



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 08:22 PM UTC

PDB ID : 2WYO / pdb_00002wyo
Title : Trypanosoma brucei glutathione synthetase
Authors : Fyfe, P.K.; Alpey, 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

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
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
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

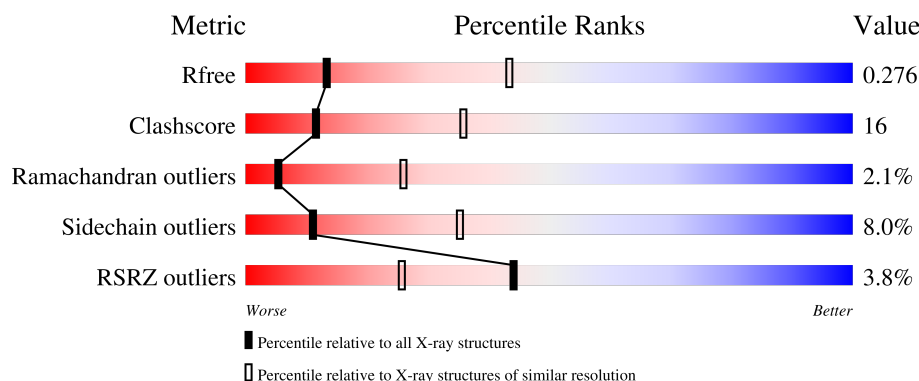
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.15 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}	180053	2361 (3.20-3.12)
Clashscore	190562	2486 (3.20-3.12)
Ramachandran outliers	187476	2405 (3.20-3.12)
Sidechain outliers	187428	2404 (3.20-3.12)
RSRZ outliers	180081	2361 (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 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	562	 4% 58% 31% 7%
1	B	562	 0% 58% 25% 13%
1	C	562	 5% 60% 23% 12%
1	D	562	 3% 59% 25% 12%

2 Entry composition [i](#)

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:

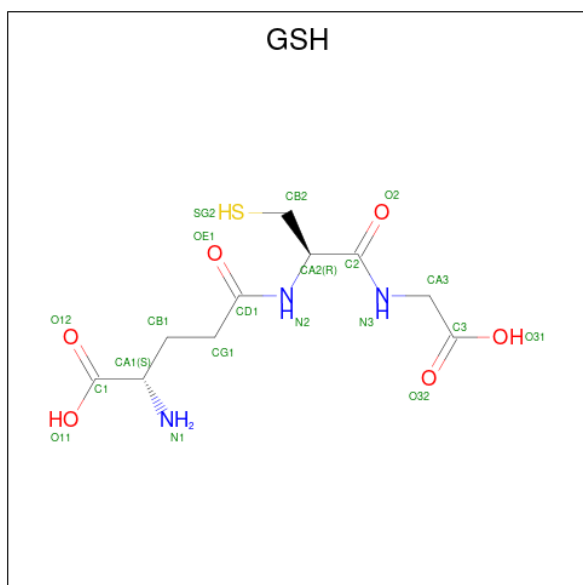
Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	ASN	-	expression tag	UNP Q57UN0
A	-5	LEU	-	expression tag	UNP Q57UN0
A	-4	TYR	-	expression tag	UNP Q57UN0
A	-3	PHE	-	expression tag	UNP Q57UN0
A	-2	GLN	-	expression tag	UNP Q57UN0
A	-1	GLY	-	expression tag	UNP Q57UN0
A	0	HIS	-	expression tag	UNP Q57UN0
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 (CCD ID: GSH) (formula: C₁₀H₁₇N₃O₆S).



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 (CCD ID: SO4) (formula: O₄S).



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		

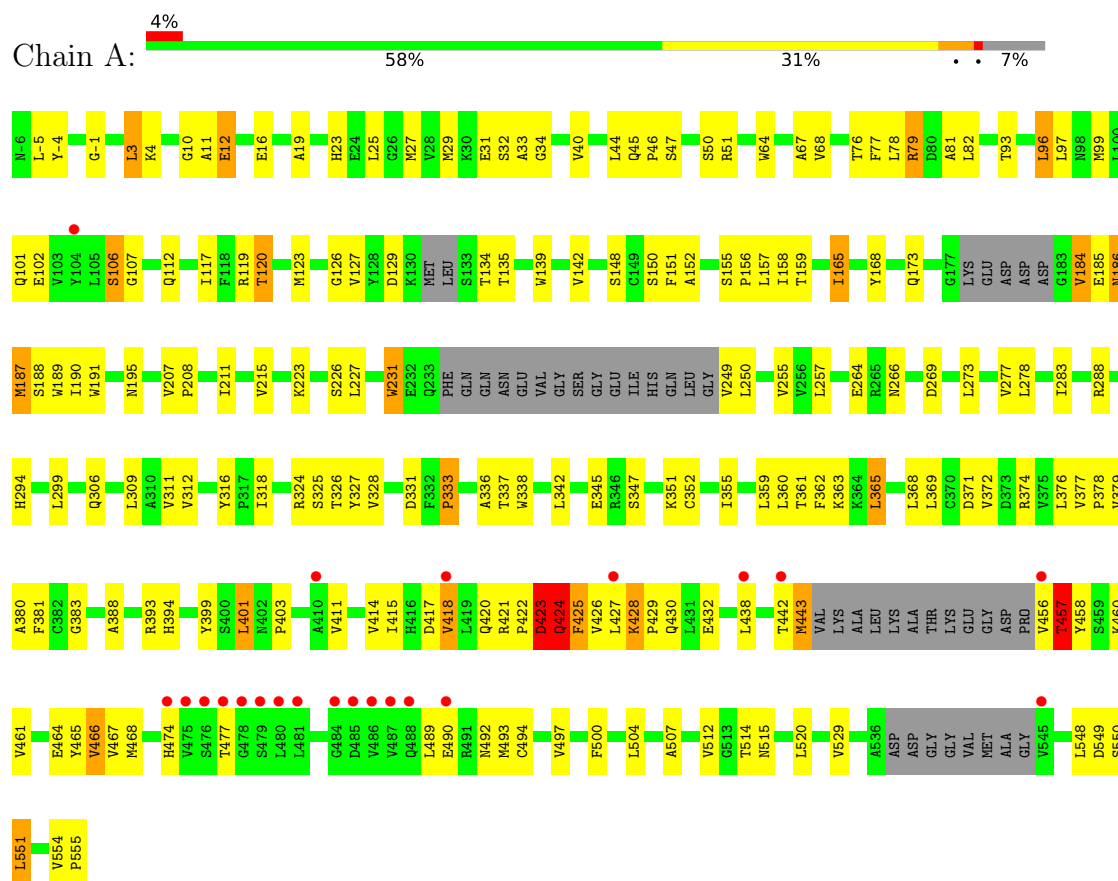
- Molecule 4 is water.

