



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 12:32 PM UTC

PDB ID : 6BAU / pdb_00006bau
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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

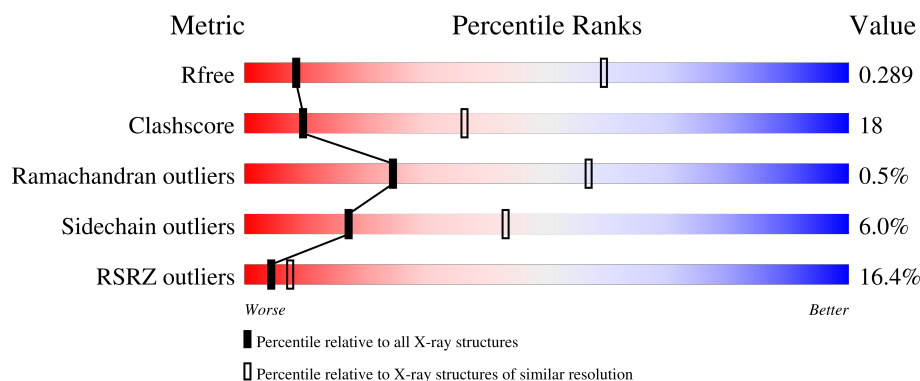
1 Overall quality at a glance

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}	180053	1065 (3.96-3.64)
Clashscore	190562	1012 (3.94-3.66)
Ramachandran outliers	187476	1048 (3.96-3.64)
Sidechain outliers	187428	1043 (3.96-3.64)
RSRZ outliers	180081	1064 (3.96-3.64)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 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	15% 62% 32% • •
1	B	420	17% 63% 31% • •
1	C	420	16% 63% 31% • •

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			

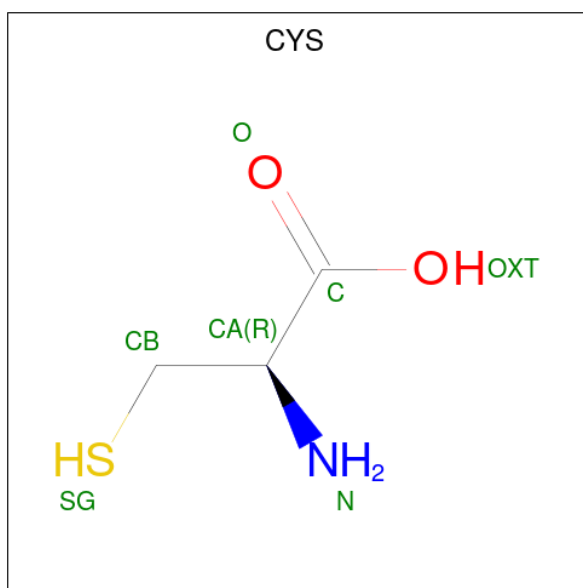
There are 12 discrepancies between the modelled and reference sequences:

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

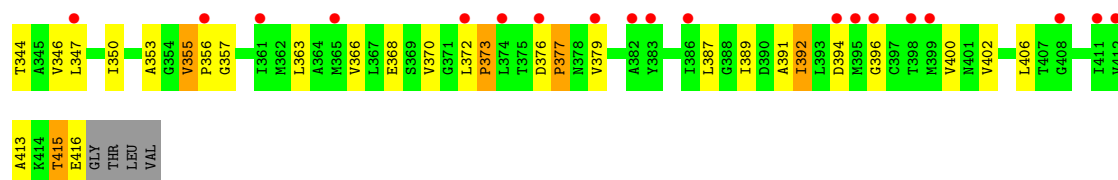
- Molecule 2 is SODIUM ION (CCD ID: NA) (formula: Na).

