Full wwPDB X-ray Structure Validation Report (i)

Aug 20, 2023 – 09:01 AM EDT

PDB ID	:	2ON5
Title	:	Structure of NaGST-2
Authors	:	Asojo, O.A.; Ngamelue, M.; Homma, H.; Goud, G.; Zhan, B.; Hotez, P.J.
Deposited on	:	2007-01-23
Resolution	:	1.90 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 (i) 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 (i)) were used in the production of this report:

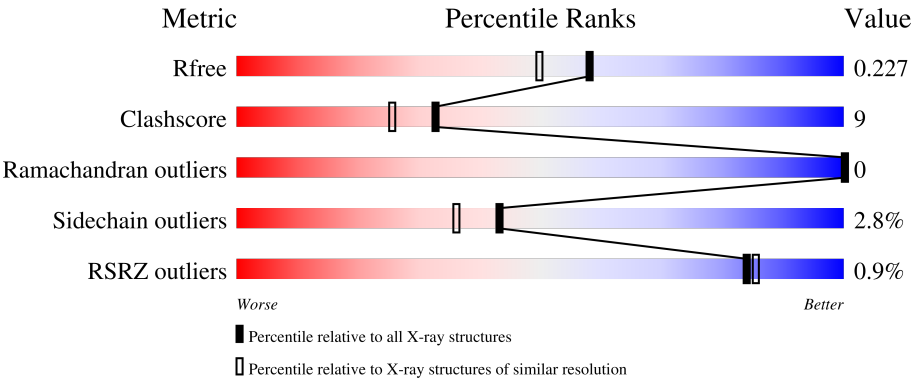
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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 <=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	206	90% 10%
1	B	206	88% 11%
1	C	206	85% 14%
1	D	206	3% 84% 15%
1	E	206	3% 78% 20%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	206	86% 12%
1	G	206	85% 13%
1	H	206	84% 15%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	EDO	A	426	-	-	X	-
2	EDO	B	426	-	-	X	-
2	EDO	D	428	-	-	X	-
2	EDO	E	454	-	-	X	-
2	EDO	F	418	-	-	X	-
2	EDO	F	450	-	-	X	-
2	EDO	H	450	-	-	X	-
2	EDO	H	451	-	-	X	-
3	GSH	A	999	X	-	-	-
3	GSH	B	999	X	-	-	-
3	GSH	C	999	X	-	-	-
3	GSH	D	999	X	-	-	-
3	GSH	E	999	X	-	-	-
3	GSH	F	999	X	-	-	-
3	GSH	G	999	X	-	-	-
3	GSH	H	999	X	-	-	-

2 Entry composition (i)

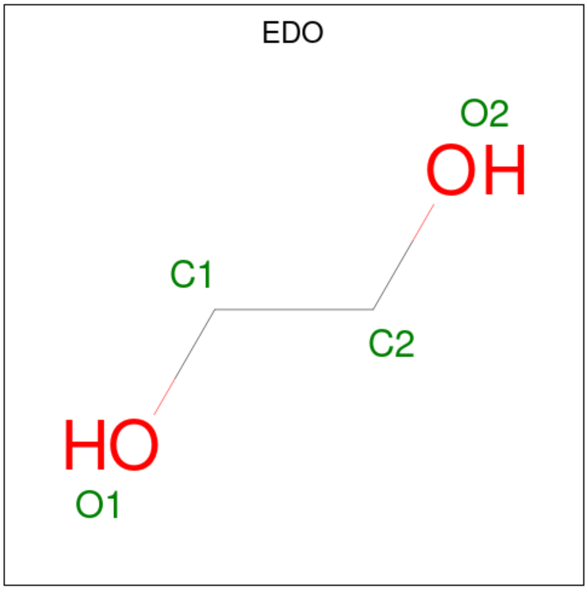
There are 4 unique types of molecules in this entry. The entry contains 15635 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Na Glutathione S-transferase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	206	Total	C	N	O	S	0	0	0
			1675	1094	276	301	4			
1	B	206	Total	C	N	O	S	0	0	0
			1675	1094	276	301	4			
1	C	206	Total	C	N	O	S	0	0	0
			1675	1094	276	301	4			
1	D	206	Total	C	N	O	S	0	0	0
			1675	1094	276	301	4			
1	E	206	Total	C	N	O	S	0	0	0
			1675	1094	276	301	4			
1	F	206	Total	C	N	O	S	0	0	0
			1675	1094	276	301	4			
1	G	206	Total	C	N	O	S	0	0	0
			1675	1094	276	301	4			
1	H	206	Total	C	N	O	S	0	0	0
			1675	1094	276	301	4			

- Molecule 2 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 4 2 2	0	0
2	A	1	Total C O 4 2 2	0	0
2	A	1	Total C O 4 2 2	0	0
2	A	1	Total C O 4 2 2	0	0
2	A	1	Total C O 4 2 2	0	0
2	A	1	Total C O 4 2 2	0	0
2	A	1	Total C O 4 2 2	0	0
2	A	1	Total C O 4 2 2	0	0
2	A	1	Total C O 4 2 2	0	0
2	A	1	Total C O 4 2 2	0	0
2	A	1	Total C O 4 2 2	0	0
2	A	1	Total C O 4 2 2	0	0
2	A	1	Total C O 4 2 2	0	0
2	B	1	Total C O 4 2 2	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total C O 4 2 2	0	0
2	B	1	Total C O 4 2 2	0	0
2	B	1	Total C O 4 2 2	0	0
2	B	1	Total C O 4 2 2	0	0
2	B	1	Total C O 4 2 2	0	0
2	B	1	Total C O 4 2 2	0	0
2	B	1	Total C O 4 2 2	0	0
2	B	1	Total C O 4 2 2	0	0
2	B	1	Total C O 4 2 2	0	0
2	B	1	Total C O 4 2 2	0	0
2	B	1	Total C O 4 2 2	0	0
2	B	1	Total C O 4 2 2	0	0
2	B	1	Total C O 4 2 2	0	0
2	C	1	Total C O 4 2 2	0	0
2	C	1	Total C O 4 2 2	0	0
2	C	1	Total C O 4 2 2	0	0
2	C	1	Total C O 4 2 2	0	0
2	C	1	Total C O 4 2 2	0	0
2	D	1	Total C O 4 2 2	0	0
2	D	1	Total C O 4 2 2	0	0
2	D	1	Total C O 4 2 2	0	0

Continued on next page...

Continued from previous page...

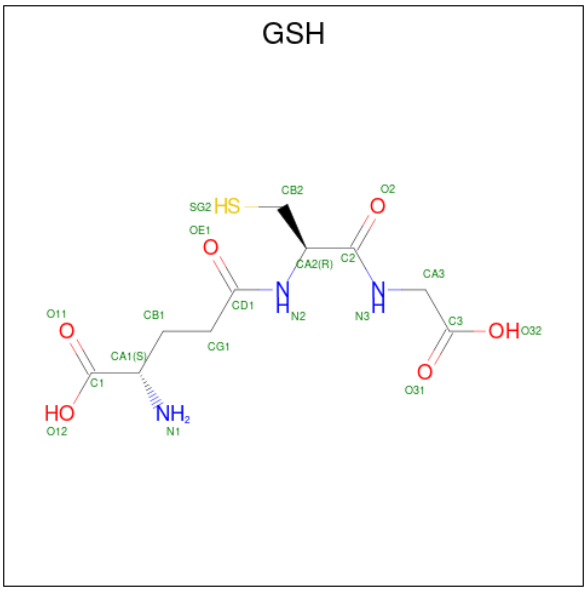
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	D	1	Total C O 4 2 2	0	0
2	D	1	Total C O 4 2 2	0	0
2	D	1	Total C O 4 2 2	0	0
2	D	1	Total C O 4 2 2	0	0
2	D	1	Total C O 4 2 2	0	0
2	D	1	Total C O 4 2 2	0	0
2	E	1	Total C O 4 2 2	0	0
2	E	1	Total C O 4 2 2	0	0
2	E	1	Total C O 4 2 2	0	0
2	E	1	Total C O 4 2 2	0	0
2	E	1	Total C O 4 2 2	0	0
2	E	1	Total C O 4 2 2	0	0
2	E	1	Total C O 4 2 2	0	0
2	E	1	Total C O 4 2 2	0	0
2	F	1	Total C O 4 2 2	0	0
2	F	1	Total C O 4 2 2	0	0
2	F	1	Total C O 4 2 2	0	0
2	F	1	Total C O 4 2 2	0	0
2	F	1	Total C O 4 2 2	0	0
2	F	1	Total C O 4 2 2	0	0
2	F	1	Total C O 4 2 2	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	F	1	Total C O 4 2 2	0	0
2	F	1	Total C O 4 2 2	0	0
2	F	1	Total C O 4 2 2	0	0
2	F	1	Total C O 4 2 2	0	0
2	G	1	Total C O 4 2 2	0	0
2	G	1	Total C O 4 2 2	0	0
2	G	1	Total C O 4 2 2	0	0
2	G	1	Total C O 4 2 2	0	0
2	G	1	Total C O 4 2 2	0	0
2	G	1	Total C O 4 2 2	0	0
2	G	1	Total C O 4 2 2	0	0
2	H	1	Total C O 4 2 2	0	0
2	H	1	Total C O 4 2 2	0	0
2	H	1	Total C O 4 2 2	0	0
2	H	1	Total C O 4 2 2	0	0
2	H	1	Total C O 4 2 2	0	0
2	H	1	Total C O 4 2 2	0	0
2	H	1	Total C O 4 2 2	0	0
2	H	1	Total C O 4 2 2	0	0
2	H	1	Total C O 4 2 2	0	0

- Molecule 3 is GLUTATHIONE (three-letter code: GSH) (formula: $C_{10}H_{17}N_3O_6S$).



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	238	Total	O	0	0
			238	238		
4	B	255	Total	O	0	0
			255	255		
4	C	242	Total	O	0	0
			242	242		
4	D	194	Total	O	0	0
			194	194		

Continued on next page...

Continued from previous page...

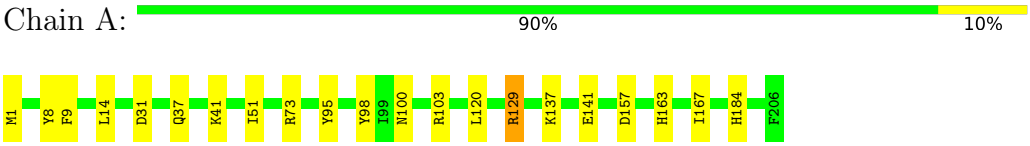
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	E	192	Total O 192 192	0	0
4	F	208	Total O 208 208	0	0
4	G	242	Total O 242 242	0	0
4	H	200	Total O 200 200	0	0

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.

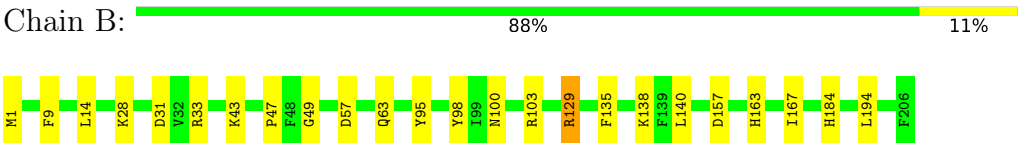
• Molecule 1: Na Glutathione S-transferase 2

Chain A:



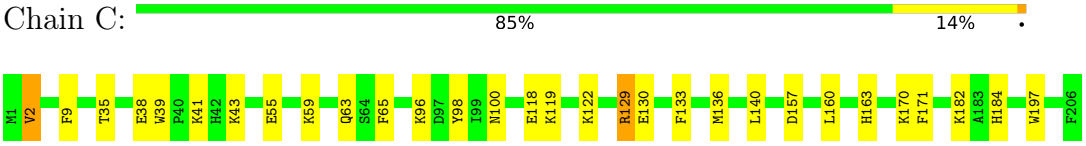
• Molecule 1: Na Glutathione S-transferase 2

Chain B:



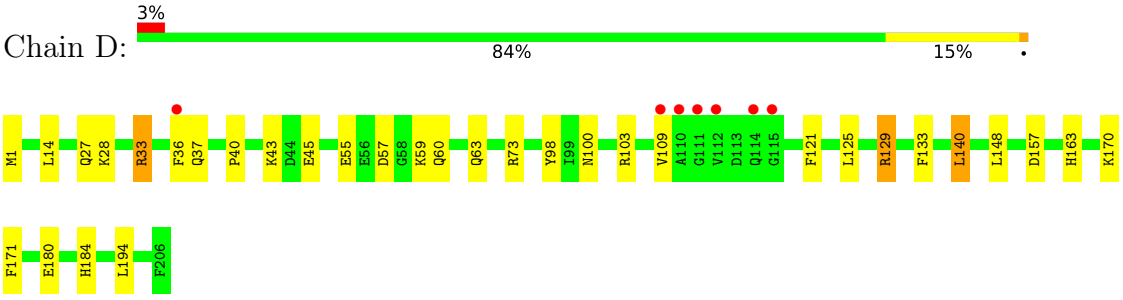
• Molecule 1: Na Glutathione S-transferase 2

Chain C:



