631:THR:CG2	1:A:640:GLN:HB3	2.44	0.47
1:A:669:TYR:HB3	1:A:670:PRO:HD2	1.96	0.47
1:A:145:ALA:HB1	1:A:224:PHE:O	2.14	0.47
1:A:154:ASN:N	1:A:154:ASN:ND2	2.63	0.47
1:A:582:GLU:O	1:A:586:ARG:HG3	2.15	0.47
1:A:618:ILE:HG23	1:A:622:THR:HG21	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:149:VAL:HG13	1:A:160:ALA:HB2	1.96	0.47
1:A:163:LEU:HD13	1:A:218:LEU:HD21	1.96	0.47
1:A:135:LEU:HD13	1:A:227:MET:SD	2.55	0.47
1:A:165:LYS:HB2	1:A:192:LEU:CD1	2.45	0.47
1:A:428:ALA:O	1:A:515:GLU:HA	2.15	0.46
1:A:594:ASP:OD2	1:A:595:ASP:N	2.48	0.46
1:A:306:LYS:NZ	1:A:519:ASN:HD22	2.14	0.46
1:A:108:ILE:HG12	1:A:527:LEU:HD13	1.96	0.46
1:A:147:PHE:CD1	1:A:200:LEU:HD13	2.51	0.45
1:A:378:HIS:HB2	1:A:383:MET:HE3	1.97	0.45
1:A:210:LYS:NZ	1:A:210:LYS:HB3	2.32	0.45
1:A:630:ALA:HB3	1:A:648:LEU:CD1	2.47	0.45
1:A:363:LEU:HB3	1:A:368:ILE:HD12	1.99	0.45
1:A:409:ASP:OD1	1:A:409:ASP:O	2.34	0.45
1:A:231:PHE:CE2	1:A:239:PRO:HB3	2.51	0.45
1:A:289:VAL:HG23	1:A:292:PHE:HD1	1.82	0.45
1:A:306:LYS:NZ	1:A:519:ASN:ND2	2.64	0.45
1:A:194:ASN:ND2	1:A:379:MET:CB	2.67	0.45
1:A:372:LYS:HB2	1:A:537:HIS:CE1	2.52	0.45
1:A:646:SER:O	1:A:649:PRO:HD2	2.17	0.44
1:A:368:ILE:HG23	1:A:537:HIS:CE1	2.52	0.44
1:A:147:PHE:O	1:A:160:ALA:N	2.50	0.44
1:A:393:ALA:O	1:A:404:ILE:HG12	2.17	0.44
1:A:564:VAL:O	1:A:593:VAL:HA	2.18	0.44
1:A:114:HIS:HD2	1:A:115:PHE:CE1	2.35	0.44
1:A:600:ILE:HG23	1:A:601:GLY:N	2.33	0.44
1:A:579:GLU:OE2	1:A:579:GLU:HA	2.18	0.44
1:A:79:PHE:O	1:A:100:GLY:HA3	2.18	0.44
1:A:277:ARG:O	1:A:279:GLU:N	2.50	0.44
1:A:343:GLU:O	1:A:345:GLY:N	2.51	0.44
1:A:277:ARG:NH2	2:A:699:DRV:H8	2.33	0.44
1:A:214:THR:O	1:A:215:GLY:C	2.57	0.44
1:A:224:PHE:HD2	1:A:280:ILE:HG12	1.83	0.44
1:A:641:ILE:HD11	1:A:666:GLU:HG2	2.00	0.44
1:A:561:LYS:HD3	1:A:656:ALA:CB	2.48	0.43
1:A:668:ARG:NH1	1:A:668:ARG:HG3	2.30	0.43
1:A:311:PHE:CD2	1:A:311:PHE:C	2.92	0.43
1:A:124:ILE:HD11	1:A:250:ILE:HG12	1.99	0.43
1:A:311:PHE:CD1	1:A:350:THR:HB	2.54	0.43
1:A:562:CYS:SG	1:A:563:SER:N	2.91	0.43
1:A:595:ASP:O	1:A:596:SER:C	2.56	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:664:ASP:HB3	1:A:668:ARG:CZ	2.48	0.43
1:A:118:GLU:HG2	1:A:358:ARG:NH1	2.33	0.43
1:A:151:ASP:OD2	1:A:153:LYS:HB2	2.19	0.43
1:A:210:LYS:NZ	1:A:215:GLY:O	2.52	0.43
1:A:336:MET:CE	1:A:341:ALA:HA	2.49	0.43
