



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 09:32 AM UTC

PDB ID : 3GST / pdb_00003gst
Title : STRUCTURE OF THE XENOBIOTIC SUBSTRATE BINDING SITE OF A GLUTATHIONE S-TRANSFERASE AS REVEALED BY X-RAY CRYSTALLOGRAPHIC ANALYSIS OF PRODUCT COMPLEXES WITH THE DIASTEREOMERS OF 9-(S-GLUTATHIONYL)-10-HYDROXY-9, 10-DIHYDROPHENANTHRENE
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Deposited on : 1993-06-07
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 ⓘ 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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

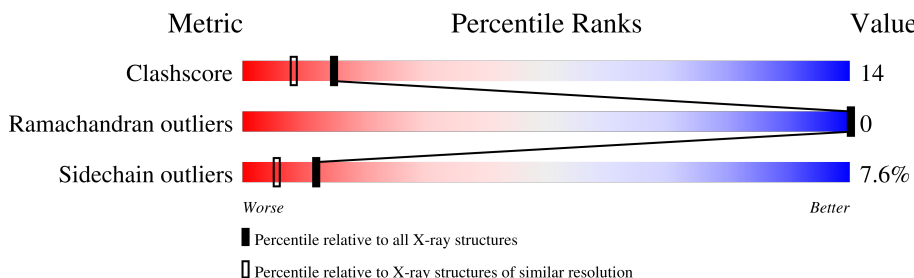
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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))
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	217	
1	B	217	

2 Entry composition [i](#)

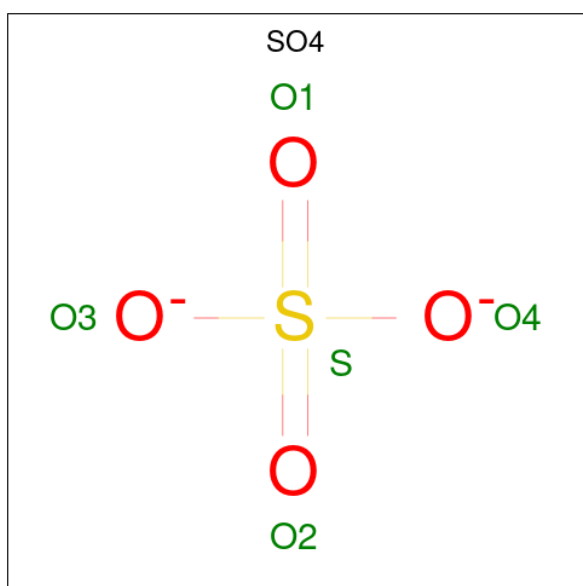
There are 4 unique types of molecules in this entry. The entry contains 4178 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 (CCD ID: SO4) (formula: O₄S).



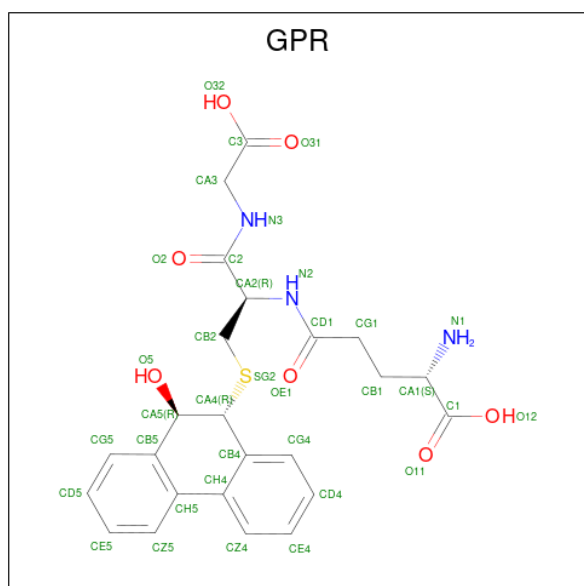
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		

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

- Molecule 3 is (9R,10R)-9-(S-GLUTATHIONYL)-10-HYDROXY-9,10-DIHYDROPHENANTHRENE (CCD ID: GPR) (formula: $C_{24}H_{27}N_3O_7S$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	
			35	24	3	7	1	0
3	B	1	Total	C	N	O	S	
			35	24	3	7	1	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	252	Total	O	0	0
			252	252		
4	B	185	Total	O	0	0
			185	185		