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

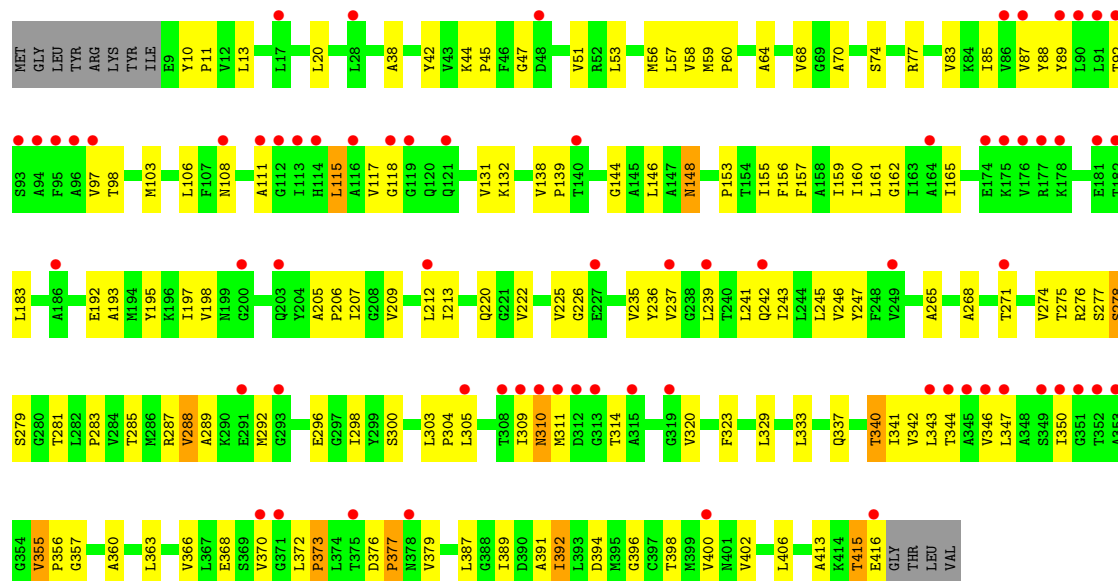
- Molecule 3 is CYSTEINE (CCD ID: CYS) (formula: $\text{C}_3\text{H}_7\text{NO}_2\text{S}$).



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



• Molecule 1: Glutamate transporter homolog



4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α , β , γ	115.31Å 115.31Å 322.27Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	40.00 – 3.80 40.00 – 3.80	Depositor EDS
% Data completeness (in resolution range)	96.8 (40.00-3.80) 96.7 (40.00-3.80)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	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 (5.26%)	wwPDB-VP
Wilson B-factor (Å ²)	135.2	Xtriage
Anisotropy	0.082	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.20 , 46.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	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 ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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: 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	0.82	0/3053	0.93	2/4162 (0.0%)
1	B	0.82	0/3053	0.93	2/4162 (0.0%)
1	C	0.82	0/3053	0.93	2/4162 (0.0%)
All	All	0.82	0/9159	0.93	6/12486 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	389	ILE	CB-CA-C	-5.19	105.25	112.36
1	A	389	ILE	CB-CA-C	-5.18	105.26	112.36
1	C	389	ILE	CB-CA-C	-5.17	105.27	112.36
1	C	310	ASN	N-CA-C	5.10	116.62	108.41
1	B	310	ASN	N-CA-C	5.08	116.60	108.41
1	A	310	ASN	N-CA-C	5.05	116.54	108.41

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	3001	0	3190	118	0
1	B	3001	0	3190	114	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	3001	0	3190	118	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	329	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 18.