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		

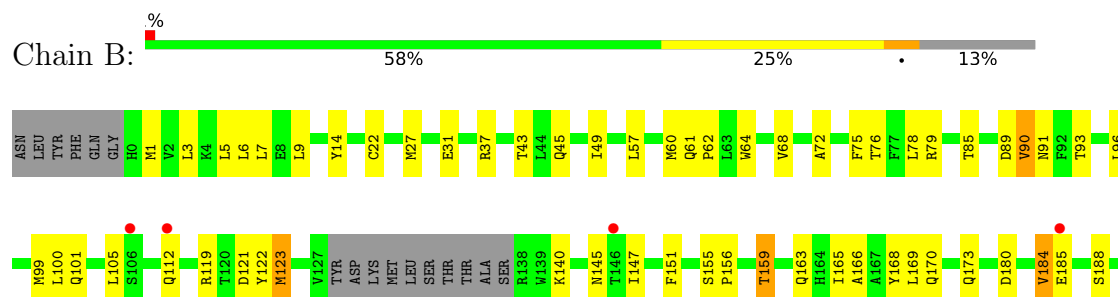
3 Residue-property plots [i](#)

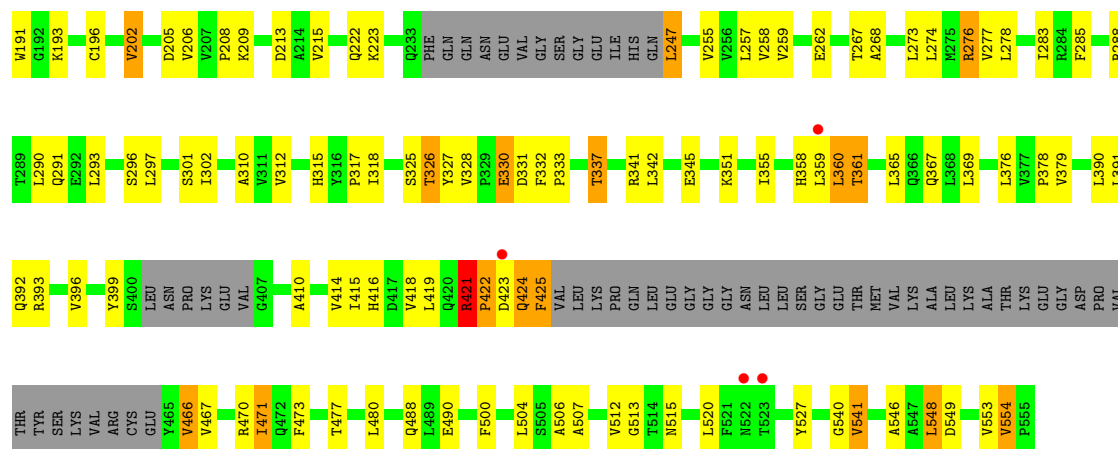
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

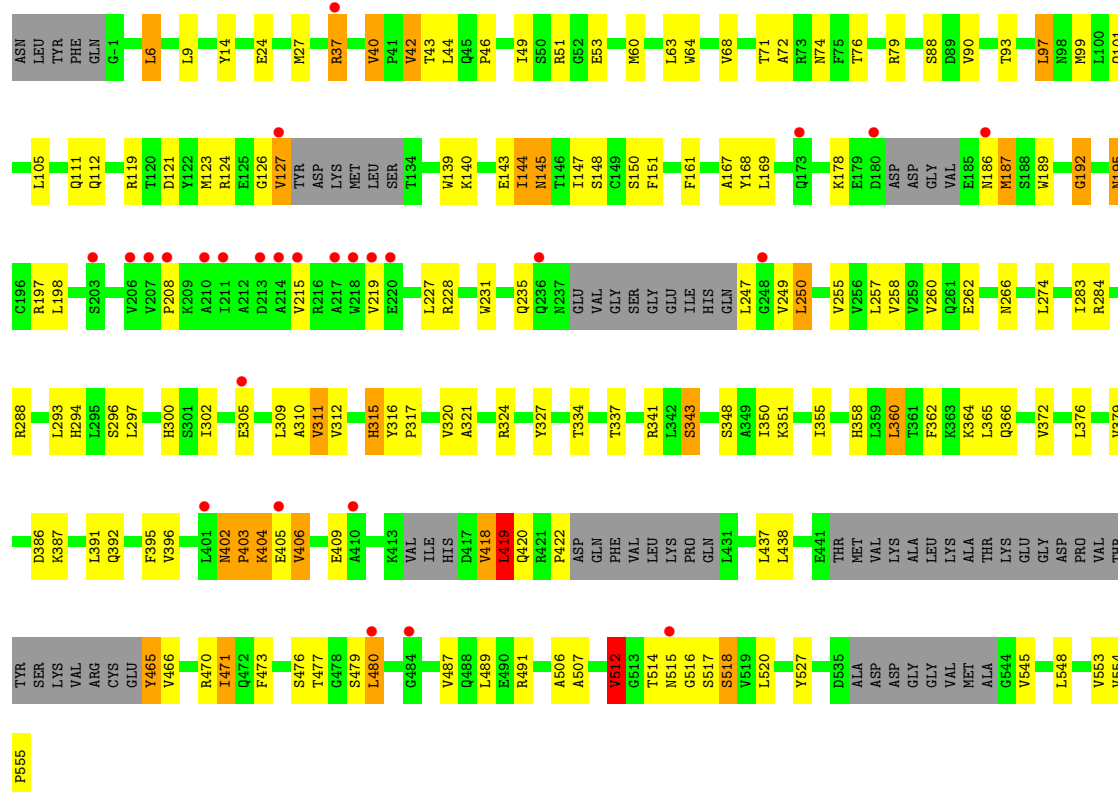


• Molecule 1: GLUTATHIONE SYNTHETASE

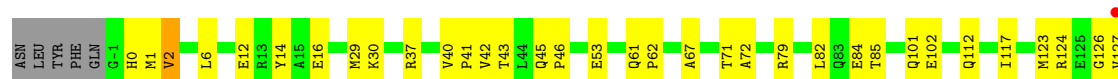




• Molecule 1: GLUTATHIONE SYNTHETASE



• Molecule 1: GLUTATHIONE SYNTHETASE





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	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) 99.8 (39.46-3.15)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	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 (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	65.1	Xtriage
Anisotropy	0.513	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 60.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	15702	wwPDB-VP
Average B, all atoms (Å ²)	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.*

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: 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	0.76	3/4145 (0.1%)	0.95	11/5615 (0.2%)
1	B	0.69	0/3880	0.88	3/5258 (0.1%)
1	C	0.85	1/3945 (0.0%)	0.98	1/5339 (0.0%)
1	D	0.83	1/3904 (0.0%)	0.99	4/5292 (0.1%)
All	All	0.79	5/15874 (0.0%)	0.95	19/21504 (0.1%)

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 (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	231	TRP	CG-CD2	-10.00	1.25	1.43
1	C	311	VAL	CA-CB	5.79	1.62	1.54
1	D	355	ILE	CA-CB	5.38	1.56	1.54
1	A	424	GLN	N-CA	5.02	1.52	1.46
1	A	423	ASP	CA-C	5.01	1.59	1.52

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	231	TRP	CD1-CG-CD2	10.19	122.60	106.30
1	A	425	PHE	N-CA-C	9.17	124.78	113.50
1	A	424	GLN	N-CA-C	7.60	126.98	110.80
1	B	421	ARG	CA-C-N	7.24	128.89	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	421	ARG	C-N-CA	7.24	128.89	119.84
1	D	540	GLY	N-CA-C	6.49	123.98	112.55
1	B	318	ILE	N-CA-C	6.26	116.40	106.88
1	C	512	VAL	N-CA-C	5.93	121.68	109.34
1	A	231	TRP	CB-CG-CD2	-5.77	118.72	126.80
1	D	420	GLN	N-CA-C	5.67	118.62	109.83
1	A	550	SER	N-CA-C	-5.51	101.06	109.65
1	A	231	TRP	CB-CG-CD1	-5.48	118.67	126.90
1	A	418	VAL	N-CA-C	5.33	115.54	110.53
1	D	545	VAL	CB-CA-C	-5.24	105.17	110.88
1	A	107	GLY	N-CA-C	-5.21	102.88	112.62
1	D	307	PRO	O-C-N	5.08	123.65	121.31
1	A	231	TRP	N-CA-C	5.05	116.47	111.07
1	A	190	ILE	CB-CA-C	-5.03	105.53	111.97
1	A	-4	TYR	N-CA-C	-5.01	107.01	112.72

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 [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	4065	0	4065	150	0
1	B	3803	0	3791	133	0
1	C	3871	0	3868	116	0
1	D	3826	0	3832	115	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	502	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 16.

