



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:04 PM GMT

PDB ID : 3SS5  
Title : Crystal structure of mouse Glutaminase C, L-glutamate-bound form  
Authors : Ambrosio, A.L.B.; Dias, S.M.G.; Cerione, R.A.  
Deposited on : 2011-07-07  
Resolution : 2.80 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 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
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) : trunk26865

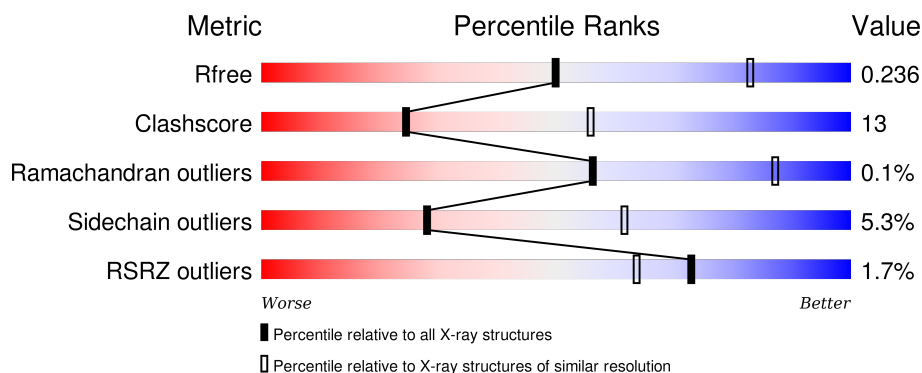
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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))
$R_{free}$	91344	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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> <div>2%</div> <div>58%</div> <div>22%</div> <div>•</div> <div>18%</div> </div> </div>
1	B	479	<div> <div>2%</div> <div>54%</div> <div>26%</div> <div>•</div> <div>19%</div> </div>
1	C	479	<div> <div>2%</div> <div>58%</div> <div>23%</div> <div>•</div> <div>17%</div> </div>
1	D	479	<div> <div>2%</div> <div>54%</div> <div>26%</div> <div>•</div> <div>18%</div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12542 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.

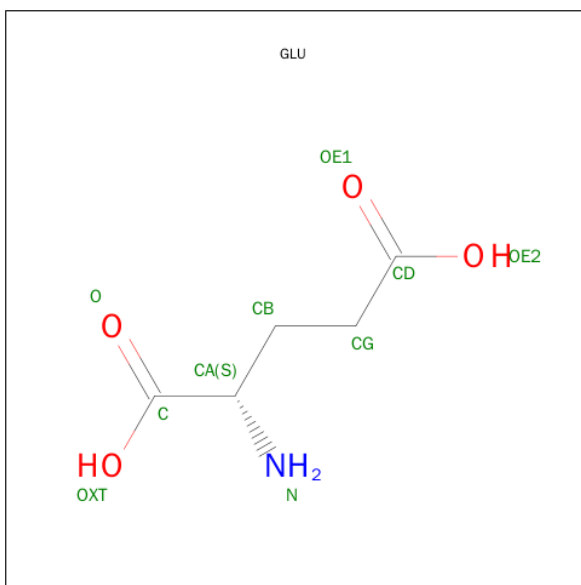
- Molecule 1 is a protein called Glutaminase C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	394	Total	C	N	O	S	1	0	0
			3080	1968	519	565	28			
1	B	390	Total	C	N	O	S	1	0	0
			3052	1951	514	559	28			
1	C	396	Total	C	N	O	S	1	0	0
			3096	1977	521	570	28			
1	D	391	Total	C	N	O	S	1	0	0
			3060	1957	515	560	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 GLUTAMIC ACID (three-letter code: GLU) (formula: C<sub>5</sub>H<sub>9</sub>NO<sub>4</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			10	5	1	4		
2	B	1	Total	C	N	O	0	0
			10	5	1	4		
2	C	1	Total	C	N	O	0	0
			10	5	1	4		
2	D	1	Total	C	N	O	0	0
			10	5	1	4		

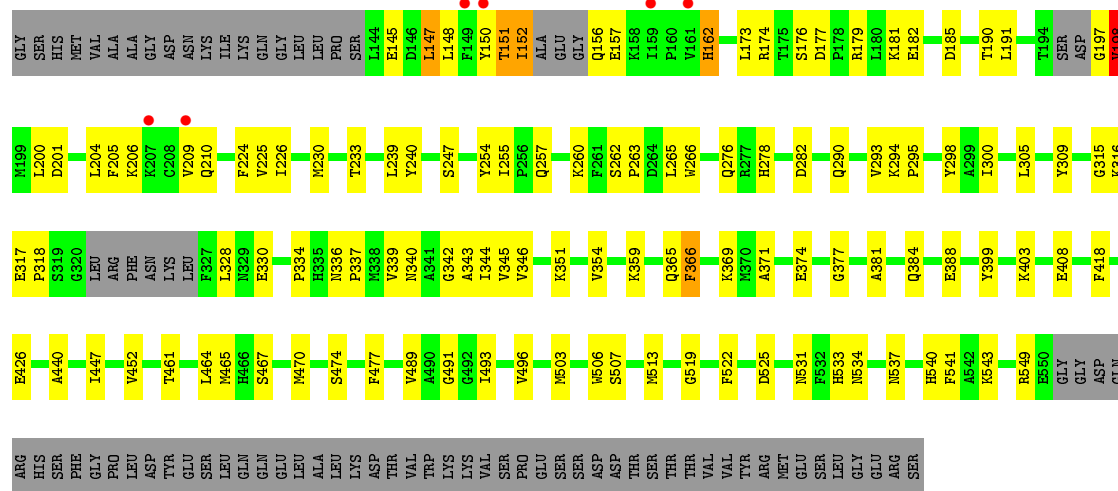
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	65	Total	O	0	0
			65	65		
3	B	56	Total	O	0	0
			56	56		
3	C	43	Total	O	0	0
			43	43		
3	D	50	Total	O	0	0
			50	50		