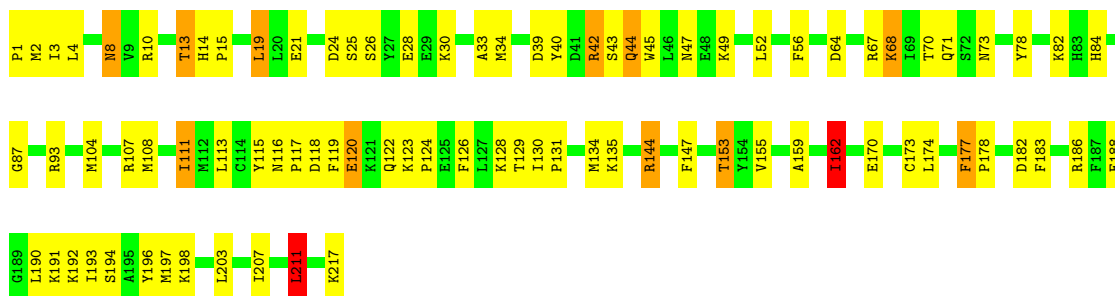
3 Residue-property plots

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. 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. 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.

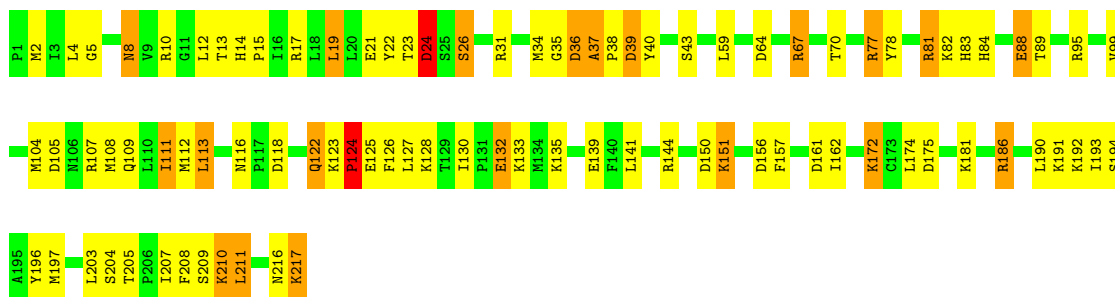
• Molecule 1: GLUTATHIONE S-TRANSFERASE

Chain A: 



• Molecule 1: GLUTATHIONE S-TRANSFERASE

Chain B: 



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore 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) – 1.90	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-1.90)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	GPRLSA	Depositor
R, R_{free}	0.159 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4178	wwPDB-VP
Average B, all atoms (Å ²)	19.0	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: GPR, 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	1.35	2/1867 (0.1%)	1.89	37/2515 (1.5%)
1	B	1.44	7/1867 (0.4%)	1.87	40/2515 (1.6%)
All	All	1.40	9/3734 (0.2%)	1.88	77/5030 (1.5%)

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	1
All	All	0	4

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	59	LEU	CA-C	6.70	1.59	1.52
1	B	4	LEU	C-N	-5.91	1.28	1.33
1	B	157	PHE	N-CA	5.60	1.53	1.46
1	B	77	ARG	NE-CZ	5.45	1.39	1.33
1	B	83	HIS	ND1-CE1	5.42	1.38	1.32
1	A	56	PHE	N-CA	5.27	1.52	1.46
1	B	31	ARG	CD-NE	5.26	1.53	1.46
1	B	5	GLY	C-O	5.22	1.30	1.23
1	A	4	LEU	N-CA	5.05	1.52	1.46