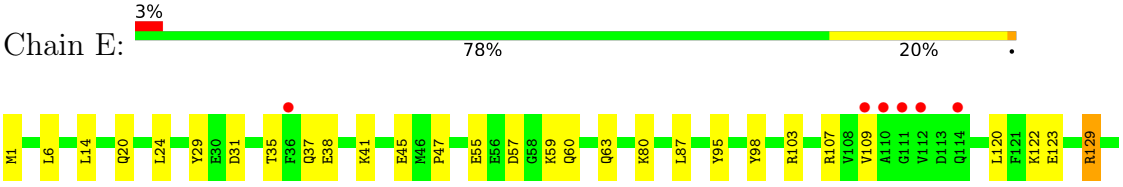
• Molecule 1: Na Glutathione S-transferase 2

Chain D:



• Molecule 1: Na Glutathione S-transferase 2

Chain E:



• Molecule 1: Na Glutathione S-transferase 2

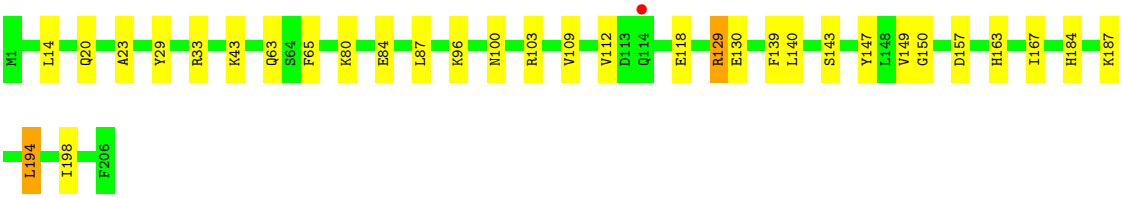
Chain F:

• Molecule 1: Na Glutathione S-transferase 2

Chain G:

• Molecule 1: Na Glutathione S-transferase 2

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	57.92Å 107.92Å 166.99Å 90.00° 90.02° 90.00°	Depositor
Resolution (Å)	25.00 – 1.90 33.04 – 1.82	Depositor EDS
% Data completeness (in resolution range)	88.1 (25.00-1.90) 83.7 (33.04-1.82)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	1.28 (at 1.82Å)	Xtriage
Refinement program	REFMAC 5.2	Depositor
R, R_{free}	0.178 , 0.227 0.180 , 0.227	Depositor DCC
R_{free} test set	7746 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	24.2	Xtriage
Anisotropy	0.163	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 27.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.468 for h,-k,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	15635	wwPDB-VP
Average B, all atoms (Å^2)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.56% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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, EDO

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	0.70	0/1721	0.63	0/2317
1	B	0.72	0/1721	0.72	2/2317 (0.1%)
1	C	0.71	0/1721	0.66	0/2317
1	D	0.69	0/1721	0.70	2/2317 (0.1%)
1	E	0.70	0/1721	0.73	0/2317
1	F	0.67	0/1721	0.72	2/2317 (0.1%)
1	G	0.68	0/1721	0.73	3/2317 (0.1%)
1	H	0.66	0/1721	0.66	0/2317
All	All	0.69	0/13768	0.69	9/18536 (0.0%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	33	ARG	NE-CZ-NH1	10.01	125.30	120.30
1	B	33	ARG	NE-CZ-NH2	-9.36	115.62	120.30
1	G	153	VAL	CB-CA-C	-7.65	96.87	111.40
1	D	33	ARG	NE-CZ-NH2	-6.83	116.88	120.30
1	D	33	ARG	NE-CZ-NH1	6.45	123.52	120.30
1	G	153	VAL	CG1-CB-CG2	6.26	120.92	110.90
1	F	153	VAL	CB-CA-C	-5.99	100.02	111.40
1	F	2	VAL	CB-CA-C	-5.69	100.59	111.40
1	G	2	VAL	CB-CA-C	-5.30	101.32	111.40

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1675	0	1672	22	0
1	B	1675	0	1672	28	0
1	C	1675	0	1672	22	0
1	D	1675	0	1672	36	0
1	E	1675	0	1672	36	0
1	F	1675	0	1672	33	0
1	G	1675	0	1672	24	0
1	H	1675	0	1672	36	0
2	A	52	0	78	10	0
2	B	56	0	84	10	0
2	C	20	0	30	2	0
2	D	36	0	54	12	0
2	E	32	0	48	13	0
2	F	44	0	66	14	0
2	G	28	0	42	6	0
2	H	36	0	54	23	0
3	A	20	0	15	2	0
3	B	20	0	15	3	0
3	C	20	0	15	3	0
3	D	20	0	15	2	0
3	E	20	0	15	1	0
3	F	20	0	15	0	0
3	G	20	0	15	2	0
3	H	20	0	15	2	0
4	A	238	0	0	3	0
4	B	255	0	0	5	0
4	C	242	0	0	3	0
4	D	194	0	0	6	0
4	E	192	0	0	7	0
4	F	208	0	0	4	0
4	G	242	0	0	6	0
4	H	200	0	0	5	0
All	All	15635	0	13952	242	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 9.