All (502) 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:D:29:MET:HE2	1:D:40:VAL:HG12	1.42	1.00
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:D:123:MET:HE3	1:D:142:VAL:HG11	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:99:MET:HE1	1:B:341:ARG:HB3	1.66	0.78
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:60:MET:HE1	1:B:390:LEU:HB3	1.66	0.75
1:B:367:GLN:HE22	1:B:466:VAL:HG21	1.50	0.75
1:B:425:PHE:C	1:B:425:PHE:CD2	2.66	0.74
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:A:27:MET:HE3	1:A:158:ILE:HD12	1.73	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
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: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:B:367:GLN:CD	1:B:466:VAL:HG11	2.19	0.67
1:B:425:PHE:C	1:B:425:PHE:HD2	2.01	0.67
1:A:27:MET:HE3	1:A:158:ILE:CD1	2.24	0.67
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:A:123:MET:HE1	1:A:494:CYS:HB2	1.77	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: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:O	1:B:247:LEU:HD12	1.96	0.66
1:B:75:PHE:HB2	1:B:105:LEU:HD21	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:82:LEU:HD11	1:A:365:LEU:CD1	2.21	0.64
1:A:504:LEU:HG	1:A:520:LEU:HD12	1.80	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:C:195:ASN:N	1:C:195:ASN:OD1	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:99:MET:HE2	1:A:342:LEU:HB2	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:C:140:LYS:HG2	1:C:471:ILE:HD12	1.81	0.63
1:B:100:LEU:HD22	1:B:359:LEU:CD1	2.28	0.62
1:D:29:MET:CE	1:D:40:VAL:HG12	2.23	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:HG12	1:A:461:VAL:O	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:C:187:MET:HE2	1:C:189:TRP:HE1	1.64	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:A:492:ASN:CG	1:A:492:ASN:O	2.45	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:423:ASP:O	1:A:424:GLN:CD	2.46	0.59
1:D:16:GLU:OE1	1:D:16:GLU:N	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:71:THR:HG22	1:C:360:LEU:HD11	1.85	0.57
1:C:402:ASN:CB	1:C:403:PRO:CD	2.83	0.57
1:C:68:VAL:HA	1:C:360:LEU:HD22	1.86	0.57
1:A:257:LEU:HB2	1:A:318:ILE:HD12	1.86	0.57
1:D:123:MET:HE2	1:D:496:GLU:OE2	2.05	0.57
1:B:554:VAL:O	1:B:554:VAL:CG2	2.52	0.56
1:D:396:VAL:HG22	1:D:471:ILE:HD12	1.87	0.56
1:A:185:GLU:CG	1:A:187:MET:HE3	2.35	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:HH11	1:B:421:ARG:CG	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:D:112:GLN:CD	1:D:507:ALA:HB2	2.31	0.56
1:A:187:MET:HE2	1:A:191:TRP:NE1	2.21	0.55
1:A:456:VAL:O	1:A:457:THR:HG22	2.05	0.55
1:A:327:TYR:CD1	1:A:328:VAL:HG13	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:185:GLU:HG3	1:A:187:MET:HE3	1.90	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:325:SER:C	1:B:326:THR:HG23	2.34	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:187:MET:HE2	1:A:191:TRP:CD1	2.44	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:64:TRP:CE2	1:A:120:THR:HG21	2.43	0.53
1:A:119:ARG:HD3	1:A:500:PHE:CE1	2.43	0.53
1:B:209:LYS:NZ	1:B:213:ASP:OD2	2.37	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:271:TYR:O	1:D:272:ALA:C	2.52	0.53
1:A:3:LEU:O	1:A:4:LYS:C	2.51	0.53
1:D:126:GLY:O	1:D:127:VAL:C	2.51	0.53
1:D:415:ILE:HG22	1:D:415:ILE:O	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:99:MET:HE1	1:C:341:ARG:CG	2.39	0.52
1:C:255:VAL:HG12	1:C:284:ARG:HB2	1.91	0.52
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:97:LEU:HD12	1:A:97:LEU:O	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:117:ILE:HD12	1:A:352:CYS:SG	2.49	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:A:112:GLN:CD	1:A:507:ALA:HB2	2.34	0.51
1:B:22:CYS:SG	1:B:27:MET:HE2	2.51	0.51
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:D:527:TYR:CD1	1:D:527:TYR:C	2.84	0.51
1:A:151:PHE:O	1:A:155:SER:HB2	2.10	0.51
1:D:1:MET:O	1:D:2:VAL:C	2.52	0.51
1:D:533:PRO:HB2	1:D:536:ALA:HB2	1.92	0.51
1:B:72:ALA:HB2	1:B:360:LEU:HD13	1.93	0.51
1:B:325:SER:O	1:B:326:THR:HG23	2.11	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:C:167:ALA:O	1:C:168:TYR:C	2.52	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:A:23:HIS:CE1	1:B:37:ARG:HD3	2.46	0.50
1:B:215:VAL:HG11	1:B:283:ILE:HD13	1.93	0.50
1:C:119:ARG:HB3	1:C:145:ASN:HD21	1.76	0.50
1:C:406:VAL:O	1:C:406:VAL:CG1	2.58	0.50
1:C:512:VAL:HG12	1:C:520:LEU:HD11	1.94	0.50
1:A:68:VAL:HG13	1:A:360:LEU:HD22	1.94	0.50
1:A:151:PHE:CD1	1:A:548:LEU:HD21	2.46	0.50
1:B:78:LEU:CD2	1:B:365:LEU:HD21	2.42	0.50
1:B:180:ASP:C	1:B:184:VAL:HG23	2.37	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:99:MET:HE1	1:B:341:ARG:CB	2.40	0.49
1:A:420:GLN:C	1:A:421:ARG:HG2	2.37	0.49
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:269:ASP:OD2	1:A:324:ARG:NH1	2.38	0.49
1:B:60:MET:HE1	1:B:390:LEU:HD22	1.95	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:D:143:GLU:CD	1:D:366:GLN:HE22	2.20	0.49
1:A:40:VAL:HG21	1:A:548:LEU:HD12	1.94	0.48
1:A:82:LEU:CD1	1:A:365:LEU:HD11	2.28	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:A:377:VAL:O	1:A:383:GLY:N	2.40	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:HD12	1:D:227:LEU:O	2.14	0.48
1:D:527:TYR:CD1	1:D:551:LEU:HD22	2.48	0.48
1:B:257:LEU:HD11	1:B:288:ARG:HB2	1.96	0.48
1:C:51:ARG:N	1:C:554:VAL:O	2.45	0.48
1:C:257:LEU:HD11	1:C:288:ARG:HB2	1.96	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:C:527:TYR:CD1	1:C:527:TYR:C	2.90	0.48
1:C:231:TRP:CD1	1:C:235:GLN:HE22	2.32	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:480:LEU:C	1:C:480:LEU:HD23	2.39	0.47
1:D:82:LEU:CD1	1:D:359:LEU:HD22	2.44	0.47
1:B:184:VAL:HG12	1:B:185:GLU:N	2.29	0.47
1:D:6:LEU:HD13	1:D:14:TYR:CD1	2.49	0.47
1:C:112:GLN:HG2	1:C:507:ALA:HB2	1.97	0.47
1:A:102:GLU:C	1:A:106:SER:HB2	2.40	0.47
1:D:311:VAL:HA	1:D:316:TYR:O	2.14	0.47
1:A:331:ASP:C	1:A:333:PRO:HD3	2.40	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:D:42:VAL:HG22	1:D:43:THR:N	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:406:VAL:HG22	1:D:408:GLU:HG2	1.97	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:46:PRO:HD2	1:A:189:TRP:CE2	2.50	0.47
1:A:93:THR:HG23	1:A:362:PHE:CE1	2.50	0.47
1:A:359:LEU:O	1:A:365:LEU:HD13	2.15	0.47
1:B:85:THR:CG2	1:B:93:THR:HG21	2.44	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:78:LEU:HD13	1:B:359:LEU:CD1	2.45	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: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: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:A:-5:LEU:HD11	1:A:186:ASN:HD22	1.80	0.46