All (329) 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:20:LEU:HD12	1:C:213:ILE:HD13	1.70	0.72
1:C:195:TYR:O	1:C:198:VAL:HG22	1.87	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:59:MET:HE2	1:B:146:LEU:HA	1.79	0.65
1:A:59:MET:HE2	1:A:146:LEU:HA	1.79	0.65
1:C:220:GLN:HE22	1:C:391:ALA:H	1.44	0.65
1:C:59:MET:HE2	1:C:146:LEU:HA	1.79	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:56:MET:HE3	1:C:157:PHE:HD1	1.66	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: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:89:TYR:CD1	1:C:310:ASN:CB	2.85	0.59
1:C:209:VAL:HG13	1:C:274:VAL:HG21	1.85	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
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:B:56:MET:HE2	1:C:157:PHE:HD1	1.71	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:157:PHE:HD1	1:C:56:MET:HE3	1.72	0.55
1:A:157:PHE:HD1	1:C:56:MET:HE2	1.71	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:97:VAL:HG11	1:A:342:VAL:HA	1.90	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: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
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:57:LEU:HD13	1:B:198:VAL:HG12	1.91	0.52
1:B:346:VAL:O	1:B:350:ILE:HG13	2.09	0.52
1:B:88:TYR:CZ	1:B:92:THR:HG21	2.45	0.52
1:C:88:TYR:CZ	1:C:92:THR:HG21	2.45	0.52
1:C:103:MET:CE	1:C:237:VAL:HG12	2.40	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:346:VAL:O	1:C:350:ILE:HG13	2.09	0.51
1:C:74:SER:HB2	1:C:77:ARG:HB2	1.92	0.51
1:C:212:LEU:CD1	1:C:274:VAL:HG12	2.40	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
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:C:83:VAL:O	1:C:87:VAL:HG23	2.11	0.50
1:C:373:PRO:O	1:C:379:VAL:HG11	2.12	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: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: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:58:VAL:HG22	1:B:283:PRO:HD3	1.95	0.48
1:B:268:ALA:CB	1:B:285:THR:HG22	2.30	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:56:MET:HE2	1:B:157:PHE:HD1	1.79	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:A:209:VAL:HA	1:A:274:VAL:HG11	1.95	0.47
1:B:225:VAL:HG12	1:B:226:GLY:N	2.29	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
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:A:56:MET:HE3	1:B:157:PHE:HD1	1.80	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:H	1:B:333:LEU:HD12	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:305:LEU:C	1:C:305:LEU:HD23	2.41	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:271:THR:HB	1:B:281:THR:HG23	1.97	0.45
1:B:276:ARG:HG3	1:B:276:ARG:HH11	1.81	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:56:MET:HE3	1:C:157:PHE:CD1	2.50	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:305:LEU:C	1:A:305:LEU:HD23	2.41	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:47:GLY:O	1:A: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:B:305:LEU:HD23	1:B:305:LEU:C	2.41	0.44
1:B:281:THR:HG22	1:B:285:THR:HG23	1.99	0.44
1:C:53:LEU:O	1:C:56:MET:HB3	2.17	0.44
1:C:276:ARG:HG3	1:C:276:ARG:HH11	1.82	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
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: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:B:376:ASP:O	1:B:377:PRO:C	2.62	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:38:ALA:O	1:B:42:TYR:HB2	2.18	0.43
1:B:115:LEU:HD12	1:B:115:LEU:H	1.84	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:376:ASP:O	1:A:377:PRO:C	2.62	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:HD12	1:C:207:ILE:H	1.85	0.42
1:B:59:MET:HB2	1:B:60:PRO:HD3	2.01	0.42
1:B:155:ILE:O	1:B:159:ILE:HG13	2.19	0.42
1:A:139:PRO:HB3	1:A:153:PRO:HB3	2.01	0.42
1:B:52:ARG:NH2	1:C:138:VAL:O	2.51	0.42
1:C:115:LEU:HD12	1:C:115:LEU:H	1.84	0.42
1:A:115:LEU:HD12	1:A:115:LEU:H	1.84	0.42
1:C:376:ASP:O	1:C:377:PRO:C	2.62	0.42
1:C:117:VAL:HG12	1:C:118:GLY:N	2.34	0.41
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
1:A:64:ALA:O	1:A:68:VAL:HG23	2.21	0.41
1:A:275:THR:O	1:A:276:ARG:HB2	2.21	0.41
1:C:44:LYS:O	1:C:45:PRO:C	2.64	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:B:44:LYS:O	1:B:45:PRO:C	2.64	0.41
1:C:64:ALA:O	1:C:68:VAL:HG23	2.21	0.41
1:C:235:VAL:HG22	1:C:320:VAL:CG1	2.34	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:A:160:ILE:CG2	1:C:197:ILE:HD12	2.44	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:HG12	1:C:197:ILE:H	1.74	0.41
1:A:44:LYS:O	1:A:45:PRO:C	2.64	0.41
1:A:144:GLY:O	1:A:148:ASN:OD1	2.38	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:C:131:VAL:HG13	1:C:132:LYS:H	1.85	0.41
1:B:353:ALA:C	1:B:355:VAL:H	2.30	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:197:ILE:HD12	1:B:160:ILE:CG2	2.48	0.40
1:C:44:LYS:N	1:C:45:PRO:HD2	2.36	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: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:A:353:ALA:C	1:A:355:VAL:H	2.30	0.40
1:B:44:LYS:N	1:B:45:PRO:HD2	2.36	0.40
1:B:144:GLY:O	1:B:148:ASN:OD1	2.38	0.40
1:A:165:ILE:CD1	1:A:183:LEU:HD23	2.51	0.40
1:B:64:ALA:O	1:B:68:VAL:HG23	2.21	0.40
1:C:292:MET:H	1:C:292:MET:HG2	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 [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	406/420 (97%)	387 (95%)	17 (4%)	2 (0%)	24	57
1	B	406/420 (97%)	387 (95%)	17 (4%)	2 (0%)	24	57
1	C	406/420 (97%)	387 (95%)	17 (4%)	2 (0%)	24	57
All	All	1218/1260 (97%)	1161 (95%)	51 (4%)	6 (0%)	24	57

