



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 03:26 am GMT

PDB ID : 2WYO  
Title : TRYPANOSOMA BRUCEI GLUTATHIONE SYNTHETASE  
Authors : Fyfe, P.K.; Alphey, M.S.; Hunter, W.N.  
Deposited on : 2009-11-17  
Resolution : 3.15 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

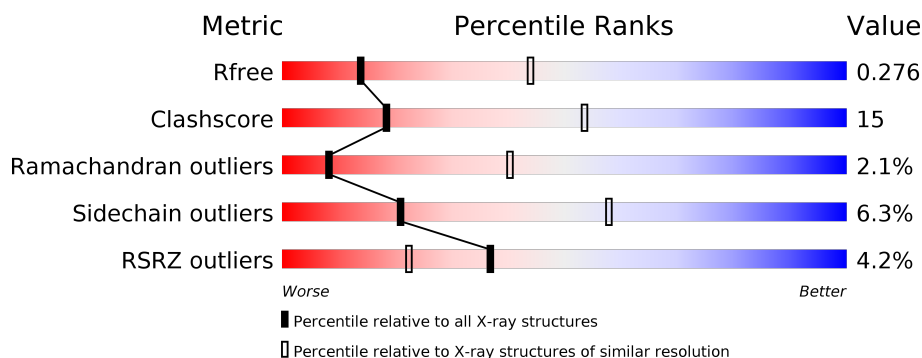
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.15 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	100719	1259 (3.20-3.12)
Clashscore	112137	1397 (3.20-3.12)
Ramachandran outliers	110173	1368 (3.20-3.12)
Sidechain outliers	110143	1367 (3.20-3.12)
RSRZ outliers	101464	1264 (3.20-3.12)

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	562	<div> <div>4%</div> <div> <div></div> <div>61%</div> <div>29%</div> <div>• 7%</div> </div> </div>
1	B	562	<div> <div>4%</div> <div> <div></div> <div>61%</div> <div>23%</div> <div>• 13%</div> </div> </div>
1	C	562	<div> <div>4%</div> <div> <div></div> <div>62%</div> <div>23%</div> <div>• 12%</div> </div> </div>
1	D	562	<div> <div>2%</div> <div> <div></div> <div>61%</div> <div>25%</div> <div>• 12%</div> </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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	GSH	C	1556	-	-	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 15702 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 GLUTATHIONE SYNTHETASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	520	Total	C	N	O	S	0	1	0
			4065	2586	703	753	23			
1	B	488	Total	C	N	O	S	0	0	0
			3803	2417	660	704	22			
1	C	496	Total	C	N	O	S	0	1	0
			3871	2458	675	717	21			
1	D	492	Total	C	N	O	S	0	0	0
			3826	2434	666	705	21			

There are 28 discrepancies between the modelled and reference sequences:

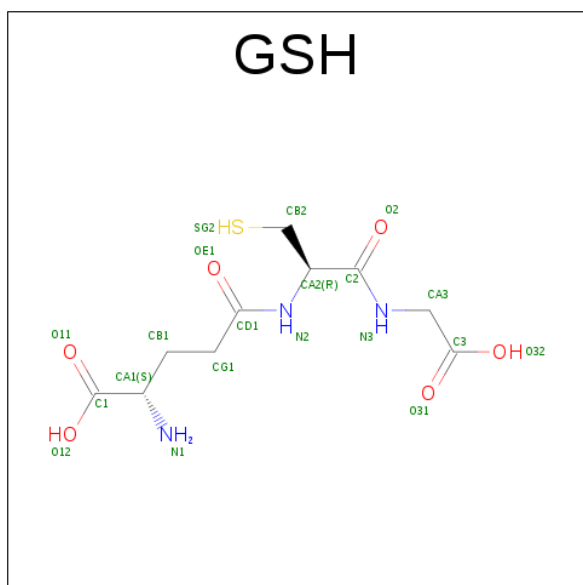
Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	ASN	-	EXPRESSION TAG	UNP Q57UN0
A	-5	LEU	-	EXPRESSION TAG	UNP Q57UN0
A	-4	TYR	-	EXPRESSION TAG	UNP Q57UN0
A	-3	PHE	-	EXPRESSION TAG	UNP Q57UN0
A	-2	GLN	-	EXPRESSION TAG	UNP Q57UN0
A	-1	GLY	-	EXPRESSION TAG	UNP Q57UN0
A	0	HIS	-	EXPRESSION TAG	UNP Q57UN0
B	-6	ASN	-	EXPRESSION TAG	UNP Q57UN0
B	-5	LEU	-	EXPRESSION TAG	UNP Q57UN0
B	-4	TYR	-	EXPRESSION TAG	UNP Q57UN0
B	-3	PHE	-	EXPRESSION TAG	UNP Q57UN0
B	-2	GLN	-	EXPRESSION TAG	UNP Q57UN0
B	-1	GLY	-	EXPRESSION TAG	UNP Q57UN0
B	0	HIS	-	EXPRESSION TAG	UNP Q57UN0
C	-6	ASN	-	EXPRESSION TAG	UNP Q57UN0
C	-5	LEU	-	EXPRESSION TAG	UNP Q57UN0
C	-4	TYR	-	EXPRESSION TAG	UNP Q57UN0
C	-3	PHE	-	EXPRESSION TAG	UNP Q57UN0
C	-2	GLN	-	EXPRESSION TAG	UNP Q57UN0
C	-1	GLY	-	EXPRESSION TAG	UNP Q57UN0
C	0	HIS	-	EXPRESSION TAG	UNP Q57UN0

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-6	ASN	-	EXPRESSION TAG	UNP Q57UN0
D	-5	LEU	-	EXPRESSION TAG	UNP Q57UN0
D	-4	TYR	-	EXPRESSION TAG	UNP Q57UN0
D	-3	PHE	-	EXPRESSION TAG	UNP Q57UN0
D	-2	GLN	-	EXPRESSION TAG	UNP Q57UN0
D	-1	GLY	-	EXPRESSION TAG	UNP Q57UN0
D	0	HIS	-	EXPRESSION TAG	UNP Q57UN0

- Molecule 2 is GLUTATHIONE (three-letter code: GSH) (formula: C<sub>10</sub>H<sub>17</sub>N<sub>3</sub>O<sub>6</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			20	10	3	6	1		
2	B	1	Total	C	N	O	S	0	0
			20	10	3	6	1		
2	C	1	Total	C	N	O	S	0	0
			20	10	3	6	1		
2	D	1	Total	C	N	O	S	0	0
			20	10	3	6	1		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		

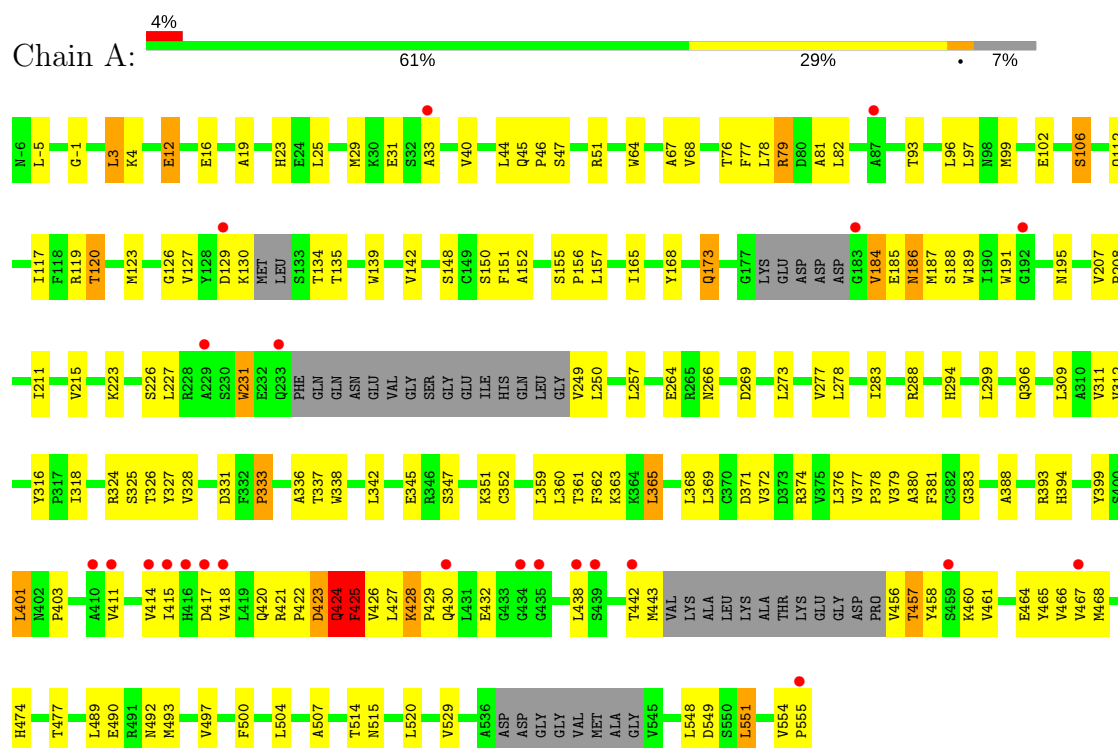
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	5	Total	O	0	0
			5	5		
4	B	4	Total	O	0	0
			4	4		
4	C	5	Total	O	0	0
			5	5		
4	D	8	Total	O	0	0
			8	8		