1:B:3:LEU:HD22	1:B:488:GLN:HB2	1.98	0.46
1:B:202:VAL:CG1	1:B:206:VAL:CG2	2.93	0.46
1:D:296:SER:O	1:D:312:VAL:HA	2.15	0.46
1:A:325:SER:C	1:A:326:THR:HG23	2.40	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: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:C:305:GLU:CG	1:C:305:GLU:O	2.63	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:68:VAL:HA	1:B:360:LEU:HD22	1.98	0.46
1:B:296:SER:HB3	1:B:312:VAL:HG13	1.97	0.46
1:B:506:ALA:CB	1:B:512:VAL:CG1	2.90	0.46
1:D:207:VAL:O	1:D:208:PRO:C	2.56	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:C:311:VAL:HA	1:C:316:TYR:O	2.16	0.46
1:B:151:PHE:CD1	1:B:548:LEU:HD11	2.51	0.45
1:B:166:ALA:O	1:B:170:GLN:HG3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:OD1	1:D:423:ASP:N	2.49	0.45
1:B:140:LYS:HG3	1:B:471:ILE:HD12	1.97	0.45
1:B:540:GLY:C	1:B:546:ALA:HB3	2.41	0.45
1:C:187:MET:HE2	1:C:189:TRP:NE1	2.31	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:89:ASP:N	1:B:89:ASP:OD1	2.50	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: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: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:99:MET:HE1	1:C:341:ARG:HG3	1.98	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: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:426:VAL:CG2	1:A:464:GLU:HA	2.46	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:42:VAL:HG21	1:C:161:PHE:CD2	2.53	0.44
1:C:324:ARG:HA	1:C:324:ARG:HD2	1.88	0.44
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:HA	1:D:488:GLN:HE21	1.81	0.44
1:B:301:SER:C	1:B:302:ILE:HD12	2.43	0.44
1:C:46:PRO:HG3	1:C:198:LEU:HD21	1.98	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:406:VAL:HG22	1:D:408:GLU:HG3	2.00	0.44
1:A:345:GLU:CD	1:A:355:ILE:HG12	2.43	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:293:LEU:O	1:C:294:HIS:C	2.61	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:A:442:THR:O	1:A:443:MET:C	2.60	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:CZ	1:D:216:ARG:HB2	2.47	0.43
1:A:277:VAL:HG12	1:A:283:ILE:HB	2.00	0.43
1:C:6:LEU:HD13	1:C:169:LEU:HD21	2.00	0.43
1:C:514:THR:HG22	1:C:515:ASN:H	1.83	0.43
1:C:49:ILE:CD1	1:C:139:TRP:CZ2	2.99	0.43
1:C:147:ILE:O	1:C:148:SER:C	2.60	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:D:224:PHE:O	1:D:227:LEU:N	2.52	0.43
1:D:271:TYR:HH	1:D:287:PHE:HE2	1.66	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:67:ALA:HB2	1:A:381:PHE:CZ	2.54	0.43
1:A:278:LEU:HD21	1:B:168:TYR:HD1	1.84	0.43
1:B:184:VAL:HG22	1:B:193:LYS:CE	2.47	0.43
1:B:421:ARG:HG3	1:B:421:ARG:NH1	2.24	0.43
1:C:93:THR:HG23	1:C:362:PHE:CE1	2.53	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:50:SER:O	1:A:51:ARG:C	2.62	0.43
1:A:155:SER:HB3	1:A:156:PRO:HD3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:96:LEU:CD2	1:B:355:ILE:HD12	2.49	0.42
1:B:259:VAL:HA	1:B:288:ARG:O	2.19	0.42
1:A:44:LEU:HD22	1:A:165:ILE:HD11	2.01	0.42
1:B:64:TRP:O	1:B:68:VAL:HG23	2.19	0.42
1:B:99:MET:HE2	1:B:342:LEU:N	2.34	0.42
1:B:327:TYR:CD1	1:B:328:VAL:HG23	2.55	0.42
1:C:72:ALA:HB2	1:C:360:LEU:HD13	2.01	0.42
1:C:231:TRP:CD1	1:C:235:GLN:NE2	2.88	0.42
1:A:425:PHE:CE2	1:A:466:VAL:HG11	2.54	0.42
1:B:173:GLN:CD	1:B:191:TRP:HZ2	2.27	0.42
1:B:399:TYR:HB2	1:B:467:VAL:CG1	2.49	0.42
1:C:186:ASN:O	1:C:187:MET:C	2.63	0.42
1:D:162:HIS:ND1	1:D:550:SER:HB3	2.35	0.42
1:A:184:VAL:O	1:A:185:GLU:HB2	2.18	0.42
1:B:49:ILE:CG2	1:B:553:VAL:HG22	2.50	0.42
1:B:358:HIS:C	1:B:358:HIS:HD1	2.26	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:151:PHE:CZ	1:B:541:VAL:HG13	2.55	0.42
1:B:274:LEU:HD22	1:B:285:PHE:CB	2.49	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:C:355:ILE:HD13	1:C:355:ILE:HA	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:42:VAL:CG2	1:D:43:THR:N	2.83	0.41
1:D:290:LEU:CB	1:D:337:THR:HG23	2.49	0.41
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:5:LEU:HD23	1:B:5:LEU:HA	1.93	0.41
1:B:123:MET:HB3	1:B:473:PHE:CD1	2.55	0.41
1:B:184:VAL:HG22	1:B:193:LYS:NZ	2.36	0.41
1:C:195:ASN:O	1:C:555:PRO:HD2	2.20	0.41
1:A:10:GLY:O	1:A:11:ALA:C	2.61	0.41
1:A:16[A]:GLU:O	1:A:19:ALA:HB3	2.20	0.41
1:A:32:SER:C	1:A:34:GLY:H	2.29	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:HD13	1:D:365:LEU:HA	1.89	0.41
1:B:43:THR:HG21	1:B:549:ASP:CG	2.44	0.41
1:B:96:LEU:HD22	1:B:355:ILE:HD12	2.02	0.41
1:B:277:VAL:HG12	1:B:283:ILE:HB	2.02	0.41
1:C:147:ILE:CD1	1:C:358:HIS:CE1	3.04	0.41
1:A:112:GLN:HG2	1:A:507:ALA:HB2	2.03	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:490:GLU:HG3	1:C:487:VAL:HG23	2.03	0.41
1:B:222:GLN:O	1:B:223:LYS:C	2.63	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:D:61:GLN:N	1:D:62:PRO:CD	2.84	0.41
1:A:99:MET:HE1	1:A:342:LEU:N	2.35	0.41
1:A:12:GLU:OE2	1:B:288:ARG:NH1	2.46	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:B:61:GLN:N	1:B:62:PRO:CD	2.84	0.41
1:B:267:THR:O	1:B:268:ALA:C	2.64	0.41
1:B:527:TYR:CD1	1:B:527:TYR:C	2.98	0.41
1:C:192:GLY:O	1:C:197:ARG:HG2	2.21	0.41
1:C:517:SER:O	1:C:518:SER:HB3	2.19	0.41
1:D:134:THR:C	1:D:136:ALA:N	2.78	0.41
1:D:191:TRP:C	1:D:193:LYS:H	2.29	0.41
1:D:224:PHE:O	1:D:225:ALA:C	2.63	0.41
1:C:27:MET:C	1:C:40:VAL:HG22	2.46	0.41
1:D:30:LYS:HA	1:D:37:ARG:CD	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:471:ILE:HG21	1:D:473:PHE:CE1	2.56	0.41
1:D:492:ASN:CG	1:D:492:ASN:O	2.63	0.41
1:B:9:LEU:HD11	1:B:173:GLN:HG2	2.03	0.40
1:A:185:GLU:HG2	1:A:187:MET:HE3	2.03	0.40
1:B:90:VAL:HG13	1:B:91:ASN:OD1	2.21	0.40
1:B:345:GLU:HA	1:B:351:LYS:HD3	2.04	0.40
1:C:111:GLN:HB2	1:C:348:SER:HA	2.03	0.40
1:D:0:HIS:O	1:D:1:MET:C	2.64	0.40
1:A:16[A]:GLU:CD	1:C:491:ARG:HH21	2.29	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
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:C:79:ARG:HG3	1:C:97:LEU:HD21	2.04	0.40
1:D:85:THR:HG22	1:D:85:THR:O	2.22	0.40
1:D:258:VAL:O	1:D:260:VAL:HG23	2.21	0.40
1:A:299:LEU:CD2	1:A:347:SER:HB3	2.52	0.40
1:B:202:VAL:HG13	1:B:202:VAL:O	2.21	0.40
1:C:300:HIS:CE1	1:C:311:VAL:CG2	3.04	0.40
1:C:418:VAL:O	1:C:419:LEU:C	2.64	0.40
1:D:318:ILE:N	1:D:318:ILE:HD13	2.36	0.40
1:C:151:PHE:CD1	1:C:548:LEU:HD21	2.57	0.40
1:C:365:LEU:N	1:C:365:LEU:HD12	2.37	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	509/562 (91%)	445 (87%)	54 (11%)	10 (2%)	6 27