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	377	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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%)	297 (94%)	19 (6%)	17	43
1	B	316/328 (96%)	297 (94%)	19 (6%)	17	43
1	C	316/328 (96%)	297 (94%)	19 (6%)	17	43
All	All	948/984 (96%)	891 (94%)	57 (6%)	17	43

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	LEU
1	A	98	THR
1	A	106	LEU
1	A	115	LEU
1	A	148	ASN
1	A	222	VAL
1	A	278	SER
1	A	279	SER
1	A	288	VAL
1	A	323	PHE
1	A	329	LEU
1	A	340	THR
1	A	355	VAL
1	A	368	GLU
1	A	370	VAL
1	A	372	LEU
1	A	387	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	392	ILE
1	A	415	THR
1	B	13	LEU
1	B	98	THR
1	B	106	LEU
1	B	115	LEU
1	B	148	ASN
1	B	222	VAL
1	B	278	SER
1	B	279	SER
1	B	288	VAL
1	B	323	PHE
1	B	329	LEU
1	B	340	THR
1	B	355	VAL
1	B	368	GLU
1	B	370	VAL
1	B	372	LEU
1	B	387	LEU
1	B	392	ILE
1	B	415	THR
1	C	13	LEU
1	C	98	THR
1	C	106	LEU
1	C	115	LEU
1	C	148	ASN
1	C	222	VAL
1	C	278	SER
1	C	279	SER
1	C	288	VAL
1	C	323	PHE
1	C	329	LEU
1	C	340	THR
1	C	355	VAL
1	C	368	GLU
1	C	370	VAL
1	C	372	LEU
1	C	387	LEU
1	C	392	ILE
1	C	415	THR

Sometimes 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 oligosaccharides 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	A	503	-	5,6,6	1.07	1 (20%)	3,7,7	1.45	1 (33%)
3	CYS	B	503	-	5,6,6	1.07	1 (20%)	3,7,7	1.46	1 (33%)
3	CYS	C	503	-	5,6,6	1.08	1 (20%)	3,7,7	1.46	1 (33%)

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	A	503	-	-	2/6/6/6	-
3	CYS	B	503	-	-	2/6/6/6	-
3	CYS	C	503	-	-	2/6/6/6	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	503	CYS	OXT-C	-2.25	1.23	1.30
3	C	503	CYS	OXT-C	-2.25	1.23	1.30
3	B	503	CYS	OXT-C	-2.24	1.23	1.30

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	503	CYS	OXT-C-O	-2.51	118.39	124.08
3	C	503	CYS	OXT-C-O	-2.50	118.40	124.08
3	A	503	CYS	OXT-C-O	-2.49	118.44	124.08

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	503	CYS	O-C-CA-N
3	B	503	CYS	O-C-CA-N
3	C	503	CYS	O-C-CA-N
3	A	503	CYS	OXT-C-CA-N
3	B	503	CYS	OXT-C-CA-N
3	C	503	CYS	OXT-C-CA-N

There are no ring outliers.