All (77) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	93	ARG	CD-NE-CZ	13.36	143.10	124.40
1	B	144	ARG	CD-NE-CZ	11.57	140.60	124.40
1	A	93	ARG	NE-CZ-NH1	11.02	132.52	121.50
1	B	84	HIS	CA-CB-CG	-10.16	103.64	113.80
1	B	24	ASP	CA-CB-CG	-9.12	103.48	112.60
1	A	120	GLU	CB-CG-CD	8.73	127.44	112.60
1	A	107	ARG	NE-CZ-NH2	7.81	126.23	119.20
1	B	205	THR	O-C-N	7.61	126.58	121.71
1	A	14	HIS	CA-CB-CG	7.54	121.34	113.80
1	B	205	THR	CA-C-O	-7.36	113.72	120.50
1	B	210	LYS	CA-C-N	7.21	130.66	120.28
1	B	210	LYS	C-N-CA	7.21	130.66	120.28
1	A	122	GLN	OE1-CD-NE2	7.15	129.75	122.60
1	A	84	HIS	CA-CB-CG	-7.08	106.72	113.80
1	B	26	SER	CB-CA-C	7.02	122.40	110.81
1	B	130	ILE	O-C-N	6.91	124.84	120.42
1	A	13	THR	CA-CB-OG1	-6.89	99.27	109.60
1	B	132	GLU	CB-CG-CD	6.87	124.27	112.60
1	B	83	HIS	CA-CB-CG	-6.65	107.15	113.80
1	B	43	SER	N-CA-C	6.58	119.30	111.33
1	B	204	SER	CA-CB-OG	-6.39	98.33	111.10
1	B	211	LEU	N-CA-C	6.37	119.04	111.71
1	B	105	ASP	N-CA-CB	6.30	119.15	110.01
1	B	141	LEU	O-C-N	6.27	128.86	122.09
1	A	117	PRO	CB-CA-C	6.25	120.81	111.68
1	B	124	PRO	CA-C-N	6.17	129.06	120.29
1	B	124	PRO	C-N-CA	6.17	129.06	120.29
1	A	120	GLU	CG-CD-OE1	6.16	132.56	118.40
1	A	162	ILE	CA-C-O	-6.14	114.34	120.85
1	B	77	ARG	CD-NE-CZ	-6.09	115.88	124.40
1	B	99	VAL	O-C-N	6.04	127.83	121.91
1	B	39	ASP	N-CA-C	6.00	117.62	111.14
1	A	183	PHE	CA-C-O	-5.98	114.55	120.82
1	B	151	LYS	O-C-N	5.94	130.36	123.17
1	A	43	SER	N-CA-C	5.84	118.40	111.33
1	B	81	ARG	NE-CZ-NH1	5.83	127.33	121.50
1	A	47	ASN	OD1-CG-ND2	5.78	128.38	122.60
1	A	144	ARG	O-C-N	5.74	127.84	121.53
1	A	87	GLY	N-CA-C	-5.72	104.76	112.14
1	B	4	LEU	CA-C-N	5.63	127.97	122.73
1	B	4	LEU	C-N-CA	5.63	127.97	122.73
1	A	42	ARG	CD-NE-CZ	-5.62	116.53	124.40
1	A	19	LEU	O-C-N	5.60	128.54	122.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	93	ARG	NE-CZ-NH2	-5.59	114.17	119.20
1	B	156	ASP	O-C-N	5.59	129.14	122.27
1	B	83	HIS	O-C-N	5.58	128.90	122.25
1	A	44	GLN	O-C-N	5.57	127.81	122.07
1	A	68	LYS	O-C-N	5.55	129.71	123.27
1	A	173	CYS	N-CA-C	5.54	119.66	113.01
1	B	211	LEU	N-CA-CB	-5.49	101.76	110.22
1	B	70	THR	CA-C-O	-5.49	115.21	121.58
1	A	15	PRO	O-C-N	5.46	128.52	122.24
1	B	2	MET	N-CA-C	-5.46	103.18	110.55
1	A	147	PHE	N-CA-C	5.44	117.21	111.28
1	B	105	ASP	CA-C-O	-5.40	115.15	120.82
1	A	135	LYS	CG-CD-CE	5.34	123.59	111.30
1	B	17	ARG	NE-CZ-NH2	-5.33	114.40	119.20
1	B	122	GLN	N-CA-C	5.30	117.97	111.82
1	A	14	HIS	CA-C-N	5.28	125.33	119.32
1	A	14	HIS	C-N-CA	5.28	125.33	119.32
1	A	211	LEU	N-CA-CB	-5.27	101.64	110.39
1	A	129	THR	CA-C-O	-5.22	112.84	119.31
1	B	161	ASP	CA-CB-CG	-5.20	107.40	112.60
1	A	73	ASN	CA-C-O	-5.17	114.25	120.10
1	A	3	ILE	CA-C-O	-5.16	115.01	120.53
1	A	134	MET	CA-C-O	5.15	125.88	120.42
1	B	95	ARG	NE-CZ-NH1	5.14	126.64	121.50
1	A	3	ILE	O-C-N	5.14	129.11	123.10
1	B	150	ASP	O-C-N	5.11	129.27	122.43
1	A	153	THR	CA-C-O	-5.10	115.73	121.40
1	B	190	LEU	CB-CA-C	5.09	117.84	109.90
1	A	182	ASP	O-C-N	5.08	127.50	122.12
1	B	89	THR	CA-CB-OG1	-5.07	102.00	109.60
1	B	17	ARG	NE-CZ-NH1	5.06	126.56	121.50
1	B	37	ALA	N-CA-C	-5.03	102.71	110.01
1	A	177	PHE	N-CA-C	5.02	118.25	108.21
1	A	159	ALA	O-C-N	5.00	127.42	122.12

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	144	ARG	Sidechain
1	A	186	ARG	Sidechain
1	A	42	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	B	186	ARG	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1818	0	1805	38	0
1	B	1818	0	1805	63	0
2	A	25	0	0	0	0
2	B	10	0	0	2	0
3	A	35	0	25	0	0
3	B	35	0	25	2	0
4	A	252	0	0	2	0
4	B	185	0	0	4	0
All	All	4178	0	3660	101	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 14.