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	478/562 (85%)	428 (90%)	42 (9%)	8 (2%)	7	30
1	C	481/562 (86%)	430 (89%)	37 (8%)	14 (3%)	3	20
1	D	482/562 (86%)	436 (90%)	37 (8%)	9 (2%)	6	28
All	All	1950/2248 (87%)	1739 (89%)	170 (9%)	41 (2%)	5	26

All (41) Ramachandran outliers are listed below:

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

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Mol	Chain	Res	Type
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 [i](#)

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%)	406 (91%)	38 (9%)	10	32
1	B	412/475 (87%)	383 (93%)	29 (7%)	14	40
1	C	420/475 (88%)	382 (91%)	38 (9%)	9	30
1	D	415/475 (87%)	384 (92%)	31 (8%)	12	38
All	All	1691/1900 (89%)	1555 (92%)	136 (8%)	11	35

All (136) 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	96	LEU
1	A	101	GLN
1	A	120	THR
1	A	134	THR
1	A	135	THR
1	A	150	SER
1	A	159	THR

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Mol	Chain	Res	Type
1	A	165	ILE
1	A	184	VAL
1	A	186	ASN
1	A	187	MET
1	A	188	SER
1	A	249	VAL
1	A	255	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
1	A	424	GLN
1	A	428	LYS
1	A	438	LEU
1	A	443	MET
1	A	457	THR
1	A	458	TYR
1	A	460	LYS
1	A	466	VAL
1	A	512	VAL
1	A	551	LEU
1	B	1	MET
1	B	45	GLN
1	B	76	THR
1	B	123	MET
1	B	159	THR
1	B	165	ILE
1	B	184	VAL
1	B	188	SER
1	B	202	VAL
1	B	247	LEU
1	B	255	VAL
1	B	276	ARG
1	B	326	THR
1	B	337	THR
1	B	360	LEU
1	B	361	THR
1	B	391	LEU

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Mol	Chain	Res	Type
1	B	392	GLN
1	B	396	VAL
1	B	415	ILE
1	B	416	HIS
1	B	421	ARG
1	B	425	PHE
1	B	466	VAL
1	B	471	ILE
1	B	477	THR
1	B	541	VAL
1	B	548	LEU
1	B	554	VAL
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	63	LEU
1	C	76	THR
1	C	88	SER
1	C	90	VAL
1	C	97	LEU
1	C	127	VAL
1	C	144	ILE
1	C	145	ASN
1	C	195	ASN
1	C	208	PRO
1	C	219	VAL
1	C	247	LEU
1	C	250	LEU
1	C	260	VAL
1	C	262	GLU
1	C	334	THR
1	C	337	THR
1	C	343	SER
1	C	360	LEU
1	C	364	LYS
1	C	386	ASP
1	C	387	LYS
1	C	396	VAL
1	C	419	LEU

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Mol	Chain	Res	Type
1	C	437	LEU
1	C	438	LEU
1	C	465	TYR
1	C	471	ILE
1	C	476	SER
1	C	480	LEU
1	C	545	VAL
1	C	553	VAL
1	D	45	GLN
1	D	84	GLU
1	D	102	GLU
1	D	134	THR
1	D	141	ASN
1	D	144	ILE
1	D	163	GLN
1	D	197	ARG
1	D	219	VAL
1	D	220	GLU
1	D	226	SER
1	D	227	LEU
1	D	230	SER
1	D	246	GLN
1	D	252	THR
1	D	297	LEU
1	D	305	GLU
1	D	326	THR
1	D	351	LYS
1	D	360	LEU
1	D	373	ASP
1	D	415	ILE
1	D	419	LEU
1	D	423	ASP
1	D	472	GLN
1	D	479	SER
1	D	488	GLN
1	D	494	CYS
1	D	545	VAL
1	D	551	LEU
1	D	554	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	-2	GLN
1	A	17	GLN
1	A	83	GLN
1	A	98	ASN
1	A	112	GLN
1	A	173	GLN
1	A	261	GLN
1	A	266	ASN
1	A	306	GLN
1	A	366	GLN
1	A	394	HIS
1	A	515	ASN
1	B	101	GLN
1	B	145	ASN
1	B	170	GLN
1	B	222	GLN
1	B	294	HIS
1	B	306	GLN
1	B	315	HIS
1	B	367	GLN
1	B	420	GLN
1	C	74	ASN
1	C	101	GLN
1	C	145	ASN
1	C	170	GLN
1	C	186	ASN
1	C	235	GLN
1	C	266	ASN
1	C	270	GLN
1	C	398	GLN
1	C	515	ASN
1	D	0	HIS
1	D	98	ASN
1	D	101	GLN
1	D	246	GLN
1	D	261	GLN
1	D	300	HIS
1	D	306	GLN
1	D	366	GLN
1	D	424	GLN
1	D	488	GLN
1	D	492	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	D	1556	-	18,19,19	3.17	3 (16%)	21,24,24	1.57	4 (19%)
2	GSH	B	1556	-	18,19,19	3.41	2 (11%)	21,24,24	1.22	3 (14%)
2	GSH	A	1556	-	18,19,19	3.26	2 (11%)	21,24,24	1.24	2 (9%)
3	SO4	D	1557	-	4,4,4	0.22	0	6,6,6	0.14	0
2	GSH	C	1556	-	18,19,19	3.41	2 (11%)	21,24,24	1.30	3 (14%)
3	SO4	B	1557	-	4,4,4	0.30	0	6,6,6	0.39	0
3	SO4	A	1557	-	4,4,4	0.22	0	6,6,6	0.31	0
3	SO4	C	1557	-	4,4,4	0.34	0	6,6,6	0.43	0
3	SO4	C	1559	-	4,4,4	0.26	0	6,6,6	0.29	0
3	SO4	A	1558	-	4,4,4	0.30	0	6,6,6	0.21	0
3	SO4	C	1558	-	4,4,4	0.31	0	6,6,6	0.47	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	C	1556	-	-	11/24/24/24	-
2	GSH	D	1556	-	-	3/24/24/24	-
2	GSH	B	1556	-	-	2/24/24/24	-
2	GSH	A	1556	-	-	9/24/24/24	-

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1556	GSH	O2-C2	10.50	1.43	1.23
2	C	1556	GSH	O2-C2	10.18	1.42	1.23
2	C	1556	GSH	OE1-CD1	9.73	1.42	1.23
2	A	1556	GSH	OE1-CD1	9.55	1.42	1.23
2	B	1556	GSH	OE1-CD1	9.46	1.42	1.23
2	A	1556	GSH	O2-C2	9.38	1.41	1.23
2	D	1556	GSH	OE1-CD1	9.14	1.41	1.23
2	D	1556	GSH	O2-C2	9.10	1.40	1.23
2	D	1556	GSH	O11-C1	-2.03	1.24	1.30