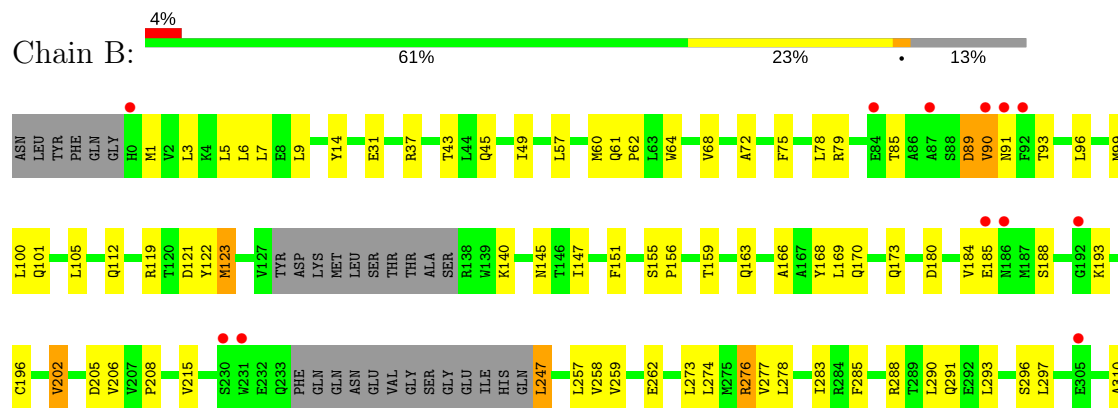
### 3 Residue-property plots [i](#)

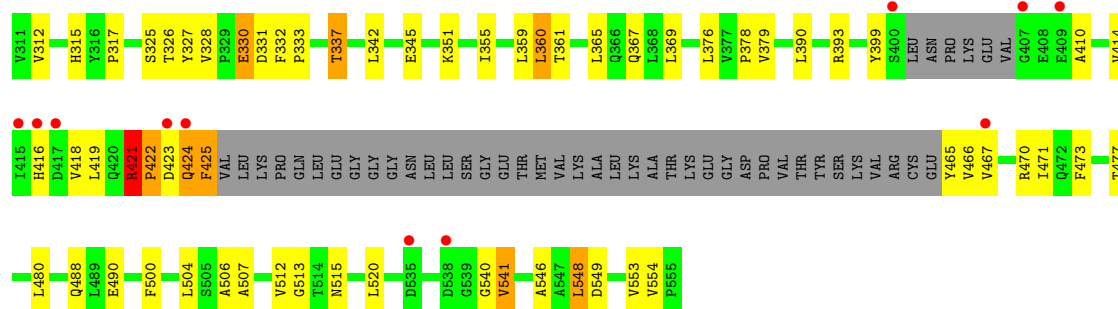
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: GLUTATHIONE SYNTHETASE

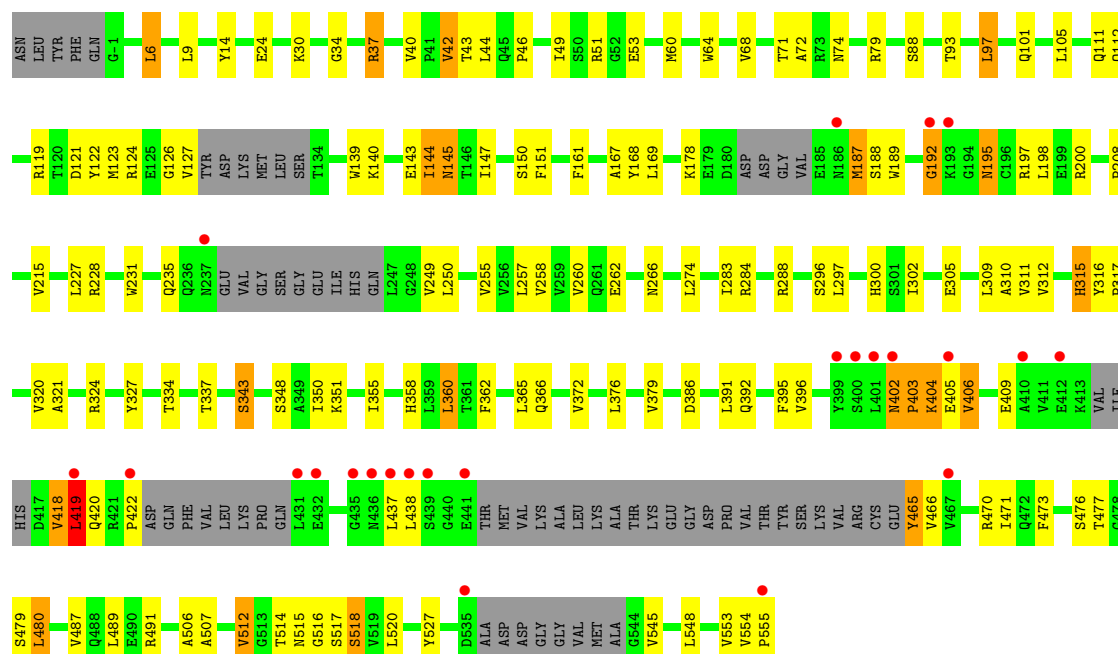


#### • Molecule 1: GLUTATHIONE SYNTHETASE

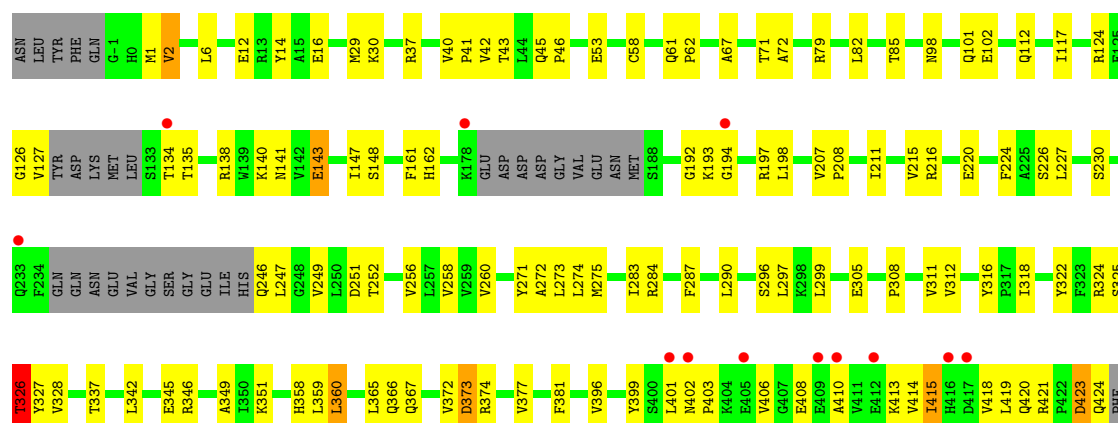




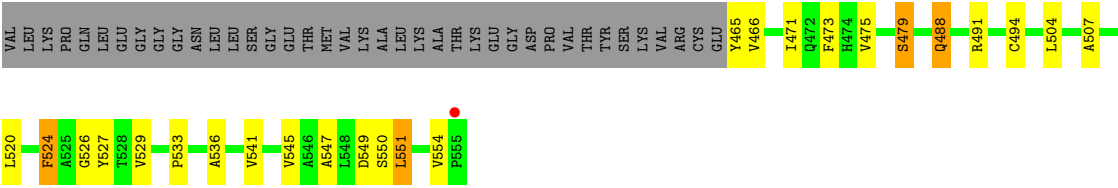
• Molecule 1: GLUTATHIONE SYNTHETASE



• Molecule 1: GLUTATHIONE SYNTHETASE







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	92.59Å 125.15Å 243.17Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.46 – 3.15 39.46 – 3.15	Depositor EDS
% Data completeness (in resolution range)	99.9 (39.46-3.15) 99.9 (39.46-3.15)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.25 (at 3.12Å)	Xtriage
Refinement program	REFMAC 5.5.0097	Depositor
R, $R_{free}$	0.203 , 0.277 0.202 , 0.276	Depositor DCC
$R_{free}$ test set	2483 reflections (5.27%)	DCC
Wilson B-factor (Å <sup>2</sup> )	65.1	Xtriage
Anisotropy	0.513	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 64.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	15702	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.50% 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: GSH, SO4

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	0.59	2/4145 (0.0%)	0.75	5/5615 (0.1%)
1	B	0.53	0/3880	0.66	1/5258 (0.0%)
1	C	0.66	0/3945	0.74	0/5339
1	D	0.66	2/3904 (0.1%)	0.74	0/5292
All	All	0.62	4/15874 (0.0%)	0.72	6/21504 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	231	TRP	CG-CD2	-10.53	1.25	1.43
1	A	231	TRP	CG-CD1	-7.80	1.25	1.36
1	D	143	GLU	CG-CD	5.73	1.60	1.51
1	D	58	CYS	CB-SG	-5.09	1.73	1.81