All (242) 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:D:59:LYS:HE2	4:D:1064:HOH:O	1.10	1.27
1:H:149:VAL:HA	2:H:450:EDO:H22	1.05	1.05
2:G:426:EDO:H21	4:G:1023:HOH:O	1.59	1.03
1:F:150:GLY:H	2:F:450:EDO:H22	1.27	1.00
1:B:100:ASN:HD22	1:B:103:ARG:HH12	1.02	0.98
1:F:150:GLY:H	2:F:450:EDO:C2	1.77	0.98
1:H:149:VAL:HA	2:H:450:EDO:C2	1.94	0.95
1:C:63:GLN:HE22	3:C:999:GSH:HN11	1.14	0.92
1:D:14:LEU:HA	2:D:426:EDO:H22	1.52	0.90
1:B:100:ASN:HD22	1:B:103:ARG:NH1	1.70	0.90
1:C:2:VAL:HG22	1:F:2:VAL:HG13	1.50	0.90
1:F:150:GLY:N	2:F:450:EDO:H22	1.87	0.89
1:H:150:GLY:H	2:H:450:EDO:H11	1.35	0.88
1:A:14:LEU:HD23	2:A:426:EDO:H11	1.53	0.88
1:F:129:ARG:HH22	2:F:418:EDO:H11	1.37	0.87
2:H:426:EDO:H22	4:H:1020:HOH:O	1.74	0.86
1:F:129:ARG:NH2	2:F:418:EDO:H11	1.91	0.84
1:D:100:ASN:HD22	1:D:103:ARG:HH12	1.26	0.83
1:H:149:VAL:CA	2:H:450:EDO:H22	2.01	0.82
1:C:119:LYS:HA	1:C:122:LYS:HE3	1.63	0.81
1:B:100:ASN:ND2	1:B:103:ARG:HH12	1.80	0.80
1:B:63:GLN:HE22	3:B:999:GSH:HN11	1.31	0.79
1:B:100:ASN:ND2	1:B:103:ARG:NH1	2.31	0.78
1:A:137:LYS:O	1:A:141:GLU:HG3	1.84	0.77
1:A:95:TYR:HE2	2:A:426:EDO:H21	1.48	0.77
1:H:63:GLN:HE22	3:H:999:GSH:HN11	1.34	0.76
1:G:38:GLU:CD	4:G:1103:HOH:O	2.22	0.76
2:H:450:EDO:H21	2:H:451:EDO:O1	1.86	0.75
1:B:95:TYR:HE2	2:B:426:EDO:H21	1.50	0.75
2:F:422:EDO:H12	4:F:1082:HOH:O	1.85	0.75
1:E:63:GLN:HE22	3:E:999:GSH:HN11	1.33	0.75
2:H:422:EDO:H11	4:H:1131:HOH:O	1.87	0.74
1:E:20:GLN:HB3	1:E:194:LEU:HD21	1.69	0.74
1:E:24:LEU:HG	1:E:194:LEU:HD23	1.70	0.74
2:G:450:EDO:O1	4:G:1100:HOH:O	2.06	0.73
1:C:59:LYS:HD2	4:C:1199:HOH:O	1.86	0.73
1:A:37:GLN:HE22	1:D:33:ARG:H	1.34	0.73
1:A:41:LYS:NZ	2:D:427:EDO:H11	2.03	0.73
1:F:129:ARG:HH22	2:F:418:EDO:C1	2.01	0.72
1:D:63:GLN:HE22	3:D:999:GSH:HN11	1.38	0.70
1:H:14:LEU:HD23	2:H:426:EDO:H12	1.74	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:129:ARG:HH12	2:B:419:EDO:H12	1.56	0.70
1:B:9:PHE:HE2	3:B:999:GSH:HB22	1.56	0.69
1:C:2:VAL:HG23	1:F:57:ASP:OD1	1.91	0.69
1:G:63:GLN:HE22	3:G:999:GSH:HN11	1.39	0.69
1:D:100:ASN:ND2	1:D:103:ARG:HH12	1.89	0.69
1:B:14:LEU:HD23	2:B:426:EDO:H11	1.74	0.68
1:E:95:TYR:OH	2:E:426:EDO:H11	1.94	0.68
1:F:150:GLY:N	2:F:450:EDO:C2	2.51	0.68
1:F:87:LEU:HD13	2:F:451:EDO:H11	1.77	0.67
1:A:41:LYS:HZ2	2:D:427:EDO:H11	1.60	0.66
1:D:100:ASN:HD22	1:D:103:ARG:NH1	1.95	0.65
1:H:87:LEU:HD13	2:H:451:EDO:H11	1.78	0.65
2:A:425:EDO:O1	2:A:426:EDO:H22	1.97	0.65
2:E:428:EDO:H22	4:E:1087:HOH:O	1.97	0.65
1:G:38:GLU:OE1	4:G:1103:HOH:O	2.15	0.64
1:H:100:ASN:ND2	1:H:103:ARG:HH12	1.96	0.63
1:E:142:LYS:HE2	2:E:450:EDO:H21	1.80	0.62
2:H:450:EDO:C2	2:H:451:EDO:O1	2.48	0.62
1:A:100:ASN:OD1	1:A:103:ARG:NH2	2.32	0.62
2:D:425:EDO:H12	2:D:426:EDO:O2	2.00	0.62
1:B:157:ASP:OD2	1:B:184:HIS:HE1	1.82	0.62
1:F:65:PHE:CD1	1:F:96:LYS:HE3	2.35	0.62
1:E:157:ASP:OD2	1:E:184:HIS:HE1	1.81	0.61
1:D:100:ASN:HA	1:D:103:ARG:HH12	1.64	0.61
1:A:14:LEU:HD23	2:A:426:EDO:C1	2.29	0.60
1:D:28:LYS:H	2:D:428:EDO:C2	2.15	0.59
1:A:157:ASP:OD2	1:A:184:HIS:HE1	1.85	0.59
1:C:157:ASP:OD2	1:C:184:HIS:HE1	1.86	0.59
1:H:139:PHE:CE2	2:H:451:EDO:H12	2.37	0.59
1:C:136:MET:HE3	1:C:160:LEU:HD22	1.84	0.59
1:E:196:LYS:O	1:E:196:LYS:HD3	2.03	0.59
1:E:31:ASP:HB2	2:E:427:EDO:H12	1.84	0.59
1:G:9:PHE:HE2	3:G:999:GSH:HB22	1.67	0.59
1:H:29:TYR:HE2	2:H:429:EDO:H12	1.67	0.59
1:D:140:LEU:HD13	1:D:148:LEU:HD23	1.85	0.58
1:E:47:PRO:HA	2:E:454:EDO:H11	1.85	0.58
1:B:43:LYS:NZ	4:B:1139:HOH:O	2.34	0.58
1:G:80:LYS:HE3	4:G:1196:HOH:O	2.03	0.57
1:D:157:ASP:OD2	1:D:184:HIS:HE1	1.87	0.57
1:D:170:LYS:HD3	1:D:171:PHE:CE1	2.40	0.57
1:F:65:PHE:CE1	1:F:96:LYS:HE3	2.39	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:100:ASN:HD22	1:H:103:ARG:NH1	2.01	0.57
1:A:1:MET:HB3	4:A:1121:HOH:O	2.04	0.56
1:B:163:HIS:HD2	4:B:1105:HOH:O	1.86	0.56
1:D:27:GLN:HA	2:D:428:EDO:H21	1.85	0.56
1:G:65:PHE:CE1	1:G:96:LYS:HE3	2.40	0.56
1:E:87:LEU:HD11	2:E:450:EDO:H22	1.87	0.55
1:E:153:VAL:HG23	4:E:1024:HOH:O	2.06	0.55
2:D:426:EDO:H11	4:D:1086:HOH:O	2.07	0.55
1:C:170:LYS:HD3	1:C:171:PHE:CE1	2.41	0.55
1:F:194:LEU:HD22	1:F:198:ILE:HD11	1.89	0.55
2:B:425:EDO:O1	2:B:426:EDO:H22	2.07	0.55
1:H:65:PHE:CE1	1:H:96:LYS:HE3	2.41	0.55
1:H:100:ASN:ND2	1:H:103:ARG:NH1	2.55	0.55
1:F:139:PHE:CE2	2:F:451:EDO:H12	2.42	0.54
1:F:150:GLY:CA	2:F:450:EDO:H22	2.38	0.54
1:A:95:TYR:CE2	2:A:426:EDO:H21	2.38	0.54
1:F:163:HIS:HD2	4:F:1151:HOH:O	1.90	0.54
1:A:31:ASP:HB2	2:A:427:EDO:H12	1.89	0.53
1:C:65:PHE:CE1	1:C:96:LYS:HE3	2.44	0.53
1:A:167:ILE:HA	2:A:422:EDO:H11	1.91	0.53
1:E:103:ARG:NH1	1:E:107:ARG:HD3	2.24	0.53
1:H:100:ASN:HD22	1:H:103:ARG:HH12	1.55	0.53
1:E:163:HIS:HD2	4:E:1128:HOH:O	1.92	0.53
1:D:60:GLN:NE2	2:D:453:EDO:O2	2.41	0.53
1:E:188:VAL:O	1:E:191:ILE:HG12	2.09	0.53
1:F:176:ASP:HB2	2:F:418:EDO:H12	1.91	0.52
1:B:95:TYR:CE2	2:B:426:EDO:H21	2.39	0.52
1:D:73:ARG:HD3	1:F:73:ARG:HH22	1.75	0.52
1:G:14:LEU:HD23	2:G:426:EDO:H11	1.91	0.52
1:G:205:LYS:H	2:G:420:EDO:C1	2.23	0.52
1:C:163:HIS:HD2	4:C:1049:HOH:O	1.92	0.52
1:D:28:LYS:H	2:D:428:EDO:H22	1.75	0.52
1:D:73:ARG:HD3	1:F:73:ARG:NH2	2.24	0.52
1:B:100:ASN:HD21	1:C:100:ASN:HD21	1.58	0.52
1:D:100:ASN:HA	1:D:103:ARG:NH1	2.25	0.51
1:D:100:ASN:ND2	1:D:103:ARG:NH1	2.56	0.51
1:G:37:GLN:H	1:G:37:GLN:HE21	1.56	0.51
1:C:35:THR:OG1	1:C:38:GLU:HG3	2.09	0.51
1:H:143:SER:HA	2:H:450:EDO:H12	1.92	0.51
1:E:45:GLU:C	2:E:454:EDO:H22	2.31	0.51
1:G:106:LEU:HD22	2:G:422:EDO:H11	1.92	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:194:LEU:HD22	1:H:198:ILE:HD11	1.92	0.51
1:H:112:VAL:O	2:H:423:EDO:H21	2.11	0.51
1:D:163:HIS:HD2	4:D:1117:HOH:O	1.93	0.51
1:B:167:ILE:HA	2:B:422:EDO:H11	1.93	0.50
1:F:135:PHE:O	1:F:138:LYS:HB2	2.12	0.50
2:D:427:EDO:H12	4:D:1070:HOH:O	2.12	0.49
1:H:29:TYR:CE2	2:H:429:EDO:H12	2.46	0.49
1:D:28:LYS:H	2:D:428:EDO:H21	1.77	0.49
1:G:103:ARG:HD2	4:G:1206:HOH:O	2.13	0.49
1:B:95:TYR:HH	2:B:426:EDO:HO1	1.55	0.49
1:G:65:PHE:CD1	1:G:96:LYS:HE3	2.48	0.49
1:E:147:TYR:CE2	1:E:153:VAL:HG22	2.47	0.49
1:C:136:MET:CE	1:C:160:LEU:HD22	2.42	0.49
1:C:118:GLU:O	1:C:122:LYS:HG2	2.12	0.49
1:E:135:PHE:O	1:E:138:LYS:HB2	2.13	0.49
1:A:129:ARG:HH12	2:A:419:EDO:H12	1.78	0.48
1:E:31:ASP:HB2	2:E:427:EDO:C1	2.43	0.48
1:G:37:GLN:H	1:G:37:GLN:NE2	2.11	0.48
1:D:43:LYS:HE2	3:D:999:GSH:O31	2.13	0.48
1:D:109:VAL:HG23	4:D:1133:HOH:O	2.13	0.48
1:G:182:LYS:HE2	1:G:186:GLU:OE1	2.14	0.48
1:C:197:TRP:HZ3	2:C:427:EDO:H21	1.79	0.48
1:F:194:LEU:HD22	1:F:198:ILE:CD1	2.43	0.48
1:F:116:ASP:O	1:F:120:LEU:HD13	2.14	0.47
1:B:57:ASP:CB	1:D:1:MET:HG2	2.44	0.47
1:A:98:TYR:HE2	1:A:163:HIS:CE1	2.32	0.47
1:D:129:ARG:HD3	1:D:133:PHE:CD2	2.50	0.47
1:A:51:ILE:O	3:A:999:GSH:HB23	2.15	0.47
1:B:1:MET:HA	1:D:57:ASP:OD2	2.13	0.47
1:D:37:GLN:O	1:D:40:PRO:HD2	2.13	0.47
1:D:170:LYS:HD3	1:D:171:PHE:HE1	1.80	0.47
1:E:35:THR:OG1	1:E:38:GLU:HG2	2.15	0.47
1:D:73:ARG:HH11	1:F:73:ARG:CZ	2.28	0.47
2:D:454:EDO:C2	1:F:138:LYS:HZ3	2.28	0.46
1:H:43:LYS:HE2	3:H:999:GSH:O31	2.15	0.46
1:F:157:ASP:OD2	1:F:184:HIS:HE1	1.98	0.46
1:G:157:ASP:OD2	1:G:184:HIS:HE1	1.99	0.46
1:E:122:LYS:HG3	1:E:123:GLU:HG3	1.98	0.46
1:A:98:TYR:OH	1:A:163:HIS:HE1	2.00	0.46
2:A:423:EDO:H22	3:A:999:GSH:HA32	1.97	0.46
1:B:31:ASP:HB2	2:B:427:EDO:H12	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:453:EDO:H12	2:C:452:EDO:O2	2.16	0.46
1:D:121:PHE:CE1	1:D:125:LEU:HD22	2.50	0.46
1:D:45:GLU:HG3	4:D:1106:HOH:O	2.16	0.45
1:H:33:ARG:NH2	4:H:1033:HOH:O	2.46	0.45
1:B:57:ASP:HB3	1:D:1:MET:HG2	1.98	0.45
1:E:29:TYR:CZ	2:E:427:EDO:H11	2.50	0.45
1:E:141:GLU:HG3	4:E:1120:HOH:O	2.17	0.45
1:H:109:VAL:HG21	2:H:422:EDO:O1	2.16	0.45
1:E:60:GLN:NE2	2:E:454:EDO:O1	2.47	0.45
1:H:157:ASP:OD2	1:H:184:HIS:HE1	2.00	0.45
1:H:184:HIS:HD2	4:H:1002:HOH:O	1.99	0.45
4:B:1135:HOH:O	1:F:80:LYS:HE3	2.16	0.45
1:D:98:TYR:OH	1:D:163:HIS:HE1	1.99	0.45
1:E:109:VAL:HG23	4:E:1110:HOH:O	2.17	0.45
1:G:98:TYR:OH	1:G:163:HIS:HE1	2.00	0.45
1:B:9:PHE:CE2	3:B:999:GSH:HB22	2.44	0.45
1:C:129:ARG:HD3	1:C:133:PHE:CD2	2.52	0.44
1:E:60:GLN:NE2	2:E:453:EDO:O2	2.46	0.44
1:A:129:ARG:HH12	2:A:419:EDO:C1	2.31	0.44
1:E:37:GLN:HG2	4:E:1123:HOH:O	2.17	0.44
1:A:1:MET:HA	1:E:57:ASP:OD2	2.16	0.44
1:C:39:TRP:CH2	1:C:43:LYS:HA	2.52	0.44
1:G:103:ARG:HB3	1:G:104:PRO:HD3	2.00	0.43
1:E:1:MET:HB3	1:E:1:MET:HE2	1.96	0.43
1:E:129:ARG:HD3	1:E:133:PHE:CD2	2.54	0.43
2:E:454:EDO:H12	2:H:452:EDO:O2	2.18	0.43
1:F:84:GLU:HG3	1:F:149:VAL:HG12	2.01	0.43
1:F:176:ASP:CB	2:F:418:EDO:H12	2.49	0.43
1:E:98:TYR:OH	1:E:163:HIS:HE1	2.00	0.43
1:G:98:TYR:HE2	1:G:163:HIS:CE1	2.35	0.43
1:F:120:LEU:HD11	4:F:1109:HOH:O	2.18	0.43
1:G:205:LYS:H	2:G:420:EDO:H12	1.84	0.43
1:C:63:GLN:NE2	3:C:999:GSH:HN11	1.98	0.43
1:E:129:ARG:HD2	1:E:129:ARG:C	2.38	0.43
1:B:129:ARG:HD2	1:B:129:ARG:C	2.39	0.42
1:H:139:PHE:HE2	2:H:451:EDO:H12	1.82	0.42
1:B:57:ASP:CG	1:D:1:MET:HG2	2.40	0.42
1:F:129:ARG:C	1:F:129:ARG:HD2	2.39	0.42
1:E:80:LYS:NZ	1:E:151:ASP:OD1	2.48	0.42
1:F:109:VAL:HG23	4:F:1083:HOH:O	2.18	0.42
1:G:170:LYS:HD3	1:G:171:PHE:CE1	2.55	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:8:TYR:CG	1:A:9:PHE:N	2.87	0.42
4:A:1208:HOH:O	1:H:80:LYS:HE3	2.18	0.42
1:F:84:GLU:O	1:F:88:VAL:HG23	2.20	0.42
1:C:9:PHE:HE2	3:C:999:GSH:HB22	1.85	0.42
1:A:98:TYR:CE2	1:A:163:HIS:CE1	3.07	0.42
1:B:47:PRO:HG3	2:B:453:EDO:H11	2.02	0.42
1:G:194:LEU:O	1:G:198:ILE:HG12	2.20	0.42
1:H:129:ARG:NH1	1:H:130:GLU:HG2	2.35	0.42
1:E:138:LYS:NZ	4:E:1125:HOH:O	2.53	0.42
1:G:55:GLU:HA	1:G:59:LYS:O	2.20	0.42
1:F:32:VAL:HG22	2:F:432:EDO:H11	2.00	0.41
1:H:23:ALA:HA	2:H:429:EDO:H11	2.02	0.41
1:H:87:LEU:HD13	2:H:451:EDO:C1	2.46	0.41
2:H:450:EDO:C2	2:H:451:EDO:HO1	2.31	0.41
1:C:182:LYS:NZ	4:C:1060:HOH:O	2.54	0.41
1:D:55:GLU:HA	1:D:59:LYS:O	2.20	0.41
1:G:121:PHE:CZ	1:G:171:PHE:HB3	2.55	0.41
1:B:43:LYS:HG3	1:B:49:GLY:O	2.20	0.41
1:H:150:GLY:H	2:H:450:EDO:C1	2.20	0.41
1:H:65:PHE:CD1	1:H:96:LYS:HE3	2.56	0.41
1:B:135:PHE:O	1:B:138:LYS:HB2	2.21	0.41
1:E:55:GLU:HA	1:E:59:LYS:O	2.20	0.41
1:H:20:GLN:NE2	1:H:194:LEU:HD21	2.36	0.41
1:H:167:ILE:HD13	2:H:422:EDO:H12	2.03	0.41
1:B:28:LYS:HE2	4:B:1130:HOH:O	2.21	0.41
4:B:1066:HOH:O	1:D:1:MET:HE2	2.21	0.41
1:C:98:TYR:OH	1:C:163:HIS:HE1	2.04	0.41
1:H:147:TYR:CZ	1:H:187:LYS:HE3	2.56	0.41
1:G:121:PHE:CE1	1:G:171:PHE:HB3	2.56	0.41
1:H:163:HIS:HD2	4:H:1156:HOH:O	2.03	0.41
1:A:163:HIS:HD2	4:A:1185:HOH:O	2.03	0.40
1:E:14:LEU:HA	2:E:426:EDO:H21	2.02	0.40
1:B:98:TYR:OH	1:B:163:HIS:HE1	2.04	0.40
1:E:194:LEU:HD12	1:E:198:ILE:HD11	2.03	0.40
1:C:55:GLU:HA	1:C:59:LYS:O	2.21	0.40
1:H:84:GLU:HG3	1:H:149:VAL:HG12	2.03	0.40
1:H:20:GLN:CD	1:H:194:LEU:HD21	2.42	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	204/206 (99%)	201 (98%)	3 (2%)	0	100	100
1	B	204/206 (99%)	202 (99%)	2 (1%)	0	100	100
1	C	204/206 (99%)	201 (98%)	3 (2%)	0	100	100
1	D	204/206 (99%)	201 (98%)	3 (2%)	0	100	100
1	E	204/206 (99%)	201 (98%)	3 (2%)	0	100	100
1	F	204/206 (99%)	201 (98%)	3 (2%)	0	100	100
1	G	204/206 (99%)	201 (98%)	3 (2%)	0	100	100
1	H	204/206 (99%)	202 (99%)	2 (1%)	0	100	100
All	All	1632/1648 (99%)	1610 (99%)	22 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	173/173 (100%)	170 (98%)	3 (2%)	60	57
1	B	173/173 (100%)	170 (98%)	3 (2%)	60	57
1	C	173/173 (100%)	168 (97%)	5 (3%)	42	35
1	D	173/173 (100%)	168 (97%)	5 (3%)	42	35
1	E	173/173 (100%)	167 (96%)	6 (4%)	36	27
1	F	173/173 (100%)	166 (96%)	7 (4%)	31	22

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	G	173/173 (100%)	167 (96%)	6 (4%)	36 27
1	H	173/173 (100%)	169 (98%)	4 (2%)	50 45
All	All	1384/1384 (100%)	1345 (97%)	39 (3%)	43 36