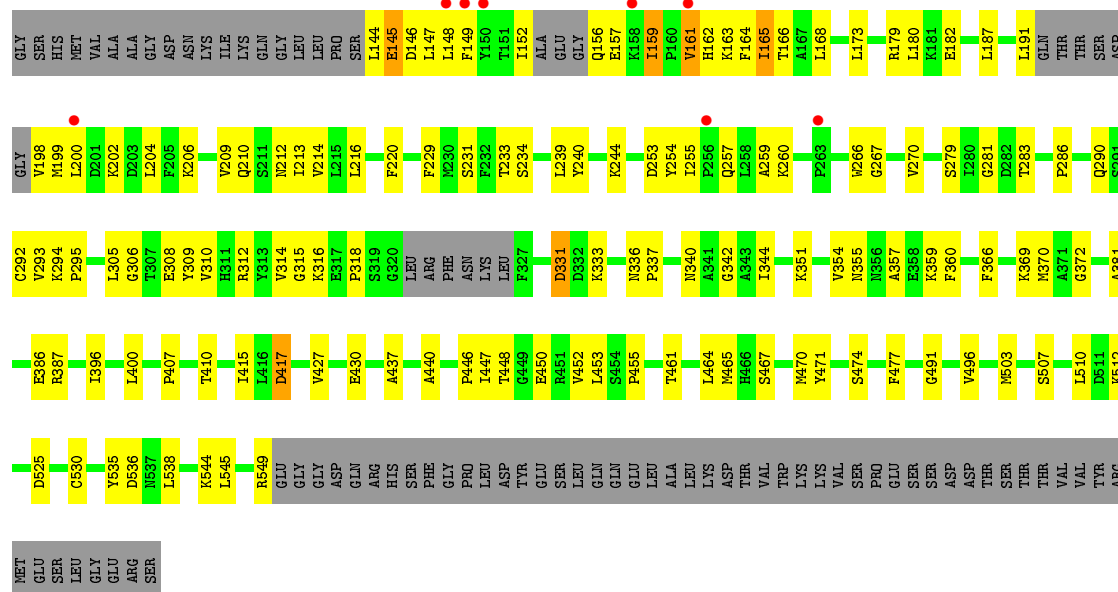


VAL  
VAL  
TYR  
ARG  
MET  
GLU  
SER  
SER  
LEU  
GLY  
GLU  
ARG  
SER

• Molecule 1: Glutaminase C



• Molecule 1: Glutaminase C



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	50.38 Å   139.43 Å   178.39 Å 90.00°   93.77°   90.00°	Depositor
Resolution (Å)	19.98 – 2.80 42.59 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.9 (19.98-2.80) 98.8 (42.59-2.80)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	0.11	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.08 (at 2.81 Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, $R_{free}$	0.206   ,   0.240 0.205   ,   0.236	Depositor DCC
$R_{free}$ test set	3017 reflections (5.33%)	DCC
Wilson B-factor (Å <sup>2</sup> )	43.1	Xtriage
Anisotropy	0.819	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 42.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 59784 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	12542	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.03% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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	0.23	0/3147	0.41	0/4244
1	B	0.23	0/3119	0.42	0/4206
1	C	0.24	0/3163	0.41	0/4266
1	D	0.24	0/3127	0.41	0/4217
All	All	0.24	0/12556	0.41	0/16933

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	3080	0	3062	75	0
1	B	3052	0	3033	89	0
1	C	3096	0	3075	72	0
1	D	3060	0	3044	86	0
2	A	10	0	8	0	0
2	B	10	0	8	1	0
2	C	10	0	8	0	0
2	D	10	0	8	0	0
3	A	65	0	0	2	0
3	B	56	0	0	5	0
3	C	43	0	0	1	0
3	D	50	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	12542	0	12246	318	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 13.