3 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	503	CYS	3	0
3	B	503	CYS	3	0
3	C	503	CYS	4	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, 95th 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 ²)	Q<0.9
1	A	408/420 (97%)	0.80	61 (14%) 5 8	92, 146, 224, 251	0
1	B	408/420 (97%)	0.95	71 (17%) 4 6	96, 162, 241, 283	0
1	C	408/420 (97%)	1.01	69 (16%) 4 7	96, 158, 242, 284	0
All	All	1224/1260 (97%)	0.92	201 (16%) 4 7	92, 155, 238, 284	0

All (201) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	90	LEU	8.3
1	B	227	GLU	8.3
1	B	12	VAL	8.2
1	C	93	SER	8.0
1	A	378	ASN	7.6
1	A	329	LEU	7.5
1	C	347	LEU	7.4
1	C	309	ILE	7.3
1	C	346	VAL	7.1
1	A	331	SER	7.1
1	C	91	LEU	7.0
1	C	94	ALA	6.9
1	C	89	TYR	6.6
1	B	226	GLY	6.5
1	C	95	PHE	6.4
1	B	324	PHE	6.3
1	B	383	TYR	6.3
1	C	343	LEU	6.2
1	C	86	VAL	6.1
1	A	414	LYS	6.1
1	B	372	LEU	5.8
1	A	379	VAL	5.8
1	B	13	LEU	5.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	33	TYR	5.5
1	A	377	PRO	5.5
1	C	177	ARG	5.4
1	A	11	PRO	5.4
1	A	118	GLY	5.4
1	C	113	ILE	5.4
1	A	22	LEU	5.3
1	C	350	ILE	5.3
1	C	370	VAL	5.2
1	C	308	THR	5.0
1	C	305	LEU	5.0
1	B	259	ILE	5.0
1	C	203	GLN	5.0
1	B	228	LEU	4.9
1	A	117	VAL	4.9
1	B	29	ILE	4.8
1	A	353	ALA	4.8
1	C	315	ALA	4.8
1	B	254	TYR	4.7
1	A	25	ILE	4.7
1	C	174	GLU	4.7
1	C	293	GLY	4.5
1	B	379	VAL	4.5
1	A	107	PHE	4.4
1	A	376	ASP	4.4
1	C	87	VAL	4.4
1	A	10	TYR	4.3
1	B	125	LYS	4.3
1	A	224	VAL	4.3
1	A	325	ILE	4.1
1	C	312	ASP	4.1
1	C	17	LEU	4.0
1	B	325	ILE	3.9
1	A	372	LEU	3.9
1	B	230	LYS	3.9
1	A	415	THR	3.9
1	B	24	ALA	3.9
1	A	134	LEU	3.8
1	C	291	GLU	3.7
1	A	21	ILE	3.7
1	C	271	THR	3.6
1	B	87	VAL	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	413	ALA	3.6
1	C	371	GLY	3.5
1	C	164	ALA	3.5
1	A	253	ILE	3.5
1	A	26	VAL	3.5
1	A	29	ILE	3.4
1	A	254	TYR	3.4
1	C	313	GLY	3.4
1	B	229	ALA	3.4
1	B	291	GLU	3.4
1	C	319	GLY	3.4
1	B	109	PRO	3.4
1	C	175	LYS	3.4
1	B	78	LEU	3.3
1	C	200	GLY	3.3
1	C	121	GLN	3.3
1	A	229	ALA	3.3
1	A	231	VAL	3.3
1	A	330	GLY	3.3
1	C	186	ALA	3.3
1	B	55	LYS	3.3
1	A	380	ALA	3.3
1	B	18	ILE	3.3
1	B	86	VAL	3.3
1	B	14	GLN	3.2
1	A	18	ILE	3.1
1	B	365	MET	3.1
1	C	378	ASN	3.0
1	A	335	VAL	3.0
1	A	106	LEU	3.0
1	C	108	ASN	3.0
1	A	14	GLN	3.0
1	C	416	GLU	3.0
1	B	79	GLY	2.9
1	C	111	ALA	2.9
1	A	12	VAL	2.9
1	C	116	ALA	2.9
1	C	212	LEU	2.9
1	C	97	VAL	2.8
1	C	237	VAL	2.8
1	C	178	LYS	2.8
