



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 13, 2020 – 11:19 PM BST

PDB ID : 6BAU  
Title : Crystal Structure of GltPh R397C in complex with L-Cysteine  
Authors : Font, J.; Scopelliti, A.J.; Vandenberg, R.J.; Boudker, O.; Ryan, R.M.  
Deposited on : 2017-10-15  
Resolution : 3.80 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

<https://www.wwpdb.org/validation/2017/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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.14.4.dev1  
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)  
Validation Pipeline (wwPDB-VP) : 2.14.4.dev1

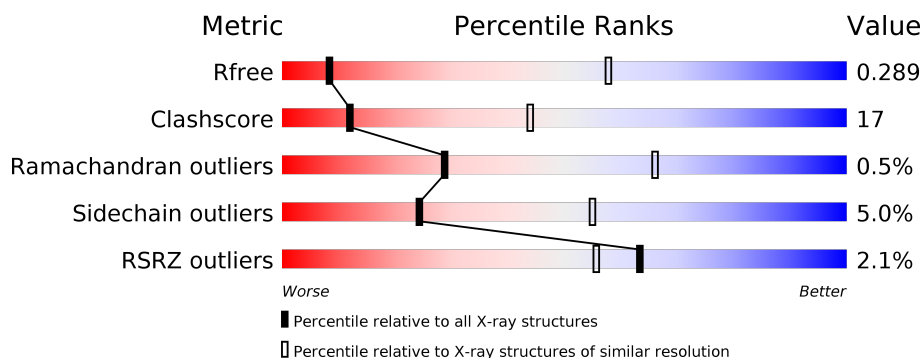
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.80 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))
$R_{free}$	130704	1212 (4.00-3.60)
Clashscore	141614	1288 (4.00-3.60)
Ramachandran outliers	138981	1243 (4.00-3.60)
Sidechain outliers	138945	1237 (4.00-3.60)
RSRZ outliers	127900	1121 (4.00-3.60)

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 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	420	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 63%, green 32%, grey 2%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>%</span> <span>63%</span> <span>32%</span> <span>• •</span> </div> </div>
1	B	420	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 3%, orange 1%, yellow 65%, green 31%, grey 2%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>3%</span> <span>65%</span> <span>31%</span> <span>• •</span> </div> </div>
1	C	420	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 2%, orange 1%, yellow 64%, green 31%, grey 2%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>2%</span> <span>64%</span> <span>31%</span> <span>• •</span> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	CYS	C	503	-	-	X	-

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9030 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 Glutamate transporter homolog.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	408	Total	C	N	O	S	0	0	0
			3001	1976	474	533	18			
1	B	408	Total	C	N	O	S	0	0	0
			3001	1976	474	533	18			
1	C	408	Total	C	N	O	S	0	0	0
			3001	1976	474	533	18			

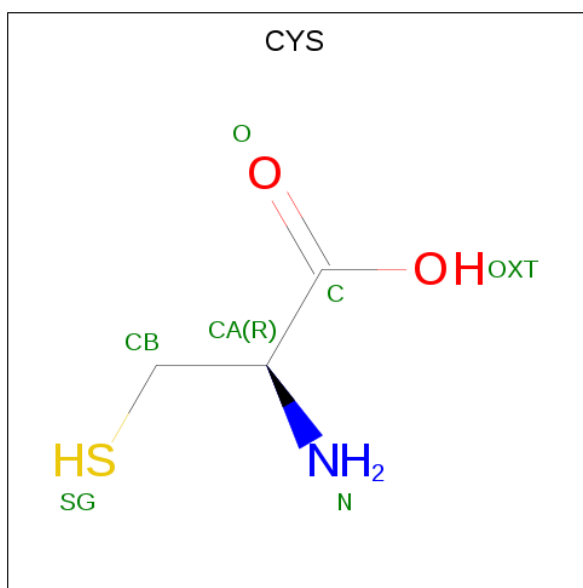
There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	397	CYS	ARG	engineered mutation	UNP O59010
A	418	THR	-	expression tag	UNP O59010
A	419	LEU	-	expression tag	UNP O59010
A	420	VAL	-	expression tag	UNP O59010
B	397	CYS	ARG	engineered mutation	UNP O59010
B	418	THR	-	expression tag	UNP O59010
B	419	LEU	-	expression tag	UNP O59010
B	420	VAL	-	expression tag	UNP O59010
C	397	CYS	ARG	engineered mutation	UNP O59010
C	418	THR	-	expression tag	UNP O59010
C	419	LEU	-	expression tag	UNP O59010
C	420	VAL	-	expression tag	UNP O59010

- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total	Na	0	0
			2	2		
2	A	2	Total	Na	0	0
			2	2		
2	C	2	Total	Na	0	0
			2	2		

- Molecule 3 is CYSTEINE (three-letter code: CYS) (formula:  $C_3H_7NO_2S$ ).

