



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 06:46 AM UTC

PDB ID : 1MTC / pdb_00001mtc
Title : GLUTATHIONE TRANSFERASE MUTANT Y115F
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Deposited on : 2002-09-20
Resolution : 2.20 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

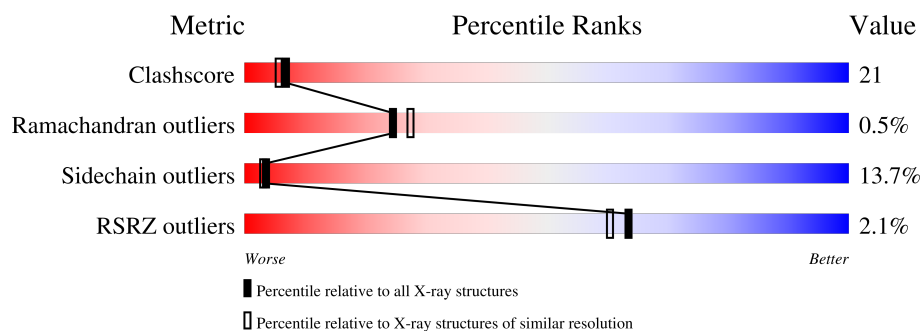
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

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

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 3887 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.

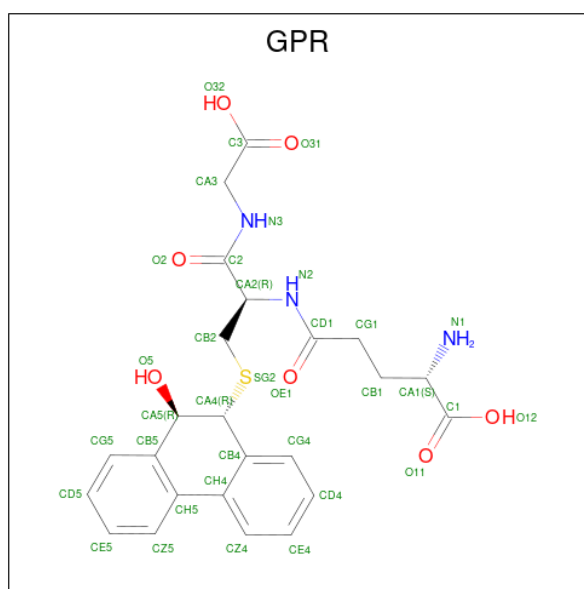
- Molecule 1 is a protein called Glutathione S-transferase YB1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	217	Total	C	N	O	S	0	0	0
			1816	1177	303	325	11			
1	B	217	Total	C	N	O	S	0	0	0
			1816	1177	303	325	11			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	115	PHE	TYR	engineered mutation	UNP P04905
B	115	PHE	TYR	engineered mutation	UNP P04905

- Molecule 2 is (9R,10R)-9-(S-GLUTATHIONYL)-10-HYDROXY-9,10-DIHYDROPHENANTHRENE (CCD ID: GPR) (formula: C₂₄H₂₇N₃O₇S).



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

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

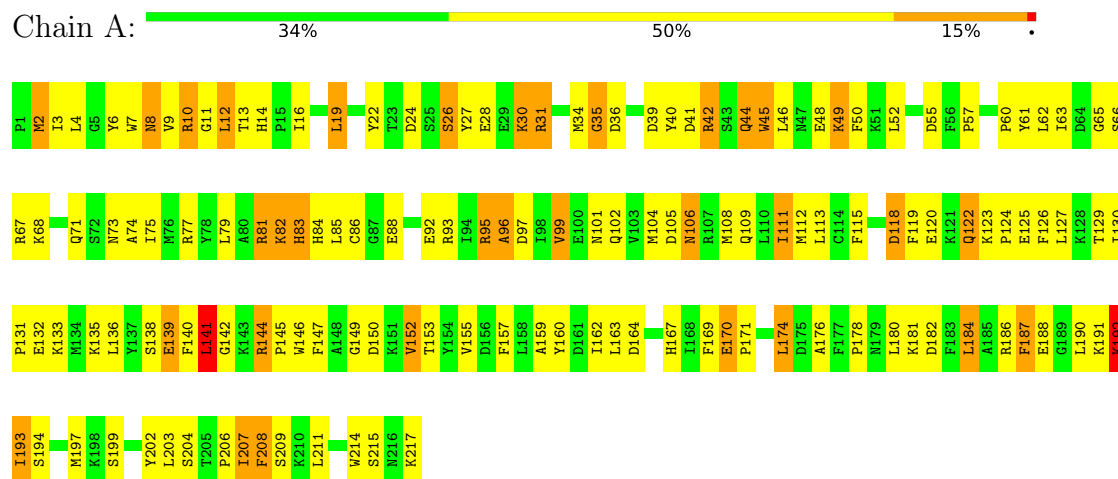
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	99	Total	O	0	0
			99	99		
3	B	86	Total	O	0	0
			86	86		

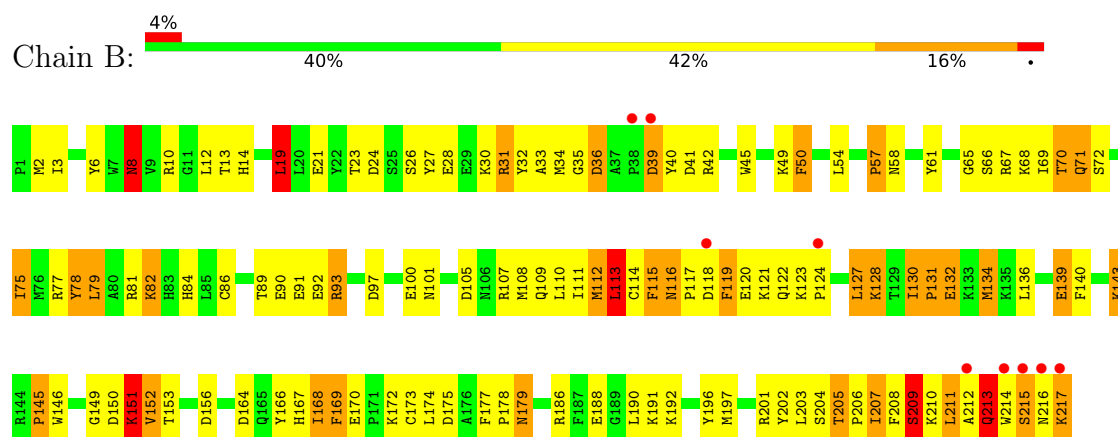
3 Residue-property plots

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 and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Glutathione S-transferase YB1



• Molecule 1: Glutathione S-transferase YB1



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	86.75Å 68.58Å 80.46Å 90.00° 105.12° 90.00°	Depositor
Resolution (Å)	10.00 – 2.20 10.00 – 2.20	Depositor EDS
% Data completeness (in resolution range)	94.6 (10.00-2.20) 93.5 (10.00-2.20)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.26 (at 2.21Å)	Xtriage
Refinement program	SHELXL-97	Depositor
R, R_{free}	0.203 , (Not available) 0.197 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	16.6	Xtriage
Anisotropy	1.161	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.44 , 92.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	3887	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.31% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.76	0/1865	2.32	110/2513 (4.4%)
1	B	0.74	0/1865	2.17	93/2513 (3.7%)
All	All	0.75	0/3730	2.24	203/5026 (4.0%)

There are no bond length outliers.