All (101) 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:34:MET:HE3	1:A:40:TYR:HB3	1.31	1.10
1:B:34:MET:HE1	1:B:209:SER:HB2	1.36	1.03
1:B:108:MET:O	1:B:112:MET:HG3	1.69	0.92
1:A:1:PRO:HG2	1:A:28:GLU:OE1	1.75	0.87
1:A:34:MET:CE	1:A:40:TYR:HB3	2.05	0.87
1:A:193:ILE:CG2	1:A:197:MET:HE3	2.10	0.81
1:B:123:LYS:HB3	1:B:124:PRO:HD3	1.64	0.79
1:A:52:LEU:O	1:A:68:LYS:NZ	2.16	0.77
1:B:88:GLU:HG2	1:B:151:LYS:NZ	2.00	0.77
1:B:36:ASP:N	1:B:36:ASP:OD1	2.18	0.75
1:A:193:ILE:HG22	1:A:197:MET:HE3	1.71	0.72
1:A:124:PRO:O	1:A:128:LYS:HE3	1.90	0.71
1:B:35:GLY:O	1:B:40:TYR:HD1	1.74	0.69
1:B:40:TYR:CE2	1:B:211:LEU:HD13	2.28	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:172:LYS:HD2	1:B:175:ASP:OD2	1.93	0.67
1:B:88:GLU:HG2	1:B:151:LYS:HZ1	1.59	0.66
1:B:109:GLN:OE1	1:B:133:LYS:HE2	1.96	0.65
1:B:34:MET:HE1	1:B:209:SER:CB	2.22	0.65
1:B:40:TYR:CD2	1:B:211:LEU:HD13	2.34	0.63
1:B:175:ASP:OD1	1:B:181:LYS:NZ	2.30	0.60
1:A:104:MET:O	1:A:108:MET:HG2	2.01	0.60
1:B:24:ASP:OD2	1:B:192:LYS:HE2	2.03	0.59
1:B:194:SER:HA	1:B:197:MET:HE2	1.86	0.58
1:B:24:ASP:OD2	1:B:192:LYS:CE	2.52	0.57
1:A:64:ASP:OD2	1:A:82:LYS:NZ	2.37	0.57
1:B:38:PRO:HG2	1:B:39:ASP:N	2.20	0.57
1:B:125:GLU:OE2	1:B:128:LYS:NZ	2.36	0.57
1:B:67:ARG:NH2	4:B:287:HOH:O	2.37	0.56
1:A:116:ASN:OD1	1:A:118:ASP:HB2	2.06	0.55
1:A:188:GLU:HG2	1:A:197:MET:HE1	1.87	0.55
1:B:22:TYR:O	1:B:192:LYS:HD2	2.07	0.54
1:B:116:ASN:OD1	1:B:118:ASP:HB2	2.08	0.53
1:A:113:LEU:HD22	1:A:126:PHE:CG	2.44	0.53
1:B:35:GLY:O	1:B:40:TYR:HA	2.09	0.53
1:B:40:TYR:CE2	1:B:211:LEU:CD1	2.91	0.53
1:B:19:LEU:HD22	1:B:23:THR:HG23	1.90	0.53
1:B:111:ILE:HG12	1:B:208:PHE:CE1	2.43	0.52
1:B:186:ARG:HD3	2:B:218:SO4:O1	2.09	0.52
1:B:135:LYS:NZ	4:B:289:HOH:O	2.42	0.52
1:A:21:GLU:HG3	1:A:196:TYR:CD1	2.44	0.52
1:B:14:HIS:N	1:B:15:PRO:CD	2.73	0.51
1:A:45:TRP:CZ2	1:A:49:LYS:HG3	2.46	0.51
1:B:8:ASN:HD22	1:B:8:ASN:H	1.57	0.51
1:B:217:LYS:NZ	4:B:352:HOH:O	2.43	0.51
1:A:10:ARG:HB3	1:A:207:ILE:HA	1.93	0.51
1:B:111:ILE:HG22	1:B:112:MET:N	2.26	0.51
1:A:190:LEU:HB2	1:A:193:ILE:HG12	1.94	0.50
1:A:111:ILE:HD13	1:A:115:TYR:CE1	2.48	0.49
1:B:193:ILE:O	1:B:197:MET:HG3	2.13	0.49
1:A:153:THR:OG1	1:A:155:VAL:HG22	2.13	0.48
1:B:135:LYS:NZ	1:B:139:GLU:OE2	2.41	0.48
1:B:108:MET:O	1:B:112:MET:CG	2.52	0.48
1:A:115:TYR:CE2	1:A:211:LEU:HD23	2.49	0.48
1:B:8:ASN:H	1:B:8:ASN:ND2	2.12	0.47
