Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 11:55 PM GMT

PDB ID	:	5GST
Title	:	REACTION COORDINATE MOTION IN AN SNAR REACTION CATALYZED BY GLUTATHIONE TRANSFERASE
Authors	:	Ji, X.; Armstrong, R.N.; Gilliland, G.L.
Deposited on	:	1993-07-20
Resolution	:	2.00 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

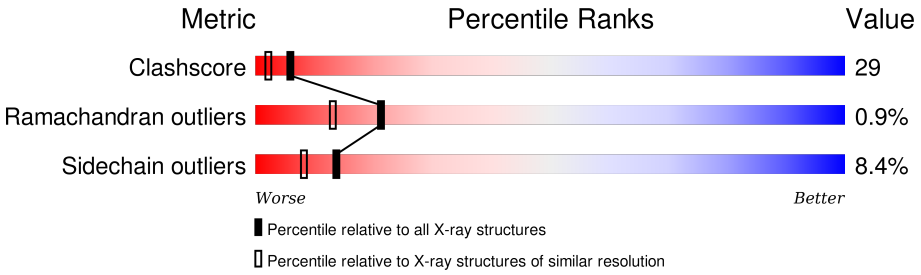
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.00 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))
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	217	55% 36% 8%
1	B	217	51% 34% 13%

2 Entry composition

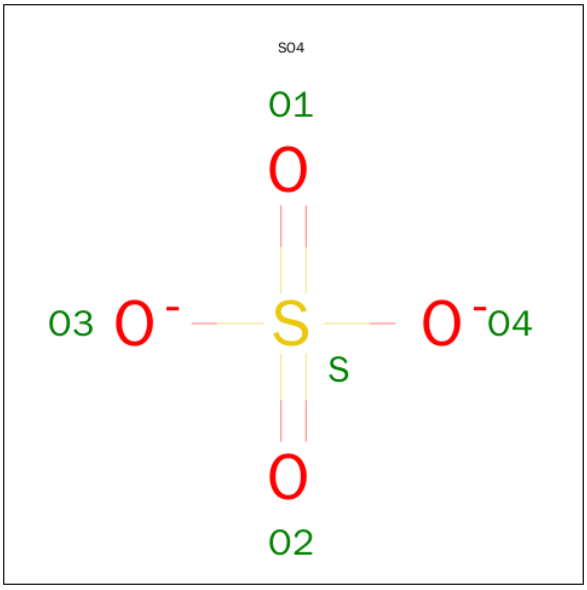
There are 4 unique types of molecules in this entry. The entry contains 4037 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 S-TRANSFERASE.

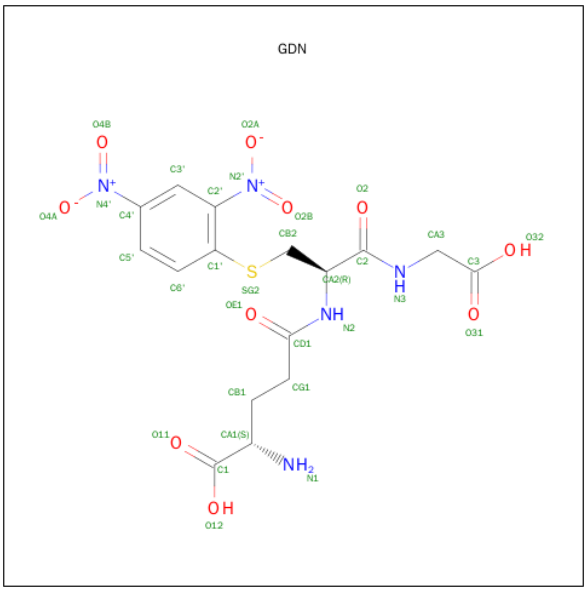
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	217	Total	C	N	O	S	0	0	0
			1818	1177	303	327	11			
1	B	217	Total	C	N	O	S	0	0	0
			1818	1177	303	327	11			

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is GLUTATHIONE S-(2,4 DINITROBENZENE) (three-letter code: GDN) (formula: $C_{16}H_{19}N_5O_{10}S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			32	16	5	10	1		
3	B	1	Total	C	N	O	S	0	0
			32	16	5	10	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	198	Total	O	0	0
			198	198		
4	B	134	Total	O	0	0
			134	134		

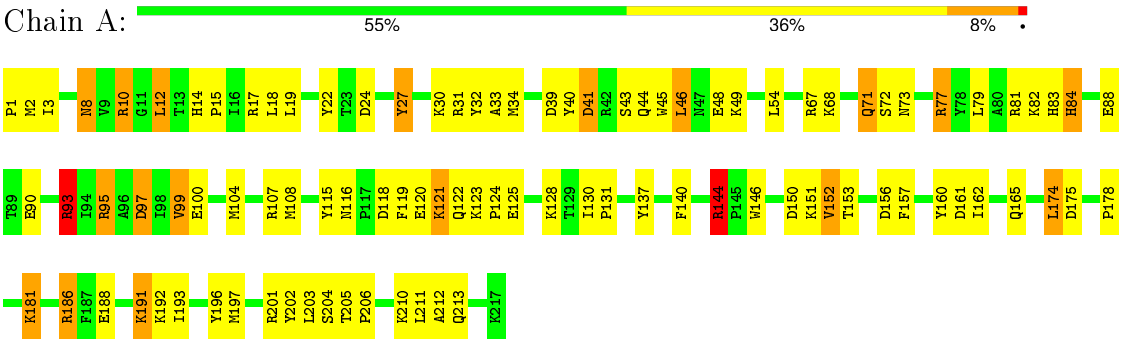
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

Note EDS was not executed.