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	73	ARG
1	A	120	LEU
1	A	129	ARG
1	B	129	ARG
1	B	140	LEU
1	B	194	LEU
1	C	2	VAL
1	C	41	LYS
1	C	129	ARG
1	C	130	GLU
1	C	140	LEU
1	D	36	PHE
1	D	129	ARG
1	D	140	LEU
1	D	180	GLU
1	D	194	LEU
1	E	6	LEU
1	E	41	LYS
1	E	120	LEU
1	E	129	ARG
1	E	194	LEU
1	E	196	LYS
1	F	2	VAL
1	F	74	LYS
1	F	118	GLU
1	F	129	ARG
1	F	140	LEU
1	F	153	VAL
1	F	194	LEU
1	G	2	VAL
1	G	37	GLN
1	G	109	VAL
1	G	124	LEU
1	G	129	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	153	VAL
1	H	118	GLU
1	H	129	ARG
1	H	140	LEU
1	H	194	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	HIS
1	A	37	GLN
1	A	60	GLN
1	A	163	HIS
1	A	184	HIS
1	B	20	GLN
1	B	50	GLN
1	B	60	GLN
1	B	63	GLN
1	B	100	ASN
1	B	163	HIS
1	B	184	HIS
1	C	50	GLN
1	C	63	GLN
1	C	163	HIS
1	C	184	HIS
1	D	3	HIS
1	D	20	GLN
1	D	50	GLN
1	D	60	GLN
1	D	63	GLN
1	D	100	ASN
1	D	163	HIS
1	D	184	HIS
1	E	20	GLN
1	E	60	GLN
1	E	63	GLN
1	E	100	ASN
1	E	114	GLN
1	E	163	HIS
1	E	184	HIS
1	F	20	GLN
1	F	27	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	163	HIS
1	F	184	HIS
1	G	37	GLN
1	G	63	GLN
1	G	100	ASN
1	G	163	HIS
1	G	184	HIS
1	H	20	GLN
1	H	27	GLN
1	H	50	GLN
1	H	63	GLN
1	H	100	ASN
1	H	163	HIS
1	H	184	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

84 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	EDO	H	450	-	3,3,3	0.55	0	2,2,2	0.68	0
3	GSH	E	999	-	18,19,19	3.08	2 (11%)	23,24,24	1.74	6 (26%)
2	EDO	E	425	-	3,3,3	0.49	0	2,2,2	0.37	0
2	EDO	F	419	-	3,3,3	0.41	0	2,2,2	0.32	0
2	EDO	H	427	-	3,3,3	0.49	0	2,2,2	0.31	0
2	EDO	E	452	-	3,3,3	0.47	0	2,2,2	0.45	0
2	EDO	B	425	-	3,3,3	0.52	0	2,2,2	0.50	0
2	EDO	G	427	-	3,3,3	0.40	0	2,2,2	0.36	0
2	EDO	A	428	-	3,3,3	0.45	0	2,2,2	0.32	0
2	EDO	G	422	-	3,3,3	0.63	0	2,2,2	0.41	0
2	EDO	A	454	-	3,3,3	0.45	0	2,2,2	0.48	0
2	EDO	F	452	-	3,3,3	0.44	0	2,2,2	0.63	0
2	EDO	E	426	-	3,3,3	0.32	0	2,2,2	0.62	0
2	EDO	H	422	-	3,3,3	0.49	0	2,2,2	0.25	0
2	EDO	H	451	-	3,3,3	0.42	0	2,2,2	0.76	0
2	EDO	D	454	-	3,3,3	0.38	0	2,2,2	0.49	0
2	EDO	A	423	-	3,3,3	0.50	0	2,2,2	0.21	0
2	EDO	F	425	-	3,3,3	0.53	0	2,2,2	0.32	0
2	EDO	G	450	-	3,3,3	0.41	0	2,2,2	0.29	0
2	EDO	G	420	-	3,3,3	0.42	0	2,2,2	0.29	0
2	EDO	H	452	-	3,3,3	0.44	0	2,2,2	0.54	0
2	EDO	B	428	-	3,3,3	0.52	0	2,2,2	0.30	0
2	EDO	D	428	-	3,3,3	0.74	0	2,2,2	0.40	0
2	EDO	H	429	-	3,3,3	0.36	0	2,2,2	0.53	0
2	EDO	D	422	-	3,3,3	0.78	0	2,2,2	0.33	0
2	EDO	G	452	-	3,3,3	0.46	0	2,2,2	0.46	0
3	GSH	F	999	-	18,19,19	3.04	2 (11%)	23,24,24	1.56	5 (21%)
2	EDO	A	429	-	3,3,3	0.47	0	2,2,2	0.25	0
2	EDO	B	422	-	3,3,3	0.69	0	2,2,2	0.64	0
2	EDO	E	428	-	3,3,3	0.36	0	2,2,2	0.72	0
3	GSH	C	999	-	18,19,19	3.04	2 (11%)	23,24,24	1.71	6 (26%)
2	EDO	F	424	-	3,3,3	0.47	0	2,2,2	0.31	0
2	EDO	F	450	-	3,3,3	0.39	0	2,2,2	0.54	0
2	EDO	A	419	-	3,3,3	0.58	0	2,2,2	0.06	0
2	EDO	C	427	-	3,3,3	0.56	0	2,2,2	0.37	0
2	EDO	B	421	-	3,3,3	0.60	0	2,2,2	0.06	0
2	EDO	D	453	-	3,3,3	0.46	0	2,2,2	0.43	0
2	EDO	A	421	-	3,3,3	0.55	0	2,2,2	0.19	0
3	GSH	H	999	-	18,19,19	2.94	2 (11%)	23,24,24	1.38	4 (17%)
2	EDO	B	453	-	3,3,3	0.40	0	2,2,2	0.60	0
2	EDO	D	426	-	3,3,3	0.43	0	2,2,2	0.36	0
2	EDO	B	423	-	3,3,3	0.51	0	2,2,2	0.19	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	EDO	F	451	-	3,3,3	0.42	0	2,2,2	0.59	0
2	EDO	D	419	-	3,3,3	0.51	0	2,2,2	0.24	0
2	EDO	D	418	-	3,3,3	0.39	0	2,2,2	0.61	0
2	EDO	C	425	-	3,3,3	0.48	0	2,2,2	0.47	0
2	EDO	H	426	-	3,3,3	0.33	0	2,2,2	0.92	0
2	EDO	B	424	-	3,3,3	0.45	0	2,2,2	0.42	0
2	EDO	B	452	-	3,3,3	0.49	0	2,2,2	0.36	0
2	EDO	F	422	-	3,3,3	0.38	0	2,2,2	0.46	0
2	EDO	B	419	-	3,3,3	0.53	0	2,2,2	0.24	0
2	EDO	B	430	-	3,3,3	0.52	0	2,2,2	0.25	0
2	EDO	F	418	-	3,3,3	0.46	0	2,2,2	0.29	0
2	EDO	A	420	-	3,3,3	0.53	0	2,2,2	0.35	0
2	EDO	F	432	-	3,3,3	0.40	0	2,2,2	0.35	0
2	EDO	E	450	-	3,3,3	0.42	0	2,2,2	0.44	0
2	EDO	E	454	-	3,3,3	0.32	0	2,2,2	0.57	0
2	EDO	C	428	-	3,3,3	0.54	0	2,2,2	0.20	0
2	EDO	C	424	-	3,3,3	0.52	0	2,2,2	0.21	0
2	EDO	F	427	-	3,3,3	0.48	0	2,2,2	0.25	0
2	EDO	F	420	-	3,3,3	0.53	0	2,2,2	0.24	0
2	EDO	D	427	-	3,3,3	0.47	0	2,2,2	0.32	0
2	EDO	B	427	-	3,3,3	0.37	0	2,2,2	0.65	0
2	EDO	B	426	-	3,3,3	0.38	0	2,2,2	0.60	0
2	EDO	C	452	-	3,3,3	0.42	0	2,2,2	0.22	0
2	EDO	H	423	-	3,3,3	0.53	0	2,2,2	0.21	0
2	EDO	E	453	-	3,3,3	0.44	0	2,2,2	0.26	0
2	EDO	E	427	-	3,3,3	0.46	0	2,2,2	0.27	0
2	EDO	B	418	-	3,3,3	0.46	0	2,2,2	0.37	0
2	EDO	G	425	-	3,3,3	0.54	0	2,2,2	0.26	0
2	EDO	G	426	-	3,3,3	0.38	0	2,2,2	0.92	0
2	EDO	A	427	-	3,3,3	0.49	0	2,2,2	0.09	0
2	EDO	D	425	-	3,3,3	0.43	0	2,2,2	0.36	0
3	GSH	A	999	-	18,19,19	3.23	2 (11%)	23,24,24	1.55	5 (21%)
2	EDO	A	422	-	3,3,3	0.60	0	2,2,2	0.34	0
2	EDO	B	420	-	3,3,3	0.48	0	2,2,2	0.24	0
2	EDO	A	424	-	3,3,3	0.49	0	2,2,2	0.25	0
2	EDO	A	426	-	3,3,3	0.38	0	2,2,2	0.54	0
3	GSH	G	999	-	18,19,19	3.02	3 (16%)	23,24,24	1.55	5 (21%)
2	EDO	H	425	-	3,3,3	0.58	0	2,2,2	0.17	0
2	EDO	A	452	-	3,3,3	0.46	0	2,2,2	0.35	0
3	GSH	B	999	-	18,19,19	3.22	2 (11%)	23,24,24	1.49	4 (17%)
3	GSH	D	999	-	18,19,19	3.02	2 (11%)	23,24,24	1.78	7 (30%)
2	EDO	A	425	-	3,3,3	0.41	0	2,2,2	0.66	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	EDO	H	450	-	-	1/1/1/1	-
3	GSH	E	999	-	1/1/6/8	6/24/24/24	-
2	EDO	E	425	-	-	1/1/1/1	-
2	EDO	F	419	-	-	1/1/1/1	-
2	EDO	H	427	-	-	1/1/1/1	-
2	EDO	E	452	-	-	0/1/1/1	-
2	EDO	B	425	-	-	0/1/1/1	-
2	EDO	G	427	-	-	0/1/1/1	-
2	EDO	A	428	-	-	1/1/1/1	-
2	EDO	G	422	-	-	1/1/1/1	-
2	EDO	A	454	-	-	1/1/1/1	-
2	EDO	F	452	-	-	0/1/1/1	-
2	EDO	E	426	-	-	0/1/1/1	-
2	EDO	H	422	-	-	1/1/1/1	-
2	EDO	H	451	-	-	1/1/1/1	-
2	EDO	D	454	-	-	1/1/1/1	-
2	EDO	A	423	-	-	1/1/1/1	-
2	EDO	F	425	-	-	1/1/1/1	-
2	EDO	G	450	-	-	1/1/1/1	-
2	EDO	G	420	-	-	1/1/1/1	-
2	EDO	H	452	-	-	1/1/1/1	-
2	EDO	B	428	-	-	0/1/1/1	-
2	EDO	D	428	-	-	1/1/1/1	-
2	EDO	H	429	-	-	1/1/1/1	-
2	EDO	D	422	-	-	0/1/1/1	-
2	EDO	G	452	-	-	1/1/1/1	-
3	GSH	F	999	-	1/1/6/8	6/24/24/24	-
2	EDO	A	429	-	-	0/1/1/1	-
2	EDO	B	422	-	-	1/1/1/1	-
2	EDO	E	428	-	-	1/1/1/1	-
3	GSH	C	999	-	1/1/6/8	7/24/24/24	-
2	EDO	F	424	-	-	1/1/1/1	-
2	EDO	F	450	-	-	0/1/1/1	-
2	EDO	A	419	-	-	1/1/1/1	-
2	EDO	C	427	-	-	0/1/1/1	-
2	EDO	B	421	-	-	1/1/1/1	-
2	EDO	D	453	-	-	0/1/1/1	-
2	EDO	A	421	-	-	1/1/1/1	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GSH	H	999	-	1/1/6/8	6/24/24/24	-
2	EDO	B	453	-	-	0/1/1/1	-
2	EDO	D	426	-	-	1/1/1/1	-
2	EDO	B	423	-	-	1/1/1/1	-
2	EDO	F	451	-	-	1/1/1/1	-
2	EDO	D	419	-	-	1/1/1/1	-
2	EDO	D	418	-	-	1/1/1/1	-
2	EDO	C	425	-	-	1/1/1/1	-
2	EDO	H	426	-	-	0/1/1/1	-
2	EDO	B	424	-	-	1/1/1/1	-
2	EDO	B	452	-	-	0/1/1/1	-
2	EDO	F	422	-	-	1/1/1/1	-
2	EDO	B	419	-	-	0/1/1/1	-
2	EDO	B	430	-	-	0/1/1/1	-
2	EDO	F	418	-	-	1/1/1/1	-
2	EDO	A	420	-	-	0/1/1/1	-
2	EDO	F	432	-	-	0/1/1/1	-
2	EDO	E	450	-	-	1/1/1/1	-
2	EDO	E	454	-	-	1/1/1/1	-
2	EDO	C	428	-	-	1/1/1/1	-
2	EDO	C	424	-	-	0/1/1/1	-
2	EDO	F	427	-	-	1/1/1/1	-
2	EDO	F	420	-	-	0/1/1/1	-
2	EDO	D	427	-	-	1/1/1/1	-
2	EDO	B	427	-	-	1/1/1/1	-
2	EDO	B	426	-	-	1/1/1/1	-
2	EDO	C	452	-	-	0/1/1/1	-
2	EDO	H	423	-	-	1/1/1/1	-
2	EDO	E	453	-	-	0/1/1/1	-
2	EDO	E	427	-	-	1/1/1/1	-
2	EDO	B	418	-	-	0/1/1/1	-
2	EDO	G	425	-	-	0/1/1/1	-
2	EDO	G	426	-	-	0/1/1/1	-
2	EDO	A	427	-	-	1/1/1/1	-
2	EDO	D	425	-	-	0/1/1/1	-
3	GSH	A	999	-	1/1/6/8	10/24/24/24	-
2	EDO	A	422	-	-	1/1/1/1	-
2	EDO	B	420	-	-	1/1/1/1	-
2	EDO	A	424	-	-	1/1/1/1	-
2	EDO	A	426	-	-	1/1/1/1	-
3	GSH	G	999	-	1/1/6/8	7/24/24/24	-
2	EDO	H	425	-	-	0/1/1/1	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	EDO	A	452	-	-	1/1/1/1	-
3	GSH	B	999	-	1/1/6/8	9/24/24/24	-
3	GSH	D	999	-	1/1/6/8	6/24/24/24	-
2	EDO	A	425	-	-	0/1/1/1	-