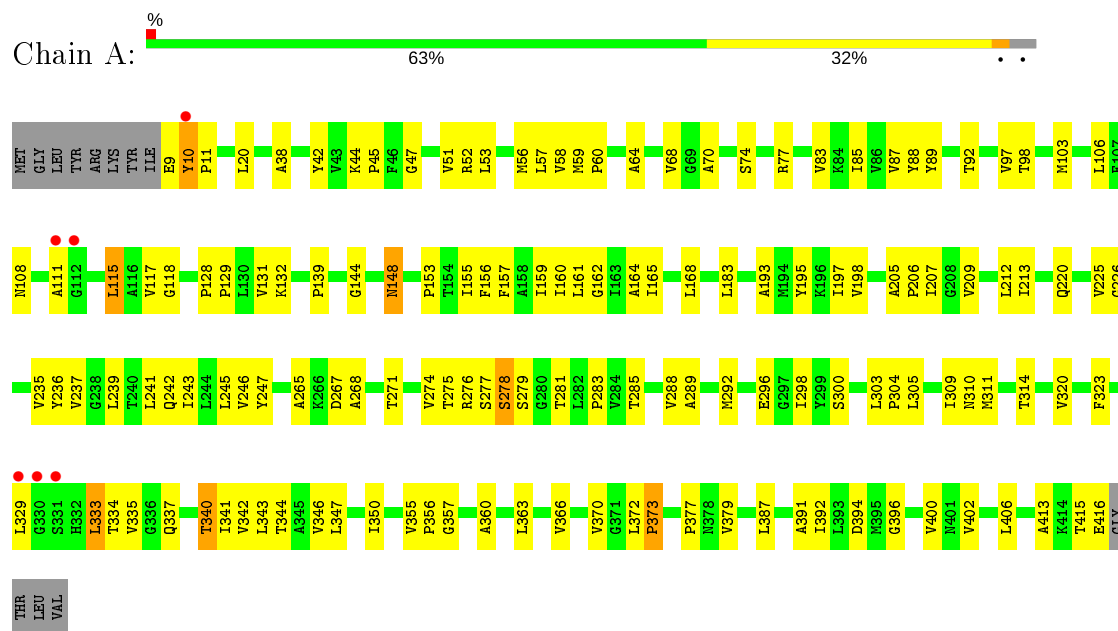


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			7	3	1	2	1		
3	B	1	Total	C	N	O	S	0	0
			7	3	1	2	1		
3	C	1	Total	C	N	O	S	0	0
			7	3	1	2	1		

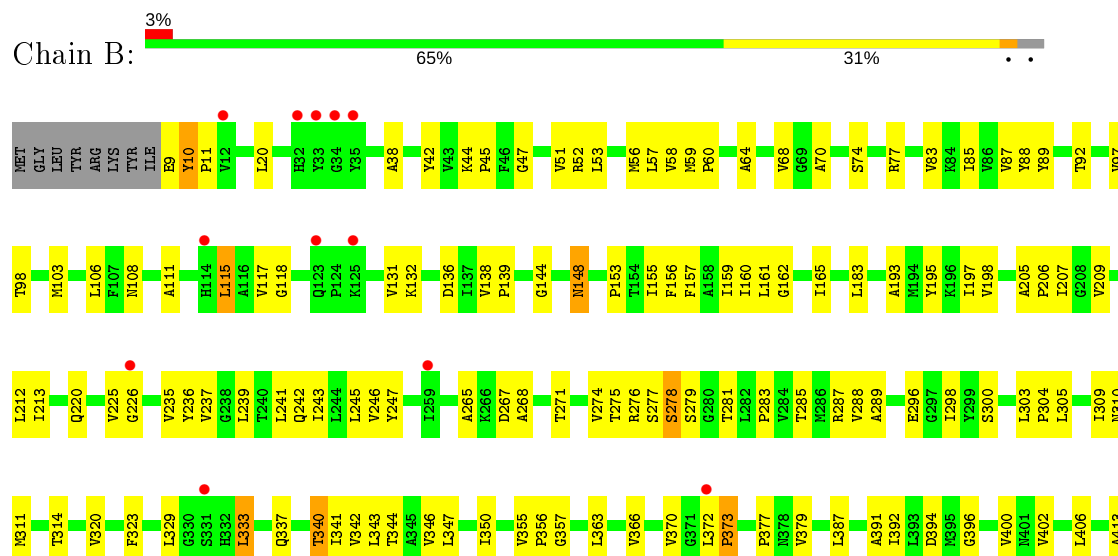
### 3 Residue-property plots

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: Glutamate transporter homolog

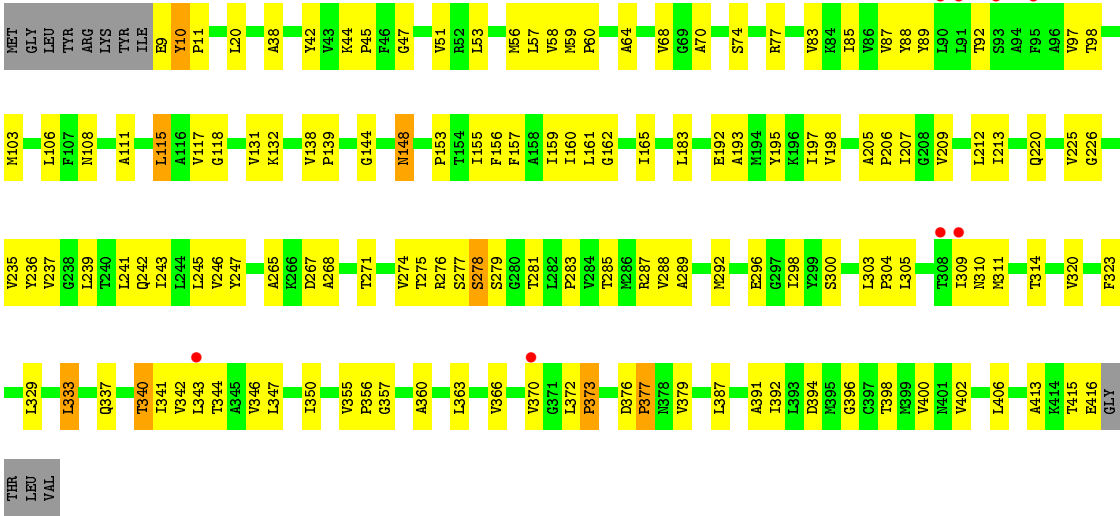


#### • Molecule 1: Glutamate transporter homolog



K414
T415
E416
GLY
THR
LEU
VAL

• Molecule 1: Glutamate transporter homolog



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	115.31Å 115.31Å 322.27Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	40.00 – 3.80 39.47 – 3.80	Depositor EDS
% Data completeness (in resolution range)	96.8 (40.00-3.80) 96.7 (39.47-3.80)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.69 (at 3.76Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.267 , 0.290 0.267 , 0.289	Depositor DCC
$R_{free}$ test set	1253 reflections (5.44%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	135.2	Xtriage
Anisotropy	0.082	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.20 , 46.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.097 for h,-h-k,-l	Xtriage
$F_o, F_c$ correlation	0.87	EDS
Total number of atoms	9030	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	160.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.32% 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