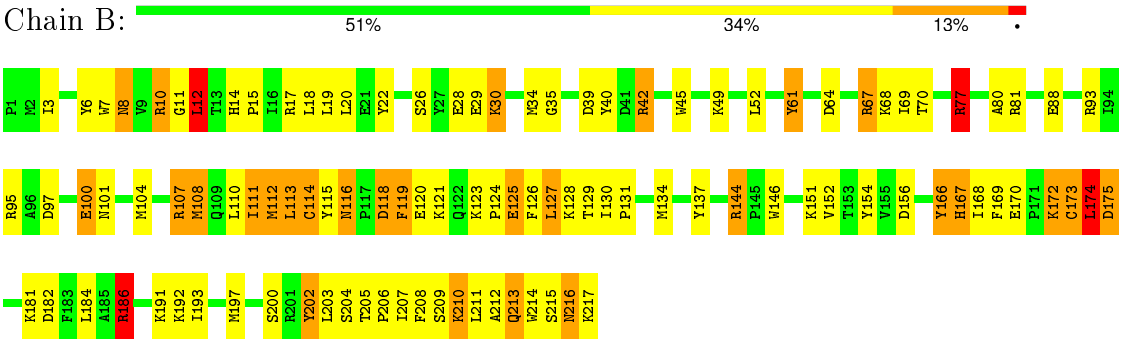
- Molecule 1: GLUTATHIONE S-TRANSFERASE

Chain A:



- Molecule 1: GLUTATHIONE S-TRANSFERASE

Chain B:



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	88.24Å 69.44Å 81.28Å 90.00° 106.01° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.00	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	GPRLSA	Depositor
R, R_{free}	0.192 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4037	wwPDB-VP
Average B, all atoms (Å^2)	24.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, GDN

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	1.04	0/1867	1.94	52/2515 (2.1%)
1	B	1.05	2/1867 (0.1%)	2.34	56/2515 (2.2%)
All	All	1.04	2/3734 (0.1%)	2.15	108/5030 (2.1%)

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	3
1	B	0	3
All	All	0	6

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	29	GLU	CD-OE1	-5.45	1.19	1.25
1	B	100	GLU	CD-OE1	-5.41	1.19	1.25