1:A:341:ALA:O	1:A:346:VAL:HB	2.19	0.43
1:A:231:PHE:CD2	1:A:239:PRO:HB3	2.54	0.43
1:A:573:PHE:CD1	1:A:573:PHE:N	2.87	0.43
1:A:245:GLU:HB2	2:A:699:DRV:HN	1.83	0.43
2:A:699:DRV:O4'	2:A:699:DRV:OAE	2.36	0.43
1:A:567:LEU:N	1:A:567:LEU:HD12	2.33	0.43
1:A:306:LYS:HZ1	1:A:519:ASN:HD22	1.67	0.43
1:A:145:ALA:HB1	1:A:224:PHE:C	2.38	0.43
1:A:657:ASN:HD22	1:A:657:ASN:N	2.17	0.42
1:A:322:TYR:CD1	1:A:333:ALA:HB2	2.54	0.42
1:A:645:ILE:O	1:A:645:ILE:HG12	2.19	0.42
1:A:118:GLU:HG3	1:A:118:GLU:O	2.18	0.42
1:A:525:PHE:N	1:A:525:PHE:CD1	2.87	0.42
1:A:182:LYS:O	1:A:186:GLU:HG3	2.19	0.42
1:A:306:LYS:O	1:A:349:ASN:HB2	2.19	0.42
1:A:320:TYR:CE1	1:A:335:LYS:HD2	2.55	0.42
1:A:224:PHE:CD2	1:A:280:ILE:HG12	2.54	0.42
1:A:542:ARG:HG3	1:A:548:ARG:HB2	2.02	0.42
1:A:138:SER:O	1:A:385:HIS:HE1	2.02	0.42
1:A:210:LYS:O	1:A:211:SER:C	2.58	0.42
1:A:296:GLU:OE2	2:A:699:DRV:N	2.53	0.42
1:A:318:HIS:ND1	1:A:337:ARG:HB2	2.35	0.42
1:A:560:PHE:O	1:A:612:VAL:HG13	2.20	0.42
1:A:211:SER:N	1:A:218:LEU:CD1	2.83	0.42
1:A:374:ARG:HD3	1:A:401:TRP:CH2	2.55	0.42
1:A:567:LEU:HD13	1:A:619:ASP:CA	2.41	0.41
1:A:79:PHE:CE2	1:A:610:ILE:HG22	2.55	0.41
1:A:651:ILE:HD11	1:A:669:TYR:CZ	2.55	0.41
1:A:247:ALA:HB1	1:A:251:PHE:CE2	2.56	0.41
1:A:648:LEU:HB2	1:A:649:PRO:HD3	2.03	0.41
1:A:201:ALA:HA	1:A:221:PRO:HG3	2.03	0.41
1:A:111:TRP:CH2	1:A:295:ALA:HB1	2.56	0.41
1:A:261:ASN:OD1	1:A:261:ASN:O	2.39	0.41
1:A:343:GLU:C	1:A:345:GLY:N	2.73	0.41
1:A:79:PHE:HA	1:A:99:VAL:HG23	2.02	0.41
1:A:220:PRO:O	1:A:222:VAL:HG13	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:560:PHE:CE2	1:A:592:LYS:HD2	2.56	0.41
1:A:606:ARG:O	1:A:609:GLU:HB2	2.19	0.41
1:A:165:LYS:HA	1:A:189:LEU:HD21	2.03	0.41
1:A:194:ASN:ND2	1:A:381:ASN:HD21	2.01	0.41
1:A:532:TYR:O	1:A:535:PHE:HB2	2.20	0.41
1:A:561:LYS:HD3	1:A:656:ALA:HB1	2.03	0.41
1:A:159:ARG:NH1	1:A:288:ARG:NH2	2.70	0.40
1:A:580:LEU:O	1:A:584:LEU:HG	2.21	0.40
1:A:151:ASP:HA	1:A:218:LEU:HA	2.03	0.40
1:A:339:GLY:O	1:A:343:GLU:HG2	2.21	0.40
1:A:151:ASP:OD2	1:A:154:ASN:ND2	2.54	0.40
1:A:242:LEU:HB3	1:A:276:PHE:CD1	2.56	0.40
1:A:375:PHE:HA	1:A:392:ASP:O	2.21	0.40
1:A:210:LYS:HB3	1:A:210:LYS:HZ3	1.85	0.40
1:A:338:LEU:HD23	1:A:338:LEU:HA	1.89	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:759:HOH:O	3:A:759:HOH:O[3_555]	2.19	0.01