### 5.1 Standard geometry

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

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	0.64	0/3053	0.57	0/4162
1	B	0.64	0/3053	0.57	0/4162
1	C	0.64	0/3053	0.57	0/4162
All	All	0.64	0/9159	0.57	0/12486

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3001	0	3190	114	0
1	B	3001	0	3190	111	0
1	C	3001	0	3190	116	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
3	A	7	0	4	3	0
3	B	7	0	4	3	0
3	C	7	0	4	4	0
All	All	9030	0	9582	320	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 17.

All (320) 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:268:ALA:HB1	1:B:285:THR:HG22	1.43	1.00
1:A:268:ALA:HB1	1:A:285:THR:HG22	1.43	1.00
1:C:268:ALA:HB1	1:C:285:THR:HG22	1.43	0.99
1:C:239:LEU:HD22	1:C:400:VAL:HG21	1.48	0.95
1:B:235:VAL:HG22	1:B:320:VAL:HG11	1.49	0.94
1:B:239:LEU:HD22	1:B:400:VAL:HG21	1.48	0.93
1:C:235:VAL:HG22	1:C:320:VAL:HG11	1.49	0.93
1:A:239:LEU:HD22	1:A:400:VAL:HG21	1.48	0.93
1:A:235:VAL:HG22	1:A:320:VAL:HG11	1.49	0.92
1:B:305:LEU:HD21	1:B:309:ILE:HD12	1.55	0.88
1:C:305:LEU:HD21	1:C:309:ILE:HD12	1.55	0.88
1:A:305:LEU:HD21	1:A:309:ILE:HD12	1.55	0.88
1:B:275:THR:HG23	1:B:277:SER:H	1.43	0.84
1:C:275:THR:HG23	1:C:277:SER:H	1.43	0.84
1:A:275:THR:HG23	1:A:277:SER:H	1.43	0.83
1:A:89:TYR:CD1	1:A:310:ASN:HB2	2.19	0.78
1:B:89:TYR:CD1	1:B:310:ASN:HB2	2.19	0.78
1:C:89:TYR:CD1	1:C:310:ASN:HB2	2.19	0.78
1:A:195:TYR:O	1:A:198:VAL:HG22	1.87	0.74
1:A:20:LEU:HD12	1:A:213:ILE:HD13	1.70	0.73
1:B:195:TYR:O	1:B:198:VAL:HG22	1.87	0.73
1:C:195:TYR:O	1:C:198:VAL:HG22	1.87	0.72
1:C:20:LEU:HD12	1:C:213:ILE:HD13	1.70	0.72
1:B:20:LEU:HD12	1:B:213:ILE:HD13	1.70	0.72
1:B:56:MET:CE	1:C:157:PHE:HD1	2.03	0.71
1:C:314:THR:OG1	3:C:503:CYS:HB3	1.89	0.71
1:C:89:TYR:HD1	1:C:310:ASN:ND2	1.89	0.71
1:B:314:THR:OG1	3:B:503:CYS:HB3	1.89	0.71
1:A:314:THR:OG1	3:A:503:CYS:HB3	1.89	0.71
1:A:89:TYR:HD1	1:A:310:ASN:ND2	1.89	0.70
1:B:89:TYR:HD1	1:B:310:ASN:ND2	1.88	0.70
1:A:160:ILE:HG22	1:C:197:ILE:HD12	1.73	0.70
1:C:343:LEU:O	1:C:347:LEU:HD23	1.93	0.69
1:A:343:LEU:O	1:A:347:LEU:HD23	1.93	0.69
1:B:343:LEU:O	1:B:347:LEU:HD23	1.93	0.69
1:C:296:GLU:O	1:C:300:SER:HB3	1.93	0.69
1:B:296:GLU:O	1:B:300:SER:HB3	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:157:PHE:HD1	1:C:56:MET:CE	2.07	0.68
1:A:296:GLU:O	1:A:300:SER:HB3	1.93	0.68
1:B:305:LEU:CD2	1:B:309:ILE:HD12	2.25	0.67
1:A:305:LEU:CD2	1:A:309:ILE:HD12	2.25	0.67
1:C:305:LEU:CD2	1:C:309:ILE:HD12	2.25	0.66
1:C:85:ILE:HG13	1:C:89:TYR:CE2	2.31	0.65
1:B:220:GLN:HE22	1:B:391:ALA:H	1.44	0.65
1:A:85:ILE:HG13	1:A:89:TYR:CE2	2.31	0.65
1:B:56:MET:HE3	1:C:157:PHE:HD1	1.61	0.65
1:C:220:GLN:HE22	1:C:391:ALA:H	1.44	0.65
1:A:197:ILE:HD12	1:B:160:ILE:HG22	1.79	0.64
1:A:220:GLN:HE22	1:A:391:ALA:H	1.44	0.64
1:B:85:ILE:HG13	1:B:89:TYR:CE2	2.31	0.64
1:A:193:ALA:O	1:A:197:ILE:HG12	1.98	0.64
1:B:193:ALA:O	1:B:197:ILE:HG12	1.98	0.64
1:C:337:GLN:O	1:C:340:THR:HG22	1.98	0.64
1:A:276:ARG:HD2	1:A:394:ASP:HB3	1.80	0.63
1:A:337:GLN:O	1:A:340:THR:HG22	1.98	0.63
1:B:337:GLN:O	1:B:340:THR:HG22	1.98	0.62
1:C:276:ARG:HD2	1:C:394:ASP:HB3	1.80	0.62
1:C:193:ALA:O	1:C:197:ILE:HG12	1.98	0.62
1:B:276:ARG:HD2	1:B:394:ASP:HB3	1.80	0.62
1:A:89:TYR:HD1	1:A:310:ASN:HD22	1.47	0.61
1:A:296:GLU:O	1:A:300:SER:CB	2.48	0.61
1:B:296:GLU:O	1:B:300:SER:CB	2.48	0.61
1:A:161:LEU:O	1:A:165:ILE:HG12	2.01	0.61
1:A:89:TYR:CD1	1:A:310:ASN:ND2	2.69	0.60
1:B:89:TYR:CD1	1:B:310:ASN:ND2	2.69	0.60
1:C:296:GLU:O	1:C:300:SER:CB	2.48	0.60
1:B:89:TYR:HD1	1:B:310:ASN:HD22	1.47	0.60
1:C:161:LEU:O	1:C:165:ILE:HG12	2.01	0.60
1:B:161:LEU:O	1:B:165:ILE:HG12	2.01	0.60
1:A:157:PHE:HD1	1:C:56:MET:HE2	1.67	0.59
1:A:89:TYR:CD1	1:A:310:ASN:CB	2.85	0.59