All (203) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	115	PHE	CA-CB-CG	12.56	126.36	113.80
1	A	50	PHE	CA-CB-CG	-11.84	101.96	113.80
1	A	67	ARG	CD-NE-CZ	11.28	140.19	124.40
1	A	84	HIS	CA-CB-CG	-11.15	102.65	113.80
1	A	45	TRP	CA-C-O	10.96	132.28	120.55
1	B	186	ARG	CD-NE-CZ	10.59	139.23	124.40
1	A	92	GLU	O-C-N	9.42	131.89	122.09
1	A	81	ARG	CD-NE-CZ	-9.42	111.21	124.40
1	A	102	GLN	CA-C-O	9.35	130.47	120.55
1	B	119	PHE	CA-C-N	9.14	132.53	120.28
1	B	119	PHE	C-N-CA	9.14	132.53	120.28
1	A	99	VAL	O-C-N	9.11	130.84	121.91
1	B	169	PHE	O-C-N	9.03	131.37	122.07
1	A	4	LEU	CA-C-N	-8.63	114.43	122.80
1	A	4	LEU	C-N-CA	-8.63	114.43	122.80
1	A	157	PHE	CA-CB-CG	-8.49	105.31	113.80
1	A	49	LYS	CA-C-O	-8.46	111.49	120.63
1	A	122	GLN	OE1-CD-NE2	8.38	130.99	122.60
1	B	31	ARG	CA-C-O	-8.36	111.95	120.98
1	B	166	TYR	CA-C-N	8.07	131.44	120.38
1	B	166	TYR	C-N-CA	8.07	131.44	120.38
1	A	147	PHE	CA-C-N	-8.05	108.34	122.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	147	PHE	C-N-CA	-8.05	108.34	122.26
1	A	36	ASP	CA-CB-CG	7.92	120.52	112.60
1	B	84	HIS	CA-CB-CG	-7.90	105.90	113.80
1	A	160	TYR	CA-C-N	7.85	131.70	120.79
1	A	160	TYR	C-N-CA	7.85	131.70	120.79
1	A	44	GLN	CA-C-O	7.84	128.86	120.55
1	B	177	PHE	CA-CB-CG	-7.78	106.02	113.80
1	A	193	ILE	O-C-N	-7.73	113.86	121.90
1	A	115	PHE	CA-C-O	7.72	127.54	119.05
1	A	83	HIS	CA-CB-CG	-7.62	106.18	113.80
1	A	97	ASP	O-C-N	-7.58	114.08	122.12
1	B	67	ARG	NE-CZ-NH2	-7.53	112.43	119.20
1	A	170	GLU	O-C-N	7.50	127.55	121.17
1	A	204	SER	CA-C-O	7.46	128.52	120.24
1	A	97	ASP	CA-C-O	7.46	128.68	120.63
1	A	187	PHE	CA-C-N	7.41	130.96	120.28
1	A	187	PHE	C-N-CA	7.41	130.96	120.28
1	A	169	PHE	CA-C-N	7.36	130.54	122.74
1	A	169	PHE	C-N-CA	7.36	130.54	122.74
1	A	44	GLN	OE1-CD-NE2	-7.33	115.27	122.60
1	B	168	ILE	CA-C-O	7.28	128.50	120.71
1	B	131	PRO	CA-C-N	-7.20	108.54	121.14
1	B	131	PRO	C-N-CA	-7.20	108.54	121.14
1	B	139	GLU	CA-C-O	7.17	128.21	120.10
1	A	144	ARG	CD-NE-CZ	7.16	134.43	124.40
1	A	115	PHE	O-C-N	-7.03	113.71	122.35
1	A	26	SER	N-CA-CB	6.97	121.78	110.42
1	A	73	ASN	CA-C-N	6.96	129.91	120.38
1	A	73	ASN	C-N-CA	6.96	129.91	120.38
1	B	27	TYR	CA-C-O	-6.94	113.56	121.40
1	B	92	GLU	CA-C-O	-6.94	113.20	120.55
1	A	130	ILE	CA-C-O	-6.91	114.06	118.69
1	B	118	ASP	CA-CB-CG	-6.90	105.70	112.60
1	B	78	TYR	O-C-N	-6.88	114.71	122.08
1	A	102	GLN	O-C-N	-6.88	114.82	122.12
1	A	39	ASP	CA-CB-CG	-6.86	105.74	112.60
1	B	54	LEU	O-C-N	-6.83	115.24	123.16
1	A	150	ASP	CA-C-N	-6.77	111.12	122.29
1	A	150	ASP	C-N-CA	-6.77	111.12	122.29
1	A	119	PHE	O-C-N	6.77	129.32	122.08
1	A	193	ILE	CA-C-O	6.74	128.53	121.05
1	B	69	ILE	CA-C-O	-6.72	112.81	120.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	156	ASP	CA-C-N	6.67	129.22	120.28
1	B	156	ASP	C-N-CA	6.67	129.22	120.28
1	A	61	TYR	CA-C-N	6.64	132.36	123.00
1	A	61	TYR	C-N-CA	6.64	132.36	123.00
1	B	151	LYS	CA-C-N	6.64	129.40	120.50
1	B	151	LYS	C-N-CA	6.64	129.40	120.50
1	B	150	ASP	CA-C-O	-6.63	114.04	121.00
1	B	118	ASP	CA-C-N	6.62	131.71	121.19
1	B	118	ASP	C-N-CA	6.62	131.71	121.19
1	B	50	PHE	CA-CB-CG	-6.57	107.23	113.80
1	A	171	PRO	CA-C-N	-6.57	112.14	122.65
1	A	171	PRO	C-N-CA	-6.57	112.14	122.65
1	B	190	LEU	CA-C-O	-6.54	113.47	120.92
1	B	32	TYR	O-C-N	6.53	130.57	122.86
1	B	149	GLY	CA-C-N	6.46	129.18	120.65
1	B	149	GLY	C-N-CA	6.46	129.18	120.65
1	A	55	ASP	CA-C-N	6.45	129.57	122.74
1	A	55	ASP	C-N-CA	6.45	129.57	122.74
1	A	207	ILE	N-CA-C	-6.41	104.61	110.82
1	B	145	PRO	CA-C-N	6.39	133.54	122.81
1	B	145	PRO	C-N-CA	6.39	133.54	122.81
1	B	36	ASP	CA-C-N	6.38	129.25	120.39
1	B	36	ASP	C-N-CA	6.38	129.25	120.39
1	A	130	ILE	O-C-N	6.36	124.49	120.42
1	B	191	LYS	O-C-N	6.35	129.41	122.11
1	A	167	HIS	CA-C-O	6.28	127.21	120.55
1	A	147	PHE	CA-CB-CG	-6.28	107.52	113.80
1	A	36	ASP	O-C-N	6.27	130.07	122.68
1	A	194	SER	CA-C-N	6.26	129.49	120.79
1	A	194	SER	C-N-CA	6.26	129.49	120.79
1	A	202	TYR	CA-C-O	-6.25	114.93	121.55
1	A	36	ASP	CA-C-N	6.24	130.15	120.60
1	A	36	ASP	C-N-CA	6.24	130.15	120.60
1	B	65	GLY	CA-C-O	6.21	131.37	120.57
1	B	213	GLN	CA-C-N	6.21	135.21	121.81
1	B	213	GLN	C-N-CA	6.21	135.21	121.81
1	B	27	TYR	O-C-N	6.19	130.66	123.17