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	999	GSH	OE1-CD1	9.72	1.43	1.23
3	A	999	GSH	OE1-CD1	9.55	1.42	1.23
3	A	999	GSH	O2-C2	9.45	1.42	1.23
3	D	999	GSH	OE1-CD1	9.38	1.42	1.23
3	E	999	GSH	OE1-CD1	9.33	1.42	1.23
3	C	999	GSH	OE1-CD1	9.30	1.42	1.23
3	G	999	GSH	OE1-CD1	9.13	1.41	1.23
3	B	999	GSH	O2-C2	9.05	1.41	1.23
3	F	999	GSH	OE1-CD1	9.00	1.41	1.23
3	F	999	GSH	O2-C2	8.79	1.40	1.23
3	H	999	GSH	OE1-CD1	8.69	1.40	1.23
3	C	999	GSH	O2-C2	8.60	1.40	1.23
3	E	999	GSH	O2-C2	8.55	1.40	1.23
3	H	999	GSH	O2-C2	8.26	1.39	1.23
3	G	999	GSH	O2-C2	8.21	1.39	1.23
3	D	999	GSH	O2-C2	7.91	1.39	1.23
3	G	999	GSH	O12-C1	-2.12	1.23	1.30

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	999	GSH	O12-C1-CA1	4.28	127.97	113.38
3	F	999	GSH	O12-C1-CA1	4.17	127.59	113.38
3	B	999	GSH	CB1-CA1-C1	4.15	120.17	110.30
3	E	999	GSH	O12-C1-CA1	3.97	126.92	113.38
3	C	999	GSH	CB1-CA1-C1	3.94	119.69	110.30
3	E	999	GSH	CB1-CA1-C1	3.86	119.50	110.30
3	D	999	GSH	CB1-CA1-C1	3.80	119.36	110.30
3	A	999	GSH	O12-C1-CA1	3.67	125.89	113.38
3	G	999	GSH	CB1-CA1-C1	3.54	118.72	110.30
3	G	999	GSH	CB2-CA2-N2	-3.39	106.45	111.28
3	F	999	GSH	CB1-CA1-C1	3.24	118.03	110.30
3	H	999	GSH	CB1-CA1-C1	3.09	117.65	110.30
3	C	999	GSH	O12-C1-O11	-2.86	117.59	124.09

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	G	999	GSH	O12-C1-O11	-2.84	117.64	124.09
3	E	999	GSH	O12-C1-O11	-2.82	117.68	124.09
3	D	999	GSH	CA2-C2-N3	2.81	122.20	116.54
3	D	999	GSH	CB2-CA2-N2	-2.80	107.30	111.28
3	D	999	GSH	CA2-CB2-SG2	-2.79	111.06	114.19
3	D	999	GSH	O32-C3-CA3	2.65	121.95	112.74
3	H	999	GSH	O12-C1-O11	-2.64	118.10	124.09
3	A	999	GSH	CA2-N2-CD1	2.58	128.29	121.65
3	F	999	GSH	O12-C1-O11	-2.55	118.31	124.09
3	E	999	GSH	CA2-CB2-SG2	-2.54	111.34	114.19
3	G	999	GSH	O32-C3-CA3	2.52	121.50	112.74
3	H	999	GSH	O32-C3-CA3	2.50	121.43	112.74
3	C	999	GSH	CB2-CA2-N2	-2.49	107.74	111.28
3	C	999	GSH	O32-C3-CA3	2.30	120.75	112.74
3	B	999	GSH	O12-C1-O11	-2.30	118.86	124.09
3	F	999	GSH	O11-C1-CA1	-2.28	114.10	122.14
3	B	999	GSH	O32-C3-CA3	2.28	120.65	112.74
3	D	999	GSH	O12-C1-O11	-2.26	118.97	124.09
3	A	999	GSH	O32-C3-CA3	2.23	120.47	112.74
3	B	999	GSH	CB2-CA2-N2	-2.21	108.13	111.28
3	E	999	GSH	CB2-CA2-N2	-2.21	108.14	111.28
3	A	999	GSH	O11-C1-CA1	-2.20	114.38	122.14
3	A	999	GSH	CB1-CA1-C1	2.19	115.52	110.30
3	C	999	GSH	O11-C1-CA1	-2.18	114.44	122.14
3	G	999	GSH	CA2-CB2-SG2	-2.13	111.80	114.19
3	D	999	GSH	O32-C3-O31	-2.08	118.10	123.30
3	H	999	GSH	CB2-CA2-N2	-2.02	108.40	111.28
3	E	999	GSH	O32-C3-CA3	2.01	119.74	112.74
3	F	999	GSH	O32-C3-O31	-2.01	118.29	123.30

All (8) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	999	GSH	CA1
3	B	999	GSH	CA1
3	C	999	GSH	CA1
3	D	999	GSH	CA1
3	E	999	GSH	CA1
3	F	999	GSH	CA1
3	G	999	GSH	CA1
3	H	999	GSH	CA1

All (105) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	999	GSH	N2-CA2-CB2-SG2
3	A	999	GSH	C2-CA2-CB2-SG2
3	B	999	GSH	O11-C1-CA1-N1
3	B	999	GSH	C1-CA1-CB1-CG1
3	B	999	GSH	C2-CA2-CB2-SG2
3	C	999	GSH	C1-CA1-CB1-CG1
3	D	999	GSH	O11-C1-CA1-N1
3	F	999	GSH	C1-CA1-CB1-CG1
3	G	999	GSH	O11-C1-CA1-N1
3	G	999	GSH	C1-CA1-CB1-CG1
3	H	999	GSH	O11-C1-CA1-N1
3	B	999	GSH	O12-C1-CA1-N1
3	E	999	GSH	O12-C1-CA1-CB1
3	F	999	GSH	CA1-CB1-CG1-CD1
3	H	999	GSH	CA1-CB1-CG1-CD1
3	F	999	GSH	O12-C1-CA1-N1
3	H	999	GSH	O12-C1-CA1-N1
3	D	999	GSH	O12-C1-CA1-N1
3	E	999	GSH	O11-C1-CA1-CB1
2	A	419	EDO	O1-C1-C2-O2
3	B	999	GSH	CA1-CB1-CG1-CD1
3	D	999	GSH	CA1-CB1-CG1-CD1
3	E	999	GSH	CA1-CB1-CG1-CD1
3	G	999	GSH	CA1-CB1-CG1-CD1
3	A	999	GSH	O12-C1-CA1-N1
3	C	999	GSH	O12-C1-CA1-N1
3	G	999	GSH	O12-C1-CA1-N1
3	C	999	GSH	O11-C1-CA1-CB1
3	A	999	GSH	CA1-CB1-CG1-CD1
3	C	999	GSH	CA1-CB1-CG1-CD1
3	B	999	GSH	N2-CA2-CB2-SG2
3	G	999	GSH	C2-CA2-CB2-SG2
3	A	999	GSH	O11-C1-CA1-CB1
3	A	999	GSH	O12-C1-CA1-CB1
3	C	999	GSH	O12-C1-CA1-CB1
3	F	999	GSH	O11-C1-CA1-CB1
3	F	999	GSH	O12-C1-CA1-CB1
2	A	426	EDO	O1-C1-C2-O2
2	A	454	EDO	O1-C1-C2-O2
2	B	421	EDO	O1-C1-C2-O2
2	B	423	EDO	O1-C1-C2-O2
2	B	424	EDO	O1-C1-C2-O2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	B	426	EDO	O1-C1-C2-O2
2	B	427	EDO	O1-C1-C2-O2
2	C	428	EDO	O1-C1-C2-O2
2	D	419	EDO	O1-C1-C2-O2
2	D	454	EDO	O1-C1-C2-O2
2	E	427	EDO	O1-C1-C2-O2
2	F	418	EDO	O1-C1-C2-O2
2	F	419	EDO	O1-C1-C2-O2
2	H	423	EDO	O1-C1-C2-O2
2	H	427	EDO	O1-C1-C2-O2
2	H	450	EDO	O1-C1-C2-O2
3	E	999	GSH	O12-C1-CA1-N1
2	D	428	EDO	O1-C1-C2-O2
2	E	428	EDO	O1-C1-C2-O2
2	H	429	EDO	O1-C1-C2-O2
3	A	999	GSH	OE1-CD1-N2-CA2
3	A	999	GSH	O11-C1-CA1-N1
3	C	999	GSH	O11-C1-CA1-N1
3	E	999	GSH	O11-C1-CA1-N1
3	F	999	GSH	O11-C1-CA1-N1
2	B	420	EDO	O1-C1-C2-O2
2	D	418	EDO	O1-C1-C2-O2
2	E	425	EDO	O1-C1-C2-O2
2	F	425	EDO	O1-C1-C2-O2
2	G	420	EDO	O1-C1-C2-O2
3	A	999	GSH	C1-CA1-CB1-CG1
3	D	999	GSH	C1-CA1-CB1-CG1
3	H	999	GSH	C1-CA1-CB1-CG1
2	A	427	EDO	O1-C1-C2-O2
2	C	425	EDO	O1-C1-C2-O2
2	D	427	EDO	O1-C1-C2-O2
2	F	451	EDO	O1-C1-C2-O2
3	E	999	GSH	C2-CA2-CB2-SG2
2	A	428	EDO	O1-C1-C2-O2
2	B	422	EDO	O1-C1-C2-O2
2	E	450	EDO	O1-C1-C2-O2
2	F	424	EDO	O1-C1-C2-O2
2	H	422	EDO	O1-C1-C2-O2
2	H	451	EDO	O1-C1-C2-O2
2	H	452	EDO	O1-C1-C2-O2
3	A	999	GSH	CG1-CD1-N2-CA2
3	G	999	GSH	O11-C1-CA1-CB1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	A	424	EDO	O1-C1-C2-O2
2	A	452	EDO	O1-C1-C2-O2
2	E	454	EDO	O1-C1-C2-O2
2	G	450	EDO	O1-C1-C2-O2
2	G	452	EDO	O1-C1-C2-O2
3	B	999	GSH	O11-C1-CA1-CB1
3	D	999	GSH	O11-C1-CA1-CB1
3	G	999	GSH	O12-C1-CA1-CB1
2	D	426	EDO	O1-C1-C2-O2
2	F	422	EDO	O1-C1-C2-O2
3	H	999	GSH	O11-C1-CA1-CB1
3	B	999	GSH	O12-C1-CA1-CB1
2	A	421	EDO	O1-C1-C2-O2
2	A	423	EDO	O1-C1-C2-O2
2	F	427	EDO	O1-C1-C2-O2
3	C	999	GSH	C2-CA2-CB2-SG2
3	D	999	GSH	O12-C1-CA1-CB1
3	H	999	GSH	O12-C1-CA1-CB1
3	B	999	GSH	O32-C3-CA3-N3
2	A	422	EDO	O1-C1-C2-O2
2	G	422	EDO	O1-C1-C2-O2

There are no ring outliers.

49 monomers are involved in 102 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	450	EDO	9	0
3	E	999	GSH	1	0
2	B	425	EDO	1	0
2	G	422	EDO	1	0
2	E	426	EDO	2	0
2	H	422	EDO	3	0
2	H	451	EDO	7	0
2	D	454	EDO	1	0
2	A	423	EDO	1	0
2	G	450	EDO	1	0
2	G	420	EDO	2	0
2	H	452	EDO	1	0
2	D	428	EDO	4	0
2	H	429	EDO	3	0
2	B	422	EDO	1	0
2	E	428	EDO	1	0

Continued on next page...

Continued from previous page...