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	231	TRP	CD1-CG-CD2	20.38	122.60	106.30
1	A	231	TRP	CB-CG-CD1	-6.40	118.67	127.00
1	A	231	TRP	CB-CG-CD2	-6.06	118.72	126.60
1	B	421	ARG	NE-CZ-NH1	6.05	123.33	120.30
1	A	424	GLN	N-CA-C	5.92	126.98	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	425	PHE	N-CA-C	5.11	124.78	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	106	SER	Peptide
1	A	423	ASP	Peptide

## 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	4065	0	4065	137	0
1	B	3803	0	3791	122	0
1	C	3871	0	3868	108	0
1	D	3826	0	3832	109	0
2	A	20	0	15	3	0
2	B	20	0	15	0	0
2	C	20	0	15	4	0
2	D	20	0	15	1	0
3	A	10	0	0	1	0
3	B	5	0	0	1	0
3	C	15	0	0	0	0
3	D	5	0	0	0	0
4	A	5	0	0	0	0
4	B	4	0	0	0	0
4	C	5	0	0	0	0
4	D	8	0	0	0	0
All	All	15702	0	15616	465	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 15.

All (465) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:231:TRP:CD2	1:A:250:LEU:HD11	1.81	1.15
1:A:529:VAL:HG21	1:A:551:LEU:HD13	1.31	1.06
1:D:325:SER:O	1:D:326:THR:HB	1.51	1.05
1:D:147:ILE:HD11	1:D:326:THR:HG22	1.41	1.01
1:A:82:LEU:HD11	1:A:365:LEU:HD11	1.42	1.01
1:B:112:GLN:HG2	1:B:507:ALA:HB2	1.48	0.96
1:A:231:TRP:CD2	1:A:250:LEU:CD1	2.50	0.95
1:D:529:VAL:HG21	1:D:551:LEU:HD13	1.49	0.94
1:D:258:VAL:HG21	1:D:274:LEU:HD11	1.51	0.92
1:C:258:VAL:HG21	1:C:274:LEU:HD11	1.54	0.89
1:A:423:ASP:O	1:A:424:GLN:NE2	2.10	0.85
1:B:410:ALA:O	1:B:414:VAL:HG23	1.76	0.84
1:D:290:LEU:HD13	1:D:337:THR:HG22	1.60	0.84
1:B:180:ASP:O	1:B:184:VAL:HG23	1.78	0.83
1:A:426:VAL:HG12	1:A:427:LEU:H	1.44	0.83
1:C:506:ALA:HB2	1:C:512:VAL:HG11	1.59	0.82
1:A:376:LEU:HD23	1:A:388:ALA:HB1	1.61	0.82
1:C:477:THR:HG22	1:C:491:ARG:HA	1.63	0.80
1:A:465:TYR:O	1:A:466:VAL:HG23	1.80	0.80
1:A:529:VAL:HG21	1:A:551:LEU:CD1	2.10	0.79
1:C:144:ILE:HG22	1:C:366:GLN:HG3	1.64	0.79
1:B:421:ARG:HG3	1:B:421:ARG:HH11	1.47	0.78
1:B:112:GLN:CG	1:B:507:ALA:HB2	2.14	0.77
1:A:227:LEU:HD21	1:A:309:LEU:HD22	1.68	0.76
1:D:147:ILE:CD1	1:D:326:THR:HG22	2.13	0.76
1:D:140:LYS:HG3	1:D:471:ILE:HD13	1.66	0.76
1:B:297:LEU:HD11	1:B:310:ALA:HB1	1.67	0.76
1:C:228:ARG:NH2	1:C:250:LEU:O	2.19	0.76
1:B:367:GLN:HE22	1:B:466:VAL:HG21	1.50	0.75
1:D:147:ILE:HD12	1:D:358:HIS:CD2	2.23	0.74
1:C:406:VAL:HG12	1:C:406:VAL:O	1.88	0.73
1:A:119:ARG:NH2	2:A:1556:GSH:O2	2.20	0.73
1:C:49:ILE:HD12	1:C:139:TRP:CZ2	2.23	0.73
1:B:506:ALA:CB	1:B:512:VAL:HG11	2.19	0.73
1:A:312:VAL:HG23	1:A:318:ILE:HD11	1.71	0.72
1:D:399:TYR:O	1:D:466:VAL:HG13	1.90	0.72
1:A:489:LEU:HD12	1:A:493:MET:HG3	1.73	0.71
1:D:290:LEU:CD1	1:D:337:THR:HG22	2.20	0.71
1:D:29:MET:HE1	1:D:40:VAL:HG12	1.72	0.70
1:A:264:GLU:OE1	2:A:1556:GSH:N1	2.24	0.70
1:B:119:ARG:NH1	1:B:121:ASP:OD1	2.25	0.70
1:C:74:ASN:ND2	1:C:379:VAL:HG13	2.06	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:425:PHE:CD2	1:B:425:PHE:C	2.66	0.69
1:B:290:LEU:CD1	1:B:337:THR:HG22	2.23	0.69
1:B:513:GLY:HA2	1:B:520:LEU:HD23	1.75	0.69
1:D:541:VAL:N	2:D:1556:GSH:O31	2.26	0.69
1:B:504:LEU:HG	1:B:520:LEU:HD12	1.74	0.69
1:D:29:MET:CE	1:D:40:VAL:HG12	2.23	0.68
1:D:258:VAL:HG12	1:D:260:VAL:HG22	1.75	0.68
1:B:290:LEU:HD13	1:B:337:THR:HG22	1.74	0.68
1:C:44:LEU:HD12	1:C:479:SER:HB3	1.75	0.68
1:D:147:ILE:HD12	1:D:358:HIS:NE2	2.09	0.67
1:D:349:ALA:O	1:D:351:LYS:HE3	1.93	0.67
1:B:6:LEU:HD12	1:B:169:LEU:HD21	1.77	0.67
1:C:406:VAL:HG13	1:C:409:GLU:HB2	1.77	0.67
1:B:99:MET:HE1	1:B:342:LEU:N	2.10	0.67
1:C:402:ASN:HB3	1:C:403:PRO:HD3	1.76	0.67
1:B:208:PRO:HD3	1:B:273:LEU:HD22	1.78	0.66
1:D:112:GLN:HG2	1:D:507:ALA:HB2	1.77	0.66
1:C:402:ASN:CB	1:C:403:PRO:HD3	2.25	0.66
1:B:247:LEU:HD12	1:B:247:LEU:O	1.96	0.66
1:B:75:PHE:HB2	1:B:105:LEU:HD21	1.77	0.65
1:B:369:LEU:HD22	1:B:376:LEU:HD12	1.78	0.65
1:C:215:VAL:HG11	1:C:283:ILE:HD13	1.79	0.65
1:B:43:THR:HG21	1:B:549:ASP:OD2	1.97	0.65
1:D:296:SER:HB3	1:D:312:VAL:HG13	1.77	0.65
1:B:332:PHE:HA	1:B:337:THR:HG21	1.79	0.65
1:C:512:VAL:CG1	1:C:520:LEU:HD11	2.27	0.65
1:A:504:LEU:HG	1:A:520:LEU:HD12	1.80	0.64
1:A:82:LEU:HD11	1:A:365:LEU:CD1	2.21	0.64
1:D:410:ALA:O	1:D:414:VAL:HG23	1.98	0.64
1:C:258:VAL:HG21	1:C:274:LEU:CD1	2.25	0.64
1:B:85:THR:HG22	1:B:93:THR:HG21	1.80	0.64
1:B:425:PHE:HD2	1:B:425:PHE:C	2.01	0.64
1:C:195:ASN:OD1	1:C:195:ASN:N	2.27	0.64
1:D:82:LEU:HD13	1:D:359:LEU:HD22	1.80	0.64
1:B:367:GLN:OE1	1:B:466:VAL:HG11	1.97	0.64
1:A:123:MET:HG3	1:A:142:VAL:HG21	1.81	0.63
1:A:79:ARG:HA	1:A:97:LEU:HD11	1.79	0.63
1:A:414:VAL:HG22	1:A:421:ARG:HG3	1.78	0.63
1:A:312:VAL:CG2	1:A:318:ILE:HD11	2.28	0.63
1:B:367:GLN:CD	1:B:466:VAL:HG11	2.19	0.63
1:C:140:LYS:HG2	1:C:471:ILE:HD12	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:100:LEU:HD22	1:B:359:LEU:CD1	2.28	0.62
1:C:126:GLY:O	1:C:127:VAL:HG22	1.99	0.62
1:D:327:TYR:CD1	1:D:328:VAL:HG13	2.34	0.62
1:A:461:VAL:O	1:A:461:VAL:HG12	1.99	0.62
1:A:25:LEU:O	1:A:157:LEU:HD13	1.99	0.62
1:A:372:VAL:O	1:A:377:VAL:HG23	1.99	0.62
1:D:258:VAL:HG21	1:D:274:LEU:CD1	2.27	0.61
1:B:421:ARG:O	1:B:422:PRO:O	2.18	0.61
1:C:119:ARG:O	1:C:145:ASN:ND2	2.32	0.61
1:A:257:LEU:HD11	1:A:288:ARG:HB2	1.83	0.61
1:B:79:ARG:HD3	1:B:101:GLN:HE21	1.66	0.61
1:B:422:PRO:HD2	1:B:470:ARG:HB2	1.82	0.61
1:C:372:VAL:HG23	1:C:376:LEU:HD23	1.83	0.61
1:B:68:VAL:HG13	1:B:360:LEU:HD22	1.83	0.61
1:D:192:GLY:O	1:D:194:GLY:N	2.33	0.61
1:A:112:GLN:CG	1:A:507:ALA:HB2	2.31	0.60
1:B:43:THR:HG23	1:B:548:LEU:O	2.02	0.60
1:B:202:VAL:CG1	1:B:206:VAL:HG23	2.31	0.60