1	A	31	ARG	CA-C-O	-6.18	114.47	121.39
1	A	10	ARG	O-C-N	-6.15	115.73	122.07
1	A	101	ASN	O-C-N	6.11	129.78	122.27
1	A	42	ARG	CD-NE-CZ	6.10	132.94	124.40
1	A	26	SER	CA-C-O	-6.08	113.86	120.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	44	GLN	O-C-N	-6.05	115.70	122.12
1	B	61	TYR	CA-CB-CG	6.05	124.80	113.90
1	B	153	THR	O-C-N	-6.00	114.80	122.78
1	B	116	ASN	CA-CB-CG	5.97	118.57	112.60
1	B	179	ASN	O-C-N	5.94	129.58	122.27
1	B	70	THR	N-CA-CB	5.92	119.93	111.05
1	B	130	ILE	N-CA-CB	-5.92	106.77	110.50
1	B	8	ASN	CA-C-N	5.91	132.02	122.68
1	B	8	ASN	C-N-CA	5.91	132.02	122.68
1	A	31	ARG	CD-NE-CZ	5.89	132.65	124.40
1	B	113	LEU	O-C-N	-5.89	114.39	122.46
1	B	50	PHE	CA-C-O	5.89	126.55	119.43
1	B	21	GLU	O-C-N	5.87	128.43	122.09
1	A	95	ARG	CA-C-O	5.87	127.18	120.90
1	A	26	SER	O-C-N	5.86	129.90	123.22
1	B	93	ARG	CA-C-N	5.85	127.93	120.56
1	B	93	ARG	C-N-CA	5.85	127.93	120.56
1	A	65	GLY	CA-C-N	5.84	129.19	120.31
1	A	65	GLY	C-N-CA	5.84	129.19	120.31
1	B	90	GLU	CA-C-O	5.83	127.14	120.90
1	B	81	ARG	CA-C-O	5.82	126.59	120.42
1	A	182	ASP	CA-C-O	5.75	126.60	120.10
1	B	13	THR	CA-CB-OG1	-5.73	101.00	109.60
1	B	97	ASP	CA-CB-CG	5.73	118.33	112.60
1	B	101	ASN	OD1-CG-ND2	-5.73	116.87	122.60
1	B	152	VAL	O-C-N	-5.72	116.56	122.63
1	A	208	PHE	CA-C-N	5.69	131.33	120.97
1	A	208	PHE	C-N-CA	5.69	131.33	120.97
1	B	190	LEU	CA-C-N	5.68	129.34	120.82
1	B	190	LEU	C-N-CA	5.68	129.34	120.82
1	B	140	PHE	CA-C-O	5.68	126.44	120.42
1	B	121	LYS	CA-C-N	-5.67	111.52	122.06
1	B	121	LYS	C-N-CA	-5.67	111.52	122.06
1	A	203	LEU	O-C-N	5.64	129.82	123.28
1	A	61	TYR	CB-CG-CD1	5.62	129.22	120.80
1	A	139	GLU	O-C-N	-5.61	115.38	122.27
1	A	193	ILE	CA-C-N	5.59	128.09	120.54
1	A	193	ILE	C-N-CA	5.59	128.09	120.54
1	A	164	ASP	O-C-N	-5.58	116.21	122.12
1	A	2	MET	CA-C-N	-5.56	115.70	123.10
1	A	2	MET	C-N-CA	-5.56	115.70	123.10
1	B	115	PHE	N-CA-C	-5.56	106.28	112.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	152	VAL	CA-C-O	-5.56	114.68	121.13
1	A	139	GLU	CA-C-O	5.55	126.35	119.97
1	A	187	PHE	O-C-N	5.51	127.75	122.07
1	A	88	GLU	CA-C-O	5.50	125.63	119.41
1	A	66	SER	O-C-N	5.47	129.00	122.27
1	A	86	CYS	CA-C-O	-5.46	115.00	121.66
1	B	75	ILE	O-C-N	5.45	127.25	121.91
1	B	191	LYS	CA-C-O	-5.44	114.83	120.92
1	A	125	GLU	O-C-N	5.42	127.94	122.09
1	B	72	SER	CA-C-O	-5.39	115.13	120.90
1	A	141	LEU	CA-C-O	5.37	126.11	120.42
1	B	150	ASP	CA-C-N	-5.36	113.35	123.27
1	B	150	ASP	C-N-CA	-5.36	113.35	123.27
1	B	67	ARG	CA-C-N	5.35	130.88	123.07
1	B	67	ARG	C-N-CA	5.35	130.88	123.07
1	B	71	GLN	O-C-N	5.32	129.66	122.59
1	B	50	PHE	O-C-N	-5.29	115.57	122.39
1	A	96	ALA	O-C-N	5.28	127.51	122.07
1	A	106	ASN	N-CA-C	-5.28	105.60	111.36
1	B	169	PHE	CA-C-O	-5.27	115.28	120.82
1	A	120	GLU	O-C-N	5.26	128.16	122.11
1	B	75	ILE	N-CA-C	-5.26	105.37	110.42
1	A	105	ASP	CB-CA-C	-5.26	102.06	110.79
1	B	131	PRO	O-C-N	-5.24	115.46	122.22
1	A	142	GLY	CA-C-N	-5.24	114.37	122.49
1	A	142	GLY	C-N-CA	-5.24	114.37	122.49
1	B	116	ASN	OD1-CG-ND2	-5.24	117.36	122.60
1	B	191	LYS	CB-CA-C	-5.22	102.08	110.74
1	A	131	PRO	O-C-N	-5.21	116.25	122.24
1	A	81	ARG	N-CA-C	-5.21	105.72	111.71
1	B	57	PRO	CB-CA-C	-5.20	105.04	111.64
1	A	84	HIS	N-CA-CB	-5.18	103.84	111.71
1	B	79	LEU	O-C-N	5.18	128.64	122.27
1	B	82	LYS	CA-C-O	5.18	126.04	120.55
1	A	184	LEU	CA-C-O	5.18	126.04	120.55
1	B	33	ALA	CA-C-N	5.17	129.65	122.77
1	B	33	ALA	C-N-CA	5.17	129.65	122.77
1	B	206	PRO	O-C-N	5.17	130.92	121.10
1	A	119	PHE	CA-CB-CG	5.16	118.96	113.80
1	B	42	ARG	NE-CZ-NH2	5.16	123.84	119.20
1	A	77	ARG	CD-NE-CZ	5.14	131.59	124.40
1	B	69	ILE	O-C-N	5.14	128.73	123.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	35	GLY	CA-C-O	5.13	126.19	121.58
1	A	67	ARG	NE-CZ-NH2	-5.12	114.59	119.20
1	A	150	ASP	CA-CB-CG	-5.10	107.50	112.60
1	B	54	LEU	CA-C-O	5.07	126.75	120.92
1	A	31	ARG	NE-CZ-NH2	-5.07	114.64	119.20
1	B	179	ASN	CA-CB-CG	5.05	117.65	112.60
1	A	182	ASP	O-C-N	-5.05	116.31	122.22
1	B	19	LEU	CA-C-N	-5.05	113.01	120.28
1	B	19	LEU	C-N-CA	-5.05	113.01	120.28
1	A	22	TYR	O-C-N	-5.05	116.77	122.12
1	A	192	LYS	O-C-N	-5.04	116.33	122.22
1	A	140	PHE	CA-C-N	-5.01	113.18	120.29
1	A	140	PHE	C-N-CA	-5.01	113.18	120.29