All (318) 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:C:156:GLN:HG2	1:C:157:GLU:H	1.27	0.94
1:B:221:ARG:HD3	1:B:223:LYS:HD3	1.56	0.83
1:D:145:GLU:HG3	1:D:206:LYS:HG3	1.61	0.83
1:A:266:TRP:HB2	1:A:518:LYS:HE3	1.61	0.81
1:C:156:GLN:HG2	1:C:157:GLU:N	1.96	0.79
1:D:144:LEU:HA	1:D:147:LEU:HD13	1.66	0.78
1:A:370:MET:HG3	1:A:452:VAL:HG11	1.66	0.77
1:A:546:ASP:OD1	1:A:548:ARG:HD3	1.84	0.77
1:B:239:LEU:HD22	1:B:525:ASP:HB3	1.70	0.74
1:C:467:SER:O	1:C:474:SER:HB3	1.90	0.71
1:A:239:LEU:HD22	1:A:525:ASP:HB3	1.73	0.71
1:B:290:GLN:HG3	1:B:489:VAL:HG12	1.74	0.70
1:B:185:ASP:OD1	1:B:188:ARG:NH1	2.23	0.69
1:D:308:GLU:OE1	1:D:312:ARG:NH2	2.25	0.69
1:C:156:GLN:CG	1:C:157:GLU:H	2.04	0.69
1:A:284:LYS:NZ	1:A:430:GLU:OE2	2.25	0.69
1:D:159:ILE:HD11	1:D:164:PHE:HB2	1.76	0.68
1:C:239:LEU:HD22	1:C:525:ASP:HB3	1.76	0.68
1:B:467:SER:O	1:B:474:SER:HB3	1.94	0.67
1:A:202:LYS:O	1:A:206:LYS:HB2	1.94	0.67
1:C:440:ALA:HB2	1:C:496:VAL:HG13	1.76	0.67
1:D:467:SER:O	1:D:474:SER:HB3	1.95	0.66
1:B:145:GLU:HG3	1:B:206:LYS:HG3	1.76	0.66
1:B:512:LYS:HD3	1:B:512:LYS:H	1.59	0.66
1:A:201:ASP:OD1	1:A:204:LEU:N	2.27	0.65
1:D:239:LEU:HD22	1:D:525:ASP:HB3	1.79	0.65
1:D:206:LYS:O	1:D:210:GLN:HG3	1.96	0.65
1:A:290:GLN:HG3	1:A:489:VAL:HG12	1.79	0.65
1:D:148:LEU:O	1:D:152:ILE:HG13	1.96	0.65
1:A:298:TYR:OH	1:A:311:HIS:NE2	2.25	0.65
1:A:467:SER:O	1:A:474:SER:HB3	1.98	0.64
1:D:279:SER:HB3	1:D:283:THR:HG21	1.78	0.64
1:A:444:PHE:CZ	1:A:451:ARG:HG3	2.32	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:470:MET:HB2	1:B:474:SER:HA	1.79	0.64
1:C:257:GLN:O	1:C:260:LYS:HG2	1.97	0.64
1:C:145:GLU:OE1	1:C:145:GLU:N	2.30	0.64
1:A:336:ASN:HB2	1:A:337:PRO:HD2	1.79	0.64
1:C:157:GLU:HG2	1:C:157:GLU:O	1.97	0.63
1:D:536:ASP:OD2	1:D:544:LYS:NZ	2.27	0.63
1:D:318:PRO:HG3	1:D:467:SER:HB2	1.81	0.63
1:B:549:ARG:NH1	3:B:120:HOH:O	2.27	0.63
1:D:369:LYS:HB3	1:D:452:VAL:HG22	1.79	0.62
1:D:440:ALA:HB2	1:D:496:VAL:HG13	1.82	0.62
1:B:160:PRO:HG2	1:B:163:LYS:HB2	1.80	0.62
1:D:315:GLY:O	1:D:336:ASN:HA	2.00	0.61
1:C:351:LYS:HB3	1:C:359:LYS:HG2	1.83	0.61
1:A:162:HIS:ND1	1:A:163:LYS:N	2.49	0.61
1:D:354:VAL:HG23	1:D:359:LYS:HG3	1.83	0.61
1:A:296:LEU:HD22	1:A:370:MET:HE1	1.82	0.60
1:B:351:LYS:O	1:B:359:LYS:HE2	2.01	0.60
1:A:318:PRO:HG3	1:A:467:SER:HB2	1.84	0.60
1:D:290:GLN:O	1:D:293:VAL:HG12	2.01	0.60
1:D:448:THR:OG1	1:D:450:GLU:HG2	2.02	0.60
1:D:182:GLU:OE1	1:D:212:ASN:ND2	2.35	0.59
1:A:482:GLY:O	1:A:534:ASN:HB2	2.03	0.59
1:A:145:GLU:OE1	1:A:145:GLU:N	2.33	0.58
1:D:257:GLN:O	1:D:260:LYS:HG2	2.04	0.58
1:D:200:LEU:HD23	1:D:204:LEU:HB3	1.86	0.58
1:A:296:LEU:HD22	1:A:370:MET:CE	2.34	0.57
1:B:534:ASN:ND2	1:C:534:ASN:OD1	2.32	0.57
1:D:198:VAL:HG13	1:D:199:MET:HG2	1.87	0.57
1:A:484:PRO:HG3	1:D:535:TYR:CE1	2.39	0.57
1:B:420:PHE:O	1:B:424:SER:OG	2.23	0.57
1:B:527:VAL:HG13	1:B:533:HIS:HB2	1.86	0.57
1:C:206:LYS:O	1:C:210:GLN:HB2	2.05	0.57
1:B:243:ALA:O	1:B:518:LYS:HG2	2.05	0.57
1:D:372:GLY:HA3	1:D:447:ILE:HD11	1.87	0.56
1:D:146:ASP:O	1:D:149:PHE:HB3	2.05	0.56
1:C:334:PRO:HG2	1:C:345:VAL:HG21	1.87	0.56
1:C:531:ASN:OD1	1:C:531:ASN:N	2.35	0.56
1:D:182:GLU:CD	1:D:182:GLU:H	2.09	0.56
1:A:365:GLN:HG3	1:A:366:PHE:N	2.20	0.56
1:C:337:PRO:HG2	1:C:464:LEU:HD13	1.87	0.56
1:D:144:LEU:CA	1:D:147:LEU:HD13	2.33	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:361:ASP:O	1:B:365:GLN:HG3	2.05	0.56
1:A:354:VAL:HB	1:A:358:GLU:OE1	2.05	0.56
1:B:437:ALA:HB1	1:B:446:PRO:HG2	1.88	0.55
1:A:532:PHE:CZ	1:A:547:PRO:HG2	2.41	0.55
