



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 02:23 am GMT

PDB ID : 3SS3  
Title : Crystal structure of mouse Glutaminase C, ligand-free form  
Authors : Ambrosio, A.L.B.; Dias, S.M.G.; Cerione, R.A.  
Deposited on : 2011-07-07  
Resolution : 2.42 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  
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

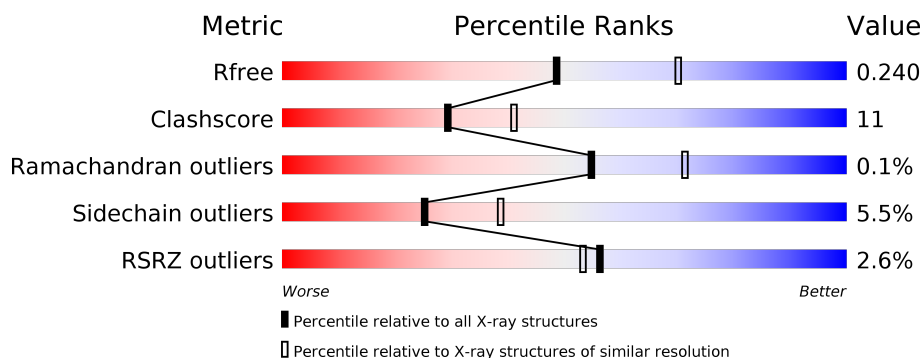
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.42 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	3709 (2.44-2.40)
Clashscore	112137	4241 (2.44-2.40)
Ramachandran outliers	110173	4178 (2.44-2.40)
Sidechain outliers	110143	4179 (2.44-2.40)
RSRZ outliers	101464	3740 (2.44-2.40)

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	479	<div> <div>2%</div> <div> <div></div> <div>66%</div> <div>14%</div> <div>•</div> <div>18%</div> </div> </div>
1	B	479	<div> <div>3%</div> <div> <div></div> <div>65%</div> <div>15%</div> <div>•</div> <div>19%</div> </div> </div>
1	C	479	<div> <div>%</div> <div> <div></div> <div>61%</div> <div>18%</div> <div>•</div> <div>20%</div> </div> </div>
1	D	479	<div> <div>3%</div> <div> <div></div> <div>62%</div> <div>17%</div> <div>•</div> <div>20%</div> </div> </div>

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 13253 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 Glutaminase C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	394	Total	C	N	O	S	3	0	0
			3083	1970	519	566	28			
1	B	390	Total	C	N	O	S	1	0	0
			3050	1948	515	559	28			
1	C	383	Total	C	N	O	S	1	0	0
			2996	1912	506	550	28			
1	D	385	Total	C	N	O	S	1	0	0
			3015	1925	509	553	28			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	125	GLY	-	EXPRESSION TAG	UNP Q69ZX9
A	126	SER	-	EXPRESSION TAG	UNP Q69ZX9
A	127	HIS	-	EXPRESSION TAG	UNP Q69ZX9
B	125	GLY	-	EXPRESSION TAG	UNP Q69ZX9
B	126	SER	-	EXPRESSION TAG	UNP Q69ZX9
B	127	HIS	-	EXPRESSION TAG	UNP Q69ZX9
C	125	GLY	-	EXPRESSION TAG	UNP Q69ZX9
C	126	SER	-	EXPRESSION TAG	UNP Q69ZX9
C	127	HIS	-	EXPRESSION TAG	UNP Q69ZX9
D	125	GLY	-	EXPRESSION TAG	UNP Q69ZX9
D	126	SER	-	EXPRESSION TAG	UNP Q69ZX9
D	127	HIS	-	EXPRESSION TAG	UNP Q69ZX9

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Cl	0	0
			1	1		
2	A	1	Total	Cl	0	0
			1	1		