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	1816	0	1805	73	0
1	B	1816	0	1805	83	0
2	A	35	0	25	5	0
2	B	35	0	25	2	0
3	A	99	0	0	4	0
3	B	86	0	0	5	0
All	All	3887	0	3660	157	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 21.

All (157) 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:2:MET:HE1	1:A:79:LEU:HD21	1.42	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:MET:HE1	2:A:5218:GPR:HD5	1.50	0.94
1:A:63:ILE:HD12	1:A:68:LYS:HD3	1.62	0.81
1:A:34:MET:HE3	1:A:40:TYR:HB3	1.64	0.79
1:B:107:ARG:O	1:B:111:ILE:HD12	1.83	0.78
1:B:114:CYS:O	1:B:213:GLN:HG2	1.83	0.77
1:B:119:PHE:HB2	1:B:213:GLN:HG3	1.64	0.77
1:A:35:GLY:O	1:A:40:TYR:HA	1.85	0.76
1:B:24:ASP:HB2	1:B:192:LYS:NZ	2.03	0.74
1:B:110:LEU:HD12	1:B:113:LEU:HD21	1.68	0.73
1:A:123:LYS:O	1:A:127:LEU:HG	1.89	0.72
1:A:2:MET:HE3	1:A:62:LEU:HD21	1.71	0.72
1:A:2:MET:HE3	1:A:62:LEU:HD11	1.72	0.72
1:A:30:LYS:HE3	1:A:48:GLU:OE2	1.89	0.71
1:A:209:SER:HB3	2:A:5218:GPR:HD4	1.73	0.70
1:B:116:ASN:HD22	1:B:117:PRO:HD2	1.56	0.70
1:A:153:THR:OG1	1:A:155:VAL:HG22	1.92	0.70
1:B:188:GLU:HG2	1:B:197:MET:SD	2.33	0.69
1:A:3:ILE:HG12	1:A:28:GLU:HG2	1.74	0.68
1:A:135:LYS:HE2	1:A:139:GLU:OE2	1.94	0.67
1:B:110:LEU:O	1:B:113:LEU:HD23	1.93	0.67
1:A:178:PRO:HA	1:A:181:LYS:HE2	1.78	0.66
1:B:170:GLU:HB3	1:B:173:CYS:HB3	1.78	0.66
1:B:196:TYR:HE1	1:B:201:ARG:HB3	1.60	0.66
1:A:16:ILE:HD13	1:A:75:ILE:HG21	1.79	0.64
1:B:151:LYS:HD2	1:B:152:VAL:H	1.63	0.63
1:A:24:ASP:OD1	1:A:192:LYS:HE2	1.99	0.62
1:A:8:ASN:HD22	1:A:8:ASN:H	1.48	0.62
1:A:138:SER:HA	1:A:180:LEU:HD21	1.82	0.61
1:B:8:ASN:HD22	1:B:8:ASN:H	1.48	0.61
1:A:184:LEU:O	1:A:188:GLU:HB2	2.01	0.60
1:B:50:PHE:CE1	1:B:57:PRO:HG2	2.36	0.60
1:B:145:PRO:HB2	1:B:146:TRP:CD1	2.36	0.60
1:B:130:ILE:HD12	1:B:170:GLU:HG3	1.83	0.60
1:A:48:GLU:HG3	1:A:52:LEU:HD11	1.82	0.59
1:B:26:SER:HA	3:B:434:HOH:O	2.01	0.59
1:B:168:ILE:HG22	1:B:214:TRP:HZ2	1.67	0.59
1:A:95:ARG:O	1:A:99:VAL:HG23	2.03	0.59
1:B:110:LEU:HA	1:B:113:LEU:HD23	1.84	0.59
1:A:124:PRO:HA	1:A:127:LEU:HD12	1.84	0.58
1:A:83:HIS:O	1:A:85:LEU:HG	2.02	0.58
1:B:115:PHE:CE1	1:B:212:ALA:HB2	2.39	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:172:LYS:HB3	1:B:172:LYS:NZ	2.19	0.57
1:B:6:TYR:O	1:B:31:ARG:HA	2.04	0.57
1:B:115:PHE:HE1	1:B:208:PHE:HB3	1.68	0.57
1:B:35:GLY:O	1:B:40:TYR:HA	2.05	0.56
1:A:8:ASN:HD22	1:A:8:ASN:N	2.03	0.56
1:B:107:ARG:HG2	1:B:111:ILE:CD1	2.35	0.56
1:A:174:LEU:HB3	1:A:181:LYS:HG3	1.88	0.56
1:B:24:ASP:HB2	1:B:192:LYS:HZ3	1.68	0.56
1:B:113:LEU:O	1:B:119:PHE:HD1	1.88	0.55
1:B:196:TYR:CE1	1:B:201:ARG:HB3	2.42	0.55
1:A:12:LEU:HD21	2:A:5218:GPR:HB11	1.87	0.55
1:A:6:TYR:OH	1:A:11:GLY:HA3	2.07	0.54
1:A:132:GLU:O	1:A:136:LEU:HG	2.07	0.54
1:B:203:LEU:HD23	1:B:205:THR:O	2.07	0.54
1:B:8:ASN:HD22	1:B:8:ASN:N	2.04	0.54
1:B:19:LEU:HD22	1:B:23:THR:HG23	1.89	0.54
1:A:12:LEU:HD11	1:A:60:PRO:HD3	1.91	0.53
1:B:39:ASP:O	1:B:40:TYR:HB2	2.08	0.53
1:B:119:PHE:CG	1:B:213:GLN:HB2	2.44	0.53
1:B:50:PHE:CD1	1:B:57:PRO:HG2	2.44	0.52
1:A:152:VAL:HG23	3:A:331:HOH:O	2.09	0.52
1:B:24:ASP:HB2	1:B:192:LYS:HZ1	1.74	0.52
1:B:89:THR:O	1:B:93:ARG:HG3	2.10	0.52
1:B:128:LYS:O	1:B:131:PRO:HD2	2.10	0.52
1:B:123:LYS:HB3	1:B:124:PRO:HD3	1.91	0.52
1:B:116:ASN:ND2	1:B:117:PRO:HD2	2.24	0.51
1:A:71:GLN:O	1:A:74:ALA:HB3	2.10	0.51
1:B:151:LYS:CD	1:B:152:VAL:H	2.23	0.51
1:B:208:PHE:H	1:B:215:SER:HB3	1.76	0.51
1:B:105:ASP:O	1:B:109:GLN:HG3	2.11	0.50
1:B:179:ASN:HA	3:B:420:HOH:O	2.11	0.50
1:A:190:LEU:HB2	1:A:193:ILE:HG12	1.93	0.50
1:B:107:ARG:HG2	1:B:111:ILE:HD11	1.93	0.50
1:B:216:ASN:O	1:B:217:LYS:HB3	2.13	0.49
1:B:120:GLU:O	1:B:124:PRO:HD3	2.12	0.49