All (108) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	81	ARG	NE-CZ-NH1	40.73	140.66	120.30
1	B	17	ARG	NE-CZ-NH1	26.88	133.74	120.30
1	B	69	ILE	CB-CG1-CD1	19.48	168.43	113.90
1	B	93	ARG	CD-NE-CZ	18.41	149.37	123.60
1	B	81	ARG	NE-CZ-NH2	-18.02	111.29	120.30
1	A	144	ARG	NE-CZ-NH1	17.03	128.81	120.30
1	B	93	ARG	NE-CZ-NH1	14.18	127.39	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	64	ASP	CB-CG-OD1	13.96	130.86	118.30
1	B	17	ARG	NE-CZ-NH2	-12.66	113.97	120.30
1	A	67	ARG	NE-CZ-NH2	-11.98	114.31	120.30
1	B	6	TYR	CB-CG-CD2	11.65	127.99	121.00
1	A	93	ARG	NE-CZ-NH2	-11.37	114.62	120.30
1	B	6	TYR	CB-CG-CD1	-11.10	114.34	121.00
1	B	95	ARG	NE-CZ-NH2	-11.01	114.80	120.30
1	B	97	ASP	CB-CG-OD1	10.87	128.08	118.30
1	B	93	ARG	NE-CZ-NH2	-10.85	114.88	120.30
1	B	95	ARG	NE-CZ-NH1	10.68	125.64	120.30
1	B	186	ARG	CD-NE-CZ	10.66	138.52	123.60
1	B	10	ARG	NE-CZ-NH1	-10.37	115.11	120.30
1	B	81	ARG	NH1-CZ-NH2	-10.32	108.04	119.40
1	B	182	ASP	CB-CG-OD1	10.08	127.37	118.30
1	B	186	ARG	NE-CZ-NH1	9.91	125.26	120.30
1	A	77	ARG	NE-CZ-NH2	9.82	125.21	120.30
1	B	42	ARG	NE-CZ-NH1	9.74	125.17	120.30
1	A	161	ASP	CB-CG-OD1	9.63	126.97	118.30
1	A	181	LYS	CB-CA-C	9.36	129.13	110.40
1	A	201	ARG	NE-CZ-NH2	9.34	124.97	120.30
1	B	144	ARG	NE-CZ-NH2	-9.30	115.65	120.30
1	A	150	ASP	CB-CG-OD2	9.18	126.56	118.30
1	B	67	ARG	NE-CZ-NH1	9.10	124.85	120.30
1	A	107	ARG	CD-NE-CZ	8.96	136.14	123.60
1	A	81	ARG	CD-NE-CZ	8.84	135.97	123.60
1	A	17	ARG	NE-CZ-NH2	8.79	124.70	120.30
1	B	26	SER	CB-CA-C	8.72	126.67	110.10
1	A	156	ASP	CB-CG-OD1	8.59	126.03	118.30
1	B	97	ASP	CB-CG-OD2	-8.41	110.73	118.30
1	B	77	ARG	NE-CZ-NH2	-8.32	116.14	120.30
1	A	160	TYR	CB-CG-CD2	-8.30	116.02	121.00
1	B	70	THR	CA-CB-OG1	-8.19	91.81	109.00
1	A	97	ASP	CB-CG-OD2	-8.04	111.07	118.30
1	A	201	ARG	NE-CZ-NH1	-7.98	116.31	120.30
1	B	202	TYR	CB-CG-CD2	-7.70	116.38	121.00
1	A	160	TYR	CB-CG-CD1	7.64	125.58	121.00
1	A	27	TYR	CB-CG-CD2	7.60	125.56	121.00
1	A	186	ARG	NE-CZ-NH2	7.58	124.09	120.30
1	A	72	SER	O-C-N	-7.54	110.63	122.70
1	B	67	ARG	CD-NE-CZ	7.36	133.91	123.60
1	B	67	ARG	CA-CB-CG	7.20	129.24	113.40
1	A	31	ARG	NE-CZ-NH2	7.09	123.85	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	12	LEU	CB-CA-C	7.09	123.67	110.20
1	A	77	ARG	CD-NE-CZ	-6.75	114.14	123.60
1	B	80	ALA	CB-CA-C	6.70	120.15	110.10
1	B	173	CYS	CA-CB-SG	6.66	126.00	114.00
1	A	17	ARG	NE-CZ-NH1	-6.65	116.97	120.30
1	A	144	ARG	NH1-CZ-NH2	-6.65	112.09	119.40
1	A	73	ASN	N-CA-CB	6.53	122.35	110.60
1	B	17	ARG	NH1-CZ-NH2	-6.46	112.29	119.40
1	B	202	TYR	CB-CG-CD1	6.46	124.88	121.00
1	A	88	GLU	OE1-CD-OE2	6.39	130.97	123.30
1	B	200	SER	CB-CA-C	-6.35	98.04	110.10
1	B	18	LEU	CA-C-O	6.19	133.11	120.10
1	B	29	GLU	CG-CD-OE1	6.15	130.60	118.30
1	B	156	ASP	N-CA-CB	-6.11	99.60	110.60
1	B	137	TYR	CB-CG-CD2	-6.04	117.38	121.00
1	A	95	ARG	CD-NE-CZ	6.03	132.04	123.60
1	A	160	TYR	CA-C-O	6.01	132.72	120.10
1	A	144	ARG	CD-NE-CZ	6.01	132.01	123.60
1	A	10	ARG	NE-CZ-NH1	-5.98	117.31	120.30
1	A	18	LEU	CB-CG-CD1	-5.97	100.84	111.00
1	B	114	CYS	CB-CA-C	5.96	122.32	110.40
1	B	200	SER	N-CA-CB	5.92	119.37	110.50
1	A	67	ARG	NE-CZ-NH1	5.90	123.25	120.30
1	A	152	VAL	CG1-CB-CG2	-5.90	101.45	110.90
1	B	175	ASP	CB-CA-C	5.90	122.20	110.40
1	B	210	LYS	CA-CB-CG	5.90	126.38	113.40
1	B	30	LYS	N-CA-CB	5.90	121.22	110.60
1	A	174	LEU	N-CA-CB	-5.88	98.65	110.40
1	A	157	PHE	CB-CG-CD1	5.80	124.86	120.80
1	A	27	TYR	CB-CG-CD1	-5.70	117.58	121.00
1	B	107	ARG	NE-CZ-NH1	-5.66	117.47	120.30
1	B	20	LEU	O-C-N	5.64	131.72	122.70
1	A	97	ASP	CB-CG-OD1	5.60	123.34	118.30
1	B	182	ASP	CB-CG-OD2	-5.56	113.29	118.30
1	B	64	ASP	OD1-CG-OD2	-5.52	112.81	123.30
1	B	156	ASP	CB-CG-OD2	-5.52	113.33	118.30
1	B	104	MET	CA-CB-CG	-5.48	103.99	113.30
1	A	108	MET	CG-SD-CE	5.43	108.89	100.20
1	A	71	GLN	OE1-CD-NE2	-5.43	109.41	121.90
1	A	72	SER	CB-CA-C	5.40	120.36	110.10
1	B	125	GLU	CA-CB-CG	5.38	125.23	113.40
1	A	77	ARG	N-CA-CB	5.35	120.22	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	48	GLU	CA-CB-CG	5.33	125.12	113.40
1	A	41	ASP	CB-CG-OD2	5.31	123.08	118.30
1	B	100	GLU	CG-CD-OE1	5.31	128.91	118.30
1	A	174	LEU	CB-CA-C	5.28	120.23	110.20
1	A	99	VAL	CA-CB-CG2	-5.28	102.98	110.90
1	A	72	SER	N-CA-CB	-5.23	102.65	110.50
1	A	72	SER	CA-C-O	5.20	131.02	120.10
1	A	153	THR	OG1-CB-CG2	5.19	121.93	110.00
1	B	100	GLU	CB-CA-C	5.18	120.77	110.40
1	B	173	CYS	CB-CA-C	5.17	120.74	110.40
1	A	165	GLN	CB-CA-C	-5.14	100.11	110.40
1	B	61	TYR	CB-CG-CD2	-5.14	117.92	121.00
1	A	104	MET	CA-CB-CG	-5.14	104.57	113.30
1	B	101	ASN	CB-CG-ND2	5.14	129.03	116.70
1	A	137	TYR	N-CA-CB	5.09	119.76	110.60
1	A	188	GLU	CG-CD-OE1	5.05	128.39	118.30
1	A	196	TYR	C-N-CA	5.01	134.23	121.70