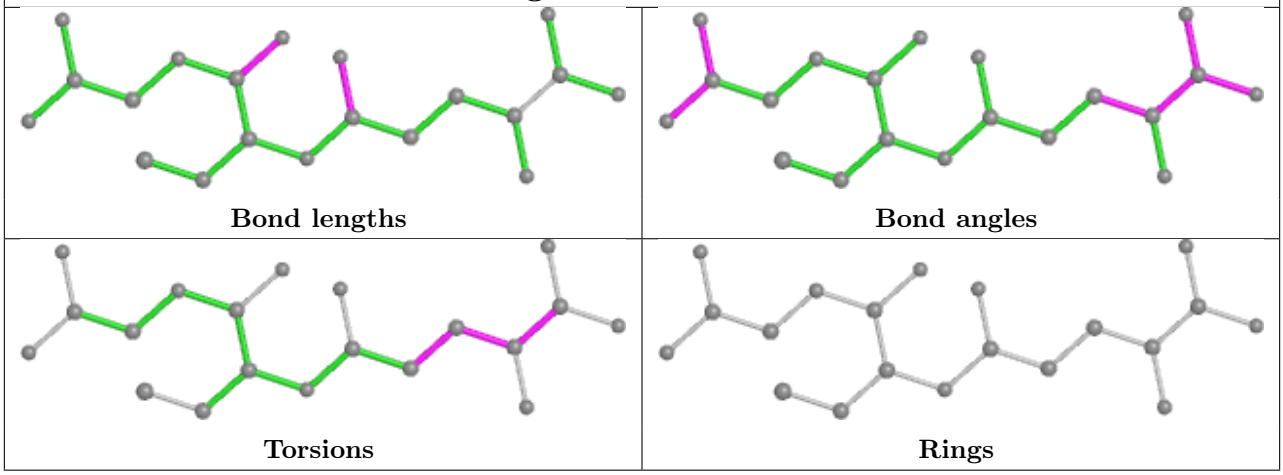
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	999	GSH	3	0
2	F	450	EDO	5	0
2	A	419	EDO	2	0
2	C	427	EDO	1	0
2	D	453	EDO	1	0
3	H	999	GSH	2	0
2	B	453	EDO	2	0
2	D	426	EDO	3	0
2	F	451	EDO	2	0
2	H	426	EDO	2	0
2	F	422	EDO	1	0
2	B	419	EDO	1	0
2	F	418	EDO	5	0
2	F	432	EDO	1	0
2	E	450	EDO	2	0
2	E	454	EDO	4	0
2	D	427	EDO	3	0
2	B	427	EDO	1	0
2	B	426	EDO	5	0
2	C	452	EDO	1	0
2	H	423	EDO	1	0
2	E	453	EDO	1	0
2	E	427	EDO	3	0
2	G	426	EDO	2	0
2	A	427	EDO	1	0
2	D	425	EDO	1	0
3	A	999	GSH	2	0
2	A	422	EDO	1	0
2	A	426	EDO	5	0
3	G	999	GSH	2	0
3	B	999	GSH	3	0
3	D	999	GSH	2	0
2	A	425	EDO	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 then 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

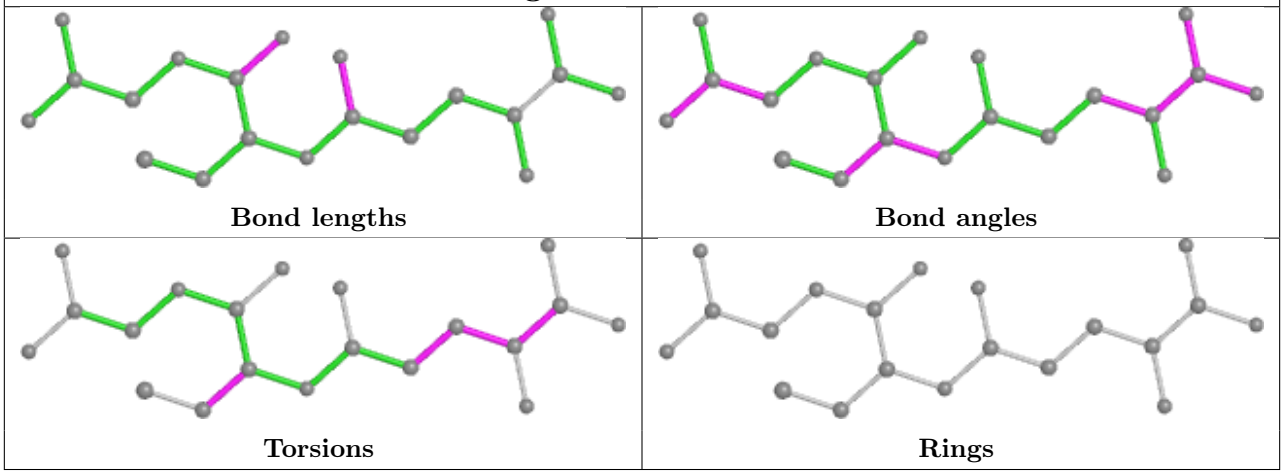
any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand GSH E 999

Ligand GSH F 999

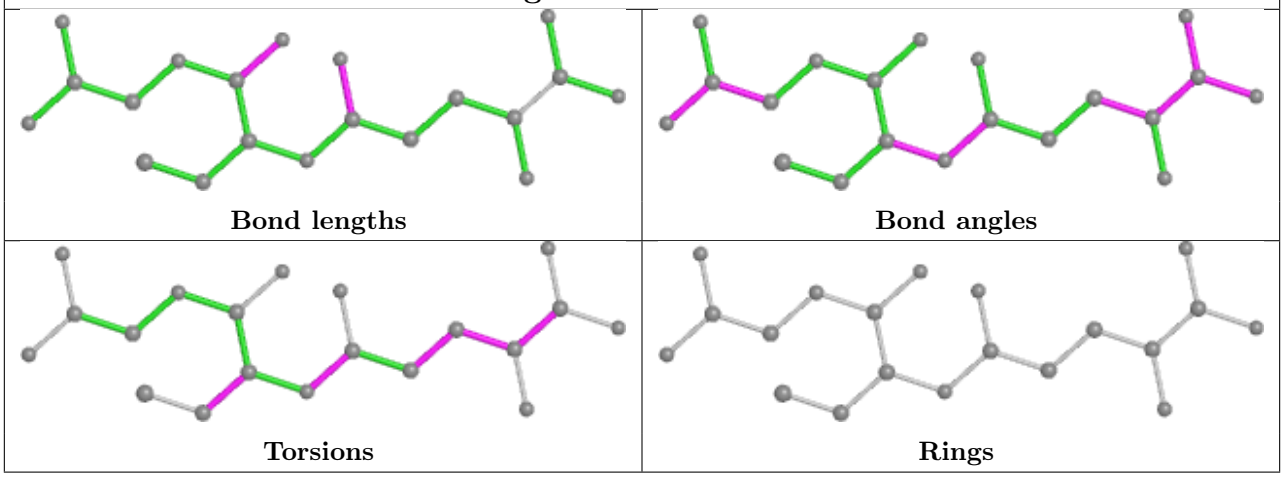


Ligand GSH C 999

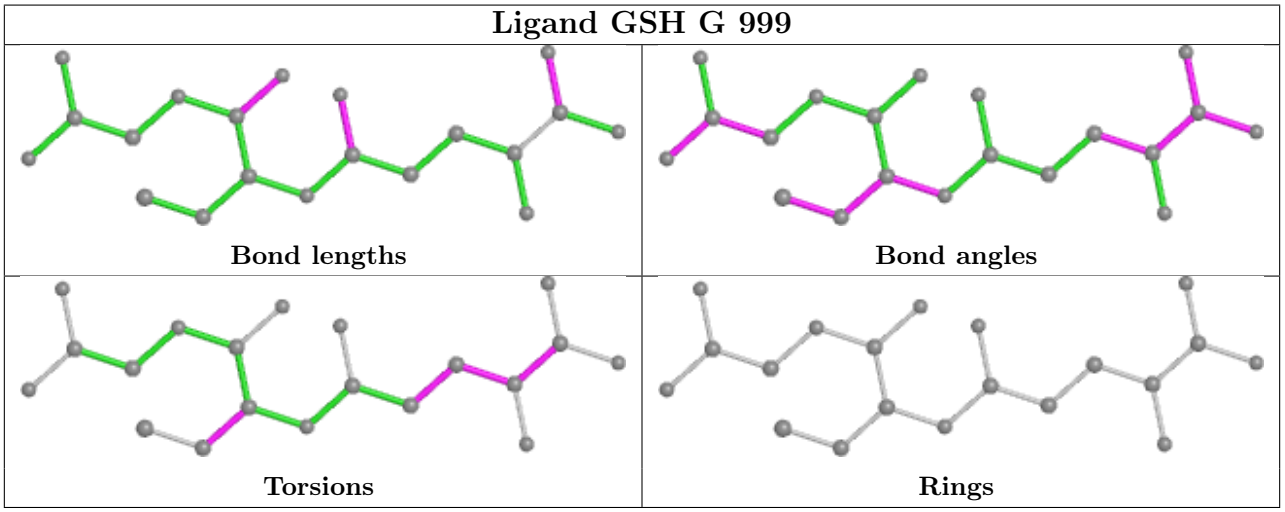


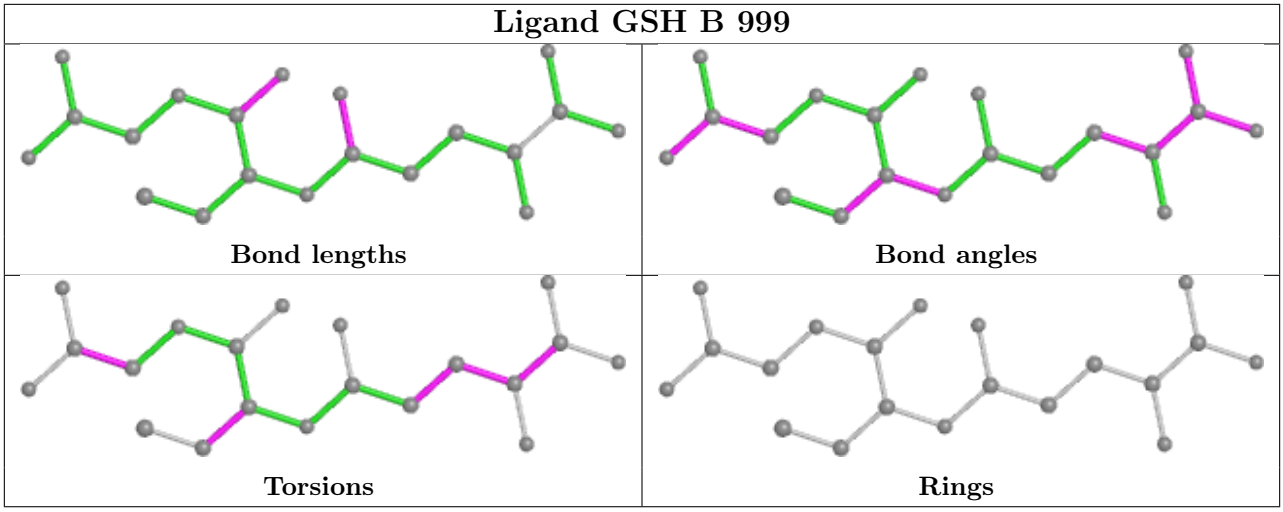
Ligand GSH H 999

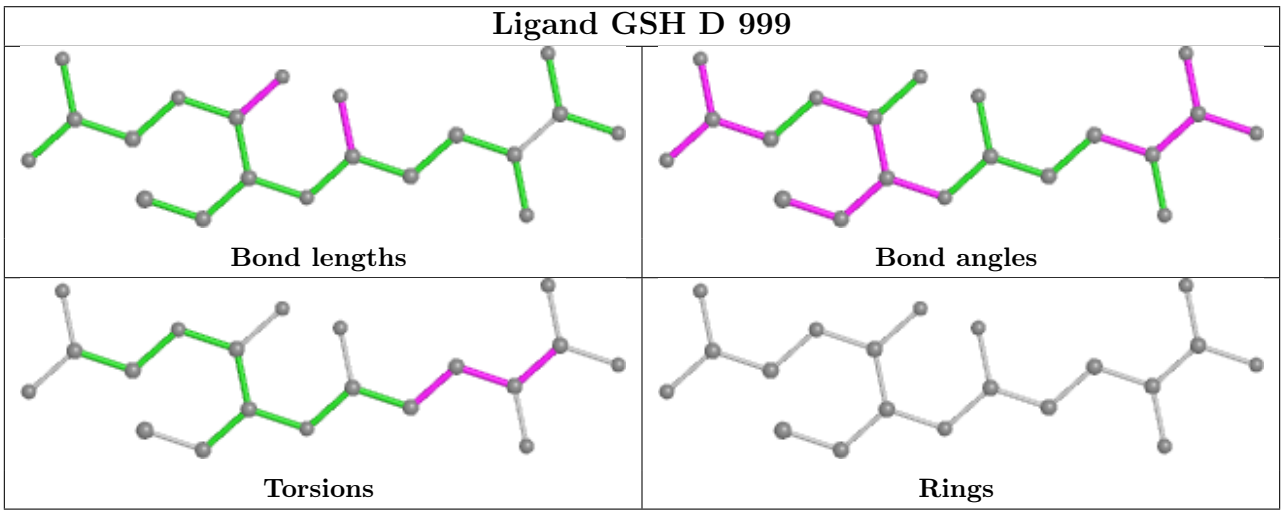
Ligand GSH A 999



Ligand GSH G 999







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^{th} 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	206/206 (100%)	-0.61	0 100 100	14, 20, 31, 38	0
1	B	206/206 (100%)	-0.58	0 100 100	14, 21, 31, 36	0
1	C	206/206 (100%)	-0.61	0 100 100	14, 22, 32, 39	0
1	D	206/206 (100%)	-0.43	7 (3%) 45 48	15, 22, 37, 43	0
1	E	206/206 (100%)	-0.39	6 (2%) 51 54	15, 22, 38, 44	0
1	F	206/206 (100%)	-0.55	1 (0%) 91 92	15, 23, 35, 42	0
1	G	206/206 (100%)	-0.60	0 100 100	14, 21, 32, 39	0
1	H	206/206 (100%)	-0.56	1 (0%) 91 92	15, 23, 36, 42	0
All	All	1648/1648 (100%)	-0.54	15 (0%) 84 85	14, 22, 34, 44	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	109	VAL	5.3
1	E	110	ALA	4.8
1	E	112	VAL	4.3
1	D	112	VAL	3.9
1	E	111	GLY	3.8
1	D	109	VAL	3.8
1	D	115	GLY	3.4
1	D	110	ALA	3.1
1	E	114	GLN	3.0
1	D	111	GLY	2.8
1	D	36	PHE	2.7
1	E	36	PHE	2.6
1	F	111	GLY	2.4
1	D	114	GLN	2.4
1	H	114	GLN	2.1