1	C	310	ASN	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	230	LYS	2.8
1	A	228	LEU	2.8
1	A	328	ALA	2.8
1	A	95	PHE	2.8
1	B	34	GLY	2.8
1	A	382	ALA	2.8
1	B	93	SER	2.7
1	C	400	VAL	2.7
1	C	311	MET	2.7
1	C	182	THR	2.7
1	C	352	THR	2.7
1	C	349	SER	2.7
1	C	28	LEU	2.7
1	A	102	ILE	2.7
1	A	233	ALA	2.7
1	B	275	THR	2.6
1	A	260	SER	2.6
1	B	292	MET	2.6
1	A	37	ASP	2.6
1	B	298	ILE	2.6
1	B	347	LEU	2.6
1	C	353	ALA	2.6
1	B	386	ILE	2.6
1	B	376	ASP	2.6
1	A	116	ALA	2.6
1	B	212	LEU	2.5
1	B	32	HIS	2.5
1	B	100	GLY	2.5
1	C	92	THR	2.5
1	C	227	GLU	2.5
1	A	324	PHE	2.5
1	B	128	PRO	2.5
1	C	118	GLY	2.5
1	B	374	LEU	2.5
1	A	355	VAL	2.5
1	B	52	ARG	2.5
1	B	398	THR	2.5
1	C	140	THR	2.5
1	B	90	LEU	2.4
1	B	262	ILE	2.4
1	C	242	GLN	2.4
1	A	341	ILE	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	109	PRO	2.4
1	A	373	PRO	2.4
1	A	130	LEU	2.4
1	B	199	ASN	2.4
1	C	344	THR	2.4
1	A	371	GLY	2.4
1	B	396	GLY	2.3
1	A	245	LEU	2.3
1	B	225	VAL	2.3
1	B	411	ILE	2.3
1	B	273	PHE	2.3
1	B	408	GLY	2.3
1	B	99	LEU	2.3
1	B	329	LEU	2.3
1	C	119	GLY	2.3
1	A	269	MET	2.3
1	A	404	GLY	2.3
1	C	239	LEU	2.3
1	B	326	ALA	2.3
1	C	345	ALA	2.2
1	B	295	SER	2.2
1	C	48	ASP	2.2
1	B	361	ILE	2.2
1	B	399	MET	2.2
1	A	256	ILE	2.2
1	B	307	ALA	2.2
1	B	395	MET	2.2
1	B	23	GLY	2.2
1	B	331	SER	2.2
1	C	112	GLY	2.2
1	C	181	GLU	2.2
1	A	175	LYS	2.2
1	B	412	VAL	2.2
1	C	176	VAL	2.2
1	B	25	ILE	2.2
1	B	356	PRO	2.2
1	B	11	PRO	2.1
1	C	351	GLY	2.1
1	A	334	THR	2.1
1	C	375	THR	2.1
1	B	84	LYS	2.1
1	B	95	PHE	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	114	HIS	2.1
1	C	249	VAL	2.1
1	B	333	LEU	2.1
1	B	394	ASP	2.1
1	B	382	ALA	2.0
1	A	416	GLU	2.0
1	A	45	PRO	2.0
1	B	85	ILE	2.0
1	A	111	ALA	2.0
1	C	96	ALA	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 oligosaccharides 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, 95th 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 ²)	Q<0.9
3	CYS	C	503	7/7	0.69	0.14	96,98,101,107	0
3	CYS	B	503	7/7	0.74	0.13	101,102,104,111	0
3	CYS	A	503	7/7	0.80	0.12	84,85,86,92	0
2	NA	C	502	1/1	0.83	0.33	104,104,104,104	0
2	NA	B	501	1/1	0.91	0.19	105,105,105,105	0
2	NA	A	501	1/1	0.95	0.20	88,88,88,88	0
2	NA	C	501	1/1	0.96	0.07	101,101,101,101	0
2	NA	A	502	1/1	0.97	0.04	91,91,91,91	0
2	NA	B	502	1/1	0.98	0.04	104,104,104,104	0

6.5 Other polymers [i](#)

There are no such residues in this entry.