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	144	ARG	Sidechain
1	A	186	ARG	Sidechain
1	A	93	ARG	Sidechain
1	B	144	ARG	Sidechain
1	B	186	ARG	Sidechain
1	B	77	ARG	Sidechain

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	1818	0	1805	78	1
1	B	1818	0	1805	126	2
2	A	5	0	0	0	0
3	A	32	0	18	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	32	0	18	3	0
4	A	198	0	0	2	0
4	B	134	0	0	4	0
All	All	4037	0	3646	210	2

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 29.

All (210) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:174:LEU:HD23	1:B:181:LYS:HG2	1.26	1.14
1:A:34:MET:HE2	1:A:40:TYR:HB3	1.23	1.11
1:B:3:ILE:HG21	1:B:30:LYS:HE3	1.11	1.08
1:B:168:ILE:HG22	1:B:214:TRP:HZ2	1.21	1.05
1:A:191:LYS:CD	1:A:191:LYS:H	1.67	1.04
1:A:95:ARG:HH12	1:A:144:ARG:HH21	1.04	1.03
1:B:127:LEU:HA	1:B:130:ILE:HG13	1.41	0.99
1:B:207:ILE:HG12	1:B:215:SER:OG	1.62	0.98
1:B:212:ALA:HB3	1:B:216:ASN:HB3	1.43	0.97
1:A:8:ASN:HD22	1:A:8:ASN:N	1.59	0.97
3:B:218:GDN:HB21	3:B:218:GDN:O2A	1.64	0.97
1:B:10:ARG:HD3	1:B:207:ILE:HD12	1.48	0.96
1:A:95:ARG:NH1	1:A:144:ARG:HH21	1.62	0.96
1:B:116:ASN:HD22	1:B:118:ASP:H	1.14	0.92
1:B:116:ASN:ND2	1:B:118:ASP:H	1.67	0.92
1:A:34:MET:CE	1:A:40:TYR:HB3	2.00	0.90
1:A:191:LYS:HD2	1:A:191:LYS:H	1.36	0.90
1:B:111:ILE:HG23	1:B:115:TYR:HD2	1.35	0.89
1:A:12:LEU:C	1:A:12:LEU:HD12	1.93	0.88
1:B:111:ILE:HG23	1:B:115:TYR:CD2	2.09	0.88
1:B:174:LEU:HD21	1:B:184:LEU:HD12	1.57	0.87
1:A:12:LEU:HD12	1:A:12:LEU:O	1.74	0.87
1:A:8:ASN:H	1:A:8:ASN:HD22	1.22	0.84
1:B:123:LYS:O	1:B:127:LEU:HG	1.78	0.84
1:B:168:ILE:HG22	1:B:214:TRP:CZ2	2.13	0.82
1:B:193:ILE:O	1:B:197:MET:HG3	1.82	0.80
1:B:125:GLU:O	1:B:128:LYS:HB2	1.82	0.79
1:A:193:ILE:O	1:A:197:MET:HG3	1.82	0.79
1:A:83:HIS:C	1:A:84:HIS:ND1	2.37	0.78
1:A:191:LYS:H	1:A:191:LYS:HD3	1.48	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:124:PRO:O	1:A:128:LYS:HD2	1.84	0.77
3:B:218:GDN:CB2	3:B:218:GDN:O2A	2.33	0.77
1:B:123:LYS:HB3	1:B:124:PRO:HD3	1.64	0.76
1:B:197:MET:SD	4:B:269:HOH:O	2.43	0.75
1:B:116:ASN:O	1:B:213:GLN:OE1	2.03	0.75
1:B:127:LEU:HD13	1:B:170:GLU:OE1	1.85	0.75
1:B:35:GLY:O	1:B:40:TYR:HA	1.87	0.74
1:B:114:CYS:HB2	1:B:208:PHE:HE2	1.51	0.74
1:B:114:CYS:CB	1:B:208:PHE:HE2	2.01	0.73
1:B:114:CYS:O	1:B:213:GLN:HG2	1.88	0.73
1:B:127:LEU:HD23	1:B:169:PHE:CE2	2.25	0.72
1:A:8:ASN:ND2	1:A:8:ASN:H	1.88	0.71
1:A:140:PHE:O	1:A:144:ARG:NH2	2.23	0.71