1:C:89:TYR:HD1	1:C:310:ASN:HD22	1.47	0.59
1:A:209:VAL:HG13	1:A:274:VAL:HG21	1.85	0.59
1:B:89:TYR:CD1	1:B:310:ASN:CB	2.85	0.59
1:C:209:VAL:HG13	1:C:274:VAL:HG21	1.85	0.59
1:C:89:TYR:CD1	1:C:310:ASN:CB	2.85	0.59
1:B:209:VAL:HG13	1:B:274:VAL:HG21	1.85	0.58
1:C:20:LEU:CD1	1:C:213:ILE:HD13	2.34	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:89:TYR:CD1	1:C:310:ASN:ND2	2.69	0.58
1:A:56:MET:CE	1:B:157:PHE:HD1	2.15	0.58
1:A:20:LEU:CD1	1:A:213:ILE:HD13	2.34	0.57
1:C:289:ALA:HB2	1:C:303:LEU:HD11	1.87	0.57
1:A:212:LEU:HD13	1:A:274:VAL:HG12	1.87	0.57
1:C:243:ILE:HA	1:C:247:TYR:CD2	2.40	0.57
1:B:197:ILE:HD12	1:C:160:ILE:HG22	1.87	0.57
1:B:212:LEU:HD13	1:B:274:VAL:HG12	1.87	0.56
1:B:289:ALA:HB2	1:B:303:LEU:HD11	1.87	0.56
1:C:236:TYR:HE1	1:C:396:GLY:HA3	1.70	0.56
1:B:243:ILE:HA	1:B:247:TYR:CD2	2.40	0.56
1:C:415:THR:O	1:C:416:GLU:HB2	2.06	0.56
1:A:289:ALA:HB2	1:A:303:LEU:HD11	1.87	0.56
1:A:415:THR:O	1:A:416:GLU:HB2	2.06	0.56
1:A:236:TYR:HE1	1:A:396:GLY:HA3	1.70	0.56
1:A:103:MET:HE3	1:A:237:VAL:HG12	1.87	0.56
1:B:344:THR:HB	1:B:366:VAL:HG23	1.87	0.56
1:C:344:THR:HB	1:C:366:VAL:HG23	1.87	0.56
1:B:415:THR:O	1:B:416:GLU:HB2	2.06	0.56
1:C:212:LEU:HD13	1:C:274:VAL:HG12	1.87	0.55
1:B:20:LEU:CD1	1:B:213:ILE:HD13	2.34	0.55
1:A:243:ILE:HA	1:A:247:TYR:CD2	2.40	0.55
1:A:344:THR:HB	1:A:366:VAL:HG23	1.87	0.55
1:B:220:GLN:HE22	1:B:391:ALA:N	2.05	0.55
1:C:415:THR:O	1:C:416:GLU:CB	2.54	0.55
1:B:236:TYR:HE1	1:B:396:GLY:HA3	1.70	0.55
1:A:415:THR:O	1:A:416:GLU:CB	2.54	0.54
1:C:355:VAL:HG13	1:C:356:PRO:HD2	1.88	0.54
1:B:355:VAL:HG13	1:B:356:PRO:HD2	1.88	0.54
1:B:205:ALA:N	1:B:206:PRO:HD2	2.23	0.54
1:A:205:ALA:N	1:A:206:PRO:HD2	2.23	0.54
1:A:355:VAL:HG13	1:A:356:PRO:HD2	1.88	0.54
1:A:97:VAL:HG11	1:A:342:VAL:HA	1.90	0.54
1:A:220:GLN:HE22	1:A:391:ALA:N	2.05	0.54
1:B:415:THR:O	1:B:416:GLU:CB	2.54	0.54
1:A:239:LEU:HD22	1:A:400:VAL:CG2	2.31	0.54
1:B:311:MET:HB3	1:B:314:THR:HB	1.91	0.53
1:C:278:SER:HB2	3:C:503:CYS:O	2.08	0.53
1:A:10:TYR:CD2	1:A:11:PRO:HD2	2.44	0.53
1:A:278:SER:HB2	3:A:503:CYS:O	2.08	0.53
1:B:10:TYR:CD2	1:B:11:PRO:HD2	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:220:GLN:HE22	1:C:391:ALA:N	2.05	0.53
1:C:10:TYR:CD2	1:C:11:PRO:HD2	2.44	0.53
1:C:205:ALA:N	1:C:206:PRO:HD2	2.23	0.53
1:C:337:GLN:O	1:C:341:ILE:HG13	2.09	0.53
1:B:278:SER:HB2	3:B:503:CYS:O	2.08	0.53
1:C:357:GLY:N	1:C:394:ASP:OD2	2.39	0.53
1:B:89:TYR:CG	1:B:310:ASN:HB2	2.44	0.53
1:B:97:VAL:HG11	1:B:342:VAL:HA	1.90	0.53
1:B:357:GLY:N	1:B:394:ASP:OD2	2.39	0.53
1:C:355:VAL:HG13	1:C:356:PRO:CD	2.39	0.53
1:A:89:TYR:CG	1:A:310:ASN:HB2	2.44	0.53
1:B:337:GLN:O	1:B:341:ILE:HG13	2.09	0.53
1:C:57:LEU:HD13	1:C:198:VAL:HG12	1.91	0.53
1:A:355:VAL:HG13	1:A:356:PRO:CD	2.39	0.52
1:C:311:MET:HB3	1:C:314:THR:HB	1.91	0.52
1:A:212:LEU:CD1	1:A:274:VAL:HG12	2.40	0.52
1:A:337:GLN:O	1:A:341:ILE:HG13	2.09	0.52
1:B:212:LEU:CD1	1:B:274:VAL:HG12	2.40	0.52
1:A:57:LEU:HD13	1:A:198:VAL:HG12	1.91	0.52
1:B:355:VAL:HG13	1:B:356:PRO:CD	2.39	0.52
1:A:88:TYR:CZ	1:A:92:THR:HG21	2.45	0.52
1:B:346:VAL:O	1:B:350:ILE:HG13	2.09	0.52
1:B:57:LEU:HD13	1:B:198:VAL:HG12	1.91	0.52
1:B:88:TYR:CZ	1:B:92:THR:HG21	2.45	0.52
1:C:103:MET:CE	1:C:237:VAL:HG12	2.40	0.52
1:C:88:TYR:CZ	1:C:92:THR:HG21	2.45	0.52
1:A:311:MET:HB3	1:A:314:THR:HB	1.91	0.52
1:C:97:VAL:HG11	1:C:342:VAL:HA	1.90	0.52
1:B:103:MET:CE	1:B:237:VAL:HG12	2.40	0.52
1:C:89:TYR:CG	1:C:310:ASN:HB2	2.44	0.52
1:A:70:ALA:HB3	1:A:162:GLY:HA3	1.93	0.51
1:A:103:MET:CE	1:A:237:VAL:HG12	2.40	0.51
1:A:346:VAL:O	1:A:350:ILE:HG13	2.09	0.51
1:B:56:MET:HE2	1:C:157:PHE:HD1	1.76	0.51
1:C:346:VAL:O	1:C:350:ILE:HG13	2.09	0.51
1:C:212:LEU:CD1	1:C:274:VAL:HG12	2.40	0.51
1:C:74:SER:HB2	1:C:77:ARG:HB2	1.92	0.51