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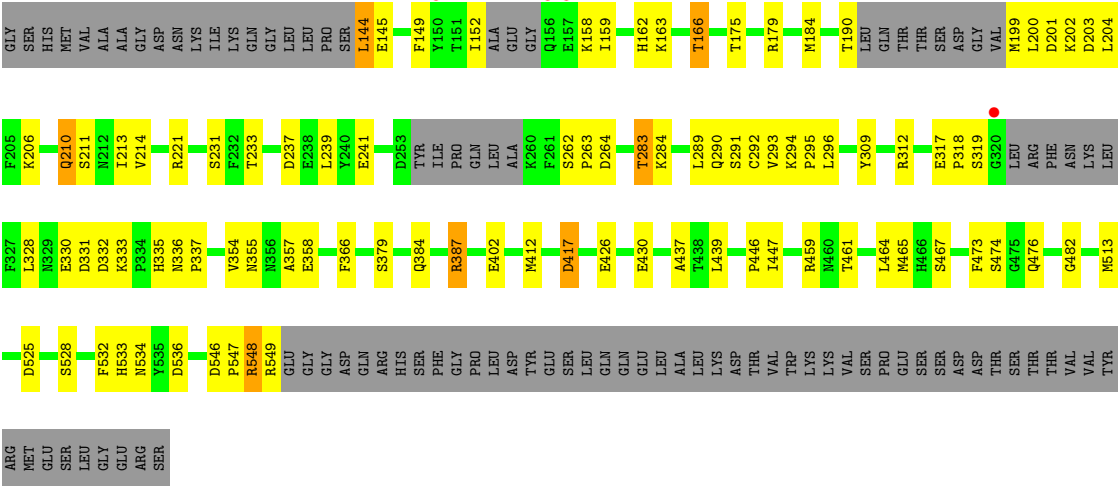
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	1	Total 1	Cl 1	0	0
2	C	1	Total 1	Cl 1	0	0

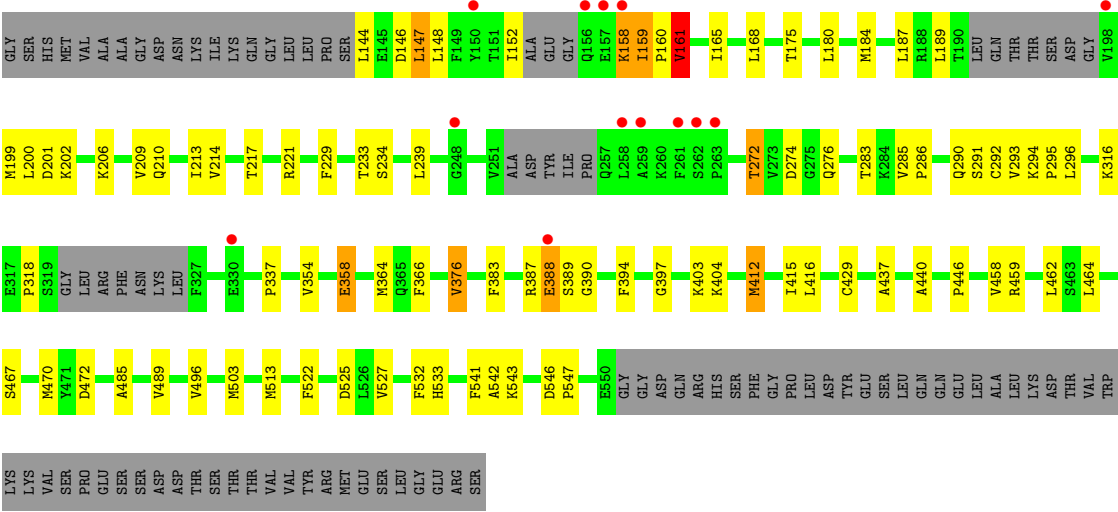
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	270	Total 270	O 270	0	0
3	B	267	Total 267	O 267	0	0
3	C	279	Total 279	O 279	0	0
3	D	289	Total 289	O 289	0	0





● Molecule 1: Glutaminase C



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	99.26Å 138.81Å 179.48Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.93 – 2.42 19.93 – 2.42	Depositor EDS
% Data completeness (in resolution range)	93.7 (19.93-2.42) 93.6 (19.93-2.42)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.14	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.12 (at 2.41Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, $R_{free}$	0.195 , 0.250 0.184 , 0.240	Depositor DCC
$R_{free}$ test set	4437 reflections (4.99%)	DCC
Wilson B-factor (Å <sup>2</sup> )	28.9	Xtriage
Anisotropy	0.195	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 54.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	13253	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 47.23 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 1.0229e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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:  
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	0.32	0/3150	0.53	0/4249
1	B	0.34	0/3114	0.53	0/4197
1	C	0.33	0/3060	0.53	0/4122
1	D	0.34	0/3079	0.54	0/4148
All	All	0.33	0/12403	0.53	0/16716

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	3083	0	3066	59	0
1	B	3050	0	3038	59	0
1	C	2996	0	2972	68	0
1	D	3015	0	2992	81	0
2	A	1	0	0	0	0
2	B	1	0	0	1	0
2	C	1	0	0	0	0
2	D	1	0	0	1	0
3	A	270	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	267	0	0	7	0
3	C	279	0	0	3	0
3	D	289	0	0	3	0
All	All	13253	0	12068	262	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 11.