1:B:554:VAL:HG23	1:B:554:VAL:O	2.02	0.60
1:A:426:VAL:HG23	1:A:464:GLU:HA	1.82	0.60
1:D:529:VAL:CG2	1:D:551:LEU:HD13	2.29	0.59
1:D:112:GLN:CG	1:D:507:ALA:HB2	2.33	0.59
1:A:82:LEU:HD21	1:A:365:LEU:HD12	1.85	0.59
1:C:151:PHE:CE1	1:C:548:LEU:HD21	2.38	0.59
1:D:67:ALA:HB2	1:D:381:PHE:CZ	2.37	0.59
1:D:16:GLU:N	1:D:16:GLU:OE1	2.36	0.59
1:D:271:TYR:CZ	1:D:287:PHE:HE2	2.21	0.58
1:D:418:VAL:HG13	1:D:419:LEU:HD13	1.85	0.58
1:B:6:LEU:CD1	1:B:169:LEU:HD21	2.32	0.58
1:C:327:TYR:OH	2:C:1556:GSH:HB13	2.04	0.58
1:B:423:ASP:O	1:B:424:GLN:CB	2.52	0.58
1:A:3:LEU:HD21	1:C:489:LEU:HD11	1.84	0.57
1:C:418:VAL:HG12	1:C:418:VAL:O	2.04	0.57
1:D:527:TYR:CE1	1:D:551:LEU:HD22	2.39	0.57
1:D:327:TYR:HD1	1:D:328:VAL:HG13	1.68	0.57
1:A:461:VAL:HG13	1:A:465:TYR:CD2	2.38	0.57
1:D:46:PRO:HG3	1:D:198:LEU:HD21	1.86	0.57
1:B:423:ASP:O	1:B:424:GLN:HB2	2.05	0.57
1:C:402:ASN:CB	1:C:403:PRO:CD	2.83	0.57
1:C:71:THR:HG22	1:C:360:LEU:HD11	1.85	0.57
1:C:68:VAL:HA	1:C:360:LEU:HD22	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:257:LEU:HB2	1:A:318:ILE:HD12	1.86	0.57
1:B:554:VAL:CG2	1:B:554:VAL:O	2.52	0.56
1:D:396:VAL:HG22	1:D:471:ILE:HD12	1.87	0.56
1:B:202:VAL:HG13	1:B:206:VAL:HG23	1.86	0.56
1:C:64:TRP:CE2	1:C:391:LEU:HD22	2.40	0.56
1:A:68:VAL:HA	1:A:360:LEU:CD2	2.35	0.56
1:B:421:ARG:CG	1:B:421:ARG:HH11	2.17	0.56
1:D:424:GLN:O	1:D:465:TYR:N	2.38	0.56
1:B:369:LEU:O	1:B:376:LEU:HD13	2.05	0.56
1:A:376:LEU:O	1:A:380:ALA:HB3	2.05	0.56
1:A:415:ILE:HD11	1:A:442:THR:HG21	1.87	0.56
1:A:456:VAL:O	1:A:457:THR:HG22	2.05	0.55
1:A:99:MET:HE1	1:A:342:LEU:N	2.21	0.55
1:A:327:TYR:CD1	1:A:328:VAL:HG13	2.42	0.55
1:A:492:ASN:CG	1:A:492:ASN:O	2.45	0.55
1:B:184:VAL:HG12	1:B:185:GLU:HG3	1.88	0.55
1:A:78:LEU:HD13	1:A:359:LEU:HD12	1.88	0.55
1:B:257:LEU:HD21	1:B:293:LEU:HD21	1.89	0.55
1:A:393:ARG:NH2	3:A:1558:SO4:O3	2.40	0.55
1:C:42:VAL:HG21	1:C:161:PHE:CE2	2.41	0.55
1:A:148:SER:OG	1:A:324:ARG:HA	2.07	0.55
1:B:184:VAL:HG22	1:B:193:LYS:HE3	1.88	0.55
1:D:41:PRO:HB2	1:D:547:ALA:HA	1.89	0.54
1:A:423:ASP:O	1:A:424:GLN:CD	2.46	0.54
1:A:152:ALA:HB3	1:A:273:LEU:HD11	1.90	0.54
1:C:296:SER:HB3	1:C:312:VAL:HG13	1.90	0.53
1:B:424:GLN:O	1:B:425:PHE:HB3	2.08	0.53
1:C:297:LEU:HD23	1:C:343:SER:HB3	1.90	0.53
1:A:497:VAL:HG22	1:A:529:VAL:HG22	1.89	0.53
1:D:406:VAL:HG22	1:D:408:GLU:CG	2.39	0.53
1:A:119:ARG:HD3	1:A:500:PHE:CE1	2.43	0.53
1:A:64:TRP:CE2	1:A:120:THR:HG21	2.43	0.53
1:B:258:VAL:HG21	1:B:274:LEU:HD11	1.91	0.53
1:B:290:LEU:HA	1:B:293:LEU:HD12	1.91	0.53
1:D:147:ILE:CD1	1:D:358:HIS:NE2	2.72	0.53
1:D:415:ILE:O	1:D:415:ILE:HG22	2.08	0.53
1:A:78:LEU:HD23	1:A:365:LEU:HD21	1.90	0.53
1:A:414:VAL:HG22	1:A:421:ARG:CG	2.39	0.53
1:B:205:ASP:OD1	1:B:276:ARG:NH2	2.41	0.53
1:D:71:THR:HB	1:D:360:LEU:HD21	1.91	0.52
1:C:255:VAL:HG12	1:C:284:ARG:HB2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:299:LEU:HD13	1:D:308:PRO:HG2	1.91	0.52
1:A:231:TRP:CD2	1:A:250:LEU:HD13	2.39	0.52
1:B:43:THR:HA	1:B:480:LEU:HD23	1.90	0.52
1:C:121:ASP:HB2	1:C:143:GLU:HB3	1.91	0.52
1:D:325:SER:O	1:D:326:THR:CB	2.36	0.52
1:C:297:LEU:HD11	1:C:310:ALA:HB1	1.92	0.52
1:A:423:ASP:HA	1:A:466:VAL:O	2.08	0.52
1:A:117:ILE:HD12	1:A:352:CYS:SG	2.49	0.52
1:A:97:LEU:HD12	1:A:97:LEU:O	2.10	0.52
1:C:24:GLU:OE1	1:D:275:MET:HG3	2.10	0.52
1:A:423:ASP:HB3	1:A:465:TYR:HB3	1.92	0.52
1:D:479:SER:OG	1:D:488:GLN:NE2	2.43	0.51
1:C:418:VAL:CG1	1:C:419:LEU:HD22	2.40	0.51
1:C:517:SER:O	1:C:518:SER:CB	2.57	0.51
1:A:47:SER:HB3	1:A:551:LEU:HD12	1.91	0.51
1:A:345:GLU:HA	1:A:351:LYS:HE2	1.91	0.51
1:C:321:ALA:HB3	1:C:351:LYS:HG2	1.93	0.51
1:A:151:PHE:O	1:A:155:SER:HB2	2.10	0.51
1:D:533:PRO:HB2	1:D:536:ALA:HB2	1.92	0.51
1:B:325:SER:O	1:B:326:THR:HG23	2.11	0.51
1:B:72:ALA:HB2	1:B:360:LEU:HD13	1.93	0.51
1:C:53:GLU:OE2	1:C:124:ARG:NH1	2.44	0.51
1:A:411:VAL:HG11	1:A:442:THR:HG23	1.93	0.51
1:D:504:LEU:HG	1:D:520:LEU:HD22	1.93	0.51
1:A:266:ASN:ND2	2:A:1556:GSH:O12	2.44	0.50
1:C:71:THR:CG2	1:C:360:LEU:HD11	2.41	0.50
1:D:112:GLN:CD	1:D:507:ALA:HB2	2.31	0.50
1:A:3:LEU:HD21	1:C:489:LEU:CD1	2.41	0.50
1:D:215:VAL:HG11	1:D:283:ILE:HD13	1.93	0.50
1:B:215:VAL:HG11	1:B:283:ILE:HD13	1.93	0.50
1:A:23:HIS:CE1	1:B:37:ARG:HD3	2.46	0.50
1:C:119:ARG:HB3	1:C:145:ASN:HD21	1.76	0.50
1:C:406:VAL:CG1	1:C:406:VAL:O	2.58	0.50
1:C:512:VAL:HG12	1:C:520:LEU:HD11	1.94	0.50
1:A:151:PHE:CD1	1:A:548:LEU:HD21	2.46	0.50
1:A:68:VAL:HG13	1:A:360:LEU:HD22	1.94	0.50
1:B:78:LEU:CD2	1:B:365:LEU:HD21	2.42	0.50
1:C:418:VAL:HG13	1:C:419:LEU:HD22	1.93	0.50
1:A:411:VAL:CG1	1:A:442:THR:HG23	2.41	0.50
1:D:271:TYR:CZ	1:D:287:PHE:CE2	2.99	0.49
1:B:60:MET:HE3	1:B:390:LEU:HB3	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:414:VAL:HG22	1:D:421:ARG:HD2	1.94	0.49
1:D:420:GLN:O	1:D:420:GLN:HG2	2.12	0.49
1:A:269:ASP:OD2	1:A:324:ARG:NH1	2.38	0.49
1:B:145:ASN:HA	1:B:361:THR:HG23	1.95	0.49
1:D:46:PRO:CG	1:D:198:LEU:HD21	2.42	0.49
1:D:401:LEU:HD13	1:D:402:ASN:N	2.28	0.49
1:A:363:LYS:HB3	1:A:425:PHE:CD1	2.48	0.49
1:A:82:LEU:CD1	1:A:365:LEU:HD11	2.28	0.48
1:A:40:VAL:HG21	1:A:548:LEU:HD12	1.94	0.48
1:B:325:SER:C	1:B:326:THR:HG23	2.34	0.48
1:A:51:ARG:N	1:A:554:VAL:O	2.39	0.48
1:C:297:LEU:CD2	1:C:343:SER:HB3	2.43	0.48
1:D:271:TYR:O	1:D:272:ALA:C	2.52	0.48
1:A:3:LEU:O	1:A:4:LYS:C	2.51	0.48
1:A:99:MET:HE2	1:A:342:LEU:HB2	1.95	0.48
1:D:126:GLY:O	1:D:127:VAL:C	2.51	0.48
1:A:377:VAL:O	1:A:383:GLY:N	2.40	0.48
1:B:60:MET:CE	1:B:390:LEU:HB3	2.43	0.48