1:A:74:SER:HB2	1:A:77:ARG:HB2	1.92	0.51
1:A:83:VAL:O	1:A:87:VAL:HG23	2.11	0.51
1:B:83:VAL:O	1:B:87:VAL:HG23	2.11	0.51
1:B:74:SER:HB2	1:B:77:ARG:HB2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:220:GLN:HB2	1:A:392:ILE:HD13	1.93	0.50
1:B:220:GLN:HB2	1:B:392:ILE:HD13	1.93	0.50
1:B:70:ALA:HB3	1:B:162:GLY:HA3	1.93	0.50
1:A:157:PHE:HD1	1:C:56:MET:HE3	1.76	0.50
1:C:373:PRO:O	1:C:379:VAL:HG11	2.12	0.50
1:C:83:VAL:O	1:C:87:VAL:HG23	2.11	0.50
1:A:373:PRO:O	1:A:379:VAL:HG11	2.12	0.50
1:A:243:ILE:HA	1:A:247:TYR:HD2	1.77	0.50
1:A:56:MET:HE3	1:B:157:PHE:HD1	1.77	0.50
1:B:243:ILE:HA	1:B:247:TYR:HD2	1.77	0.50
1:A:268:ALA:CB	1:A:285:THR:HG22	2.30	0.49
1:C:70:ALA:HB3	1:C:162:GLY:HA3	1.93	0.49
1:B:56:MET:HE3	1:C:157:PHE:CD1	2.46	0.49
1:C:239:LEU:HD22	1:C:400:VAL:CG2	2.31	0.49
1:A:156:PHE:O	1:A:160:ILE:HG12	2.13	0.49
1:A:357:GLY:N	1:A:394:ASP:OD2	2.39	0.49
1:B:373:PRO:O	1:B:379:VAL:HG11	2.12	0.49
1:C:58:VAL:HG22	1:C:283:PRO:HD3	1.95	0.49
1:B:156:PHE:O	1:B:160:ILE:HG12	2.13	0.49
1:C:243:ILE:HA	1:C:247:TYR:HD2	1.77	0.49
1:C:156:PHE:O	1:C:160:ILE:HG12	2.13	0.49
1:C:220:GLN:HB2	1:C:392:ILE:HD13	1.93	0.49
1:B:239:LEU:HD22	1:B:400:VAL:CG2	2.31	0.48
1:B:268:ALA:CB	1:B:285:THR:HG22	2.30	0.48
1:B:58:VAL:HG22	1:B:283:PRO:HD3	1.95	0.48
1:A:58:VAL:HG22	1:A:283:PRO:HD3	1.95	0.48
1:C:242:GLN:O	1:C:246:VAL:HB	2.14	0.48
1:A:52:ARG:NH2	1:B:136:ASP:HA	2.29	0.48
1:C:209:VAL:HA	1:C:274:VAL:HG11	1.95	0.48
1:C:303:LEU:HD21	1:C:406:LEU:HD23	1.96	0.48
1:A:303:LEU:HD21	1:A:406:LEU:HD23	1.96	0.48
1:B:242:GLN:O	1:B:246:VAL:HB	2.14	0.47
1:A:225:VAL:HG12	1:A:226:GLY:N	2.30	0.47
1:A:333:LEU:HD12	1:A:333:LEU:H	1.79	0.47
1:B:303:LEU:HD21	1:B:406:LEU:HD23	1.96	0.47
1:A:242:GLN:O	1:A:246:VAL:HB	2.14	0.47
1:B:209:VAL:HA	1:B:274:VAL:HG11	1.95	0.47
1:B:225:VAL:HG12	1:B:226:GLY:N	2.29	0.47
1:A:209:VAL:HA	1:A:274:VAL:HG11	1.95	0.47
1:A:271:THR:HB	1:A:281:THR:HG23	1.97	0.47
1:C:225:VAL:HG12	1:C:226:GLY:N	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:363:LEU:O	1:A:366:VAL:HG12	2.15	0.47
1:C:363:LEU:O	1:C:366:VAL:HG12	2.15	0.47
1:C:271:THR:HB	1:C:281:THR:HG23	1.97	0.47
1:A:343:LEU:O	1:A:343:LEU:HD23	2.15	0.46
1:B:155:ILE:HD11	1:B:304:PRO:HB2	1.97	0.46
1:A:155:ILE:HD11	1:A:304:PRO:HB2	1.97	0.46
1:B:333:LEU:HD12	1:B:333:LEU:H	1.79	0.46
1:B:343:LEU:O	1:B:343:LEU:HD23	2.15	0.46
1:B:363:LEU:O	1:B:366:VAL:HG12	2.15	0.46
1:C:108:ASN:HB3	1:C:111:ALA:HB2	1.98	0.46
1:C:343:LEU:O	1:C:343:LEU:HD23	2.15	0.46
1:A:241:LEU:O	1:A:245:LEU:HB3	2.16	0.46
1:C:241:LEU:O	1:C:245:LEU:HB3	2.16	0.46
1:C:333:LEU:HD12	1:C:333:LEU:H	1.79	0.46
1:C:394:ASP:OD1	3:C:503:CYS:N	2.49	0.46
1:B:241:LEU:O	1:B:245:LEU:HB3	2.16	0.46
1:B:108:ASN:HB3	1:B:111:ALA:HB2	1.98	0.46
1:C:268:ALA:CB	1:C:285:THR:HG22	2.30	0.46
1:C:155:ILE:HD11	1:C:304:PRO:HB2	1.97	0.46
1:B:394:ASP:OD1	3:B:503:CYS:N	2.49	0.46
1:A:235:VAL:HG22	1:A:320:VAL:CG1	2.34	0.45
1:B:235:VAL:HG22	1:B:320:VAL:CG1	2.34	0.45
1:B:276:ARG:HG3	1:B:276:ARG:HH11	1.81	0.45
1:B:271:THR:HB	1:B:281:THR:HG23	1.97	0.45
1:A:275:THR:HG21	1:A:281:THR:OG1	2.17	0.45
1:A:394:ASP:OD1	3:A:503:CYS:N	2.49	0.45
1:B:275:THR:HG21	1:B:281:THR:OG1	2.17	0.45
1:A:292:MET:H	1:A:292:MET:HG2	1.66	0.45
1:B:165:ILE:HD12	1:B:183:LEU:HD23	1.99	0.45
1:C:47:GLY:O	1:C:51:VAL:HG23	2.16	0.45
1:C:275:THR:HG21	1:C:281:THR:OG1	2.17	0.45
1:A:164:ALA:HB2	1:C:197:ILE:HD11	1.99	0.45
1:B:47:GLY:O	1:B:51:VAL:HG23	2.16	0.44
1:A:108:ASN:HB3	1:A:111:ALA:HB2	1.98	0.44
1:A:276:ARG:HG3	1:A:276:ARG:HH11	1.81	0.44
1:A:47:GLY:O	1:A:51:VAL:HG23	2.16	0.44
1:B:281:THR:HG22	1:B:285:THR:HG23	1.99	0.44
1:C:276:ARG:HG3	1:C:276:ARG:HH11	1.82	0.44
1:C:53:LEU:O	1:C:56:MET:HB3	2.17	0.44
1:A:53:LEU:O	1:A:56:MET:HB3	2.17	0.44