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:B:406:PHE:HB3	1:B:410:THR:HG21	1.37	1.01
1:D:159:ILE:HD13	1:D:161:VAL:H	1.25	0.99
1:C:145:GLU:HG3	1:C:206:LYS:HG3	1.41	0.98
1:D:272:THR:HG22	1:D:274:ASP:H	1.26	0.96
1:D:158:LYS:CG	1:D:199:MET:HB3	1.97	0.94
1:A:209:VAL:HG22	1:A:216:LEU:HD13	1.59	0.84
1:D:158:LYS:HD2	1:D:200:LEU:C	1.98	0.84
1:C:461:THR:HG22	1:C:465:MET:HE2	1.60	0.84
1:D:158:LYS:HG2	1:D:199:MET:HB3	1.58	0.81
1:D:272:THR:CG2	1:D:274:ASP:H	1.95	0.80
1:D:158:LYS:HG3	1:D:199:MET:HB3	1.63	0.80
1:B:272:THR:HG22	1:B:274:ASP:H	1.45	0.79
1:D:383:PHE:O	1:D:387:ARG:HG3	1.83	0.79
1:A:512:LYS:H	1:A:512:LYS:HD2	1.49	0.78
1:C:355:ASN:HD21	1:C:357:ALA:HB3	1.50	0.77
1:B:406:PHE:HB3	1:B:410:THR:CG2	2.12	0.77
1:A:145:GLU:HG3	1:A:206:LYS:HG3	1.65	0.77
1:A:546:ASP:OD1	1:A:548:ARG:HD2	1.85	0.77
1:B:272:THR:CG2	1:B:274:ASP:H	2.00	0.75
1:A:412:MET:HE2	1:A:413:VAL:HA	1.68	0.74
1:D:272:THR:HG22	1:D:274:ASP:N	2.03	0.74
1:C:461:THR:HG22	1:C:465:MET:CE	2.19	0.73
1:A:412:MET:HE1	1:A:416:LEU:HD12	1.69	0.72
1:B:407:PRO:O	1:B:410:THR:HG22	1.89	0.71
1:C:152:ILE:HG22	1:C:163:LYS:HD3	1.72	0.71
1:C:295:PRO:HB2	1:C:465:MET:HE2	1.73	0.70
1:C:162:HIS:O	1:C:166:THR:HG23	1.91	0.70
1:C:354:VAL:CG1	1:C:358:GLU:HB2	2.22	0.70
1:B:272:THR:HG21	1:B:276:GLN:OE1	1.91	0.70
1:C:221:ARG:NH1	3:C:874:HOH:O	2.25	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:239:LEU:HD22	1:C:525:ASP:HB3	1.74	0.67
1:C:461:THR:CG2	1:C:465:MET:HE2	2.24	0.67
1:D:158:LYS:HZ3	1:D:201:ASP:H	1.42	0.67
1:C:290:GLN:O	1:C:293:VAL:HG22	1.95	0.67
1:D:158:LYS:HZ3	1:D:201:ASP:N	1.93	0.67
1:C:283:THR:HG23	1:C:430:GLU:HG3	1.76	0.67
1:A:512:LYS:CD	1:A:512:LYS:H	2.05	0.66
1:C:437:ALA:HB1	1:C:446:PRO:HG2	1.76	0.66
1:D:158:LYS:HG2	1:D:199:MET:CB	2.26	0.66
1:B:153:ALA:HA	1:B:159:ILE:HD11	1.78	0.66
1:A:412:MET:HE2	1:A:413:VAL:CA	2.25	0.66
1:B:277:ARG:NH2	1:B:374:GLU:OE2	2.28	0.64
1:B:326:LEU:HB2	3:B:767:HOH:O	1.98	0.62
1:B:362:TYR:O	1:B:365:GLN:HG3	2.00	0.62
1:B:272:THR:HG22	1:B:274:ASP:N	2.15	0.62
1:C:461:THR:O	1:C:465:MET:HG3	1.99	0.61
1:A:354:VAL:CG1	1:A:358:GLU:HB2	2.30	0.61
1:D:472:ASP:HB2	1:D:513:MET:HE2	1.82	0.61
1:B:174:ARG:NH2	3:B:51:HOH:O	2.33	0.61
1:C:289:LEU:HD13	1:C:293:VAL:HG12	1.81	0.61
1:A:144:LEU:HD23	1:A:145:GLU:OE1	2.00	0.61
1:A:239:LEU:HD22	1:A:525:ASP:HB3	1.82	0.61
1:D:159:ILE:CD1	1:D:161:VAL:H	2.06	0.61
1:C:355:ASN:ND2	1:C:357:ALA:HB3	2.16	0.60
1:C:295:PRO:HB2	1:C:465:MET:CE	2.32	0.59
1:D:144:LEU:N	1:D:147:LEU:HD23	2.17	0.59
1:D:291:SER:OG	1:D:294:LYS:HE2	2.02	0.59
1:C:354:VAL:HG11	1:C:358:GLU:HB2	1.85	0.59
1:A:148:LEU:O	1:A:152:ILE:HG13	2.03	0.59
1:D:472:ASP:HB2	1:D:513:MET:CE	2.33	0.59
1:A:144:LEU:HB3	1:A:145:GLU:OE1	2.03	0.59
1:B:153:ALA:CA	1:B:159:ILE:HD11	2.33	0.58
1:B:239:LEU:HD22	1:B:525:ASP:HB3	1.84	0.58
1:C:387:ARG:NH1	1:C:417:ASP:OD1	2.36	0.58
1:D:229:PHE:O	1:D:233:THR:HG23	2.03	0.58
1:A:512:LYS:NZ	3:A:744:HOH:O	2.35	0.58