1:B:123:LYS:HB3	1:B:124:PRO:CD	2.39	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:8:ASN:HD22	1:B:8:ASN:N	2.12	0.47
1:B:81:ARG:HD3	2:B:219:SO4:O4	2.15	0.47
1:A:8:ASN:HD22	1:A:8:ASN:N	2.13	0.47
1:A:30:LYS:NZ	4:A:318:HOH:O	2.42	0.47
1:A:2:MET:CE	1:A:25:SER:HB3	2.45	0.46
1:B:123:LYS:HE2	1:B:127:LEU:HD11	1.97	0.46
1:A:33:ALA:H	1:A:44:GLN:NE2	2.14	0.46
1:B:12:LEU:HB3	1:B:107:ARG:HD3	1.96	0.46
1:B:113:LEU:HD22	1:B:126:PHE:CG	2.50	0.46
1:B:21:GLU:HG3	1:B:196:TYR:CD1	2.51	0.46
1:B:38:PRO:CG	1:B:39:ASP:N	2.79	0.46
1:B:111:ILE:HG13	3:B:220:GPR:CE5	2.46	0.46
1:B:123:LYS:CB	1:B:124:PRO:HD3	2.42	0.46
1:B:64:ASP:OD2	1:B:78:TYR:OH	2.34	0.45
1:B:77:ARG:HH11	1:B:77:ARG:HD3	1.57	0.45
1:B:37:ALA:HB2	1:B:40:TYR:CZ	2.51	0.45
1:A:177:PHE:HA	1:A:178:PRO:HD2	1.83	0.45
1:B:88:GLU:CG	1:B:151:LYS:NZ	2.77	0.45
1:A:78:TYR:OH	1:A:82:LYS:NZ	2.36	0.45
1:B:24:ASP:OD2	1:B:192:LYS:NZ	2.49	0.45
1:B:88:GLU:CG	1:B:151:LYS:HZ1	2.26	0.44
1:B:203:LEU:HD23	1:B:203:LEU:C	2.43	0.44
1:A:13:THR:HG22	1:A:13:THR:O	2.17	0.44
1:B:10:ARG:HB3	1:B:207:ILE:HA	2.00	0.44
1:B:111:ILE:HG13	3:B:220:GPR:CD5	2.48	0.44
1:B:124:PRO:O	1:B:128:LYS:HG3	2.19	0.43
1:A:70:THR:O	1:A:71:GLN:HB2	2.19	0.43
1:B:38:PRO:HG2	1:B:39:ASP:OD2	2.19	0.43
1:A:8:ASN:HD22	1:A:8:ASN:H	1.65	0.42
1:B:104:MET:O	1:B:108:MET:HG2	2.19	0.42
1:B:111:ILE:CG2	1:B:112:MET:N	2.81	0.42
1:A:34:MET:HE2	1:A:40:TYR:CD1	2.55	0.42
1:B:122:GLN:HE21	1:B:122:GLN:HB3	1.67	0.42
1:A:123:LYS:N	1:A:124:PRO:CD	2.81	0.42
1:A:24:ASP:OD2	1:A:192:LYS:HE3	2.20	0.42
1:B:82:LYS:HE3	4:B:327:HOH:O	2.20	0.42
1:A:194:SER:O	1:A:198:LYS:HD2	2.19	0.41
1:A:2:MET:HG2	1:A:64:ASP:HB2	2.03	0.41
1:A:119:PHE:CZ	1:A:123:LYS:HD3	2.56	0.41
1:A:162:ILE:HD12	1:A:162:ILE:HA	1.87	0.41
1:B:209:SER:O	1:B:216:ASN:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:40:TYR:CE1	1:B:210:LYS:HB3	2.55	0.41
1:A:108:MET:HE3	1:A:108:MET:HB3	1.72	0.41
1:A:130:ILE:N	1:A:131:PRO:CD	2.84	0.41
1:A:192:LYS:HD3	4:A:286:HOH:O	2.21	0.41
1:B:13:THR:HG22	1:B:13:THR:O	2.21	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	215/217 (99%)	212 (99%)	3 (1%)	0	100	100
1	B	215/217 (99%)	211 (98%)	4 (2%)	0	100	100
All	All	430/434 (99%)	423 (98%)	7 (2%)	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	197/197 (100%)	183 (93%)	14 (7%)	13	7
1	B	197/197 (100%)	181 (92%)	16 (8%)	11	5
All	All	394/394 (100%)	364 (92%)	30 (8%)	12	5