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1556	GSH	CA2-CB2-SG2	-3.44	110.28	114.16
2	D	1556	GSH	O31-C3-CA3	2.90	123.84	112.81
2	D	1556	GSH	O31-C3-O32	-2.80	116.12	123.33
2	A	1556	GSH	O11-C1-O12	-2.66	118.04	124.08
2	D	1556	GSH	O11-C1-O12	-2.60	118.17	124.08
2	C	1556	GSH	O11-C1-O12	-2.39	118.65	124.08
2	C	1556	GSH	C2-CA2-N2	2.32	117.39	111.11
2	B	1556	GSH	O31-C3-CA3	2.16	121.01	112.81
2	A	1556	GSH	CA2-CB2-SG2	-2.15	111.74	114.16
2	B	1556	GSH	CB2-CA2-C2	2.14	114.15	109.50
2	B	1556	GSH	O31-C3-O32	-2.12	117.88	123.33
2	C	1556	GSH	OE1-CD1-CG1	-2.06	118.29	122.02

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1556	GSH	CA2-C2-N3-CA3
2	A	1556	GSH	O2-C2-N3-CA3
2	B	1556	GSH	CA2-C2-N3-CA3

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Mol	Chain	Res	Type	Atoms
2	B	1556	GSH	O2-C2-N3-CA3
2	C	1556	GSH	CG1-CD1-N2-CA2
2	C	1556	GSH	OE1-CD1-N2-CA2
2	C	1556	GSH	CA2-C2-N3-CA3
2	C	1556	GSH	O2-C2-N3-CA3
2	C	1556	GSH	O32-C3-CA3-N3
2	D	1556	GSH	CA2-C2-N3-CA3
2	D	1556	GSH	O2-C2-N3-CA3
2	A	1556	GSH	CG1-CD1-N2-CA2
2	C	1556	GSH	C2-CA2-N2-CD1
2	C	1556	GSH	O31-C3-CA3-N3
2	A	1556	GSH	OE1-CD1-N2-CA2
2	A	1556	GSH	O31-C3-CA3-N3
2	A	1556	GSH	O32-C3-CA3-N3
2	C	1556	GSH	CA1-CB1-CG1-CD1
2	A	1556	GSH	O11-C1-CA1-N1
2	A	1556	GSH	C1-CA1-CB1-CG1
2	C	1556	GSH	O2-C2-CA2-N2
2	C	1556	GSH	N3-C2-CA2-N2
2	D	1556	GSH	C3-CA3-N3-C2
2	A	1556	GSH	O2-C2-CA2-N2
2	C	1556	GSH	O11-C1-CA1-N1

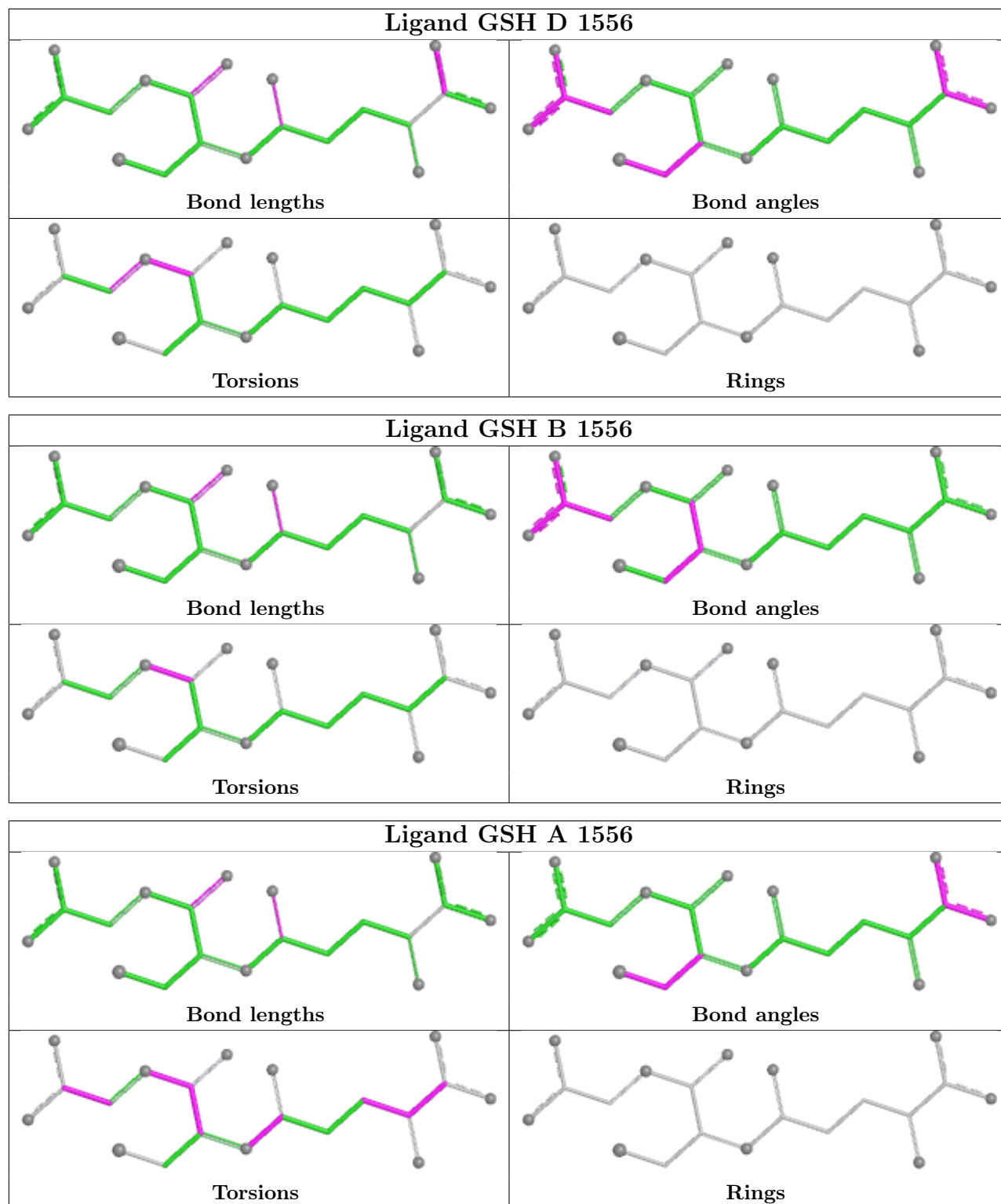
There are no ring outliers.

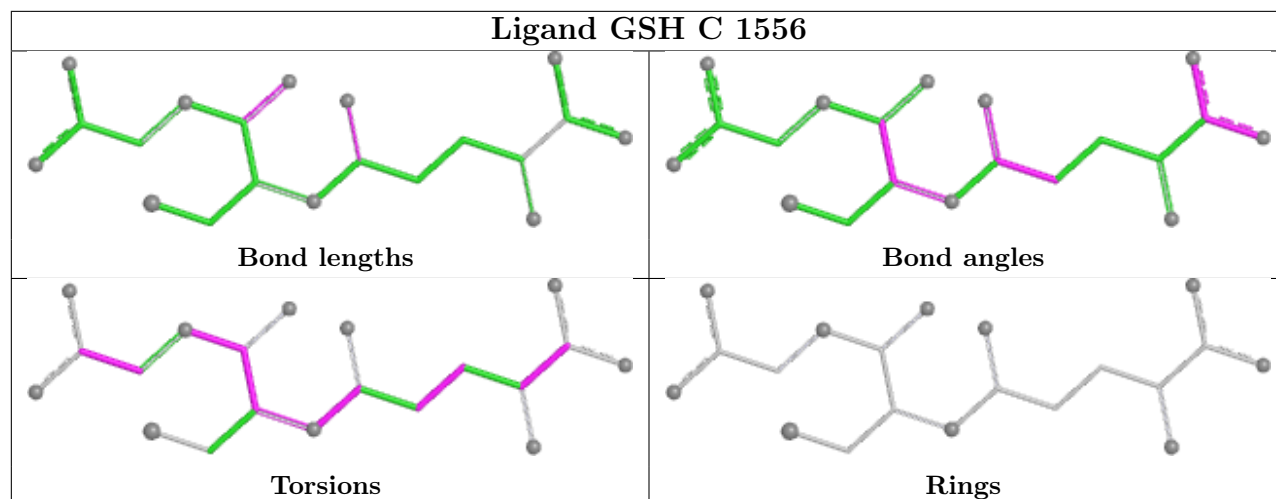
5 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1556	GSH	1	0
2	A	1556	GSH	3	0
2	C	1556	GSH	4	0
3	B	1557	SO4	1	0
3	A	1558	SO4	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