1:C:532:PHE:CZ	1:C:547:PRO:HG2	2.38	0.58
1:A:254:TYR:CD1	1:A:255:ILE:HG23	2.39	0.58
1:B:364:MET:HE2	1:B:425:ILE:HG12	1.85	0.58
1:A:412:MET:HE2	1:A:413:VAL:N	2.19	0.57
1:C:546:ASP:OD1	1:C:548:ARG:HD2	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:158:LYS:HG2	1:B:201:ASP:HA	1.86	0.57
1:D:239:LEU:HD22	1:D:525:ASP:HB3	1.86	0.57
1:D:144:LEU:HD22	1:D:213:ILE:HG13	1.86	0.57
1:C:211:SER:HB3	3:C:927:HOH:O	2.04	0.57
1:D:412:MET:CE	1:D:416:LEU:CD1	2.83	0.57
1:C:312:ARG:O	1:C:333:LYS:HE2	2.05	0.56
1:D:148:LEU:HD11	1:D:152:ILE:HD11	1.87	0.56
1:D:159:ILE:HD13	1:D:159:ILE:C	2.26	0.56
1:D:412:MET:HE1	1:D:416:LEU:CD1	2.36	0.56
1:A:437:ALA:HB1	1:A:446:PRO:HG2	1.86	0.56
1:B:546:ASP:OD2	1:B:548:ARG:HD3	2.06	0.56
1:C:336:ASN:HB2	1:C:337:PRO:CD	2.36	0.56
1:A:149:PHE:CE2	1:A:202:LYS:HG2	2.41	0.56
1:D:532:PHE:CZ	1:D:547:PRO:HG2	2.40	0.56
1:B:294:LYS:HE3	1:B:343:ALA:CB	2.36	0.56
1:D:412:MET:CE	1:D:416:LEU:HD11	2.37	0.55
1:D:318:PRO:HG3	1:D:467:SER:HB2	1.86	0.55
1:D:161:VAL:HG23	1:D:200:LEU:HD11	1.87	0.55
1:A:512:LYS:N	1:A:512:LYS:HD2	2.19	0.55
1:A:144:LEU:N	3:A:610:HOH:O	2.39	0.54
1:D:161:VAL:HG23	1:D:200:LEU:CD1	2.37	0.54
1:C:200:LEU:HD12	1:C:204:LEU:HB3	1.90	0.54
1:B:470:MET:HE1	1:B:486:LYS:CA	2.38	0.54
1:D:158:LYS:NZ	1:D:201:ASP:N	2.56	0.53
1:A:412:MET:CE	1:A:413:VAL:HA	2.37	0.53
1:D:290:GLN:O	1:D:293:VAL:HG12	2.09	0.53
1:B:244:LYS:NZ	3:B:940:HOH:O	2.39	0.53
1:B:312:ARG:O	1:B:333:LYS:HE2	2.08	0.53
1:A:501:MET:SD	1:A:503:MET:HE2	2.49	0.53
1:B:410:THR:HB	3:B:619:HOH:O	2.08	0.53
1:D:159:ILE:HD13	1:D:161:VAL:N	2.09	0.53
1:D:354:VAL:HG21	1:D:358:GLU:HB3	1.91	0.53
1:A:160:PRO:HG2	1:A:163:LYS:HB2	1.91	0.52
1:B:279:SER:HB3	1:B:283:THR:HG21	1.91	0.52
1:C:263:PRO:O	1:C:264:ASP:HB2	2.10	0.52
1:A:354:VAL:O	1:A:359:LYS:HE3	2.10	0.52
1:A:351:LYS:HB3	1:A:359:LYS:HG2	1.92	0.52
1:B:277:ARG:HH22	1:B:374:GLU:CD	2.13	0.52
1:A:257:GLN:OE1	1:A:257:GLN:N	2.40	0.52
1:C:295:PRO:CB	1:C:465:MET:HE2	2.40	0.52
1:A:533:HIS:CG	1:C:459:ARG:HD2	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:160:PRO:O	1:D:161:VAL:HG12	2.10	0.51
1:C:283:THR:HG23	1:C:430:GLU:CG	2.40	0.51
1:C:439:LEU:HD13	1:C:465:MET:HE3	1.93	0.51
1:D:147:LEU:H	1:D:147:LEU:CD2	2.23	0.51
1:D:206:LYS:O	1:D:210:GLN:HB2	2.11	0.51
1:B:470:MET:CE	1:B:486:LYS:HA	2.41	0.51
1:A:534:ASN:OD1	1:C:534:ASN:ND2	2.37	0.51
1:C:175:THR:O	1:C:184:MET:HG3	2.10	0.51
1:D:158:LYS:HD2	1:D:201:ASP:N	2.25	0.50
1:D:272:THR:HG21	1:D:276:GLN:OE1	2.11	0.50
1:C:237:ASP:O	1:C:241:GLU:HG2	2.11	0.50
1:C:292:CYS:O	1:C:295:PRO:HD2	2.12	0.50
1:C:337:PRO:CD	1:C:464:LEU:HD13	2.41	0.50
1:C:384:GLN:O	1:C:387:ARG:HG2	2.12	0.50
1:D:470:MET:HE3	1:D:485:ALA:CB	2.42	0.49
1:A:255:ILE:HG12	1:A:258:LEU:HD12	1.94	0.49
1:B:546:ASP:OD2	1:B:548:ARG:CD	2.60	0.49
1:D:388:GLU:HG2	1:D:389:SER:N	2.27	0.49
1:D:503:MET:HE1	1:D:522:PHE:CE2	2.48	0.49
1:A:459:ARG:HD2	1:C:533:HIS:CG	2.47	0.49
1:C:206:LYS:O	1:C:210:GLN:HB3	2.13	0.48
1:C:548:ARG:HB3	3:C:677:HOH:O	2.12	0.48