1:C:376:ASP:HA	1:C:377:PRO:HD2	1.84	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:53:LEU:O	1:B:56:MET:HB3	2.17	0.44
1:C:281:THR:HG22	1:C:285:THR:HG23	1.99	0.44
1:A:281:THR:HG22	1:A:285:THR:HG23	1.99	0.43
1:C:265:ALA:HA	1:C:288:VAL:HG11	2.00	0.43
1:A:52:ARG:NH2	1:B:138:VAL:O	2.51	0.43
1:C:165:ILE:HD12	1:C:183:LEU:HD23	1.99	0.43
1:C:103:MET:HE3	1:C:237:VAL:HG12	1.99	0.43
1:A:265:ALA:HA	1:A:288:VAL:HG11	2.00	0.43
1:C:271:THR:O	1:C:275:THR:HG22	2.19	0.43
1:A:271:THR:O	1:A:275:THR:HG22	2.19	0.43
1:B:265:ALA:HA	1:B:288:VAL:HG11	2.00	0.43
1:C:38:ALA:O	1:C:42:TYR:HB2	2.19	0.43
1:A:165:ILE:HD12	1:A:183:LEU:HD23	1.99	0.43
1:A:164:ALA:HB2	1:C:197:ILE:CD1	2.49	0.43
1:B:285:THR:HG21	1:B:402:VAL:CG1	2.48	0.43
1:A:168:LEU:HD21	1:C:192:GLU:HB2	2.01	0.43
1:A:38:ALA:O	1:A:42:TYR:HB2	2.18	0.43
1:C:59:MET:HB2	1:C:60:PRO:HD3	2.01	0.43
1:A:117:VAL:HG12	1:A:118:GLY:N	2.34	0.43
1:A:128:PRO:HA	1:A:129:PRO:HD3	1.90	0.43
1:B:115:LEU:HD12	1:B:115:LEU:H	1.84	0.43
1:B:38:ALA:O	1:B:42:TYR:HB2	2.18	0.43
1:B:139:PRO:HB3	1:B:153:PRO:HB3	2.01	0.42
1:B:271:THR:O	1:B:275:THR:HG22	2.19	0.42
1:A:285:THR:HG21	1:A:402:VAL:CG1	2.48	0.42
1:C:155:ILE:O	1:C:159:ILE:HG13	2.19	0.42
1:C:285:THR:HG21	1:C:402:VAL:CG1	2.48	0.42
1:B:117:VAL:HG12	1:B:118:GLY:N	2.34	0.42
1:B:207:ILE:HD12	1:B:207:ILE:H	1.85	0.42
1:A:131:VAL:HG13	1:A:132:LYS:H	1.85	0.42
1:C:207:ILE:H	1:C:207:ILE:HD12	1.85	0.42
1:B:155:ILE:O	1:B:159:ILE:HG13	2.19	0.42
1:B:59:MET:HB2	1:B:60:PRO:HD3	2.01	0.42
1:A:139:PRO:HB3	1:A:153:PRO:HB3	2.01	0.42
1:C:115:LEU:HD12	1:C:115:LEU:H	1.84	0.42
1:B:52:ARG:NH2	1:C:138:VAL:O	2.51	0.42
1:A:115:LEU:H	1:A:115:LEU:HD12	1.84	0.42
1:C:117:VAL:HG12	1:C:118:GLY:N	2.34	0.42
1:C:139:PRO:HB3	1:C:153:PRO:HB3	2.01	0.41
1:A:59:MET:HB2	1:A:60:PRO:HD3	2.01	0.41
1:A:155:ILE:O	1:A:159:ILE:HG13	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:103:MET:HE3	1:B:237:VAL:HG12	2.02	0.41
1:A:275:THR:O	1:A:276:ARG:HB2	2.21	0.41
1:A:64:ALA:O	1:A:68:VAL:HG23	2.21	0.41
1:C:275:THR:O	1:C:276:ARG:HB2	2.21	0.41
1:A:207:ILE:HD12	1:A:207:ILE:H	1.85	0.41
1:C:235:VAL:HG22	1:C:320:VAL:CG1	2.34	0.41
1:C:305:LEU:HD23	1:C:305:LEU:C	2.41	0.41
1:C:64:ALA:O	1:C:68:VAL:HG23	2.21	0.41
1:B:131:VAL:HG13	1:B:132:LYS:H	1.85	0.41
1:B:165:ILE:CD1	1:B:183:LEU:HD23	2.51	0.41
1:C:298:ILE:HD13	1:C:413:ALA:HA	2.03	0.41
1:B:197:ILE:HG12	1:B:197:ILE:H	1.74	0.41
1:B:275:THR:O	1:B:276:ARG:HB2	2.21	0.41
1:C:144:GLY:O	1:C:148:ASN:OD1	2.38	0.41
1:C:197:ILE:H	1:C:197:ILE:HG12	1.74	0.41
1:A:160:ILE:CG2	1:C:197:ILE:HD12	2.44	0.41
1:A:144:GLY:O	1:A:148:ASN:OD1	2.38	0.41
1:C:131:VAL:HG13	1:C:132:LYS:H	1.85	0.41
1:A:298:ILE:HD13	1:A:413:ALA:HA	2.03	0.41
1:B:198:VAL:HG23	1:B:287:ARG:HD3	2.03	0.41
1:A:56:MET:HE2	1:B:157:PHE:HD1	1.82	0.41
1:A:197:ILE:HD12	1:B:160:ILE:CG2	2.48	0.40
1:C:165:ILE:CD1	1:C:183:LEU:HD23	2.51	0.40
1:C:198:VAL:HG23	1:C:287:ARG:HD3	2.03	0.40
1:C:44:LYS:N	1:C:45:PRO:HD2	2.36	0.40
1:B:298:ILE:HD13	1:B:413:ALA:HA	2.03	0.40
1:A:44:LYS:N	1:A:45:PRO:HD2	2.36	0.40
1:B:144:GLY:O	1:B:148:ASN:OD1	2.38	0.40
1:B:44:LYS:N	1:B:45:PRO:HD2	2.36	0.40
1:A:165:ILE:CD1	1:A:183:LEU:HD23	2.51	0.40
1:B:305:LEU:C	1:B:305:LEU:HD23	2.41	0.40
1:B:64:ALA:O	1:B:68:VAL:HG23	2.21	0.40
1:C:292:MET:HG2	1:C:292:MET:H	1.66	0.40
1:C:360:ALA:O	1:C:363:LEU:HB3	2.22	0.40
1:A:334:THR:HG22	1:A:335:VAL:N	2.37	0.40
1:A:360:ALA:O	1:A:363:LEU:HB3	2.22	0.40
1:C:398:THR:HG23	3:C:503:CYS:O	2.22	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	406/420 (97%)	387 (95%)	17 (4%)	2 (0%)	29	66
1	B	406/420 (97%)	387 (95%)	17 (4%)	2 (0%)	29	66
1	C	406/420 (97%)	387 (95%)	17 (4%)	2 (0%)	29	66
All	All	1218/1260 (97%)	1161 (95%)	51 (4%)	6 (0%)	29	66