1:A:118:ASP:O	1:A:122:GLN:HG2	1.90	0.71
1:B:42:ARG:HH12	1:B:45:TRP:HD1	1.37	0.71
1:B:125:GLU:O	1:B:128:LYS:CB	2.39	0.71
1:B:125:GLU:HA	1:B:128:LYS:HD2	1.72	0.70
1:A:95:ARG:HH12	1:A:144:ARG:NH2	1.84	0.70
1:B:113:LEU:HG	1:B:119:PHE:HE1	1.57	0.69
1:B:123:LYS:CG	1:B:127:LEU:HD21	2.22	0.69
1:B:30:LYS:HD2	1:B:61:TYR:OH	1.93	0.68
1:B:205:THR:HG23	1:B:206:PRO:HA	1.76	0.67
1:B:119:PHE:CG	1:B:213:GLN:HG3	2.30	0.66
1:A:34:MET:CE	1:A:211:LEU:HD23	2.26	0.66
1:B:42:ARG:NH1	1:B:45:TRP:HD1	1.94	0.66
1:A:39:ASP:OD1	1:A:39:ASP:N	2.28	0.66
1:B:34:MET:CE	1:B:40:TYR:HB3	2.25	0.65
1:B:174:LEU:CD2	1:B:181:LYS:HG2	2.17	0.65
1:B:52:LEU:O	1:B:68:LYS:NZ	2.20	0.65
1:A:124:PRO:O	1:A:128:LYS:CD	2.44	0.65
1:A:175:ASP:OD1	1:A:181:LYS:NZ	2.30	0.65
1:A:84:HIS:ND1	1:A:84:HIS:N	2.44	0.64
1:B:173:CYS:O	1:B:175:ASP:N	2.30	0.64
1:A:24:ASP:OD2	1:A:192:LYS:HE2	1.98	0.64
1:B:216:ASN:HD22	1:B:216:ASN:C	2.01	0.64
1:B:168:ILE:CG2	1:B:214:TRP:HZ2	2.05	0.63
1:A:191:LYS:N	1:A:191:LYS:CD	2.49	0.63
1:A:144:ARG:HH11	1:A:144:ARG:HG3	1.63	0.63
1:B:34:MET:HE3	1:B:40:TYR:HB3	1.79	0.63
1:A:30:LYS:HE2	1:A:32:TYR:CE1	2.33	0.63
1:B:123:LYS:HG2	1:B:127:LEU:HD21	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:119:PHE:CE2	1:B:214:TRP:HB2	2.35	0.61
1:B:172:LYS:HA	1:B:175:ASP:OD2	2.00	0.61
1:B:113:LEU:HG	1:B:119:PHE:CE1	2.34	0.61
3:A:219:GDN:C6'	3:A:219:GDN:HA2	2.30	0.61
1:B:130:ILE:N	1:B:131:PRO:CD	2.63	0.60
1:B:12:LEU:CB	1:B:107:ARG:HD3	2.33	0.59
1:B:116:ASN:C	1:B:116:ASN:HD22	2.06	0.59
1:A:119:PHE:HB2	1:A:213:GLN:HG3	1.85	0.58
1:B:114:CYS:HB2	1:B:208:PHE:CE2	2.36	0.58
1:A:202:TYR:CE2	1:A:204:SER:OG	2.54	0.58
1:B:40:TYR:HE1	1:B:210:LYS:HB2	1.70	0.57
1:B:146:TRP:CH2	1:B:186:ARG:HG2	2.39	0.57
1:A:95:ARG:NH1	1:A:144:ARG:NH2	2.44	0.57
1:B:8:ASN:HD22	1:B:8:ASN:N	2.02	0.57
1:A:118:ASP:OD2	1:A:122:GLN:OE1	2.22	0.57
1:B:12:LEU:HB2	1:B:107:ARG:HD3	1.87	0.56
1:B:130:ILE:N	1:B:131:PRO:HD2	2.21	0.56
1:B:119:PHE:HB2	1:B:213:GLN:HG3	1.86	0.55
1:B:3:ILE:CG2	1:B:30:LYS:HE3	2.07	0.55
1:A:146:TRP:CE2	1:A:152:VAL:HG22	2.41	0.55
1:A:95:ARG:CZ	1:A:144:ARG:HE	2.20	0.55
1:A:115:TYR:CZ	1:A:212:ALA:HB2	2.41	0.55
1:B:120:GLU:OE1	1:B:120:GLU:HA	2.06	0.54
1:A:191:LYS:N	1:A:191:LYS:HD2	2.16	0.54
1:B:116:ASN:HD22	1:B:118:ASP:N	1.96	0.54
1:B:120:GLU:O	1:B:124:PRO:HD3	2.08	0.54
1:A:174:LEU:HD23	1:A:181:LYS:CG	2.37	0.54
1:B:113:LEU:HD22	1:B:126:PHE:CD2	2.44	0.53
1:B:45:TRP:CZ2	1:B:49:LYS:HG3	2.43	0.53