1:D:159:ILE:HG23	1:D:200:LEU:HB2	1.96	0.48
1:B:182:GLU:CD	1:B:182:GLU:H	2.17	0.48
1:B:167:ALA:HB1	1:B:220:PHE:HE2	1.78	0.48
1:B:498:PRO:O	1:B:499:ASN:HB2	2.14	0.48
1:A:412:MET:HE3	1:A:416:LEU:HG	1.95	0.48
1:C:283:THR:HG22	1:C:284:LYS:HG3	1.96	0.47
1:B:153:ALA:HA	1:B:159:ILE:CD1	2.43	0.47
1:D:337:PRO:HG2	1:D:464:LEU:HD13	1.96	0.47
1:B:326:LEU:HD13	1:B:328:LEU:O	2.14	0.47
1:A:257:GLN:HE21	1:A:381:ALA:HB1	1.79	0.47
1:B:298:TYR:OH	1:B:460:ASN:HB3	2.14	0.47
1:A:204:LEU:HD12	1:A:204:LEU:HA	1.75	0.47
1:A:317:GLU:HB2	1:A:318:PRO:HD2	1.96	0.47
1:B:153:ALA:CB	1:B:159:ILE:HD11	2.44	0.47
1:B:548:ARG:HB3	3:B:679:HOH:O	2.15	0.47
1:A:354:VAL:HG11	1:A:358:GLU:HB2	1.96	0.47
1:D:187:LEU:HD11	1:D:200:LEU:HD11	1.96	0.47
1:B:360:PHE:CZ	1:B:364:MET:HE2	2.50	0.46
1:D:470:MET:CE	1:D:485:ALA:CB	2.93	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:153:ALA:HB2	1:B:159:ILE:HD11	1.96	0.46
1:A:387:ARG:NH2	3:A:608:HOH:O	2.49	0.46
1:B:387:ARG:NH1	1:B:417:ASP:OD1	2.47	0.46
1:C:159:ILE:HG23	1:C:163:LYS:HD2	1.98	0.46
1:C:379:SER:HB2	1:C:426:GLU:OE2	2.15	0.46
1:D:159:ILE:HA	1:D:160:PRO:HD3	1.74	0.46
1:D:458:VAL:O	1:D:462:LEU:HG	2.15	0.46
1:B:500:VAL:HG12	1:B:501:MET:HE3	1.97	0.46
1:D:364:MET:SD	1:D:376:VAL:HG22	2.56	0.46
1:A:265:LEU:HD13	1:A:506:TRP:CH2	2.50	0.46
1:D:159:ILE:HG22	1:D:200:LEU:O	2.15	0.46
1:A:337:PRO:HD2	1:A:464:LEU:HD13	1.98	0.46
1:D:527:VAL:CG1	1:D:533:HIS:HB2	2.45	0.46
1:B:437:ALA:HB1	1:B:446:PRO:HG2	1.98	0.46
1:B:482:GLY:O	1:B:534:ASN:HB2	2.16	0.46
1:B:148:LEU:HD11	1:B:152:ILE:HD11	1.98	0.46
1:C:289:LEU:CB	1:C:293:VAL:HG13	2.46	0.46
1:A:437:ALA:CB	1:A:446:PRO:HG2	2.45	0.45
1:C:263:PRO:O	1:C:264:ASP:CB	2.63	0.45
1:C:152:ILE:CG2	1:C:163:LYS:HD3	2.43	0.45
1:A:467:SER:O	1:A:474:SER:HB3	2.17	0.45
1:C:317:GLU:HB2	1:C:318:PRO:HD2	1.97	0.45
1:C:467:SER:O	1:C:474:SER:HB3	2.15	0.45
1:D:158:LYS:NZ	1:D:201:ASP:H	2.12	0.45
1:B:291:SER:HB2	2:B:2:CL:CL	2.54	0.45
1:A:305:LEU:HD13	1:A:309:TYR:CE2	2.52	0.45
1:D:292:CYS:O	1:D:295:PRO:HD2	2.17	0.45
1:D:532:PHE:HZ	1:D:547:PRO:HG2	1.79	0.45
1:C:289:LEU:HB3	1:C:293:VAL:HG13	1.99	0.45
1:D:175:THR:O	1:D:184:MET:HG3	2.17	0.45
1:A:146:ASP:HB2	3:A:610:HOH:O	2.16	0.45
1:C:149:PHE:CE2	1:C:202:LYS:HB2	2.52	0.45
1:D:489:VAL:HG13	2:D:4:CL:CL	2.53	0.45
1:D:146:ASP:OD2	1:D:202:LYS:HE3	2.17	0.44
1:C:262:SER:OG	1:C:263:PRO:O	2.33	0.44
1:D:147:LEU:N	1:D:147:LEU:CD2	2.80	0.44
1:D:161:VAL:O	1:D:165:ILE:HG12	2.17	0.44
1:D:470:MET:CE	1:D:485:ALA:HB3	2.48	0.44
1:A:412:MET:CE	1:A:416:LEU:HD12	2.43	0.44
1:B:191:LEU:HA	1:B:191:LEU:HD12	1.78	0.44
1:C:331:ASP:O	1:C:332:ASP:HB2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:158:LYS:HB3	1:A:199:MET:HB3	1.98	0.44
1:B:532:PHE:CZ	1:B:547:PRO:HG2	2.53	0.44
1:A:148:LEU:HA	1:A:151:THR:HG23	2.00	0.44
1:B:470:MET:CE	1:B:486:LYS:CA	2.96	0.43
1:D:390:GLY:O	1:D:394:PHE:HD2	2.00	0.43
1:A:159:ILE:HG22	1:A:160:PRO:O	2.18	0.43
1:C:317:GLU:HB2	1:C:318:PRO:CD	2.48	0.43