1:C:227:LEU:HD11	1:C:302:ILE:HD12	1.96	0.48
1:C:60:MET:HG3	1:C:391:LEU:HD23	1.96	0.48
1:D:227:LEU:O	1:D:227:LEU:HD12	2.14	0.48
1:D:527:TYR:CD1	1:D:551:LEU:HD22	2.48	0.48
1:A:112:GLN:CD	1:A:507:ALA:HB2	2.34	0.48
1:B:257:LEU:HD11	1:B:288:ARG:HB2	1.96	0.48
1:C:257:LEU:HD11	1:C:288:ARG:HB2	1.96	0.48
1:C:51:ARG:N	1:C:554:VAL:O	2.45	0.48
1:D:140:LYS:HG3	1:D:471:ILE:CD1	2.39	0.48
1:A:168:TYR:HD1	1:B:278:LEU:HD21	1.79	0.48
1:A:461:VAL:O	1:A:461:VAL:CG1	2.62	0.48
1:C:266:ASN:HD22	2:C:1556:GSH:HA1	1.79	0.48
1:C:506:ALA:HB2	1:C:512:VAL:CG1	2.40	0.48
1:A:423:ASP:O	1:A:424:GLN:CG	2.61	0.48
1:A:490:GLU:OE2	1:C:14:TYR:OH	2.09	0.48
1:B:184:VAL:HG12	1:B:185:GLU:N	2.29	0.47
1:C:167:ALA:O	1:C:168:TYR:C	2.52	0.47
1:A:414:VAL:O	1:A:418:VAL:HA	2.15	0.47
1:C:150:SER:OG	2:C:1556:GSH:CG1	2.61	0.47
1:C:30:LYS:NZ	1:C:34:GLY:O	2.40	0.47
1:D:271:TYR:HH	1:D:287:PHE:HE2	1.61	0.47
1:D:82:LEU:CD1	1:D:359:LEU:HD22	2.44	0.47
1:D:6:LEU:HD13	1:D:14:TYR:CD1	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:305:GLU:O	1:C:305:GLU:CG	2.63	0.47
1:C:112:GLN:HG2	1:C:507:ALA:HB2	1.97	0.47
1:D:311:VAL:HA	1:D:316:TYR:O	2.14	0.47
1:D:406:VAL:HG22	1:D:408:GLU:HG2	1.97	0.47
1:D:42:VAL:HG22	1:D:43:THR:N	2.29	0.47
1:B:506:ALA:HB3	1:B:512:VAL:CG1	2.45	0.47
1:C:315:HIS:O	1:C:317:PRO:HD3	2.14	0.47
1:A:425:PHE:CD2	1:A:466:VAL:HB	2.50	0.47
1:A:529:VAL:HB	1:A:549:ASP:HB3	1.96	0.47
1:A:359:LEU:O	1:A:365:LEU:HD13	2.15	0.47
1:A:93:THR:HG23	1:A:362:PHE:CE1	2.50	0.47
1:A:46:PRO:HD2	1:A:189:TRP:CE2	2.50	0.47
1:B:85:THR:CG2	1:B:93:THR:HG21	2.44	0.47
1:C:64:TRP:HE1	1:C:122:TYR:HH	1.63	0.47
1:C:514:THR:HG22	1:C:515:ASN:N	2.30	0.47
1:D:53:GLU:OE2	1:D:124:ARG:NH1	2.47	0.47
1:D:211:ILE:CG2	1:D:256:VAL:HG21	2.44	0.46
1:B:159:THR:HG22	1:B:163:GLN:OE1	2.16	0.46
1:B:196:CYS:SG	1:B:554:VAL:HG12	2.56	0.46
1:B:78:LEU:HD13	1:B:359:LEU:CD1	2.45	0.46
1:D:418:VAL:CG1	1:D:419:LEU:HD13	2.44	0.46
1:A:168:TYR:CD1	1:B:278:LEU:HD21	2.50	0.46
1:B:290:LEU:HD12	1:B:337:THR:HG22	1.98	0.46
1:D:527:TYR:CD1	1:D:527:TYR:C	2.84	0.46
1:A:208:PRO:HD3	1:A:273:LEU:HD22	1.97	0.46
1:B:147:ILE:HD13	1:B:327:TYR:HB3	1.97	0.46
1:D:1:MET:O	1:D:2:VAL:C	2.52	0.46
1:A:-5:LEU:HD11	1:A:186:ASN:HD22	1.80	0.46
1:B:202:VAL:CG1	1:B:206:VAL:CG2	2.93	0.46
1:B:3:LEU:HD22	1:B:488:GLN:HB2	1.98	0.46
1:D:296:SER:O	1:D:312:VAL:HA	2.15	0.46
1:B:202:VAL:CG1	1:B:202:VAL:O	2.63	0.46
1:B:262:GLU:HG3	1:B:291:GLN:NE2	2.30	0.46
1:C:187:MET:HE2	1:C:189:TRP:HE1	1.79	0.46
1:C:288:ARG:NH1	1:D:12:GLU:OE2	2.49	0.46
1:A:399:TYR:O	1:A:466:VAL:HG13	2.16	0.46
1:B:155:SER:N	1:B:156:PRO:CD	2.78	0.46
1:D:290:LEU:CD1	1:D:337:THR:CG2	2.92	0.46
1:A:426:VAL:HG12	1:A:427:LEU:N	2.20	0.46
1:B:296:SER:HB3	1:B:312:VAL:HG13	1.97	0.46
1:B:68:VAL:HA	1:B:360:LEU:HD22	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:506:ALA:CB	1:B:512:VAL:CG1	2.90	0.46
1:A:68:VAL:HG13	1:A:360:LEU:CD2	2.44	0.46
1:C:419:LEU:O	1:C:419:LEU:HD23	2.15	0.46
1:D:345:GLU:OE1	1:D:351:LYS:HD2	2.16	0.46
1:A:185:GLU:HG2	1:A:187:MET:HE3	1.97	0.46
1:C:311:VAL:HA	1:C:316:TYR:O	2.16	0.46
1:B:166:ALA:O	1:B:170:GLN:HG3	2.16	0.45
1:B:151:PHE:CD1	1:B:548:LEU:HD11	2.51	0.45
1:A:414:VAL:HG22	1:A:421:ARG:CD	2.46	0.45
1:D:79:ARG:HD3	1:D:101:GLN:HE22	1.81	0.45
1:B:422:PRO:CD	1:B:470:ARG:HB2	2.45	0.45
1:B:418:VAL:HG12	1:B:419:LEU:HD23	1.99	0.45
1:B:180:ASP:C	1:B:184:VAL:HG23	2.37	0.45
1:C:249:VAL:HG12	1:C:250:LEU:N	2.31	0.45
1:C:422:PRO:HD3	1:C:470:ARG:HB2	1.98	0.45
1:D:423:ASP:N	1:D:423:ASP:OD1	2.49	0.45
1:B:140:LYS:HG3	1:B:471:ILE:HD12	1.97	0.45
1:D:42:VAL:HG21	1:D:161:PHE:CD2	2.51	0.45
1:A:461:VAL:HG22	1:A:465:TYR:CE2	2.51	0.45
1:B:3:LEU:O	1:B:7:LEU:HG	2.16	0.45
1:D:367:GLN:HG3	1:D:466:VAL:HG11	1.98	0.45
1:D:406:VAL:O	1:D:408:GLU:HG2	2.17	0.45
1:B:257:LEU:HD12	1:B:258:VAL:N	2.32	0.45
1:B:331:ASP:O	1:B:337:THR:HG21	2.16	0.45
1:B:89:ASP:N	1:B:89:ASP:OD1	2.50	0.45
1:C:392:GLN:HA	1:C:395:PHE:CD1	2.52	0.45
1:A:81:ALA:HB1	1:A:368:LEU:CD1	2.47	0.45
1:D:147:ILE:O	1:D:147:ILE:HG23	2.17	0.45
1:A:420:GLN:C	1:A:421:ARG:HG2	2.37	0.44
1:A:414:VAL:HG13	1:A:421:ARG:HB2	1.97	0.44
1:B:315:HIS:O	1:B:317:PRO:HD3	2.17	0.44
1:C:231:TRP:CD2	1:C:250:LEU:HD13	2.53	0.44
1:D:342:LEU:HD21	1:D:346:ARG:CZ	2.47	0.44
1:A:426:VAL:CG2	1:A:464:GLU:HA	2.46	0.44
1:A:77:PHE:CD1	1:A:379:VAL:HG11	2.52	0.44
1:A:96:LEU:HD13	1:A:338:TRP:HH2	1.82	0.44
1:A:173:GLN:HG3	1:A:191:TRP:CH2	2.51	0.44
1:A:514:THR:HG22	1:A:515:ASN:HD22	1.82	0.44
1:B:78:LEU:HD13	1:B:359:LEU:HD12	2.00	0.44
1:C:324:ARG:HA	1:C:324:ARG:HD2	1.88	0.44
1:C:42:VAL:HG21	1:C:161:PHE:CD2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:465:TYR:O	1:A:466:VAL:CG2	2.60	0.44
1:C:42:VAL:CG2	1:C:43:THR:N	2.79	0.44
1:D:488:GLN:HE21	1:D:488:GLN:HA	1.81	0.44
1:A:184:VAL:O	1:A:185:GLU:HB2	2.18	0.44
1:C:150:SER:OG	2:C:1556:GSH:HG12	2.18	0.44
1:C:231:TRP:CG	1:C:250:LEU:HD13	2.53	0.44
1:C:46:PRO:HG3	1:C:198:LEU:HD21	1.98	0.44
1:D:143:GLU:CD	1:D:366:GLN:HE22	2.20	0.44
1:D:406:VAL:HG22	1:D:408:GLU:HG3	2.00	0.44
1:A:401:LEU:HD11	1:A:467:VAL:HG23	1.98	0.44
1:C:404:LYS:O	1:C:406:VAL:N	2.50	0.44
1:D:117:ILE:HD12	1:D:322:TYR:CE2	2.53	0.44
1:D:524:PHE:CZ	1:D:526:GLY:HA2	2.53	0.44
1:C:418:VAL:O	1:C:420:GLN:N	2.51	0.44
1:D:72:ALA:HB2	1:D:360:LEU:HD13	2.00	0.44
1:B:393:ARG:NH2	3:B:1557:SO4:O3	2.51	0.43
1:D:549:ASP:OD1	1:D:550:SER:N	2.46	0.43
1:A:139:TRP:O	1:A:394:HIS:HD2	2.01	0.43
1:B:119:ARG:HD3	1:B:500:PHE:CE1	2.53	0.43