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	ASN
1	A	19	LEU
1	A	26	SER
1	A	39	ASP
1	A	67	ARG
1	A	111	ILE
1	A	120	GLU
1	A	162	ILE
1	A	170	GLU
1	A	174	LEU
1	A	191	LYS
1	A	203	LEU
1	A	211	LEU
1	A	217	LYS
1	B	8	ASN
1	B	19	LEU
1	B	24	ASP
1	B	26	SER
1	B	36	ASP
1	B	67	ARG
1	B	88	GLU
1	B	111	ILE
1	B	113	LEU
1	B	124	PRO
1	B	132	GLU
1	B	162	ILE
1	B	172	LYS
1	B	174	LEU
1	B	191	LYS
1	B	217	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	ASN
1	A	44	GLN
1	A	106	ASN
1	B	8	ASN
1	B	106	ASN
1	B	122	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

9 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	220	-	4,4,4	0.89	0	6,6,6	0.32	0
2	SO4	B	218	-	4,4,4	0.75	0	6,6,6	0.39	0
3	GPR	B	220	-	35,37,37	2.20	11 (31%)	46,51,51	1.90	14 (30%)
2	SO4	A	222	-	4,4,4	0.86	0	6,6,6	0.33	0
3	GPR	A	223	-	35,37,37	1.86	7 (20%)	46,51,51	1.58	8 (17%)
2	SO4	A	218	-	4,4,4	0.88	0	6,6,6	0.29	0
2	SO4	B	219	-	4,4,4	1.07	0	6,6,6	0.37	0
2	SO4	A	221	-	4,4,4	0.93	0	6,6,6	0.47	0
2	SO4	A	219	-	4,4,4	0.84	0	6,6,6	0.21	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
3	GPR	A	223	-	-	2/27/43/43	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GPR	B	220	-	-	2/27/43/43	0/3/3/3

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	220	GPR	CA4-SG2	-6.15	1.68	1.84
3	B	220	GPR	O11-C1	5.60	1.38	1.22
3	A	223	GPR	CB2-SG2	-5.45	1.76	1.82
3	A	223	GPR	CA4-SG2	-5.25	1.70	1.84
3	A	223	GPR	O11-C1	3.80	1.33	1.22
3	B	220	GPR	O5-CA5	3.66	1.49	1.42
3	B	220	GPR	CB1-CA1	3.53	1.60	1.53
3	B	220	GPR	CG4-CB4	3.33	1.43	1.39
3	B	220	GPR	O12-C1	-3.21	1.20	1.30
3	B	220	GPR	C2-N3	-2.73	1.27	1.33
3	B	220	GPR	CA2-N2	2.61	1.51	1.45
3	B	220	GPR	CZ5-CH5	2.44	1.43	1.40
3	A	223	GPR	O12-C1	-2.42	1.23	1.30
3	B	220	GPR	CA3-N3	2.40	1.51	1.45
3	A	223	GPR	CB1-CA1	2.28	1.58	1.53
3	A	223	GPR	CG4-CB4	2.26	1.42	1.39
3	B	220	GPR	CH4-CB4	2.18	1.43	1.40
3	A	223	GPR	CZ5-CH5	2.06	1.43	1.40