1:A:190:THR:O	1:A:194:THR:HB	2.17	0.43
1:A:482:GLY:O	1:A:534:ASN:HB2	2.17	0.43
1:D:546:ASP:HA	1:D:547:PRO:HD2	1.91	0.43
1:A:466:HIS:CD2	1:A:466:HIS:C	2.92	0.43
1:A:160:PRO:HB3	1:A:199:MET:HE1	2.00	0.43
1:D:532:PHE:CZ	1:D:547:PRO:CG	3.02	0.43
1:D:470:MET:HE3	1:D:485:ALA:HB3	2.00	0.43
1:B:327:PHE:O	1:B:328:LEU:HD23	2.19	0.43
1:C:354:VAL:CG1	1:C:355:ASN:N	2.82	0.43
1:C:291:SER:HB3	1:C:294:LYS:HD2	2.01	0.43
1:D:294:LYS:N	1:D:295:PRO:HD2	2.34	0.43
1:B:455:PRO:HG2	1:D:542:ALA:HB2	2.01	0.42
1:B:403:LYS:HD3	1:B:403:LYS:HA	1.84	0.42
1:B:470:MET:HE1	1:B:486:LYS:N	2.35	0.42
1:A:459:ARG:HD2	1:C:533:HIS:CD2	2.54	0.42
1:B:159:ILE:HG22	1:B:160:PRO:O	2.19	0.42
1:B:548:ARG:NH2	3:B:742:HOH:O	2.43	0.42
1:D:144:LEU:N	3:D:945:HOH:O	2.52	0.42
1:B:149:PHE:CE1	1:B:159:ILE:HG12	2.55	0.42
1:B:265:LEU:HD12	1:B:265:LEU:H	1.83	0.42
1:C:213:ILE:HG23	1:C:214:VAL:N	2.34	0.42
1:C:482:GLY:O	1:C:534:ASN:HB2	2.20	0.42
1:B:513:MET:O	3:B:643:HOH:O	2.21	0.42
1:A:210:GLN:O	1:A:210:GLN:HG2	2.19	0.42
1:A:265:LEU:HD13	1:A:506:TRP:HH2	1.85	0.42
1:B:467:SER:O	1:B:474:SER:HB3	2.19	0.42
1:D:147:LEU:HD23	1:D:147:LEU:H	1.84	0.42
1:D:285:VAL:HA	1:D:286:PRO:HD3	1.91	0.42
1:D:412:MET:CE	1:D:416:LEU:HG	2.50	0.42
1:D:503:MET:HE3	1:D:503:MET:HB3	1.88	0.42
1:A:336:ASN:HB2	1:A:337:PRO:CD	2.49	0.42
1:D:217:THR:O	1:D:221:ARG:HB2	2.19	0.42
1:D:459:ARG:NH2	3:D:741:HOH:O	2.53	0.41
1:D:415:ILE:HD13	1:D:415:ILE:HA	1.76	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:437:ALA:HB1	1:D:446:PRO:HG2	2.03	0.41
1:B:258:LEU:N	1:B:258:LEU:HD12	2.35	0.41
1:C:533:HIS:HB3	1:C:536:ASP:OD2	2.20	0.41
1:D:283:THR:HA	1:D:429:CYS:HB2	2.02	0.41
1:A:339:VAL:HG23	1:A:342:GLY:H	1.86	0.41
1:C:144:LEU:HD13	1:C:213:ILE:HG13	2.01	0.41
1:C:179:ARG:HG3	1:C:447:ILE:O	2.21	0.41
1:C:437:ALA:CB	1:C:446:PRO:HG2	2.49	0.41
1:A:225:VAL:HG21	1:A:500:VAL:HA	2.03	0.41
1:B:432:ALA:HB3	1:B:504:MET:HG2	2.03	0.41
1:C:210:GLN:HG2	1:C:211:SER:N	2.36	0.41
1:D:397:GLY:HA3	1:D:412:MET:CE	2.51	0.41
1:A:445:CYS:HA	1:A:446:PRO:HD3	1.92	0.41
1:C:319:SER:HB3	1:C:335:HIS:CG	2.56	0.41
1:C:473:PHE:CE2	1:C:476:GLN:HG2	2.55	0.41
1:A:294:LYS:N	1:A:295:PRO:HD2	2.35	0.41
1:B:294:LYS:N	1:B:295:PRO:HD2	2.36	0.41
1:C:309:TYR:O	1:C:312:ARG:HB2	2.21	0.41
1:C:337:PRO:HD2	1:C:464:LEU:HD13	2.03	0.41
1:D:144:LEU:HD22	1:D:213:ILE:CG1	2.51	0.41
1:A:246:GLN:O	1:A:518:LYS:HE3	2.20	0.40
1:D:403:LYS:HE3	3:D:1045:HOH:O	2.21	0.40
1:D:168:LEU:HD21	1:D:180:LEU:HD13	2.03	0.40
1:D:209:VAL:CG1	1:D:213:ILE:HD13	2.52	0.40
1:D:440:ALA:HB2	1:D:496:VAL:HG13	2.03	0.40
1:B:469:GLY:O	1:B:470:MET:HE2	2.22	0.40
1:C:158:LYS:HG2	1:C:201:ASP:HA	2.03	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	386/479 (81%)	380 (98%)	6 (2%)	0	100	100
1	B	380/479 (79%)	376 (99%)	4 (1%)	0	100	100
1	C	373/479 (78%)	365 (98%)	8 (2%)	0	100	100
1	D	375/479 (78%)	367 (98%)	7 (2%)	1 (0%)	44	59
All	All	1514/1916 (79%)	1488 (98%)	25 (2%)	1 (0%)	55	71