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} 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
2	EDO	D	419	4/4	0.60	0.23	54,55,56,56	0
2	EDO	A	423	4/4	0.65	0.18	77,78,78,78	0
2	EDO	D	428	4/4	0.74	0.23	26,32,34,37	0
2	EDO	B	423	4/4	0.75	0.14	59,59,59,59	0
2	EDO	C	428	4/4	0.78	0.16	53,54,55,55	0
2	EDO	F	424	4/4	0.79	0.15	58,58,58,59	0
2	EDO	H	422	4/4	0.79	0.35	42,46,46,49	0
2	EDO	D	422	4/4	0.80	0.15	32,36,37,39	0
2	EDO	B	421	4/4	0.80	0.12	46,47,47,48	0
2	EDO	D	453	4/4	0.81	0.23	25,31,33,33	4
2	EDO	A	420	4/4	0.81	0.27	34,34,35,35	0
2	EDO	C	427	4/4	0.81	0.17	39,40,41,43	0
2	EDO	G	427	4/4	0.82	0.23	50,50,50,52	0
2	EDO	A	419	4/4	0.82	0.14	39,40,41,41	0
3	GSH	B	999	20/20	0.82	0.21	24,36,40,40	0
3	GSH	A	999	20/20	0.83	0.24	24,37,41,44	0
2	EDO	E	453	4/4	0.83	0.29	29,31,32,33	4
2	EDO	H	427	4/4	0.84	0.17	43,44,44,45	0
2	EDO	B	453	4/4	0.85	0.22	36,37,39,39	4
2	EDO	A	454	4/4	0.85	0.14	28,33,33,38	4
2	EDO	A	452	4/4	0.86	0.15	30,31,33,36	4
2	EDO	H	423	4/4	0.86	0.30	45,45,45,47	0
2	EDO	F	450	4/4	0.86	0.23	24,30,30,31	4
2	EDO	G	422	4/4	0.86	0.21	32,36,38,43	0
2	EDO	B	428	4/4	0.86	0.24	55,56,57,57	0
2	EDO	A	428	4/4	0.87	0.13	59,59,60,60	0
2	EDO	A	421	4/4	0.87	0.16	46,49,50,52	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	EDO	B	422	4/4	0.87	0.21	31,33,34,34	0
2	EDO	C	424	4/4	0.87	0.15	48,50,52,53	0
2	EDO	B	419	4/4	0.88	0.11	37,40,41,44	0
2	EDO	E	427	4/4	0.88	0.17	25,32,34,39	0
2	EDO	A	422	4/4	0.88	0.23	30,34,36,36	0
3	GSH	C	999	20/20	0.88	0.15	24,36,41,47	0
2	EDO	B	430	4/4	0.89	0.17	30,31,32,32	0
2	EDO	F	420	4/4	0.89	0.15	41,41,42,43	0
2	EDO	C	425	4/4	0.89	0.14	30,31,31,33	0
2	EDO	B	425	4/4	0.89	0.12	28,30,32,32	0
3	GSH	G	999	20/20	0.89	0.14	23,34,39,46	0
2	EDO	B	418	4/4	0.90	0.14	56,56,56,56	0
2	EDO	F	427	4/4	0.91	0.10	39,40,40,40	0
2	EDO	D	426	4/4	0.91	0.38	23,28,31,36	0
2	EDO	H	450	4/4	0.91	0.13	18,19,24,29	4
2	EDO	E	425	4/4	0.91	0.16	37,37,37,39	0
2	EDO	F	422	4/4	0.91	0.34	46,47,47,48	0
2	EDO	G	450	4/4	0.91	0.26	32,37,38,40	4
2	EDO	A	429	4/4	0.91	0.17	28,31,33,35	0
2	EDO	F	451	4/4	0.92	0.18	20,23,24,26	4
2	EDO	A	426	4/4	0.92	0.31	24,25,27,29	0
3	GSH	H	999	20/20	0.92	0.11	24,28,31,42	0
2	EDO	A	424	4/4	0.93	0.12	65,65,65,65	0
2	EDO	C	452	4/4	0.93	0.14	39,40,41,41	4
2	EDO	H	426	4/4	0.93	0.20	26,29,31,31	0
3	GSH	E	999	20/20	0.93	0.14	19,31,39,44	0
2	EDO	D	418	4/4	0.93	0.11	34,35,36,37	0
2	EDO	B	426	4/4	0.93	0.35	28,28,29,32	0
2	EDO	E	428	4/4	0.94	0.18	23,34,35,37	0
2	EDO	B	420	4/4	0.94	0.14	33,33,34,36	0
2	EDO	H	451	4/4	0.94	0.21	19,24,24,26	4
2	EDO	E	454	4/4	0.94	0.24	30,32,33,33	4
2	EDO	E	450	4/4	0.94	0.22	20,26,28,31	4
2	EDO	B	424	4/4	0.94	0.11	55,55,55,55	0
3	GSH	D	999	20/20	0.94	0.13	22,31,36,43	0
2	EDO	D	425	4/4	0.94	0.10	32,32,32,34	0
3	GSH	F	999	20/20	0.94	0.11	24,31,36,44	0
2	EDO	E	426	4/4	0.94	0.32	34,34,35,36	0
2	EDO	B	427	4/4	0.94	0.19	32,32,36,37	0
2	EDO	F	452	4/4	0.95	0.10	32,32,33,34	4
2	EDO	D	454	4/4	0.95	0.22	23,26,29,33	4
2	EDO	H	452	4/4	0.95	0.07	34,34,35,36	4

Continued on next page...

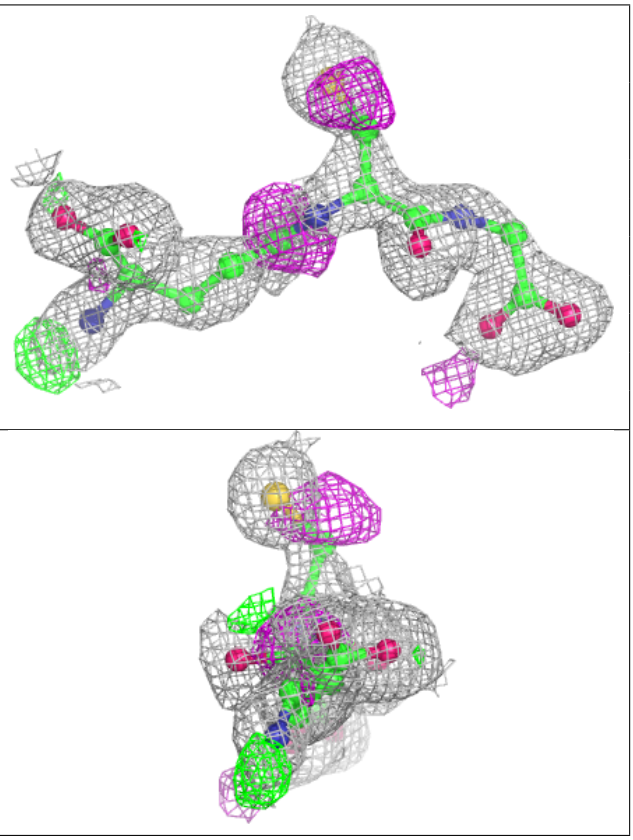
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	EDO	G	425	4/4	0.95	0.10	29,30,31,32	0
2	EDO	A	427	4/4	0.95	0.15	32,33,35,36	0
2	EDO	F	425	4/4	0.95	0.12	28,28,30,31	0
2	EDO	G	452	4/4	0.95	0.09	32,32,34,35	4
2	EDO	E	452	4/4	0.95	0.12	37,37,39,39	4
2	EDO	F	432	4/4	0.95	0.18	39,39,40,42	0
2	EDO	F	418	4/4	0.95	0.15	32,32,33,34	0
2	EDO	D	427	4/4	0.95	0.10	31,36,37,38	0
2	EDO	H	429	4/4	0.96	0.24	39,39,40,41	0
2	EDO	G	426	4/4	0.96	0.25	26,29,29,29	0
2	EDO	G	420	4/4	0.96	0.26	31,32,35,38	0
2	EDO	H	425	4/4	0.96	0.18	28,29,29,30	0
2	EDO	F	419	4/4	0.96	0.24	26,31,32,34	0
2	EDO	A	425	4/4	0.96	0.11	29,30,31,33	0
2	EDO	B	452	4/4	0.97	0.09	36,37,38,39	4

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.

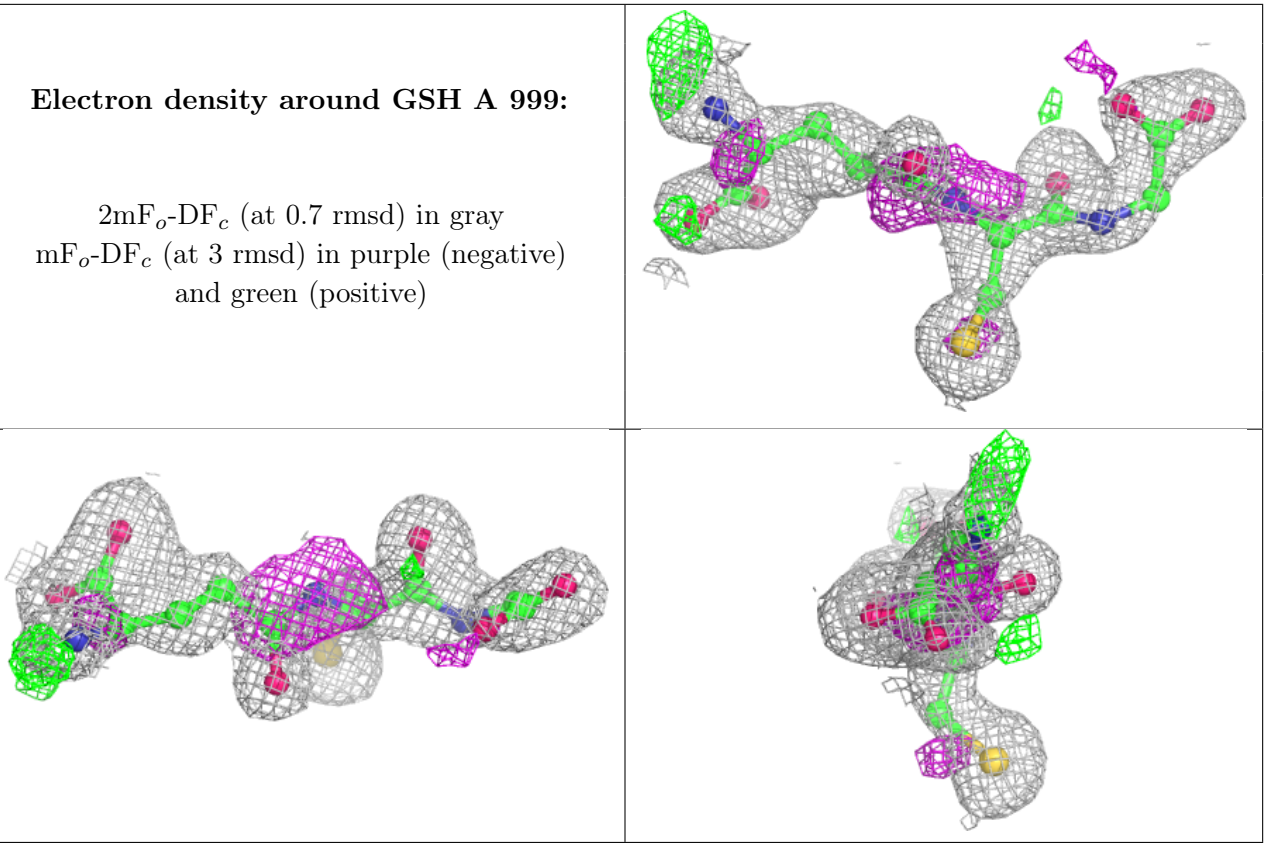
Electron density around GSH B 999:

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



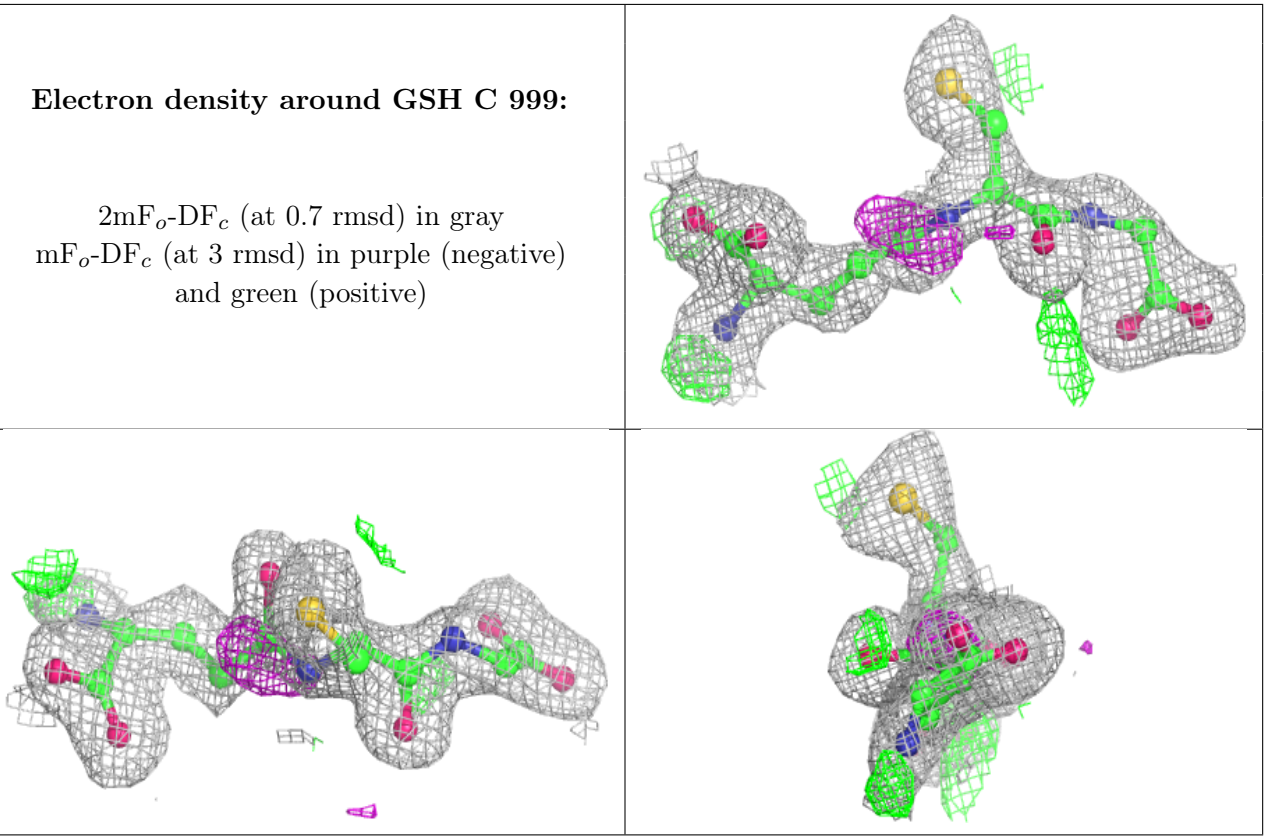
Electron density around GSH A 999:

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



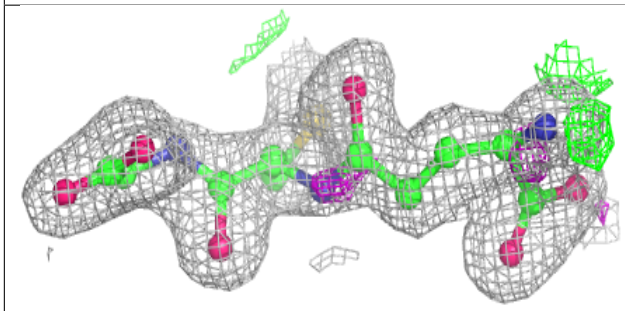
Electron density around GSH C 999:

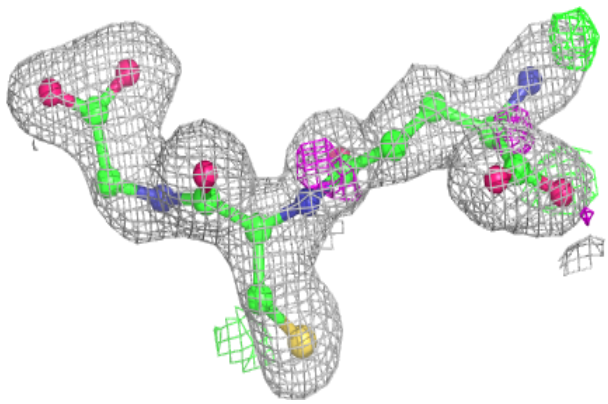
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

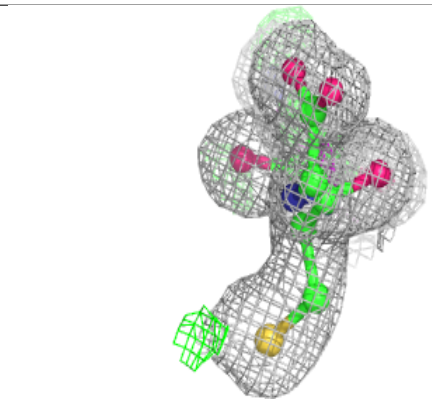


Electron density around GSH G 999:

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

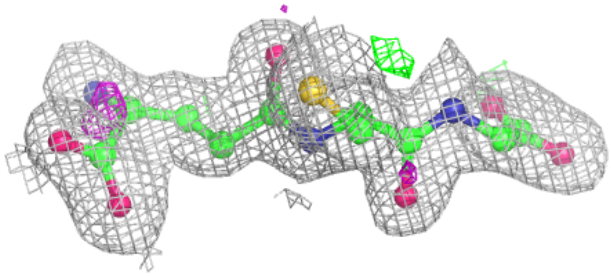


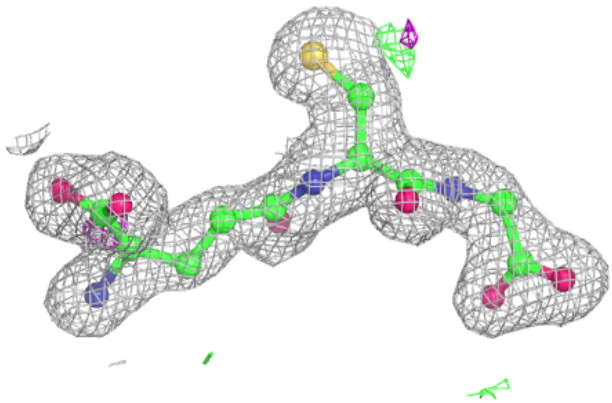


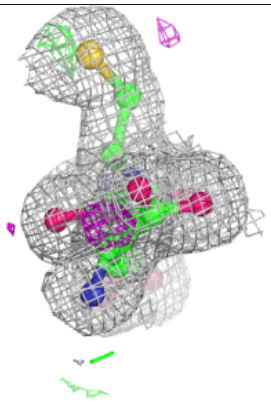


Electron density around GSH H 999:

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

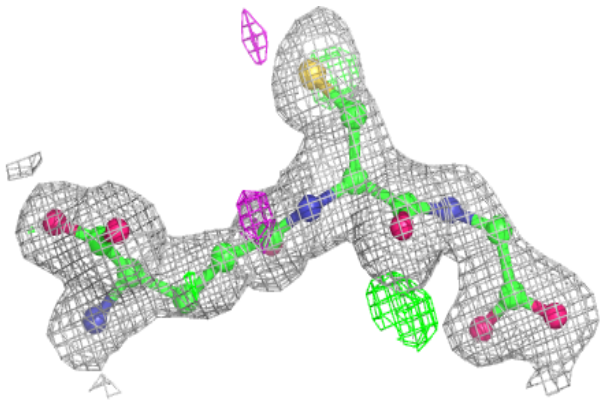


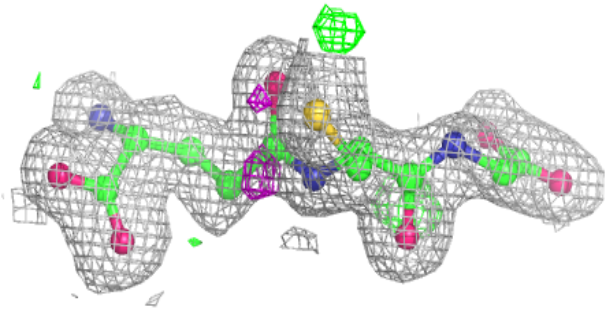


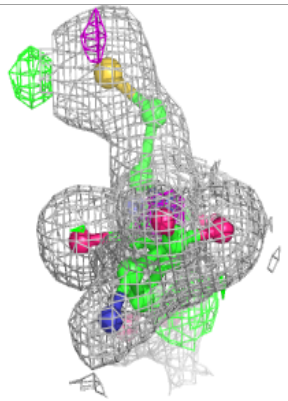


Electron density around GSH E 999:

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

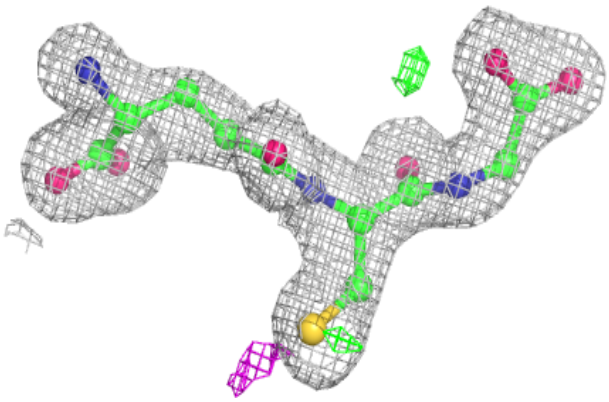


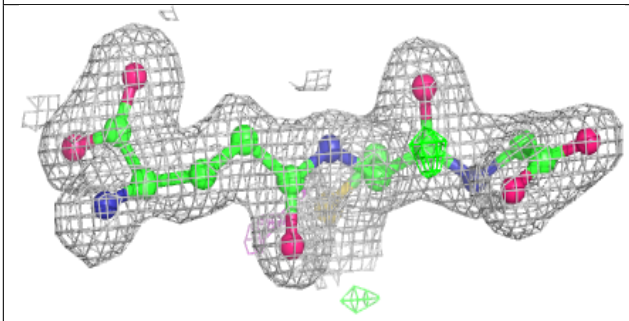


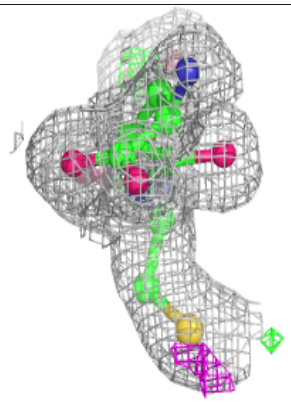


Electron density around GSH D 999:

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

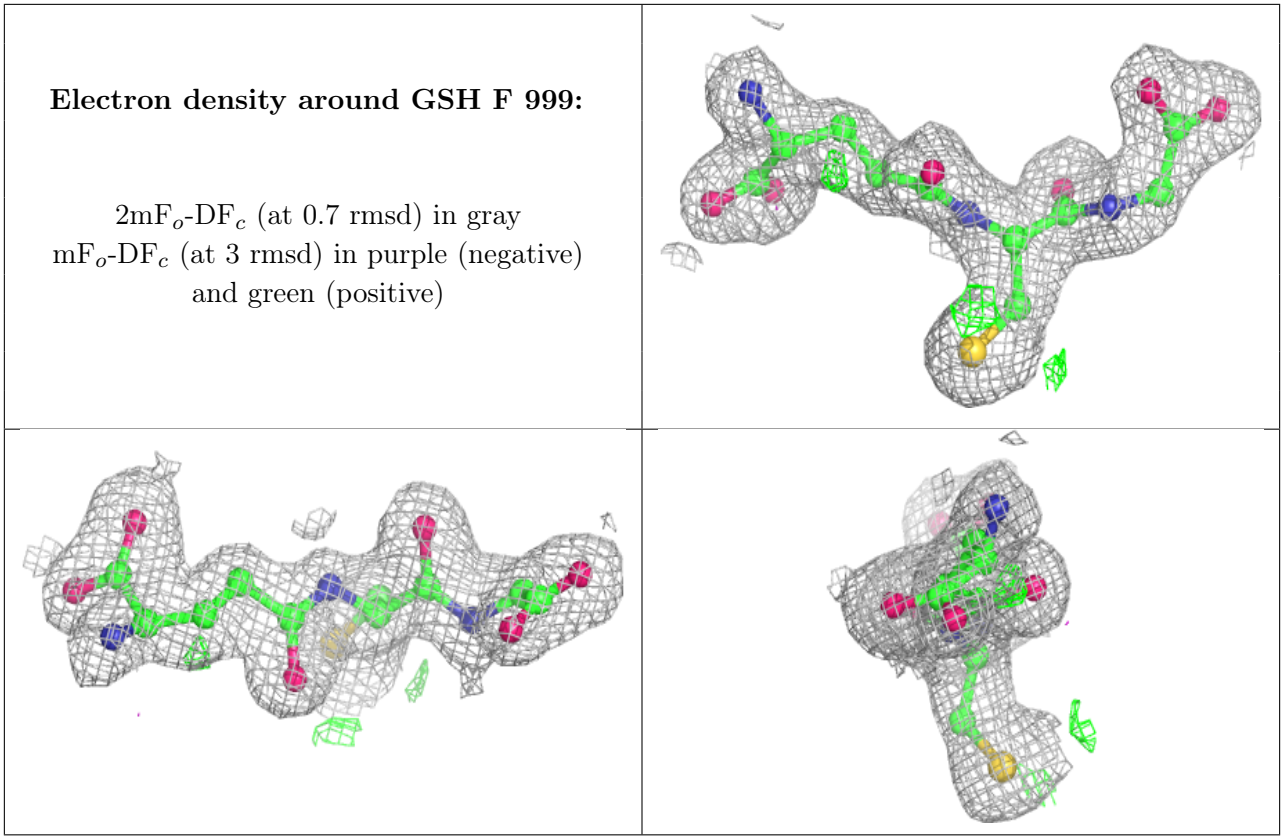






Electron density around GSH F 999:

$2mF_o$-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.