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	220	GPR	O32-C3-O31	-4.54	111.66	123.33
3	B	220	GPR	O5-CA5-CB5	-4.10	102.60	110.42
3	A	223	GPR	O32-C3-O31	-3.89	113.34	123.33
3	B	220	GPR	OE1-CD1-N2	3.89	129.53	122.95
3	A	223	GPR	OE1-CD1-CG1	-3.68	115.35	122.02
3	B	220	GPR	CG1-CB1-CA1	-3.40	106.07	113.86
3	B	220	GPR	O2-C2-CA2	-3.08	114.03	120.48
3	B	220	GPR	OE1-CD1-CG1	-3.07	116.47	122.02
3	A	223	GPR	CG1-CB1-CA1	-3.01	106.96	113.86
3	A	223	GPR	O5-CA5-CB5	-2.84	105.01	110.42
3	A	223	GPR	CB1-CG1-CD1	2.66	119.00	113.06
3	A	223	GPR	CA5-CA4-SG2	-2.65	102.78	110.88
3	B	220	GPR	CB1-CA1-C1	-2.45	103.96	110.45
3	B	220	GPR	O2-C2-N3	2.37	128.00	122.98
3	A	223	GPR	CB1-CA1-C1	-2.36	104.19	110.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	220	GPR	CG5-CB5-CH5	2.35	122.23	119.35
3	B	220	GPR	O32-C3-CA3	2.35	121.75	112.81
3	B	220	GPR	CA2-N2-CD1	-2.28	115.97	121.68
3	B	220	GPR	C3-CA3-N3	-2.14	106.41	113.06
3	B	220	GPR	CA2-CB2-SG2	-2.14	105.87	113.66
3	A	223	GPR	OE1-CD1-N2	2.07	126.46	122.95
3	B	220	GPR	CG5-CB5-CA5	-2.06	116.83	120.94

There are no chirality outliers.

All (4) torsion outliers are listed below:

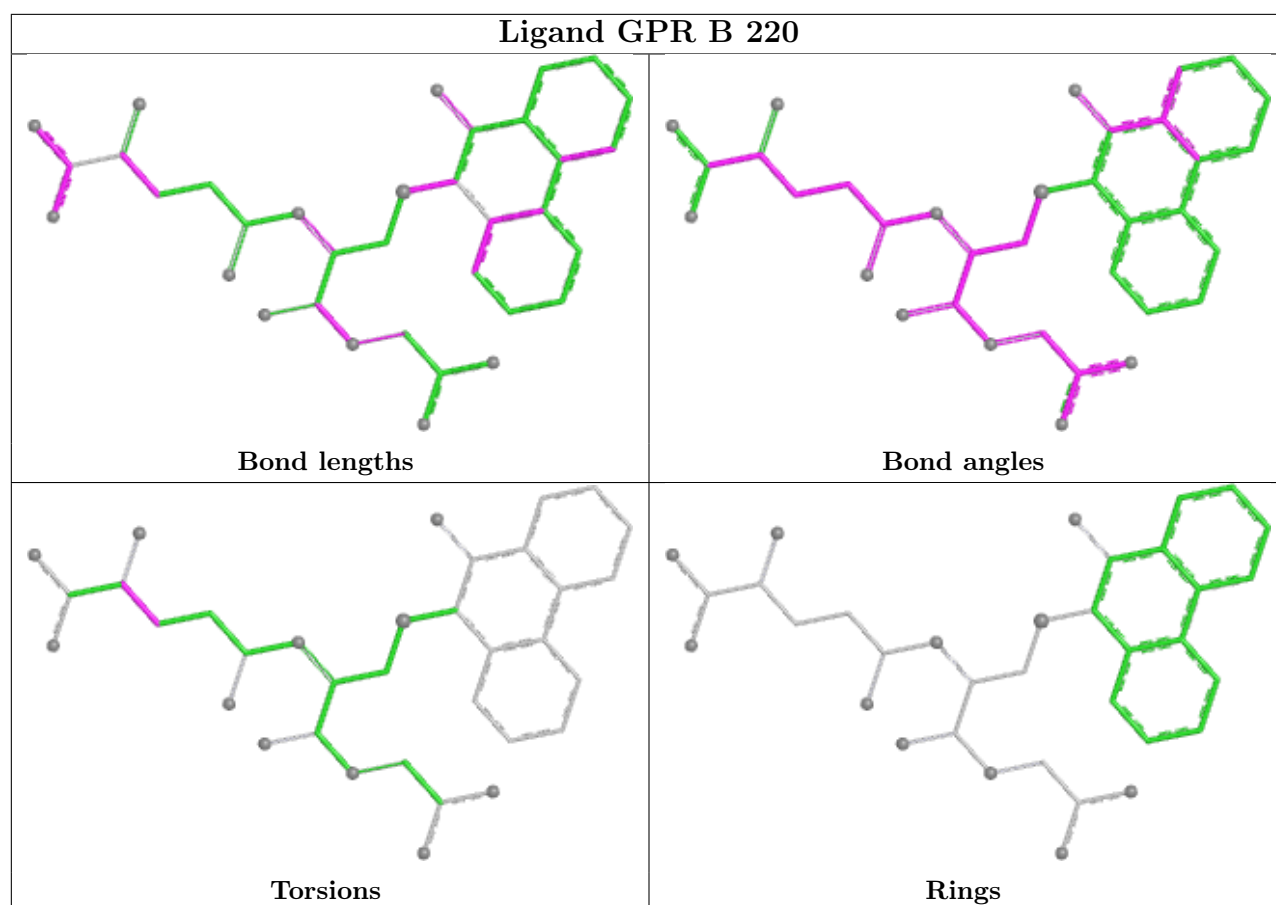
Mol	Chain	Res	Type	Atoms
3	A	223	GPR	C1-CA1-CB1-CG1
3	B	220	GPR	N1-CA1-CB1-CG1
3	B	220	GPR	C1-CA1-CB1-CG1
3	A	223	GPR	N1-CA1-CB1-CG1