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	161	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	343/415 (83%)	324 (94%)	19 (6%)	25	39
1	B	339/415 (82%)	323 (95%)	16 (5%)	30	47
1	C	333/415 (80%)	312 (94%)	21 (6%)	21	32
1	D	335/415 (81%)	317 (95%)	18 (5%)	26	40
All	All	1350/1660 (81%)	1276 (94%)	74 (6%)	25	39

All (74) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	144	LEU
1	A	145	GLU
1	A	151	THR
1	A	157	GLU
1	A	173	LEU
1	A	190	THR
1	A	194	THR
1	A	201	ASP
1	A	209	VAL
1	A	221	ARG

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Mol	Chain	Res	Type
1	A	293	VAL
1	A	319	SER
1	A	330	GLU
1	A	365	GLN
1	A	412	MET
1	A	417	ASP
1	A	512	LYS
1	A	528	SER
1	A	548	ARG
1	B	144	LEU
1	B	151	THR
1	B	175	THR
1	B	191	LEU
1	B	194	THR
1	B	211	SER
1	B	262	SER
1	B	272	THR
1	B	296	LEU
1	B	326	LEU
1	B	365	GLN
1	B	366	PHE
1	B	392	ARG
1	B	410	THR
1	B	504	MET
1	B	512	LYS
1	C	144	LEU
1	C	166	THR
1	C	190	THR
1	C	199	MET
1	C	203	ASP
1	C	210	GLN
1	C	231	SER
1	C	233	THR
1	C	283	THR
1	C	296	LEU
1	C	328	LEU
1	C	330	GLU
1	C	366	PHE
1	C	387	ARG
1	C	402	GLU
1	C	412	MET
1	C	417	ASP