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	520/562 (92%)	0.08	22 (4%) 40 23	3, 27, 37, 47	2 (0%)
1	B	488/562 (86%)	0.25	8 (1%) 70 50	13, 27, 37, 46	0
1	C	496/562 (88%)	0.22	27 (5%) 31 18	6, 24, 33, 46	1 (0%)
1	D	492/562 (87%)	0.02	18 (3%) 45 26	14, 24, 38, 67	0
All	All	1996/2248 (88%)	0.14	75 (3%) 44 26	3, 25, 36, 67	3 (0%)

All (75) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	484	GLY	4.3
1	D	523	THR	4.3
1	C	218	TRP	4.3
1	D	417	ASP	4.2
1	A	481	LEU	4.1
1	C	211	ILE	4.1
1	A	410	ALA	4.0
1	D	511	SER	3.9
1	C	410	ALA	3.9
1	D	521	PHE	3.9
1	D	501	GLY	3.8
1	C	215	VAL	3.8
1	C	213	ASP	3.4
1	A	488	GLN	3.4
1	B	185	GLU	3.4
1	A	545	VAL	3.3
1	D	502	VAL	3.2
1	A	474	HIS	3.1
1	A	490	GLU	3.1
1	A	478	GLY	3.1
1	D	522	ASN	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	479	SER	3.0
1	B	106	SER	3.0
1	B	423	ASP	3.0
1	C	515	ASN	3.0
1	B	523	THR	2.9
1	C	217	ALA	2.8
1	A	486	VAL	2.7
1	D	526	GLY	2.7
1	C	248	GLY	2.6
1	B	112	GLN	2.6
1	C	186	ASN	2.6
1	C	37[A]	ARG	2.6
1	A	480	LEU	2.6
1	C	180	ASP	2.6
1	A	487	VAL	2.6
1	C	207	VAL	2.6
1	D	509	GLY	2.5
1	A	418	VAL	2.5
1	C	405	GLU	2.5
1	C	203	SER	2.4
1	C	208	PRO	2.4
1	D	416	HIS	2.4
1	C	206	VAL	2.4
1	A	438	LEU	2.4
1	D	504	LEU	2.3
1	A	485	ASP	2.3
1	C	173	GLN	2.3
1	C	210	ALA	2.3
1	D	503	ILE	2.3
1	D	520	LEU	2.2
1	C	305	GLU	2.2
1	A	475	VAL	2.2
1	A	477	THR	2.1
1	A	476	SER	2.1
1	C	214	ALA	2.1
1	A	104	TYR	2.1
1	C	480	LEU	2.1
1	C	484	GLY	2.1
1	A	442	THR	2.1
1	B	359	LEU	2.1
1	D	516	GLY	2.1
1	A	456	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	127	VAL	2.1
1	D	127	VAL	2.1
1	B	146	THR	2.1
1	C	219	VAL	2.1
1	D	519	VAL	2.0
1	B	522	ASN	2.0
1	C	236	GLN	2.0
1	C	220	GLU	2.0
1	D	512	VAL	2.0
1	A	427	LEU	2.0
1	C	401	LEU	2.0
1	D	401	LEU	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](#)

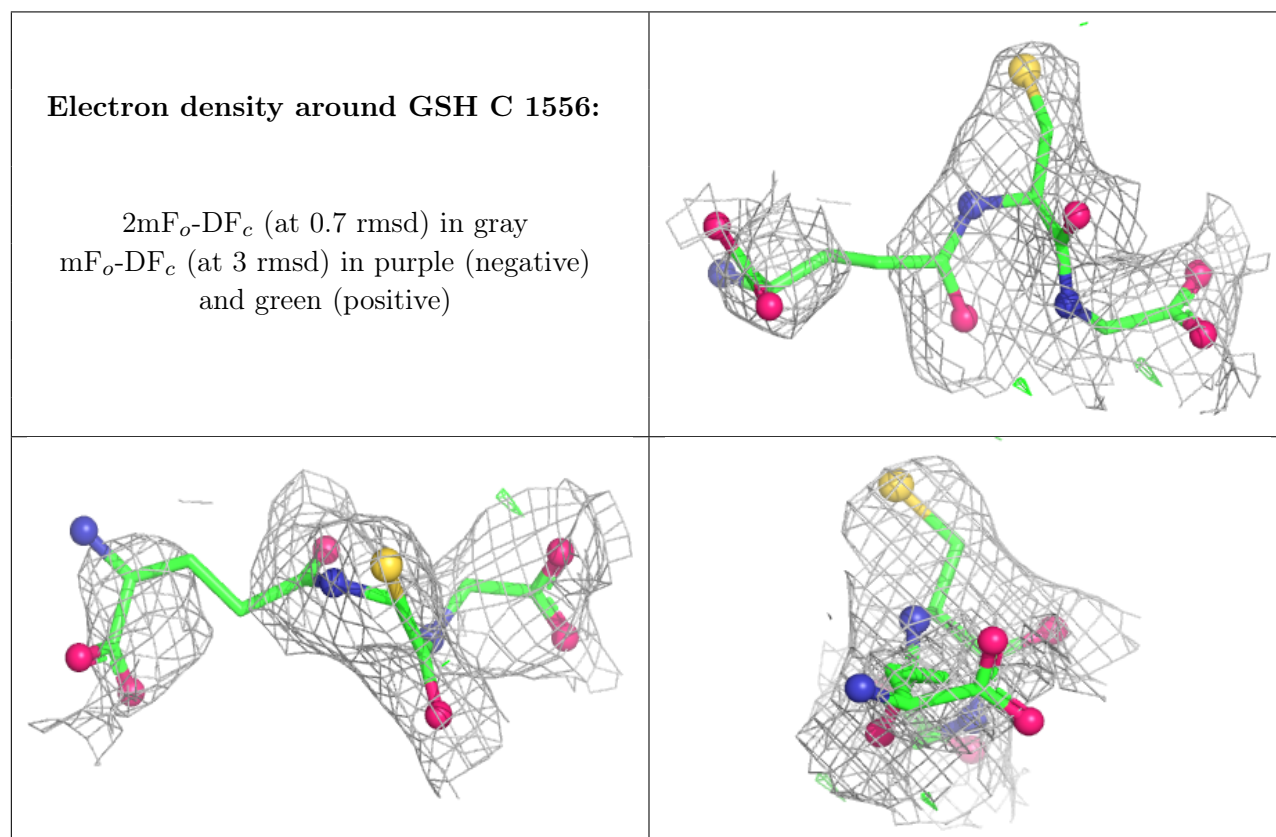
There are no oligosaccharides in this entry.

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.