1:A:2:MET:CE	1:A:62:LEU:HD11	2.40	0.49
1:B:164:ASP:O	1:B:167:HIS:HB3	2.13	0.48
1:B:115:PHE:CE1	1:B:208:PHE:HB3	2.47	0.48
1:A:118:ASP:O	1:A:122:GLN:HB2	2.13	0.48
1:B:2:MET:HE3	3:B:355:HOH:O	2.12	0.48
1:B:114:CYS:SG	1:B:214:TRP:HB3	2.53	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:35:GLY:HA3	1:B:41:ASP:HB3	1.95	0.48
1:A:96:ALA:HB1	1:A:155:VAL:HG11	1.95	0.48
1:A:176:ALA:C	1:A:178:PRO:HD3	2.38	0.48
1:B:213:GLN:N	1:B:213:GLN:HE21	2.12	0.48
1:A:111:ILE:HG13	1:A:208:PHE:CE1	2.49	0.48
1:A:2:MET:O	1:A:27:TYR:HA	2.14	0.47
1:A:133:LYS:HG2	3:A:393:HOH:O	2.14	0.47
1:A:146:TRP:CH2	1:A:186:ARG:HG2	2.49	0.47
1:B:115:PHE:HE1	1:B:212:ALA:HB2	1.78	0.47
1:B:208:PHE:HE2	1:B:214:TRP:HE3	1.61	0.47
1:A:113:LEU:CD1	1:A:122:GLN:HB3	2.45	0.47
1:A:188:GLU:HG2	1:A:197:MET:SD	2.54	0.47
1:A:42:ARG:O	1:A:46:LEU:HG	2.15	0.47
1:B:10:ARG:HB3	1:B:207:ILE:HA	1.97	0.47
1:B:70:THR:O	1:B:71:GLN:HB2	2.14	0.47
1:B:8:ASN:H	1:B:8:ASN:ND2	2.12	0.47
1:A:159:ALA:O	1:A:163:LEU:HD12	2.15	0.46
1:A:10:ARG:HB3	1:A:207:ILE:HA	1.97	0.46
1:B:39:ASP:N	1:B:39:ASP:OD1	2.47	0.46
1:B:45:TRP:CZ2	1:B:49:LYS:HG3	2.51	0.46
1:B:112:MET:HE2	1:B:112:MET:N	2.30	0.46
1:B:19:LEU:HD22	1:B:23:THR:CG2	2.45	0.46
1:B:77:ARG:NE	1:B:100:GLU:OE1	2.49	0.46
1:A:145:PRO:HG2	1:A:149:GLY:O	2.16	0.45
1:A:8:ASN:H	1:A:8:ASN:ND2	2.13	0.45
1:A:82:LYS:HE2	1:A:82:LYS:HB2	1.24	0.45
1:A:45:TRP:CZ2	1:A:49:LYS:HG3	2.52	0.45
1:B:58:ASN:HB3	3:B:367:HOH:O	2.17	0.45
1:B:123:LYS:HG2	1:B:127:LEU:HD21	1.99	0.45
1:A:16:ILE:HD13	1:A:75:ILE:CG2	2.44	0.45
1:B:66:SER:O	1:B:68:LYS:HE3	2.17	0.45
1:A:141:LEU:HD11	1:A:144:ARG:O	2.17	0.44
1:B:2:MET:HE2	1:B:82:LYS:NZ	2.32	0.44
1:B:110:LEU:HA	1:B:113:LEU:CD2	2.47	0.44
1:B:209:SER:CB	2:B:6218:GPR:HE4	2.47	0.44
1:A:6:TYR:O	1:A:31:ARG:HA	2.17	0.44
1:A:12:LEU:CD1	1:A:60:PRO:HD3	2.48	0.44
1:B:132:GLU:O	1:B:136:LEU:HG	2.18	0.44
1:B:151:LYS:HD3	1:B:151:LYS:HA	1.62	0.44
1:A:45:TRP:CD1	1:A:46:LEU:HD23	2.53	0.44
1:A:7:TRP:HH2	1:A:42:ARG:HB3	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:9:VAL:HG12	1:A:206:PRO:HG2	2.00	0.43
1:B:178:PRO:HG2	3:B:453:HOH:O	2.18	0.43
1:A:35:GLY:HA3	1:A:41:ASP:HB3	2.00	0.43
1:A:2:MET:CE	1:A:62:LEU:HD21	2.45	0.43
1:A:174:LEU:O	1:A:181:LYS:NZ	2.50	0.43
1:A:187:PHE:O	1:A:190:LEU:HG	2.18	0.43
1:A:207:ILE:HD12	1:A:214:TRP:CZ3	2.54	0.43
1:A:113:LEU:HD22	1:A:126:PHE:CG	2.54	0.42
2:A:5218:GPR:HG11	3:A:415:HOH:O	2.18	0.42
1:B:209:SER:OG	2:B:6218:GPR:HE4	2.19	0.42
1:A:104:MET:O	1:A:108:MET:HG2	2.19	0.42
1:B:115:PHE:CD1	1:B:212:ALA:HB2	2.55	0.42
1:A:81:ARG:HH11	1:A:81:ARG:HD3	1.59	0.42
1:B:8:ASN:HB3	1:B:31:ARG:HB3	2.01	0.42
1:A:132:GLU:HB2	3:A:438:HOH:O	2.18	0.42
1:B:19:LEU:HD13	1:B:79:LEU:HB2	2.01	0.42
1:B:172:LYS:NZ	1:B:175:ASP:OD2	2.50	0.42
1:B:110:LEU:HD12	1:B:113:LEU:CD2	2.42	0.42
1:B:123:LYS:HE3	1:B:169:PHE:CZ	2.55	0.42
1:A:207:ILE:HD13	1:A:207:ILE:HG21	1.80	0.42
1:B:202:TYR:CE2	1:B:204:SER:HB3	2.55	0.42
1:A:24:ASP:CG	1:A:192:LYS:HE2	2.45	0.41
1:A:106:ASN:HA	1:A:109:GLN:OE1	2.19	0.41
1:B:3:ILE:HA	1:B:28:GLU:O	2.20	0.41
1:B:143:LYS:HB3	1:B:143:LYS:HE3	1.91	0.41
1:A:3:ILE:HG12	1:A:28:GLU:CG	2.46	0.41
1:A:19:LEU:HD13	1:A:79:LEU:HB2	2.03	0.41
1:A:34:MET:HE2	1:A:40:TYR:CD1	2.56	0.41
2:A:5218:GPR:HN12	1:B:105:ASP:CG	2.28	0.41
1:B:75:ILE:O	1:B:78:TYR:HB3	2.21	0.41
1:B:134:MET:HE2	1:B:134:MET:N	2.36	0.40
1:A:40:TYR:CE2	1:A:211:LEU:HD13	2.56	0.40
1:A:30:LYS:HZ3	1:A:30:LYS:HG2	1.48	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	215/217 (99%)	209 (97%)	6 (3%)	0	100	100
1	B	215/217 (99%)	201 (94%)	12 (6%)	2 (1%)	14	14
All	All	430/434 (99%)	410 (95%)	18 (4%)	2 (0%)	24	27