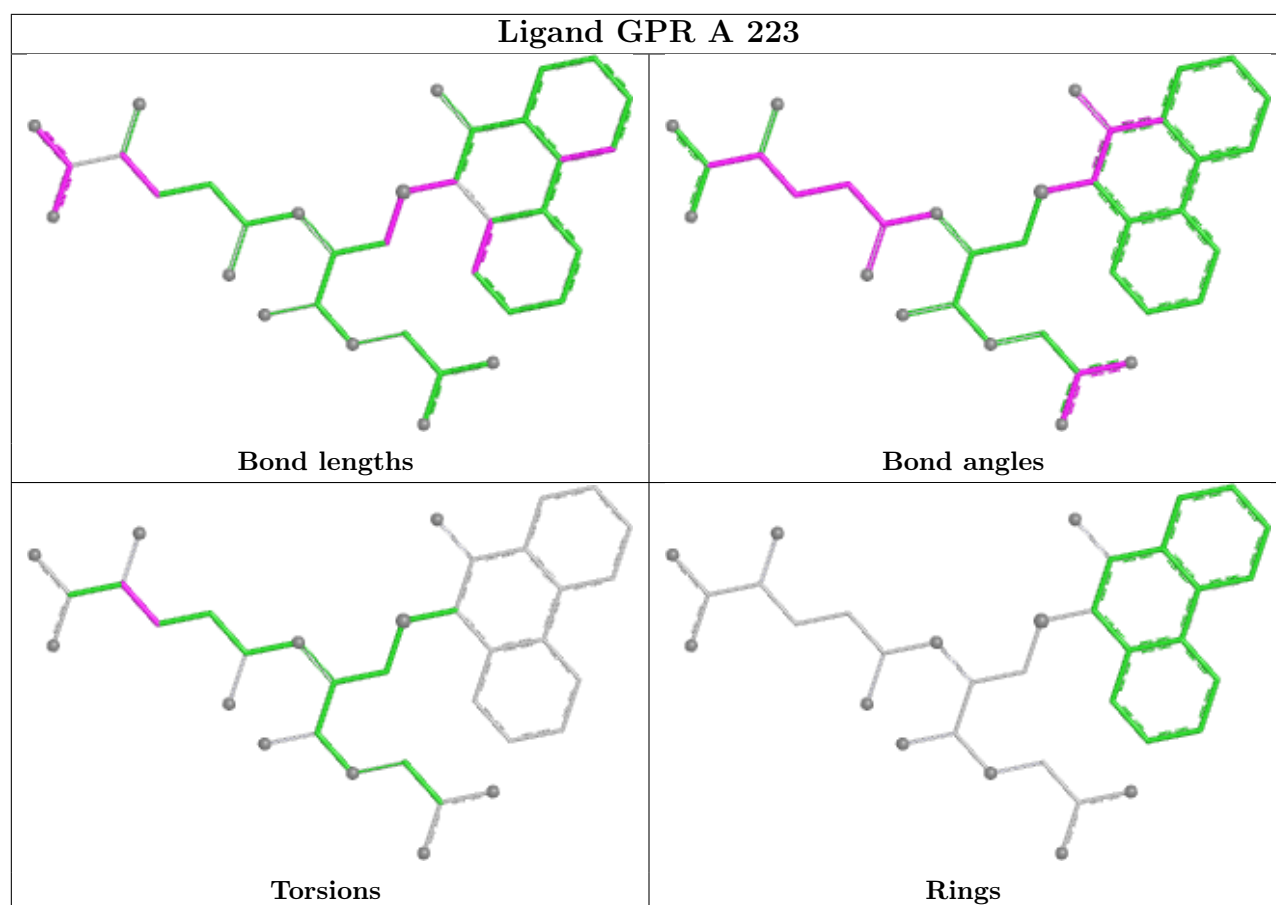
There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	218	SO4	1	0
3	B	220	GPR	2	0
2	B	219	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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.