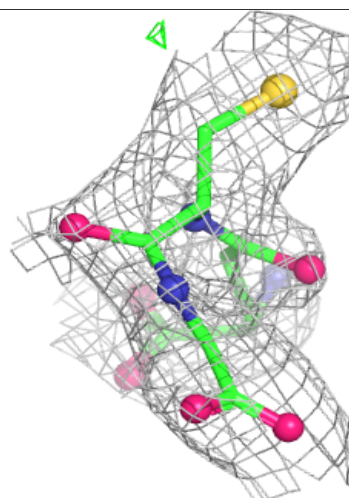
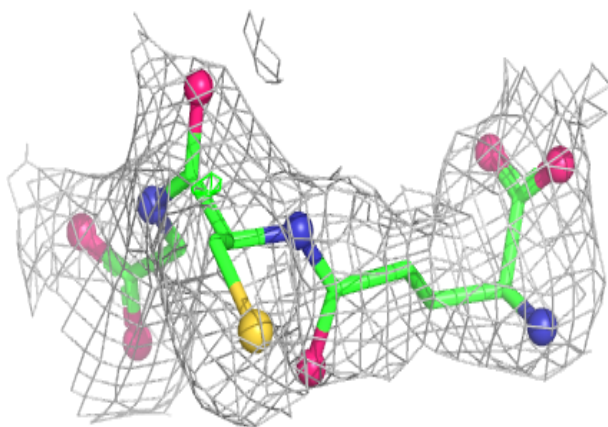
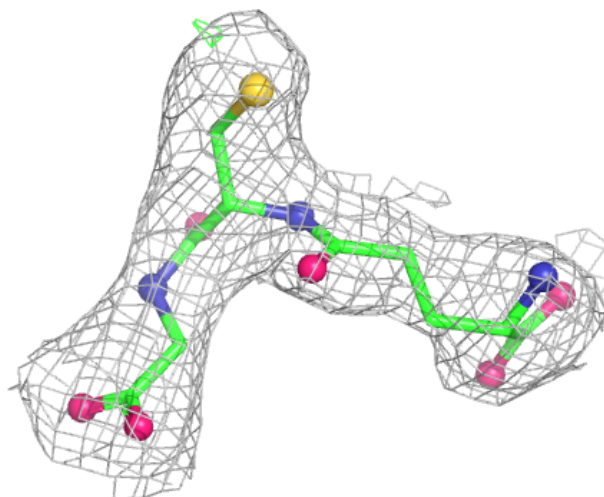
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	SO4	D	1557	5/5	0.72	0.29	117,117,117,118	0
2	GSH	C	1556	20/20	0.76	0.17	89,93,94,94	0
3	SO4	B	1557	5/5	0.85	0.15	86,87,87,88	0
2	GSH	B	1556	20/20	0.86	0.10	56,59,61,62	0
3	SO4	C	1559	5/5	0.86	0.24	99,99,99,99	0
3	SO4	A	1557	5/5	0.86	0.12	78,79,79,79	0
3	SO4	A	1558	5/5	0.89	0.10	93,93,94,94	0
2	GSH	A	1556	20/20	0.89	0.11	63,73,79,80	0
3	SO4	C	1557	5/5	0.91	0.11	62,64,64,64	0
2	GSH	D	1556	20/20	0.93	0.10	46,48,52,54	0
3	SO4	C	1558	5/5	0.97	0.05	48,49,50,50	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



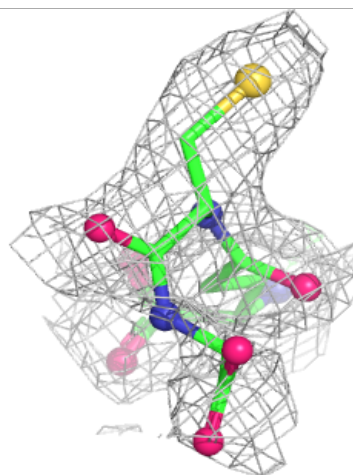
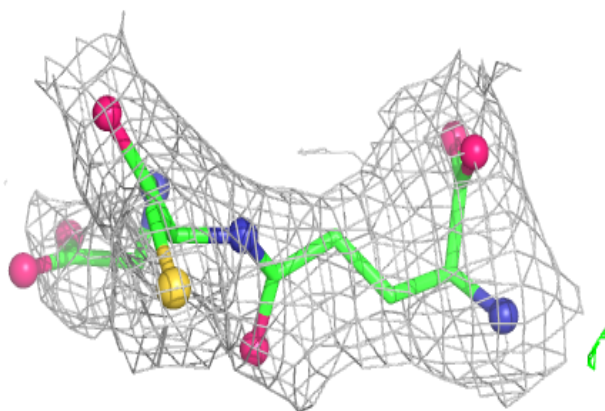
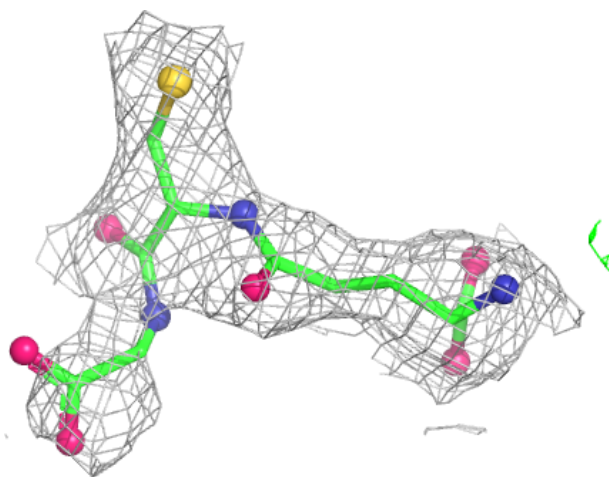
Electron density around GSH B 1556:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



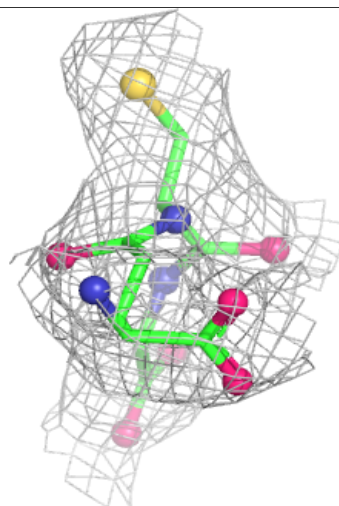
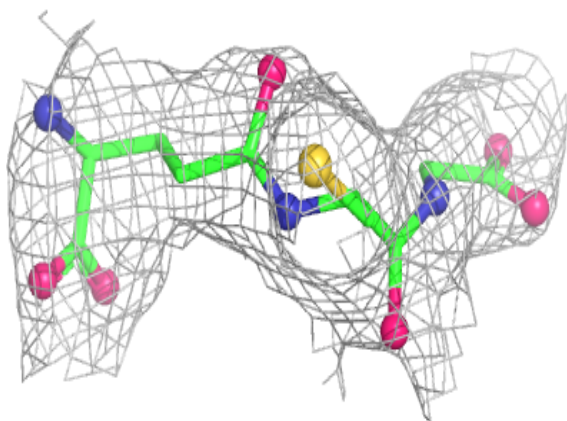
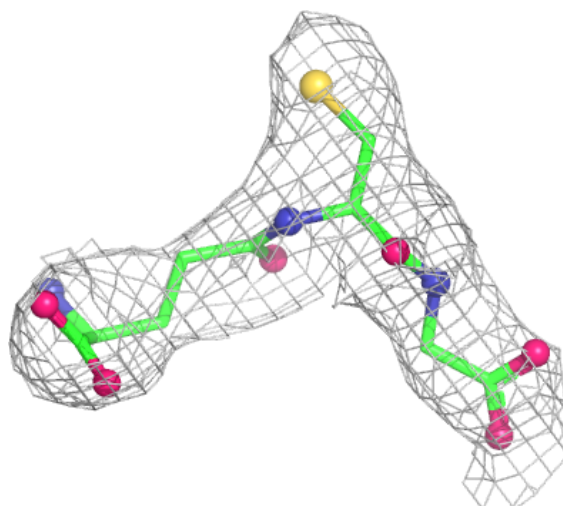
Electron density around GSH A 1556:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around GSH D 1556:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.