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	209	SER
1	B	211	LEU

5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	197/197 (100%)	173 (88%)	24 (12%)	5	4
1	B	197/197 (100%)	167 (85%)	30 (15%)	3	2
All	All	394/394 (100%)	340 (86%)	54 (14%)	3	3

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	ASN
1	A	12	LEU
1	A	13	THR
1	A	14	HIS

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Mol	Chain	Res	Type
1	A	19	LEU
1	A	26	SER
1	A	30	LYS
1	A	44	GLN
1	A	57	PRO
1	A	82	LYS
1	A	93	ARG
1	A	111	ILE
1	A	112	MET
1	A	118	ASP
1	A	129	THR
1	A	141	LEU
1	A	162	ILE
1	A	170	GLU
1	A	174	LEU
1	A	191	LYS
1	A	192	LYS
1	A	199	SER
1	A	215	SER
1	A	217	LYS
1	B	8	ASN
1	B	12	LEU
1	B	14	HIS
1	B	19	LEU
1	B	30	LYS
1	B	34	MET
1	B	36	ASP
1	B	39	ASP
1	B	86	CYS
1	B	91	GLU
1	B	108	MET
1	B	112	MET
1	B	113	LEU
1	B	122	GLN
1	B	127	LEU
1	B	128	LYS
1	B	132	GLU
1	B	134	MET
1	B	139	GLU
1	B	143	LYS
1	B	151	LYS
1	B	174	LEU

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Mol	Chain	Res	Type
1	B	205	THR
1	B	207	ILE
1	B	209	SER
1	B	210	LYS
1	B	211	LEU
1	B	213	GLN
1	B	215	SER
1	B	217	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	ASN
1	A	44	GLN
1	A	73	ASN
1	A	83	HIS
1	B	8	ASN
1	B	101	ASN
1	B	106	ASN
1	B	116	ASN
1	B	122	GLN
1	B	213	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 ⓘ

2 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	GPR	A	5218	-	35,37,37	1.82	9 (25%)	46,51,51	2.64	20 (43%)
2	GPR	B	6218	-	35,37,37	2.22	9 (25%)	46,51,51	2.94	23 (50%)

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	GPR	A	5218	-	-	5/27/43/43	0/3/3/3
2	GPR	B	6218	-	-	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)
2	B	6218	GPR	CA4-SG2	-5.70	1.69	1.84
2	B	6218	GPR	CG4-CB4	5.37	1.46	1.39
2	A	5218	GPR	CA4-SG2	-5.10	1.71	1.84
2	B	6218	GPR	CH5-CB5	-3.61	1.36	1.40
2	A	5218	GPR	CG4-CB4	3.57	1.44	1.39
2	B	6218	GPR	CZ5-CH5	3.53	1.45	1.40
2	B	6218	GPR	CG1-CD1	-3.41	1.44	1.51
2	A	5218	GPR	CG1-CD1	-3.22	1.44	1.51
2	A	5218	GPR	CZ5-CH5	3.01	1.44	1.40
2	B	6218	GPR	CA2-N2	2.84	1.51	1.45
2	B	6218	GPR	CH4-CB4	2.80	1.44	1.40
2	B	6218	GPR	CB1-CA1	2.69	1.59	1.53
2	B	6218	GPR	CA3-N3	2.52	1.51	1.45
2	A	5218	GPR	CB2-SG2	-2.42	1.79	1.82
2	A	5218	GPR	CA2-C2	2.29	1.58	1.52
2	A	5218	GPR	CH4-CB4	2.22	1.43	1.40
2	A	5218	GPR	O12-C1	2.11	1.37	1.30
2	A	5218	GPR	CA3-N3	2.04	1.50	1.45