1:C:399:TYR:O	1:C:403:LYS:HG2	2.06	0.55
1:D:305:LEU:HD13	1:D:309:TYR:CE1	2.41	0.55
1:B:337:PRO:HD2	1:B:464:LEU:HD13	1.88	0.55
1:A:233:THR:HG23	1:A:278:HIS:CE1	2.42	0.55
1:B:386:GLU:OE2	2:B:1:GLU:N	2.23	0.55
1:B:283:THR:HB	1:B:430:GLU:HG3	1.88	0.55
1:C:254:TYR:CD1	1:C:255:ILE:HG23	2.42	0.55
1:B:221:ARG:HB3	1:B:223:LYS:HD2	1.89	0.54
1:C:148:LEU:O	1:C:152:ILE:HG22	2.07	0.54
1:D:179:ARG:HG3	1:D:447:ILE:O	2.06	0.54
1:B:256:PRO:O	1:B:260:LYS:HG3	2.07	0.54
1:D:187:LEU:O	1:D:191:LEU:HD13	2.08	0.54
1:C:233:THR:HG23	1:C:278:HIS:CE1	2.42	0.54
1:B:246:GLN:O	1:B:518:LYS:HE3	2.08	0.54
1:A:484:PRO:HD2	1:A:496:VAL:O	2.08	0.54
1:A:384:GLN:O	1:A:388:GLU:HG3	2.08	0.54
1:C:290:GLN:O	1:C:293:VAL:HG12	2.08	0.54
1:D:370:MET:HG2	1:D:452:VAL:HG11	1.90	0.53
1:A:283:THR:HB	1:A:430:GLU:HG3	1.89	0.53
1:A:351:LYS:O	1:A:359:LYS:HE2	2.08	0.53
1:C:290:GLN:HG3	1:C:489:VAL:HG12	1.90	0.53
1:C:315:GLY:O	1:C:336:ASN:HA	2.07	0.53
1:D:254:TYR:OH	1:D:386:GLU:OE1	2.23	0.53
1:B:233:THR:OG1	1:B:278:HIS:ND1	2.42	0.53
1:A:150:TYR:HE1	1:A:202:LYS:HE3	1.73	0.53
1:D:244:LYS:HG3	1:D:266:TRP:HD1	1.73	0.53
1:D:156:GLN:O	1:D:156:GLN:HG2	2.09	0.53
1:A:527:VAL:HG13	1:A:533:HIS:HB2	1.90	0.53
1:D:337:PRO:HD2	1:D:464:LEU:HD13	1.91	0.53
1:D:351:LYS:HB3	1:D:359:LYS:HG2	1.90	0.53
1:C:224:PHE:HB3	1:C:276:GLN:OE1	2.09	0.53
1:B:482:GLY:O	1:B:534:ASN:HB2	2.10	0.52
1:C:162:HIS:C	1:C:162:HIS:ND1	2.63	0.52
1:A:145:GLU:HB2	1:A:206:LYS:HG2	1.90	0.52
1:C:182:GLU:H	1:C:182:GLU:CD	2.12	0.52
1:A:542:ALA:HB2	1:D:455:PRO:HG2	1.92	0.52
1:C:377:GLY:O	1:C:426:GLU:N	2.31	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:179:ARG:HG3	1:B:447:ILE:O	2.10	0.52
1:D:146:ASP:OD2	1:D:202:LYS:HD3	2.10	0.52
1:C:369:LYS:HB3	1:C:452:VAL:HG22	1.91	0.52
1:C:181:LYS:HE3	1:C:185:ASP:OD2	2.09	0.52
1:B:290:GLN:O	1:B:293:VAL:HG12	2.11	0.51
1:B:512:LYS:HD3	1:B:512:LYS:N	2.24	0.51
1:A:470:MET:HB2	1:A:474:SER:HA	1.90	0.51
1:B:144:LEU:CD2	1:B:213:ILE:HG12	2.40	0.51
1:D:144:LEU:N	3:D:607:HOH:O	2.42	0.51
1:C:317:GLU:HB2	1:C:318:PRO:HD2	1.92	0.51
1:B:145:GLU:HG3	1:B:206:LYS:CG	2.40	0.51
1:B:512:LYS:CD	1:B:512:LYS:H	2.24	0.51
1:D:530:CYS:O	1:D:544:LYS:HE2	2.11	0.51
1:B:209:VAL:HG22	1:B:216:LEU:HD13	1.91	0.51
1:A:470:MET:HG3	1:A:477:PHE:CG	2.45	0.51
1:D:530:CYS:HA	1:D:545:LEU:O	2.11	0.51
1:A:440:ALA:HB2	1:A:496:VAL:HG13	1.92	0.51
1:D:231:SER:O	1:D:234:SER:OG	2.21	0.51
1:B:380:ASN:O	1:B:384:GLN:HG2	2.11	0.51
1:B:477:PHE:CE1	1:B:481:VAL:HG21	2.46	0.51
1:C:201:ASP:C	1:C:201:ASP:OD2	2.50	0.51
1:D:209:VAL:CG1	1:D:213:ILE:HD13	2.41	0.51
1:A:200:LEU:HA	1:A:204:LEU:HD23	1.93	0.50
1:D:538:LEU:O	1:D:549:ARG:NH2	2.43	0.50
1:A:337:PRO:CG	1:A:464:LEU:HD13	2.41	0.50
1:D:452:VAL:HG12	1:D:453:LEU:HG	1.94	0.50
1:A:354:VAL:O	1:A:359:LYS:HE3	2.12	0.50
1:A:529:LEU:HD11	1:A:545:LEU:HD22	1.94	0.50
1:B:225:VAL:N	1:B:274:ASP:OD2	2.39	0.49
1:C:205:PHE:O	1:C:209:VAL:HG22	2.12	0.49
1:C:257:GLN:N	1:C:257:GLN:OE1	2.43	0.49
1:B:532:PHE:CZ	1:B:547:PRO:HG2	2.47	0.49
1:C:305:LEU:HD13	1:C:309:TYR:CE1	2.47	0.49
1:C:316:LYS:NZ	3:C:606:HOH:O	2.38	0.49
1:B:284:LYS:HE3	1:B:430:GLU:OE2	2.12	0.49
1:B:527:VAL:CG1	1:B:533:HIS:HB2	2.43	0.49
1:A:355:ASN:OD1	1:A:357:ALA:HB3	2.12	0.49
1:D:387:ARG:HD2	1:D:417:ASP:OD2	2.12	0.49
1:A:290:GLN:O	1:A:293:VAL:HG12	2.13	0.49
1:C:257:GLN:HE21	1:C:381:ALA:HB1	1.78	0.49
1:C:179:ARG:HG3	1:C:447:ILE:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:253:ASP:HA	1:B:259:ALA:HB2	1.94	0.49