1:A:34:MET:HE1	1:A:211:LEU:HD23	1.91	0.53
1:B:7:TRP:HZ2	1:B:42:ARG:NH1	2.07	0.53
1:A:95:ARG:NH2	1:A:144:ARG:NE	2.57	0.52
1:B:112:MET:O	1:B:116:ASN:HB2	2.08	0.52
1:A:12:LEU:C	1:A:12:LEU:CD1	2.71	0.52
1:B:118:ASP:OD2	1:B:121:LYS:HB2	2.08	0.52
1:B:123:LYS:HG3	1:B:127:LEU:HD21	1.91	0.52
1:B:119:PHE:CB	1:B:213:GLN:HG3	2.40	0.52
1:B:35:GLY:C	1:B:40:TYR:HA	2.30	0.52
1:A:14:HIS:N	1:A:15:PRO:CD	2.73	0.51
1:A:121:LYS:HD2	1:A:121:LYS:N	2.22	0.51
1:B:114:CYS:CB	1:B:208:PHE:CE2	2.88	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:24:ASP:CG	1:A:192:LYS:HE2	2.31	0.51
1:B:173:CYS:C	1:B:175:ASP:H	2.14	0.51
1:B:8:ASN:H	1:B:8:ASN:HD22	1.59	0.51
1:B:111:ILE:HG22	1:B:112:MET:N	2.26	0.51
1:A:95:ARG:CZ	1:A:144:ARG:HH21	2.23	0.51
1:A:118:ASP:OD2	1:A:122:GLN:HG2	2.12	0.50
1:A:34:MET:HE3	1:A:211:LEU:HD23	1.93	0.50
1:A:32:TYR:HD1	1:A:44:GLN:HG2	1.75	0.50
1:B:203:LEU:HD23	1:B:203:LEU:C	2.32	0.50
1:A:54:LEU:HD23	1:A:68:LYS:HB3	1.94	0.50
1:A:93:ARG:NH2	4:A:322:HOH:O	2.37	0.50
1:B:125:GLU:HA	1:B:128:LYS:HB2	1.94	0.49
1:B:119:PHE:O	1:B:123:LYS:HB2	2.12	0.49
1:B:7:TRP:CZ2	1:B:42:ARG:NH1	2.80	0.49
1:A:174:LEU:HD23	1:A:181:LYS:HG3	1.94	0.49
1:A:8:ASN:O	1:A:8:ASN:CG	2.51	0.49
1:B:22:TYR:O	1:B:192:LYS:HD2	2.13	0.48
1:A:191:LYS:N	1:A:191:LYS:HD3	2.20	0.48
1:A:77:ARG:NH2	1:A:97:ASP:OD1	2.47	0.48
1:B:40:TYR:CE1	1:B:210:LYS:HB2	2.48	0.48
1:B:111:ILE:CG2	1:B:115:TYR:HD2	2.18	0.48
1:B:10:ARG:HD3	1:B:207:ILE:CD1	2.34	0.48
1:B:34:MET:HE2	1:B:40:TYR:HB3	1.95	0.47
1:B:118:ASP:OD2	1:B:121:LYS:HD3	2.13	0.47
1:B:209:SER:C	1:B:211:LEU:N	2.68	0.47
1:B:119:PHE:CD2	1:B:213:GLN:HB2	2.49	0.47
1:B:202:TYR:CE2	1:B:204:SER:HB3	2.50	0.47
1:B:10:ARG:HD2	1:B:204:SER:O	2.14	0.47
1:B:100:GLU:OE1	1:B:154:TYR:OH	2.21	0.47
1:B:113:LEU:HD22	1:B:126:PHE:CG	2.50	0.47
1:B:116:ASN:ND2	1:B:116:ASN:C	2.68	0.47
1:B:114:CYS:SG	1:B:119:PHE:CE1	3.04	0.47
3:B:218:GDN:O2A	3:B:218:GDN:SG2	2.72	0.47
1:B:129:THR:C	1:B:131:PRO:HD2	2.35	0.46
1:A:34:MET:HE3	1:A:211:LEU:CD2	2.45	0.46
1:B:192:LYS:HG3	4:B:263:HOH:O	2.15	0.46
1:B:123:LYS:CB	1:B:124:PRO:HD3	2.38	0.46
1:A:193:ILE:N	1:A:193:ILE:HD12	2.30	0.46
1:B:12:LEU:HB3	1:B:107:ARG:HD3	1.97	0.46
1:B:209:SER:C	1:B:211:LEU:H	2.18	0.46
1:A:8:ASN:ND2	1:A:8:ASN:C	2.68	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:14:HIS:N	1:B:15:PRO:CD	2.79	0.45
1:B:119:PHE:CZ	1:B:169:PHE:HE1	2.35	0.45
1:B:39:ASP:O	1:B:40:TYR:C	2.55	0.45