1:C:42:VAL:HG22	1:C:43:THR:O	2.18	0.43
1:B:57:LEU:HD23	1:B:122:TYR:CZ	2.53	0.43
1:C:37[A]:ARG:HH11	1:C:37[A]:ARG:CG	2.31	0.43
1:A:195:ASN:O	1:A:555:PRO:HD3	2.18	0.43
1:B:6:LEU:HD23	1:B:14:TYR:CD1	2.54	0.43
1:D:216:ARG:HB2	1:D:216:ARG:CZ	2.47	0.43
1:A:277:VAL:HG12	1:A:283:ILE:HB	2.00	0.43
1:C:514:THR:HG22	1:C:515:ASN:H	1.83	0.43
1:C:6:LEU:HD13	1:C:169:LEU:HD21	2.00	0.43
1:C:49:ILE:CD1	1:C:139:TRP:CZ2	2.99	0.43
1:C:123:MET:HB3	1:C:473:PHE:CD1	2.53	0.43
1:C:255:VAL:HG22	1:C:317:PRO:O	2.18	0.43
1:C:320:VAL:HA	1:C:350:ILE:O	2.18	0.43
1:C:527:TYR:C	1:C:527:TYR:CD1	2.90	0.43
1:D:224:PHE:O	1:D:227:LEU:N	2.52	0.43
1:A:-5:LEU:CD1	1:A:186:ASN:HD22	2.31	0.43
1:B:78:LEU:HD21	1:B:365:LEU:HD21	2.01	0.43
1:A:102:GLU:C	1:A:106:SER:HB2	2.40	0.43
1:A:278:LEU:HD21	1:B:168:TYR:HD1	1.84	0.43
1:A:67:ALA:HB2	1:A:381:PHE:CZ	2.54	0.43
1:B:184:VAL:HG22	1:B:193:LYS:CE	2.47	0.43
1:B:421:ARG:NH1	1:B:421:ARG:HG3	2.24	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:93:THR:HG23	1:C:362:PHE:CE1	2.53	0.43
1:C:480:LEU:C	1:C:480:LEU:HD23	2.39	0.43
1:D:147:ILE:HD13	1:D:327:TYR:HA	2.01	0.43
1:D:415:ILE:HG12	1:D:418:VAL:HG23	2.01	0.43
1:A:155:SER:HB3	1:A:156:PRO:HD3	2.00	0.43
1:B:79:ARG:CD	1:B:101:GLN:HE21	2.32	0.43
1:D:208:PRO:HD3	1:D:273:LEU:CD2	2.49	0.43
1:C:402:ASN:HB2	1:C:403:PRO:CD	2.47	0.42
1:D:148:SER:OG	1:D:324:ARG:HA	2.19	0.42
1:A:211:ILE:O	1:A:215:VAL:HG23	2.19	0.42
1:B:259:VAL:HA	1:B:288:ARG:O	2.19	0.42
1:B:96:LEU:CD2	1:B:355:ILE:HD12	2.49	0.42
1:A:44:LEU:HD22	1:A:165:ILE:HD11	2.01	0.42
1:B:327:TYR:CD1	1:B:328:VAL:HG23	2.55	0.42
1:B:64:TRP:O	1:B:68:VAL:HG23	2.19	0.42
1:C:231:TRP:CD1	1:C:235:GLN:NE2	2.88	0.42
1:C:72:ALA:HB2	1:C:360:LEU:HD13	2.01	0.42
1:A:331:ASP:C	1:A:333:PRO:HD3	2.40	0.42
1:A:425:PHE:CE2	1:A:466:VAL:HG11	2.54	0.42
1:B:399:TYR:HB2	1:B:467:VAL:CG1	2.49	0.42
1:D:162:HIS:ND1	1:D:550:SER:HB3	2.35	0.42
1:B:49:ILE:CG2	1:B:553:VAL:HG22	2.50	0.42
1:C:517:SER:O	1:C:518:SER:HB3	2.19	0.42
1:D:258:VAL:HG12	1:D:260:VAL:CG2	2.46	0.42
1:A:81:ALA:HB1	1:A:368:LEU:HD11	2.01	0.42
1:A:428:LYS:N	1:A:429:PRO:CD	2.83	0.42
1:B:274:LEU:HD22	1:B:285:PHE:CB	2.49	0.42
1:B:151:PHE:CZ	1:B:541:VAL:HG13	2.55	0.42
1:A:126:GLY:HA2	1:A:474:HIS:HB2	2.01	0.42
1:A:312:VAL:HB	1:A:316:TYR:HB2	2.00	0.42
1:D:373:ASP:OD1	1:D:373:ASP:N	2.52	0.42
1:D:29:MET:HE2	1:D:40:VAL:HG12	1.99	0.42
1:C:355:ILE:HA	1:C:355:ILE:HD13	1.90	0.42
1:A:-1:GLY:HA3	1:A:477:THR:O	2.19	0.42
1:B:290:LEU:HB2	1:B:337:THR:HG23	2.01	0.42
1:A:333:PRO:HD2	1:A:337:THR:HG21	2.01	0.42
1:D:475:VAL:O	1:D:491:ARG:NH1	2.53	0.42
1:C:227:LEU:HA	1:C:227:LEU:HD12	1.73	0.41
1:C:465:TYR:O	1:C:466:VAL:HG13	2.20	0.41
1:D:290:LEU:CB	1:D:337:THR:HG23	2.49	0.41
1:D:42:VAL:CG2	1:D:43:THR:N	2.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:139:TRP:O	1:A:394:HIS:CD2	2.73	0.41
1:C:309:LEU:HD12	1:C:310:ALA:N	2.36	0.41
1:D:372:VAL:HG13	1:D:377:VAL:HG23	2.02	0.41
1:A:325:SER:C	1:A:326:THR:HG23	2.40	0.41
1:B:184:VAL:HG22	1:B:193:LYS:NZ	2.36	0.41
1:B:123:MET:HB3	1:B:473:PHE:CD1	2.55	0.41
1:B:5:LEU:HA	1:B:5:LEU:HD23	1.93	0.41
1:C:195:ASN:O	1:C:555:PRO:HD2	2.20	0.41
1:A:16[A]:GLU:O	1:A:19:ALA:HB3	2.20	0.41
1:A:294:HIS:CG	1:A:336:ALA:HB1	2.56	0.41
1:A:415:ILE:HD11	1:A:442:THR:CG2	2.49	0.41
1:C:300:HIS:ND1	1:C:311:VAL:HG22	2.35	0.41
1:C:512:VAL:HG12	1:C:520:LEU:CD1	2.50	0.41
1:D:30:LYS:HA	1:D:37:ARG:HD2	2.02	0.41
1:D:365:LEU:HA	1:D:365:LEU:HD13	1.89	0.41
1:B:277:VAL:HG12	1:B:283:ILE:HB	2.02	0.41
1:B:96:LEU:HD22	1:B:355:ILE:HD12	2.02	0.41
1:C:147:ILE:CD1	1:C:358:HIS:CE1	3.04	0.41
1:A:424:GLN:HG2	1:A:432:GLU:HG2	2.03	0.41
1:A:461:VAL:HG13	1:A:465:TYR:CG	2.55	0.41
1:A:112:GLN:HG2	1:A:507:ALA:HB2	2.03	0.41
1:D:207:VAL:O	1:D:208:PRO:C	2.56	0.41
1:B:328:VAL:HG12	1:B:330:GLU:H	1.85	0.41
1:B:378:PRO:HG2	1:B:379:VAL:HG23	2.03	0.41
1:C:101:GLN:HA	1:C:105:LEU:HB2	2.03	0.41
1:A:490:GLU:HG3	1:C:487:VAL:HG23	2.03	0.41
1:D:61:GLN:N	1:D:62:PRO:CD	2.84	0.41
1:A:12:GLU:OE2	1:B:288:ARG:NH1	2.46	0.41
1:B:61:GLN:N	1:B:62:PRO:CD	2.84	0.41
1:C:192:GLY:O	1:C:197:ARG:HG2	2.21	0.41
1:A:148:SER:CB	1:A:324:ARG:HA	2.51	0.41
1:A:223:LYS:O	1:A:226:SER:N	2.49	0.41
1:A:421:ARG:HA	1:A:468:MET:O	2.21	0.41
1:D:30:LYS:HA	1:D:37:ARG:CD	2.51	0.41
1:D:471:ILE:HG21	1:D:473:PHE:CE1	2.56	0.41
1:B:9:LEU:HD11	1:B:173:GLN:HG2	2.03	0.40
1:B:345:GLU:HA	1:B:351:LYS:HD3	2.04	0.40
1:B:90:VAL:HG13	1:B:91:ASN:OD1	2.21	0.40
1:C:111:GLN:HB2	1:C:348:SER:HA	2.03	0.40
1:A:207:VAL:HG11	1:A:273:LEU:HD13	2.02	0.40
1:A:369:LEU:O	1:A:376:LEU:HD13	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:377:VAL:N	1:A:378:PRO:HD2	2.36	0.40
1:A:461:VAL:HA	1:A:465:TYR:CD2	2.56	0.40
1:B:480:LEU:HD23	1:B:480:LEU:HA	1.86	0.40
1:B:540:GLY:C	1:B:546:ALA:HB3	2.41	0.40
1:C:79:ARG:HG3	1:C:97:LEU:HD21	2.04	0.40
1:D:258:VAL:O	1:D:260:VAL:HG23	2.21	0.40
1:D:85:THR:O	1:D:85:THR:HG22	2.22	0.40
1:A:299:LEU:CD2	1:A:347:SER:HB3	2.52	0.40
1:B:202:VAL:O	1:B:202:VAL:HG13	2.21	0.40
1:C:300:HIS:CE1	1:C:311:VAL:CG2	3.04	0.40
1:D:318:ILE:HD13	1:D:318:ILE:N	2.36	0.40
1:C:365:LEU:HD12	1:C:365:LEU:N	2.37	0.40
1:C:151:PHE:CD1	1:C:548:LEU:HD21	2.57	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	509/562 (91%)	445 (87%)	54 (11%)	10 (2%)	9	42
1	B	478/562 (85%)	428 (90%)	42 (9%)	8 (2%)	11	46
1	C	481/562 (86%)	430 (89%)	37 (8%)	14 (3%)	5	31
1	D	482/562 (86%)	436 (90%)	37 (8%)	9 (2%)	9	43
All	All	1950/2248 (87%)	1739 (89%)	170 (9%)	41 (2%)	8	40