1:D:267:GLY:HA2	1:D:281:GLY:HA3	1.95	0.49
1:D:351:LYS:O	1:D:359:LYS:HE2	2.13	0.48
1:A:491:GLY:HA3	1:A:507:SER:O	2.13	0.48
1:B:144:LEU:HD22	1:B:213:ILE:HG12	1.95	0.48
1:C:543:LYS:NZ	1:C:543:LYS:HB3	2.28	0.48
1:B:230:MET:O	1:B:233:THR:HG22	2.13	0.48
1:B:209:VAL:CG1	1:B:213:ILE:HD13	2.44	0.48
1:C:225:VAL:HG13	1:C:226:ILE:HG13	1.96	0.48
1:B:293:VAL:O	1:B:297:LYS:HG2	2.13	0.48
1:D:470:MET:HB2	1:D:474:SER:HA	1.96	0.47
1:D:254:TYR:CD1	1:D:255:ILE:HG23	2.49	0.47
1:D:437:ALA:HB1	1:D:446:PRO:HG3	1.96	0.47
1:B:533:HIS:HB3	1:B:536:ASP:OD2	2.14	0.47
1:C:317:GLU:HB2	1:C:318:PRO:CD	2.43	0.47
1:C:191:LEU:HD23	1:C:191:LEU:O	2.14	0.47
1:B:387:ARG:NH1	3:B:10:HOH:O	2.46	0.47
1:D:294:LYS:HB2	1:D:295:PRO:HD3	1.96	0.47
1:D:491:GLY:HA2	1:D:510:LEU:HD21	1.96	0.47
1:A:149:PHE:CE2	1:A:202:LYS:HG2	2.49	0.47
1:A:200:LEU:HD23	1:A:205:PHE:HA	1.97	0.47
1:A:336:ASN:O	1:A:342:GLY:HA3	2.14	0.47
1:B:254:TYR:CD1	1:B:255:ILE:HG23	2.50	0.47
1:A:179:ARG:HD2	1:A:447:ILE:O	2.15	0.47
1:C:371:ALA:O	1:C:374:GLU:HG3	2.15	0.47
1:D:312:ARG:O	1:D:333:LYS:HE2	2.16	0.46
1:B:546:ASP:OD1	1:B:548:ARG:NH1	2.48	0.46
1:D:355:ASN:OD1	1:D:357:ALA:HB3	2.15	0.46
1:A:254:TYR:CD1	1:A:255:ILE:HG23	2.50	0.46
1:D:292:CYS:O	1:D:295:PRO:HD2	2.16	0.46
1:C:174:ARG:O	1:C:177:ASP:HB2	2.15	0.46
1:C:503:MET:HE3	1:C:503:MET:HB3	1.73	0.46
1:B:531:ASN:HA	1:B:544:LYS:HD3	1.97	0.46
1:B:185:ASP:HA	1:B:188:ARG:NH1	2.31	0.46
1:A:441:ASN:ND2	1:A:444:PHE:O	2.46	0.46
1:B:354:VAL:HG23	1:B:355:ASN:O	2.16	0.46
1:C:461:THR:O	1:C:465:MET:HG3	2.16	0.45
1:B:149:PHE:CZ	1:B:159:ILE:HD11	2.51	0.45
1:A:527:VAL:CG1	1:A:533:HIS:HB2	2.47	0.45
1:C:340:ASN:O	1:C:344:ILE:HG13	2.16	0.45
1:B:294:LYS:N	1:B:295:PRO:HD2	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:168:LEU:HD21	1:B:180:LEU:HD13	1.97	0.45
1:D:152:ILE:HG22	1:D:163:LYS:NZ	2.31	0.45
1:C:148:LEU:O	1:C:152:ILE:CG2	2.64	0.45
1:A:351:LYS:O	1:A:354:VAL:HG22	2.16	0.45
1:B:224:PHE:HB2	3:B:612:HOH:O	2.16	0.45
1:C:147:LEU:HD13	1:C:147:LEU:HA	1.82	0.45
1:B:437:ALA:CB	1:B:446:PRO:HG2	2.46	0.45
1:D:161:VAL:HG12	1:D:162:HIS:N	2.30	0.45
1:A:201:ASP:H	1:A:204:LEU:HB3	1.81	0.45
1:D:470:MET:HG3	1:D:477:PHE:CG	2.52	0.45
1:C:265:LEU:HD13	1:C:506:TRP:CH2	2.52	0.45
1:C:359:LYS:HB3	1:C:418:PHE:CZ	2.52	0.45
1:D:286:PRO:HA	1:D:427:VAL:O	2.16	0.45
1:D:240:TYR:OH	1:D:281:GLY:HA2	2.16	0.45
1:C:351:LYS:O	1:C:354:VAL:HG22	2.17	0.44
1:A:533:HIS:HB3	1:A:536:ASP:OD2	2.17	0.44
1:D:270:VAL:HG22	1:D:503:MET:HE2	1.97	0.44
1:C:470:MET:HG3	1:C:477:PHE:CG	2.52	0.44
1:B:470:MET:HG3	1:B:477:PHE:CG	2.52	0.44
1:B:369:LYS:HB3	1:B:452:VAL:HG22	1.98	0.44
1:A:149:PHE:CD2	1:A:202:LYS:HG2	2.52	0.44
1:A:169:LYS:HE2	3:A:619:HOH:O	2.17	0.44
1:D:314:VAL:HG22	1:D:315:GLY:N	2.32	0.44
1:A:310:VAL:O	1:A:314:VAL:HG12	2.18	0.44
1:B:312:ARG:O	1:B:333:LYS:HE2	2.17	0.44
1:C:197:GLY:O	1:C:198:VAL:HB	2.18	0.44
1:C:503:MET:HE1	1:C:522:PHE:CE2	2.52	0.44
1:B:318:PRO:HG3	1:B:467:SER:HB2	2.00	0.44
1:A:372:GLY:HA3	1:A:447:ILE:HD11	1.98	0.44
1:D:340:ASN:O	1:D:344:ILE:HG13	2.17	0.44
1:A:340:ASN:O	1:A:344:ILE:HG13	2.18	0.44
1:C:493:ILE:HD12	1:C:519:GLY:HA3	2.00	0.43
1:B:267:GLY:HA2	1:B:281:GLY:HA3	2.00	0.43
1:A:253:ASP:HA	1:A:259:ALA:HB2	1.99	0.43
1:B:221:ARG:HD3	1:B:223:LYS:CD	2.37	0.43
1:D:491:GLY:HA3	1:D:507:SER:O	2.17	0.43
1:C:147:LEU:O	1:C:151:THR:HG23	2.19	0.43
1:C:298:TYR:HA	1:C:346:VAL:HG11	2.00	0.43
1:D:461:THR:O	1:D:465:MET:HG3	2.18	0.43
1:B:262:SER:O	1:B:508:PRO:HG2	2.19	0.43