## 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	526/693 (76%)	431 (82%)	69 (13%)	26 (5%)	2	20

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	215	GLY

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Mol	Chain	Res	Type
1	A	348	ASN
1	A	412	CYS
1	A	545	ASP
1	A	624	ASN
1	A	86	ILE
1	A	132	GLU
1	A	323	SER
1	A	330	GLY
1	A	344	GLN
1	A	410	ARG
1	A	421	ALA
1	A	191	GLN
1	A	278	ASN
1	A	547	GLN
1	A	570	ASN
1	A	596	SER
1	A	671	LEU
1	A	546	GLU
1	A	161	ASP
1	A	306	LYS
1	A	312	GLN
1	A	420	ARG
1	A	68	ALA
1	A	98	PRO
1	A	152	VAL

### 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	460/600 (77%)	425 (92%)	35 (8%)	15	49

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	64	ILE

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Mol	Chain	Res	Type
1	A	98	PRO
1	A	154	ASN
1	A	163	LEU
1	A	164	LEU
1	A	170	LYS
1	A	191	GLN
1	A	200	LEU
1	A	204	PHE
1	A	206	ASN
1	A	217	ASP
1	A	218	LEU
1	A	230	THR
1	A	237	ASN
1	A	255	LYS
1	A	259	GLU
1	A	264	LYS
1	A	288	ARG
1	A	307	ASP
1	A	319	LEU
1	A	348	ASN
1	A	364	THR
1	A	379	MET
1	A	381	ASN
1	A	383	MET
1	A	396	LYS
1	A	415	LEU
1	A	517	VAL
1	A	545	ASP
1	A	556	VAL
1	A	570	ASN
1	A	621	ASP
1	A	644	GLU
1	A	655	LEU
1	A	660	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	105	ASN
1	A	106	ASN
1	A	154	ASN
1	A	169	GLN

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Mol	Chain	Res	Type
1	A	191	GLN
1	A	194	ASN
1	A	197	GLN
1	A	206	ASN
1	A	208	ASN
1	A	261	ASN
1	A	271	GLN
1	A	278	ASN
1	A	299	HIS
1	A	381	ASN
1	A	519	ASN
1	A	624	ASN
1	A	640	GLN
1	A	657	ASN
1	A	659	ASN

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

1 ligand is 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	DRV	A	699	-	25,29,29	3.69	6 (24%)	28,43,43	3.10	8 (28%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	DRV	A	699	-	-	0/12/33/33	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	699	DRV	O5'-SBA	-11.15	1.43	1.59
2	A	699	DRV	C-NAO	-2.59	1.33	1.38
2	A	699	DRV	O4'-C1'	2.30	1.44	1.41
2	A	699	DRV	SBA-NAO	3.21	1.63	1.59
2	A	699	DRV	OAD-SBA	9.59	1.50	1.42
2	A	699	DRV	OAE-SBA	9.73	1.50	1.42

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	699	DRV	OAE-SBA-OAD	-11.72	109.32	121.30
2	A	699	DRV	N3-C2-N1	-8.19	121.72	128.86
2	A	699	DRV	C4'-O4'-C1'	-3.08	106.49	109.77
2	A	699	DRV	C2'-C3'-C4'	-2.74	97.29	102.62
2	A	699	DRV	C-NAO-SBA	-2.58	119.93	124.23
2	A	699	DRV	C4-C5-N7	-2.05	107.43	109.41
2	A	699	DRV	O5'-C5'-C4'	2.08	111.64	107.67
2	A	699	DRV	O-C-NAO	3.65	123.95	121.56

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	699	DRV	6	0

## 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	530/693 (76%)	0.42	29 (5%) 26 26	94, 133, 163, 172	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	512	TYR	5.9
1	A	218	LEU	3.9
1	A	274	ASN	3.5
1	A	293	THR	3.3
1	A	541	VAL	3.2
1	A	518	PRO	3.1
1	A	513	VAL	2.9
1	A	347	ILE	2.8
1	A	126	CYS	2.7
1	A	521	ILE	2.7
1	A	125	ASP	2.6
1	A	549	THR	2.6
1	A	618	ILE	2.5
1	A	672	PHE	2.5
1	A	209	VAL	2.5
1	A	319	LEU	2.4
1	A	567	LEU	2.4
1	A	300	PHE	2.3
1	A	273	GLY	2.3
1	A	427	VAL	2.3
1	A	346	VAL	2.2
1	A	164	LEU	2.1
1	A	207	TYR	2.1
1	A	175	LYS	2.1
1	A	566	PRO	2.1
1	A	338	LEU	2.1
1	A	662	TRP	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	212	PRO	2.0
1	A	640	GLN	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	DRV	A	699	27/27	0.95	0.32	0.21	108,111,115,116	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.