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	5218	GPR	CG5-CB5-CA5	-7.21	106.56	120.94
2	B	6218	GPR	O32-C3-O31	-6.30	107.13	123.33
2	A	5218	GPR	O32-C3-O31	-6.04	107.80	123.33
2	A	5218	GPR	O5-CA5-CA4	5.92	127.42	109.58
2	B	6218	GPR	CD5-CE5-CZ5	5.90	127.52	120.24
2	B	6218	GPR	CA2-N2-CD1	-5.76	107.24	121.68
2	B	6218	GPR	CG5-CB5-CH5	5.19	125.70	119.35
2	B	6218	GPR	O2-C2-CA2	-5.17	109.65	120.48
2	B	6218	GPR	CE5-CZ5-CH5	-4.87	112.16	120.23
2	B	6218	GPR	O12-C1-O11	-4.76	113.28	124.08
2	B	6218	GPR	CH5-CH4-CB4	-4.23	113.57	119.64
2	B	6218	GPR	CD5-CG5-CB5	-4.23	115.92	120.99
2	A	5218	GPR	CD5-CE5-CZ5	4.21	125.43	120.24
2	B	6218	GPR	CA5-CA4-SG2	-4.20	98.03	110.88
2	B	6218	GPR	CG5-CB5-CA5	-4.13	112.71	120.94
2	A	5218	GPR	CG1-CB1-CA1	-3.80	105.13	113.86
2	B	6218	GPR	CB1-CG1-CD1	3.65	121.21	113.06
2	A	5218	GPR	CE5-CZ5-CH5	-3.58	114.29	120.23
2	A	5218	GPR	CB1-CG1-CD1	3.55	120.98	113.06
2	B	6218	GPR	CG1-CB1-CA1	-3.54	105.74	113.86
2	A	5218	GPR	CA2-N2-CD1	-3.47	112.99	121.68
2	A	5218	GPR	CH5-CH4-CB4	-3.30	114.91	119.64
2	B	6218	GPR	CB1-CA1-N1	-3.23	101.71	110.12
2	A	5218	GPR	CD5-CG5-CB5	-3.21	117.15	120.99
2	A	5218	GPR	O2-C2-CA2	-3.16	113.85	120.48
2	A	5218	GPR	CD4-CG4-CB4	-3.01	117.39	120.99
2	B	6218	GPR	CZ5-CH5-CH4	-2.97	115.58	121.61
2	B	6218	GPR	CH4-CH5-CB5	2.83	123.69	119.64
2	A	5218	GPR	CG5-CB5-CH5	2.71	122.67	119.35
2	A	5218	GPR	CA5-CA4-SG2	-2.68	102.69	110.88
2	B	6218	GPR	O32-C3-CA3	2.61	122.72	112.81
2	B	6218	GPR	CB5-CA5-CA4	-2.59	103.96	110.64
2	A	5218	GPR	O5-CA5-CB5	-2.51	105.64	110.42
2	A	5218	GPR	O2-C2-N3	2.49	128.26	122.98
2	A	5218	GPR	O32-C3-CA3	2.48	122.23	112.81
2	B	6218	GPR	C3-CA3-N3	-2.34	105.80	113.06
2	B	6218	GPR	O2-C2-N3	2.32	127.88	122.98
2	A	5218	GPR	CH5-CB5-CA5	-2.24	115.86	118.64
2	B	6218	GPR	CB1-CA1-C1	-2.22	104.57	110.45
2	A	5218	GPR	CB2-CA2-N2	-2.08	105.61	111.06
2	B	6218	GPR	CD4-CE4-CZ4	2.07	122.79	120.24
2	B	6218	GPR	C2-CA2-N2	-2.03	105.61	111.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	5218	GPR	CA2-CB2-SG2	-2.03	106.27	113.66

There are no chirality outliers.

All (7) torsion outliers are listed below:

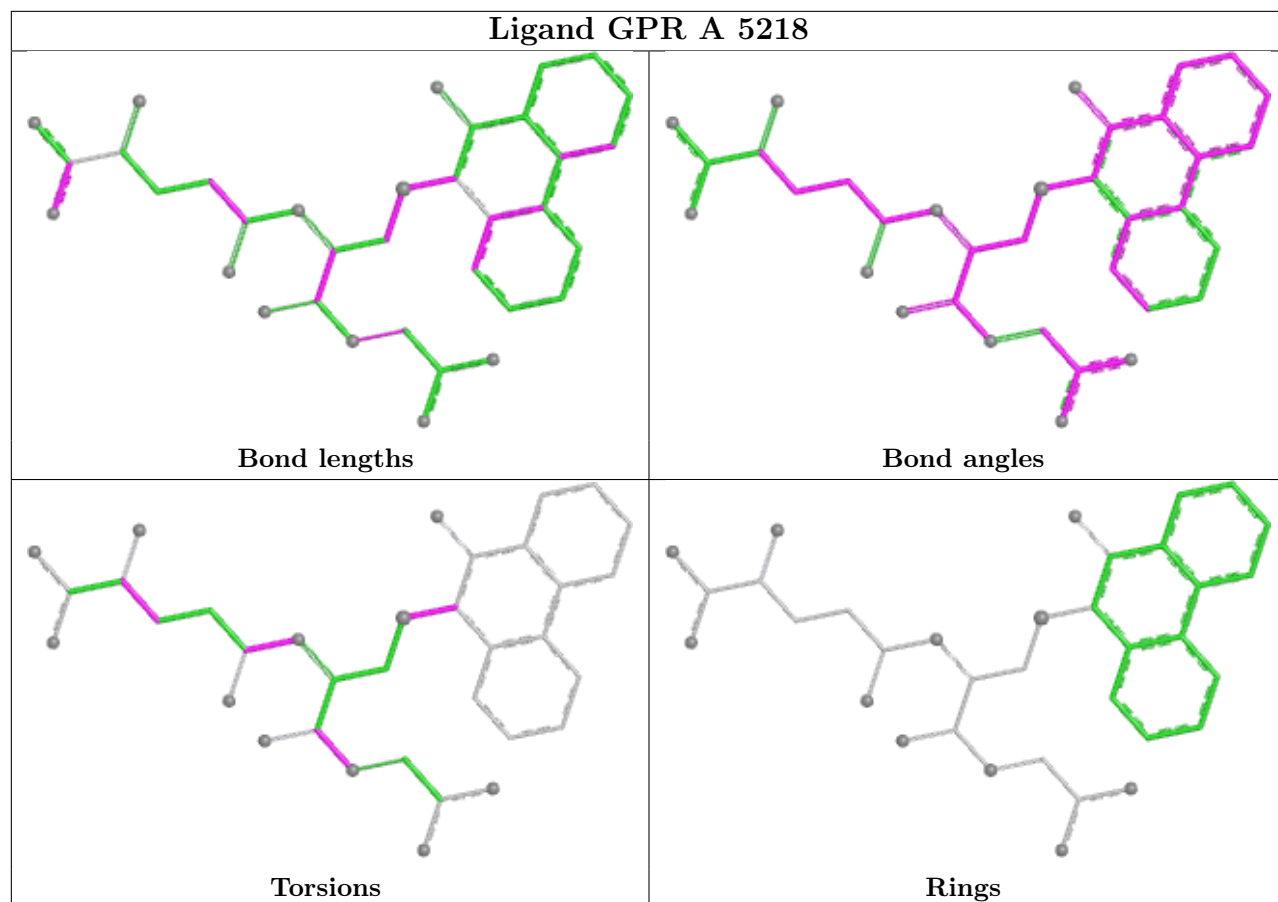
Mol	Chain	Res	Type	Atoms
2	A	5218	GPR	N1-CA1-CB1-CG1
2	A	5218	GPR	CB4-CA4-SG2-CB2
2	B	6218	GPR	N1-CA1-CB1-CG1
2	A	5218	GPR	OE1-CD1-N2-CA2
2	A	5218	GPR	C1-CA1-CB1-CG1
2	B	6218	GPR	C1-CA1-CB1-CG1
2	A	5218	GPR	CA2-C2-N3-CA3