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Mol	Chain	Res	Type
1	C	513	MET
1	C	528	SER
1	C	548	ARG
1	C	549	ARG
1	D	147	LEU
1	D	158	LYS
1	D	159	ILE
1	D	161	VAL
1	D	189	LEU
1	D	214	VAL
1	D	234	SER
1	D	272	THR
1	D	296	LEU
1	D	316	LYS
1	D	358	GLU
1	D	366	PHE
1	D	376	VAL
1	D	388	GLU
1	D	404	LYS
1	D	412	MET
1	D	541	PHE
1	D	543	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	355	ASN
1	D	335	HIS

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 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, 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	394/479 (82%)	-0.44	11 (2%) 53 50	16, 26, 55, 73	4 (1%)
1	B	390/479 (81%)	-0.36	13 (3%) 47 44	15, 26, 55, 73	2 (0%)
1	C	383/479 (79%)	-0.47	4 (1%) 82 80	15, 26, 56, 83	2 (0%)
1	D	385/479 (80%)	-0.38	13 (3%) 46 43	13, 26, 56, 91	4 (1%)
All	All	1552/1916 (81%)	-0.41	41 (2%) 56 53	13, 26, 56, 91	12 (0%)

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	258	LEU	5.2
1	B	247	SER	5.1
1	B	262	SER	3.9
1	B	326	LEU	3.8
1	B	261	PHE	3.7
1	D	262	SER	3.7
1	B	248	GLY	3.5
1	B	150	TYR	3.5
1	D	157	GLU	3.5
1	D	150	TYR	3.3
1	D	261	PHE	3.2
1	A	254	TYR	3.2
1	D	158	LYS	3.1
1	D	330	GLU	3.0
1	B	258	LEU	3.0
1	C	156	GLN	3.0
1	A	256	PRO	2.9
1	B	263	PRO	2.9
1	C	150	TYR	2.9
1	C	157	GLU	2.8
1	B	249	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	263	PRO	2.6
1	D	156	GLN	2.6
1	D	198	VAL	2.5
1	A	150	TYR	2.5
1	A	151	THR	2.5
1	D	259	ALA	2.5
1	B	330	GLU	2.5
1	A	260	LYS	2.4
1	A	259	ALA	2.4
1	B	543	LYS	2.4
1	A	144	LEU	2.4
1	B	259	ALA	2.4
1	A	257	GLN	2.3
1	B	245	LYS	2.3
1	C	320	GLY	2.3
1	D	248	GLY	2.3
1	A	330	GLU	2.3
1	A	255	ILE	2.2
1	D	388	GLU	2.2
1	A	253	ASP	2.1

## 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	CL	B	2	1/1	0.99	0.07	-1.14	36,36,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	CL	C	3	1/1	0.99	0.06	-1.60	25,25,25,25	0
2	CL	D	4	1/1	0.99	0.04	-5.91	29,29,29,29	0
2	CL	A	1	1/1	0.99	0.05	-	27,27,27,27	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.