All (41) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	31	GLU
1	A	424	GLN

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Mol	Chain	Res	Type
1	B	422	PRO
1	B	424	GLN
1	C	402	ASN
1	C	404	LYS
1	C	405	GLU
1	C	512	VAL
1	D	193	LYS
1	A	33	ALA
1	A	457	THR
1	C	419	LEU
1	D	249	VAL
1	D	326	THR
1	A	129	ASP
1	A	403	PRO
1	A	430	GLN
1	B	330	GLU
1	C	187	MET
1	C	192	GLY
1	C	518	SER
1	D	247	LEU
1	A	422	PRO
1	C	178	LYS
1	D	135	THR
1	A	333	PRO
1	B	490	GLU
1	B	515	ASN
1	D	2	VAL
1	D	251	ASP
1	D	415	ILE
1	B	31	GLU
1	B	333	PRO
1	C	315	HIS
1	C	418	VAL
1	C	516	GLY
1	C	406	VAL
1	B	90	VAL
1	C	403	PRO
1	D	403	PRO
1	A	127	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	444/475 (94%)	412 (93%)	32 (7%)	17	51
1	B	412/475 (87%)	395 (96%)	17 (4%)	35	71
1	C	420/475 (88%)	390 (93%)	30 (7%)	17	52
1	D	415/475 (87%)	387 (93%)	28 (7%)	19	55
All	All	1691/1900 (89%)	1584 (94%)	107 (6%)	21	58

All (107) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LEU
1	A	12	GLU
1	A	29	MET
1	A	45	GLN
1	A	76	THR
1	A	79	ARG
1	A	120	THR
1	A	130	LYS
1	A	134	THR
1	A	135	THR
1	A	150	SER
1	A	173	GLN
1	A	184	VAL
1	A	186	ASN
1	A	188	SER
1	A	249	VAL
1	A	306	GLN
1	A	311	VAL
1	A	361	THR
1	A	365	LEU
1	A	371	ASP
1	A	374	ARG
1	A	401	LEU
1	A	417	ASP

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Mol	Chain	Res	Type
1	A	424	GLN
1	A	425	PHE
1	A	428	LYS
1	A	438	LEU
1	A	443	MET
1	A	458	TYR
1	A	460	LYS
1	A	551	LEU
1	B	1	MET
1	B	45	GLN
1	B	89	ASP
1	B	123	MET
1	B	188	SER
1	B	202	VAL
1	B	247	LEU
1	B	276	ARG
1	B	337	THR
1	B	360	LEU
1	B	416	HIS
1	B	421	ARG
1	B	425	PHE
1	B	465	TYR
1	B	477	THR
1	B	541	VAL
1	B	548	LEU
1	C	6	LEU
1	C	9	LEU
1	C	37[A]	ARG
1	C	37[B]	ARG
1	C	40	VAL
1	C	42	VAL
1	C	88	SER
1	C	97	LEU
1	C	144	ILE
1	C	145	ASN
1	C	188	SER
1	C	195	ASN
1	C	200	ARG
1	C	208	PRO
1	C	260	VAL
1	C	262	GLU
1	C	334	THR