1:B:148:LEU:O	1:B:152:ILE:HG13	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:198:VAL:HG22	1:B:199:MET:N	2.33	0.43
1:A:392:ARG:NE	3:A:628:HOH:O	2.52	0.43
1:B:511:ASP:HB3	1:B:517:VAL:HG22	1.99	0.43
1:D:470:MET:O	1:D:471:TYR:HB2	2.18	0.43
1:B:548:ARG:NE	3:B:107:HOH:O	2.51	0.43
1:A:294:LYS:N	1:A:295:PRO:HD2	2.34	0.43
1:D:240:TYR:CE2	1:D:266:TRP:CD1	3.06	0.43
1:B:144:LEU:N	1:B:144:LEU:HD13	2.34	0.43
1:A:189:LEU:O	1:A:192:GLN:HB2	2.18	0.43
1:D:229:PHE:O	1:D:233:THR:HG23	2.19	0.43
1:B:286:PRO:HA	1:B:427:VAL:O	2.19	0.43
1:A:206:LYS:O	1:A:210:GLN:HB2	2.18	0.42
1:D:354:VAL:O	1:D:359:LYS:HE3	2.19	0.42
1:A:319:SER:HB3	1:A:335:HIS:CG	2.53	0.42
1:B:470:MET:O	1:B:471:TYR:HB2	2.20	0.42
1:B:392:ARG:O	1:B:396:ILE:HG13	2.19	0.42
1:A:265:LEU:HD13	1:A:506:TRP:HH2	1.85	0.42
1:C:300:ILE:HG23	1:C:366:PHE:CE1	2.55	0.42
1:A:417:ASP:O	1:A:421:GLN:HG3	2.19	0.42
1:A:549:ARG:HB2	1:A:549:ARG:CZ	2.48	0.42
1:C:294:LYS:N	1:C:295:PRO:HD2	2.35	0.42
1:A:304:ASP:OD2	1:A:362:TYR:OH	2.35	0.42
1:A:315:GLY:O	1:A:336:ASN:HA	2.19	0.42
1:D:165:ILE:HG22	1:D:166:THR:N	2.34	0.42
1:B:491:GLY:HA3	1:B:507:SER:O	2.19	0.42
1:C:156:GLN:CG	1:C:157:GLU:N	2.67	0.42
1:B:290:GLN:CG	1:B:489:VAL:HG12	2.45	0.42
1:D:209:VAL:CG1	1:D:209:VAL:O	2.68	0.42
1:D:407:PRO:O	1:D:410:THR:OG1	2.29	0.42
1:A:288:CYS:HA	1:A:426:GLU:HA	2.01	0.41
1:B:377:GLY:O	1:B:426:GLU:N	2.34	0.41
1:C:537:ASN:HB3	1:C:540:HIS:O	2.20	0.41
1:D:144:LEU:HD12	1:D:144:LEU:O	2.21	0.41
1:D:336:ASN:O	1:D:342:GLY:HA3	2.20	0.41
1:C:262:SER:HA	1:C:263:PRO:HD3	1.91	0.41
1:D:168:LEU:HD21	1:D:180:LEU:HD13	2.02	0.41
1:D:331:ASP:N	1:D:331:ASP:OD1	2.53	0.41
1:A:507:SER:HA	1:A:508:PRO:HD3	1.91	0.41
1:A:240:TYR:CE2	1:A:266:TRP:CD1	3.08	0.41
1:C:359:LYS:HB3	1:C:418:PHE:CE2	2.56	0.41
1:B:336:ASN:HB2	1:B:337:PRO:CD	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:327:PHE:CZ	1:B:396:ILE:HG12	2.55	0.41
1:B:175:THR:O	3:B:9:HOH:O	2.22	0.41
1:C:305:LEU:HD13	1:C:309:TYR:HE1	1.84	0.41
1:B:310:VAL:O	1:B:314:VAL:HG12	2.20	0.41
1:B:206:LYS:O	1:B:210:GLN:HB3	2.19	0.41
1:C:150:TYR:C	1:C:152:ILE:H	2.24	0.41
1:A:285:VAL:HA	1:A:286:PRO:HD3	1.88	0.41
1:B:257:GLN:H	1:B:257:GLN:CD	2.23	0.41
1:D:415:ILE:HD13	1:D:415:ILE:HA	1.93	0.41
1:C:384:GLN:O	1:C:388:GLU:HG3	2.21	0.41
1:A:293:VAL:O	1:A:297:LYS:HG2	2.21	0.41
1:D:336:ASN:HB2	1:D:337:PRO:CD	2.51	0.41
1:C:316:LYS:HE2	1:C:316:LYS:HB3	1.93	0.41
1:B:541:PHE:CE1	1:B:544:LYS:O	2.74	0.41
1:B:157:GLU:OE1	1:B:157:GLU:N	2.54	0.41
1:A:367:LEU:HB3	1:A:435:MET:CE	2.51	0.41
1:C:339:VAL:HG23	1:C:342:GLY:H	1.85	0.41
1:B:459:ARG:HD2	1:C:533:HIS:CG	2.56	0.41
1:B:486:LYS:HD2	1:B:486:LYS:HA	1.94	0.41
1:D:308:GLU:O	1:D:312:ARG:HG3	2.21	0.41
1:D:257:GLN:HE21	1:D:381:ALA:HB1	1.86	0.41
1:D:283:THR:OG1	1:D:430:GLU:OE2	2.38	0.40
1:D:306:GLY:O	1:D:310:VAL:HG23	2.21	0.40
1:B:177:ASP:HA	1:B:178:PRO:HD3	1.95	0.40
1:D:396:ILE:O	1:D:400:LEU:HG	2.21	0.40
1:D:213:ILE:HG23	1:D:214:VAL:N	2.36	0.40
1:D:253:ASP:HA	1:D:259:ALA:HB2	2.03	0.40
1:A:209:VAL:HG12	1:A:209:VAL:O	2.21	0.40
1:C:200:LEU:HG	1:C:204:LEU:HD23	2.03	0.40
1:B:481:VAL:O	1:B:527:VAL:HG21	2.22	0.40
1:B:255:ILE:HD11	1:B:258:LEU:HG	2.03	0.40
1:C:294:LYS:HG2	1:C:343:ALA:HB2	2.03	0.40
1:B:440:ALA:HB2	1:B:496:VAL:HG13	2.02	0.40
1:B:444:PHE:CE1	1:B:451:ARG:HB2	2.57	0.40
1:C:240:TYR:CE2	1:C:266:TRP:CD1	3.10	0.40
1:B:445:CYS:HA	1:B:446:PRO:HD3	1.96	0.40
1:D:216:LEU:O	1:D:220:PHE:HD1	2.04	0.40
1:C:491:GLY:HA3	1:C:507:SER:O	2.21	0.40
1:A:355:ASN:H	1:A:355:ASN:HD22	1.69	0.40