1:A:2:MET:CE	1:A:82:LYS:NZ	2.80	0.45
1:A:202:TYR:CZ	1:A:204:SER:OG	2.70	0.45
1:A:45:TRP:CZ2	1:A:49:LYS:HG3	2.52	0.45
1:A:2:MET:O	1:A:27:TYR:HA	2.17	0.44
1:B:120:GLU:O	1:B:124:PRO:CD	2.65	0.44
1:B:123:LYS:HB3	1:B:124:PRO:CD	2.43	0.44
1:A:10:ARG:HD2	1:A:10:ARG:HH11	1.58	0.44
1:A:12:LEU:CD1	1:A:12:LEU:O	2.56	0.44
1:A:24:ASP:OD2	1:A:192:LYS:CE	2.66	0.44
1:B:173:CYS:C	1:B:175:ASP:N	2.69	0.44
1:A:122:GLN:O	1:A:125:GLU:HB2	2.18	0.43
1:B:8:ASN:ND2	4:B:254:HOH:O	2.51	0.43
1:A:123:LYS:N	1:A:124:PRO:HD2	2.33	0.43
1:A:43:SER:HA	1:A:46:LEU:HB2	1.99	0.43
1:B:110:LEU:O	1:B:111:ILE:C	2.56	0.43
1:B:125:GLU:C	1:B:128:LYS:HB2	2.38	0.43
1:B:146:TRP:CE2	1:B:152:VAL:HG22	2.54	0.43
1:B:203:LEU:CD2	1:B:203:LEU:C	2.87	0.43
1:B:10:ARG:O	1:B:11:GLY:C	2.57	0.43
1:B:114:CYS:HB3	1:B:208:PHE:CE2	2.54	0.43
1:A:115:TYR:HE2	1:A:211:LEU:CD1	2.30	0.42
1:B:127:LEU:HG	1:B:127:LEU:H	1.67	0.42
1:B:113:LEU:C	1:B:115:TYR:N	2.73	0.42
1:A:205:THR:HB	1:A:206:PRO:HA	2.01	0.42
1:A:99:VAL:O	1:A:100:GLU:C	2.57	0.42
1:A:130:ILE:N	1:A:131:PRO:CD	2.83	0.42
1:B:123:LYS:CB	1:B:124:PRO:CD	2.97	0.42
1:A:2:MET:HE3	4:A:293:HOH:O	2.19	0.42
1:A:162:ILE:HD12	1:A:162:ILE:HA	1.74	0.42
1:B:110:LEU:O	1:B:113:LEU:HB3	2.20	0.42
1:B:216:ASN:ND2	1:B:217:LYS:HG2	2.35	0.42
1:B:152:VAL:HG23	4:B:258:HOH:O	2.19	0.42
1:A:79:LEU:HD23	1:A:79:LEU:HA	1.87	0.42
1:B:108:MET:HE3	1:B:108:MET:HB2	1.92	0.42
1:B:126:PHE:C	1:B:128:LYS:H	2.21	0.41
1:A:116:ASN:C	1:A:118:ASP:H	2.24	0.41
1:B:111:ILE:O	1:B:115:TYR:N	2.53	0.41
1:B:119:PHE:HE2	1:B:214:TRP:HB2	1.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:77:ARG:CZ	1:B:100:GLU:OE1	2.69	0.41
1:A:210:LYS:HG2	1:A:210:LYS:H	1.49	0.41
1:B:168:ILE:CG2	1:B:214:TRP:CZ2	2.91	0.41
1:B:107:ARG:HG3	1:B:107:ARG:HH11	1.85	0.41
1:B:167:HIS:O	1:B:167:HIS:CG	2.74	0.41
1:B:216:ASN:HD22	1:B:217:LYS:N	2.18	0.41
1:A:22:TYR:HB2	1:A:193:ILE:HD11	2.03	0.41
1:B:40:TYR:HE1	1:B:210:LYS:CB	2.33	0.41
1:B:172:LYS:HE2	1:B:172:LYS:HB3	1.89	0.41
1:A:71:GLN:OE1	3:A:219:GDN:N1	2.54	0.41
1:A:24:ASP:OD1	1:A:192:LYS:HE2	2.21	0.41
3:A:219:GDN:HA2	3:A:219:GDN:H6'	2.01	0.40
1:A:33:ALA:H	1:A:44:GLN:NE2	2.19	0.40
1:B:118:ASP:OD2	1:B:121:LYS:CD	2.70	0.40
3:A:219:GDN:SG2	3:A:219:GDN:O2A	2.79	0.40
1:B:134:MET:CE	1:B:166:TYR:CD2	3.04	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:67:ARG:NH2	1:B:67:ARG:NH2[2_555]	1.70	0.50
1:A:90:GLU:CB	1:B:67:ARG:NH1[2_555]	2.00	0.20