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	377	PRO
1	B	377	PRO
1	C	377	PRO
1	A	373	PRO
1	B	373	PRO
1	C	373	PRO

### 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	316/328 (96%)	300 (95%)	16 (5%)	24	54
1	B	316/328 (96%)	300 (95%)	16 (5%)	24	54
1	C	316/328 (96%)	300 (95%)	16 (5%)	24	54
All	All	948/984 (96%)	900 (95%)	48 (5%)	24	54

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	GLU
1	A	10	TYR
1	A	98	THR
1	A	106	LEU
1	A	115	LEU
1	A	148	ASN
1	A	267	ASP
1	A	278	SER
1	A	279	SER
1	A	323	PHE
1	A	329	LEU
1	A	333	LEU
1	A	340	THR
1	A	370	VAL
1	A	372	LEU
1	A	387	LEU
1	B	9	GLU
1	B	10	TYR
1	B	98	THR
1	B	106	LEU
1	B	115	LEU
1	B	148	ASN
1	B	267	ASP
1	B	278	SER
1	B	279	SER
1	B	323	PHE
1	B	329	LEU
1	B	333	LEU
1	B	340	THR
1	B	370	VAL
1	B	372	LEU
1	B	387	LEU
1	C	9	GLU
1	C	10	TYR
1	C	98	THR
1	C	106	LEU
1	C	115	LEU
1	C	148	ASN
1	C	267	ASP
1	C	278	SER
1	C	279	SER
1	C	323	PHE