There are no symmetry-related clashes.



## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	386/479 (81%)	378 (98%)	8 (2%)	0	100	100
1	B	382/479 (80%)	369 (97%)	13 (3%)	0	100	100
1	C	388/479 (81%)	378 (97%)	9 (2%)	1 (0%)	46	79
1	D	383/479 (80%)	375 (98%)	8 (2%)	0	100	100
All	All	1539/1916 (80%)	1500 (98%)	38 (2%)	1 (0%)	56	87

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	198	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	342/415 (82%)	321 (94%)	21 (6%)	23	55
1	B	339/415 (82%)	319 (94%)	20 (6%)	24	57
1	C	344/415 (83%)	325 (94%)	19 (6%)	27	59
1	D	340/415 (82%)	328 (96%)	12 (4%)	43	77
All	All	1365/1660 (82%)	1293 (95%)	72 (5%)	28	61

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	148	LEU
1	A	152	ILE
1	A	162	HIS
1	A	190	THR
1	A	193	THR
1	A	201	ASP
1	A	206	LYS
1	A	226	ILE
1	A	231	SER
1	A	233	THR
1	A	260	LYS
1	A	317	GLU
1	A	338	MET
1	A	366	PHE
1	A	408	GLU
1	A	417	ASP
1	A	451	ARG
1	A	507	SER
1	A	541	PHE
1	A	548	ARG
1	A	549	ARG
1	B	144	LEU
1	B	145	GLU
1	B	147	LEU
1	B	156	GLN
1	B	157	GLU
1	B	159	ILE
1	B	161	VAL
1	B	165	ILE
1	B	173	LEU
1	B	199	MET
1	B	209	VAL
1	B	211	SER
1	B	223	LYS
1	B	233	THR
1	B	241	GLU
1	B	282	ASP
1	B	366	PHE
1	B	367	LEU
1	B	413	VAL
1	B	424	SER
1	C	147	LEU
1	C	151	THR