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	215/217 (99%)	201 (94%)	14 (6%)	0	100 100
1	B	215/217 (99%)	196 (91%)	15 (7%)	4 (2%)	10 4
All	All	430/434 (99%)	397 (92%)	29 (7%)	4 (1%)	21 13

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	111	ILE
1	B	112	MET
1	B	174	LEU
1	B	119	PHE

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	197/197 (100%)	182 (92%)	15 (8%)	16 10
1	B	197/197 (100%)	179 (91%)	18 (9%)	12 6
All	All	394/394 (100%)	361 (92%)	33 (8%)	14 8

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	PRO
1	A	3	ILE
1	A	8	ASN
1	A	12	LEU
1	A	19	LEU
1	A	41	ASP
1	A	46	LEU
1	A	84	HIS
1	A	120	GLU
1	A	121	LYS
1	A	144	ARG
1	A	151	LYS
1	A	178	PRO
1	A	191	LYS
1	A	203	LEU
1	B	8	ASN
1	B	12	LEU
1	B	19	LEU
1	B	28	GLU

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Mol	Chain	Res	Type
1	B	88	GLU
1	B	108	MET
1	B	113	LEU
1	B	116	ASN
1	B	118	ASP
1	B	127	LEU
1	B	151	LYS
1	B	166	TYR
1	B	167	HIS
1	B	172	LYS
1	B	174	LEU
1	B	191	LYS
1	B	213	GLN
1	B	216	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	ASN
1	A	44	GLN
1	A	122	GLN
1	A	216	ASN
1	B	8	ASN
1	B	116	ASN
1	B	216	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 carbohydrates in this entry.

5.6 Ligand geometry (i)

3 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	SO4	A	218	-	4,4,4	1.20	0	6,6,6	0.42	0
3	GDN	A	219	-	22,32,32	2.26	3 (13%)	25,43,43	2.12	10 (40%)
3	GDN	B	218	-	22,32,32	1.72	4 (18%)	25,43,43	2.33	9 (36%)

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	SO4	A	218	-	-	0/0/0/0	0/0/0/0
3	GDN	A	219	-	-	0/28/35/35	0/1/1/1
3	GDN	B	218	-	-	0/28/35/35	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	218	GDN	C1'-SG2	-5.59	1.69	1.77
3	A	219	GDN	C1'-SG2	-5.01	1.70	1.77
3	B	218	GDN	CB2-SG2	-3.31	1.74	1.81
3	A	219	GDN	CB2-SG2	-2.63	1.75	1.81
3	B	218	GDN	C2-N3	-2.28	1.28	1.33
3	B	218	GDN	CB1-CG1	2.15	1.59	1.52
3	A	219	GDN	O4B-N4'	7.90	1.38	1.22

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	218	GDN	C3'-C2'-C1'	-4.04	118.52	122.92
3	A	219	GDN	C3'-C2'-C1'	-4.02	118.54	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	219	GDN	CA3-N3-C2	-3.56	117.44	122.34
3	A	219	GDN	OE1-CD1-CG1	-2.53	117.62	121.98
3	A	219	GDN	CB1-CG1-CD1	-2.36	107.65	113.27
3	B	218	GDN	C3-CA3-N3	-2.35	105.67	111.74
3	B	218	GDN	CB1-CG1-CD1	-2.34	107.71	113.27
3	A	219	GDN	CG1-CD1-N2	-2.21	112.23	115.83
3	A	219	GDN	O2-C2-CA2	-2.20	115.49	120.36
3	B	218	GDN	O2-C2-CA2	-2.17	115.57	120.36
3	B	218	GDN	CG1-CD1-N2	-2.05	112.50	115.83
3	A	219	GDN	CA2-C2-N3	2.46	121.55	116.72
3	A	219	GDN	C6'-C1'-C2'	2.60	122.22	118.30
3	B	218	GDN	CA3-N3-C2	2.64	125.97	122.34
3	B	218	GDN	C6'-C1'-C2'	2.98	122.79	118.30
3	A	219	GDN	CB2-SG2-C1'	3.15	109.34	102.09
3	B	218	GDN	O4B-N4'-C4'	3.61	125.37	118.89
3	A	219	GDN	OE1-CD1-N2	4.13	130.02	123.01
3	B	218	GDN	CB2-SG2-C1'	7.07	118.36	102.09

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	219	GDN	4	0
3	B	218	GDN	3	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.