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Mol	Chain	Res	Type
1	C	329	LEU
1	C	333	LEU
1	C	340	THR
1	C	370	VAL
1	C	372	LEU
1	C	387	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	220	GLN
1	A	327	ASN
1	B	220	GLN
1	B	310	ASN
1	B	327	ASN
1	C	220	GLN
1	C	310	ASN
1	C	327	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 monosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

Of 9 ligands modelled in this entry, 6 are monoatomic - leaving 3 for Mogul analysis.

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	$\# Z  > 2$
3	CYS	C	503	-	3,6,6	0.31	0	1,7,7	0.02	0
3	CYS	B	503	-	3,6,6	0.28	0	1,7,7	0.02	0
3	CYS	A	503	-	3,6,6	0.28	0	1,7,7	0.01	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
3	CYS	C	503	-	-	0/2/6/6	-
3	CYS	B	503	-	-	0/2/6/6	-
3	CYS	A	503	-	-	0/2/6/6	-

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.

3 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	503	CYS	4	0
3	B	503	CYS	3	0
3	A	503	CYS	3	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	408/420 (97%)	-0.45	6 (1%) 73 66	92, 146, 224, 251	0
1	B	408/420 (97%)	-0.44	12 (2%) 51 42	96, 162, 241, 283	0
1	C	408/420 (97%)	-0.60	8 (1%) 65 58	96, 158, 242, 284	0
All	All	1224/1260 (97%)	-0.50	26 (2%) 63 55	92, 155, 238, 284	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	33	TYR	5.9
1	B	125	LYS	4.6
1	C	93	SER	3.7
1	B	12	VAL	3.4
1	A	331	SER	3.4
1	B	35	TYR	3.0
1	B	114	HIS	2.9
1	A	330	GLY	2.9
1	B	226	GLY	2.8
1	B	34	GLY	2.8
1	C	90	LEU	2.6
1	B	331	SER	2.6
1	C	309	ILE	2.5
1	B	259	ILE	2.5
1	A	329	LEU	2.5
1	C	91	LEU	2.4
1	C	95	PHE	2.4
1	C	308	THR	2.3
1	B	32	HIS	2.3
1	A	112	GLY	2.2
1	C	370	VAL	2.2
1	B	372	LEU	2.2
1	C	343	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	10	TYR	2.1
1	A	111	ALA	2.1
1	B	123	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 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(Å <sup>2</sup> )	Q<0.9
3	CYS	A	503	7/7	0.75	0.18	84,85,86,92	0
3	CYS	B	503	7/7	0.78	0.13	101,102,104,111	0
3	CYS	C	503	7/7	0.81	0.12	96,98,101,107	0
2	NA	B	502	1/1	0.96	0.04	104,104,104,104	0
2	NA	B	501	1/1	0.97	0.16	105,105,105,105	0
2	NA	A	502	1/1	0.97	0.06	91,91,91,91	0
2	NA	C	501	1/1	0.98	0.21	101,101,101,101	0
2	NA	A	501	1/1	0.99	0.14	88,88,88,88	0
2	NA	C	502	1/1	0.99	0.35	104,104,104,104	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.