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Mol	Chain	Res	Type
1	C	152	ILE
1	C	162	HIS
1	C	173	LEU
1	C	176	SER
1	C	190	THR
1	C	198	VAL
1	C	230	MET
1	C	247	SER
1	C	282	ASP
1	C	328	LEU
1	C	330	GLU
1	C	365	GLN
1	C	366	PHE
1	C	408	GLU
1	C	513	MET
1	C	541	PHE
1	C	549	ARG
1	D	145	GLU
1	D	157	GLU
1	D	159	ILE
1	D	161	VAL
1	D	165	ILE
1	D	173	LEU
1	D	316	LYS
1	D	331	ASP
1	D	360	PHE
1	D	366	PHE
1	D	417	ASP
1	D	512	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	355	ASN

### 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 ⓘ

4 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	GLU	A	1	-	3,9,9	0.37	0	2,11,11	0.07	0
2	GLU	B	1	-	3,9,9	0.37	0	2,11,11	0.10	0
2	GLU	C	1	-	3,9,9	0.37	0	2,11,11	0.08	0
2	GLU	D	1	-	3,9,9	0.38	0	2,11,11	0.06	0

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	GLU	A	1	-	-	0/3/9/9	0/0/0/0
2	GLU	B	1	-	-	0/3/9/9	0/0/0/0
2	GLU	C	1	-	-	0/3/9/9	0/0/0/0
2	GLU	D	1	-	-	0/3/9/9	0/0/0/0

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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1	GLU	1	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	394/479 (82%)	-0.26	3 (0%) 87 81	28, 39, 71, 92	1 (0%)
1	B	390/479 (81%)	-0.08	10 (2%) 59 47	27, 41, 72, 97	1 (0%)
1	C	396/479 (82%)	-0.18	6 (1%) 76 68	31, 43, 72, 93	1 (0%)
1	D	391/479 (81%)	-0.10	8 (2%) 68 58	31, 43, 71, 90	1 (0%)
All	All	1571/1916 (81%)	-0.16	27 (1%) 73 63	27, 42, 72, 97	4 (0%)

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	159	ILE	4.5
1	B	150	TYR	4.2
1	B	158	LYS	3.9
1	B	149	PHE	3.2
1	B	151	THR	3.2
1	D	150	TYR	3.2
1	D	256	PRO	2.9
1	A	150	TYR	2.7
1	B	148	LEU	2.6
1	B	201	ASP	2.6
1	D	161	VAL	2.6
1	C	207	LYS	2.5
1	C	150	TYR	2.5
1	B	205	PHE	2.4
1	C	149	PHE	2.4
1	D	200	LEU	2.3
1	D	149	PHE	2.3
1	A	203	ASP	2.3
1	C	161	VAL	2.2
1	A	199	MET	2.2
1	D	158	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	159	ILE	2.2
1	D	148	LEU	2.2
1	B	390	GLY	2.2
1	C	209	VAL	2.1
1	D	263	PRO	2.1
1	B	157	GLU	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( $\text{\AA}^2$ )	Q<0.9
2	GLU	C	1	10/10	0.94	0.16	0.07	41,51,55,56	0
2	GLU	B	1	10/10	0.93	0.18	-0.07	41,50,55,59	0
2	GLU	D	1	10/10	0.94	0.17	-0.38	42,52,57,63	0
2	GLU	A	1	10/10	0.94	0.15	-0.77	41,44,49,50	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.