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Mol	Chain	Res	Type
1	C	337	THR
1	C	343	SER
1	C	360	LEU
1	C	386	ASP
1	C	396	VAL
1	C	419	LEU
1	C	437	LEU
1	C	438	LEU
1	C	465	TYR
1	C	476	SER
1	C	480	LEU
1	C	545	VAL
1	C	553	VAL
1	D	45	GLN
1	D	98	ASN
1	D	102	GLU
1	D	134	THR
1	D	138	ARG
1	D	141	ASN
1	D	197	ARG
1	D	220	GLU
1	D	226	SER
1	D	230	SER
1	D	246	GLN
1	D	252	THR
1	D	284	ARG
1	D	297	LEU
1	D	305	GLU
1	D	326	THR
1	D	360	LEU
1	D	373	ASP
1	D	374	ARG
1	D	413	LYS
1	D	423	ASP
1	D	479	SER
1	D	488	GLN
1	D	494	CYS
1	D	524	PHE
1	D	545	VAL
1	D	551	LEU
1	D	554	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	-2	GLN
1	A	98	ASN
1	A	266	ASN
1	A	306	GLN
1	A	394	HIS
1	A	515	ASN
1	B	101	GLN
1	B	145	ASN
1	B	186	ASN
1	B	222	GLN
1	B	367	GLN
1	B	488	GLN
1	C	74	ASN
1	C	98	ASN
1	C	145	ASN
1	C	186	ASN
1	C	235	GLN
1	C	266	ASN
1	C	515	ASN
1	D	0	HIS
1	D	101	GLN
1	D	261	GLN
1	D	366	GLN
1	D	488	GLN

### 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

11 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	GSH	A	1556	-	11,19,19	3.92	2 (18%)	14,24,24	1.08	1 (7%)
3	SO4	A	1557	-	4,4,4	0.14	0	6,6,6	0.30	0
3	SO4	A	1558	-	4,4,4	0.21	0	6,6,6	0.20	0
2	GSH	B	1556	-	11,19,19	4.14	2 (18%)	14,24,24	1.14	1 (7%)
3	SO4	B	1557	-	4,4,4	0.24	0	6,6,6	0.47	0
2	GSH	C	1556	-	11,19,19	4.13	2 (18%)	14,24,24	1.29	1 (7%)
3	SO4	C	1557	-	4,4,4	0.28	0	6,6,6	0.47	0
3	SO4	C	1558	-	4,4,4	0.25	0	6,6,6	0.49	0
3	SO4	C	1559	-	4,4,4	0.20	0	6,6,6	0.29	0
2	GSH	D	1556	-	11,19,19	3.80	2 (18%)	14,24,24	1.35	2 (14%)
3	SO4	D	1557	-	4,4,4	0.14	0	6,6,6	0.14	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	GSH	A	1556	-	-	0/18/24/24	0/0/0/0
3	SO4	A	1557	-	-	0/0/0/0	0/0/0/0
3	SO4	A	1558	-	-	0/0/0/0	0/0/0/0
2	GSH	B	1556	-	-	0/18/24/24	0/0/0/0
3	SO4	B	1557	-	-	0/0/0/0	0/0/0/0
2	GSH	C	1556	-	-	0/18/24/24	0/0/0/0
3	SO4	C	1557	-	-	0/0/0/0	0/0/0/0
3	SO4	C	1558	-	-	0/0/0/0	0/0/0/0
3	SO4	C	1559	-	-	0/0/0/0	0/0/0/0
2	GSH	D	1556	-	-	0/18/24/24	0/0/0/0
3	SO4	D	1557	-	-	0/0/0/0	0/0/0/0

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1556	GSH	OE1-CD1	8.67	1.41	1.23
2	D	1556	GSH	O2-C2	8.91	1.40	1.23
2	B	1556	GSH	OE1-CD1	8.98	1.42	1.23
2	A	1556	GSH	OE1-CD1	9.06	1.42	1.23
2	A	1556	GSH	O2-C2	9.18	1.41	1.23
2	C	1556	GSH	OE1-CD1	9.23	1.42	1.23
2	C	1556	GSH	O2-C2	9.97	1.42	1.23
2	B	1556	GSH	O2-C2	10.29	1.43	1.23

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1556	GSH	CA2-CB2-SG2	-3.32	110.28	114.15
2	A	1556	GSH	CA2-CB2-SG2	-2.07	111.74	114.15
2	B	1556	GSH	CB2-CA2-C2	2.06	114.15	109.60
2	C	1556	GSH	C2-CA2-N2	2.25	117.39	111.20
2	D	1556	GSH	CA3-N3-C2	2.64	125.97	122.39

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1556	GSH	3	0
3	A	1558	SO4	1	0
3	B	1557	SO4	1	0
2	C	1556	GSH	4	0
2	D	1556	GSH	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	520/562 (92%)	-0.11	23 (4%)	35 20	3, 27, 37, 47	1 (0%)
1	B	488/562 (86%)	-0.05	23 (4%)	32 18	13, 27, 37, 46	0
1	C	496/562 (88%)	-0.24	24 (4%)	31 17	6, 24, 33, 46	0
1	D	492/562 (87%)	-0.23	13 (2%)	56 40	14, 24, 38, 67	0
All	All	1996/2248 (88%)	-0.16	83 (4%)	37 22	3, 25, 36, 67	1 (0%)

All (83) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	401	LEU	5.0
1	B	0	HIS	4.6
1	C	410	ALA	4.4
1	A	410	ALA	4.3
1	B	185	GLU	4.2
1	B	423	ASP	4.2
1	C	436	ASN	4.2
1	B	416	HIS	3.9
1	A	418	VAL	3.9
1	A	430	GLN	3.9
1	A	415	ILE	3.9
1	D	412	GLU	3.8
1	B	417	ASP	3.8
1	B	305	GLU	3.7
1	C	435	GLY	3.7
1	A	416	HIS	3.7
1	A	414	VAL	3.7
1	D	417	ASP	3.6
1	D	416	HIS	3.6
1	C	405	GLU	3.6
1	C	431	LEU	3.5

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Mol	Chain	Res	Type	RSRZ
1	C	412	GLU	3.5
1	B	91	ASN	3.5
1	A	555	PRO	3.5
1	A	438	LEU	3.4
1	B	192	GLY	3.2
1	C	400	SER	3.1
1	C	437	LEU	3.1
1	A	442	THR	3.1
1	C	555	PRO	3.0
1	A	417	ASP	3.0
1	B	186	ASN	3.0
1	C	192	GLY	2.9
1	C	237	ASN	2.9
1	D	178	LYS	2.8
1	C	419	LEU	2.8
1	B	84	GLU	2.8
1	B	409	GLU	2.7
1	C	432	GLU	2.7
1	A	435	GLY	2.7
1	B	415	ILE	2.7
1	B	424	GLN	2.7
1	C	441	GLU	2.7
1	D	410	ALA	2.7
1	B	400	SER	2.7
1	A	129	ASP	2.7
1	C	439	SER	2.7
1	B	87	ALA	2.6
1	B	90	VAL	2.6
1	A	439	SER	2.6
1	D	134	THR	2.6
1	A	467	VAL	2.6
1	B	538	ASP	2.6
1	C	467	VAL	2.6
1	D	409	GLU	2.5
1	A	411	VAL	2.5
1	A	233	GLN	2.5
1	C	401	LEU	2.4
1	A	459	SER	2.4
1	A	33	ALA	2.4
1	A	434	GLY	2.4
1	D	233	GLN	2.4
1	C	399	TYR	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	438	LEU	2.4
1	B	535	ASP	2.3
1	C	193	LYS	2.3
1	B	92	PHE	2.3
1	B	230	SER	2.3
1	A	87	ALA	2.3
1	C	186	ASN	2.2
1	C	422	PRO	2.2
1	C	402	ASN	2.2
1	D	194	GLY	2.2
1	D	405	GLU	2.2
1	D	555	PRO	2.1
1	B	231	TRP	2.1
1	B	467	VAL	2.1
1	A	183	GLY	2.1
1	A	192	GLY	2.1
1	B	407	GLY	2.1
1	A	229	ALA	2.0
1	D	402	ASN	2.0
1	C	535	ASP	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	GSH	C	1556	20/20	0.73	0.32	5.72	89,93,94,94	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	SO4	C	1559	5/5	0.94	0.24	0.84	99,99,99,99	0
2	GSH	D	1556	20/20	0.96	0.19	0.56	46,48,52,54	0
2	GSH	A	1556	20/20	0.92	0.18	0.04	63,73,79,80	0
3	SO4	B	1557	5/5	0.93	0.17	-0.27	86,87,87,88	0
3	SO4	C	1558	5/5	0.98	0.15	-0.29	48,49,50,50	0
2	GSH	B	1556	20/20	0.94	0.17	-0.57	56,59,61,62	0
3	SO4	A	1557	5/5	0.96	0.14	-0.64	78,79,79,79	0
3	SO4	A	1558	5/5	0.94	0.18	-1.14	93,93,94,94	0
3	SO4	C	1557	5/5	0.98	0.09	-1.66	62,64,64,64	0
3	SO4	D	1557	5/5	0.80	0.55	-	117,117,117,118	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.