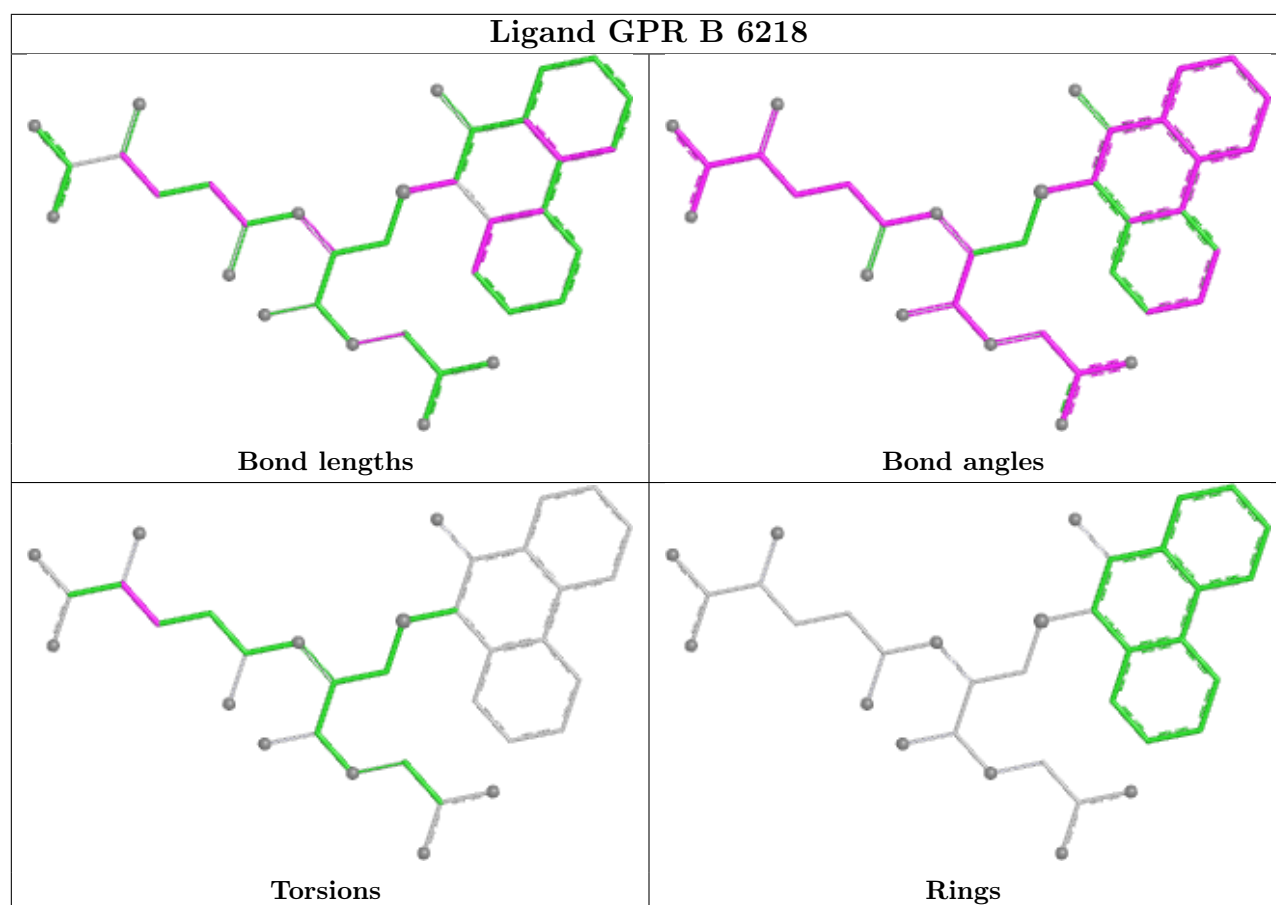
There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	5218	GPR	5	0
2	B	6218	GPR	2	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	217/217 (100%)	-0.16	0 100 100	14, 26, 45, 53	0
1	B	217/217 (100%)	-0.01	9 (4%) 41 38	13, 25, 70, 91	0
All	All	434/434 (100%)	-0.08	9 (2%) 63 60	13, 26, 55, 91	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	39	ASP	3.1
1	B	214	TRP	3.0
1	B	216	ASN	2.9
1	B	212	ALA	2.5
1	B	217	LYS	2.4
1	B	215	SER	2.4
1	B	124	PRO	2.2
1	B	38	PRO	2.1
1	B	118	ASP	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

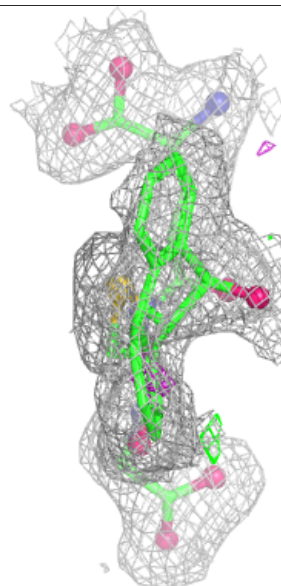
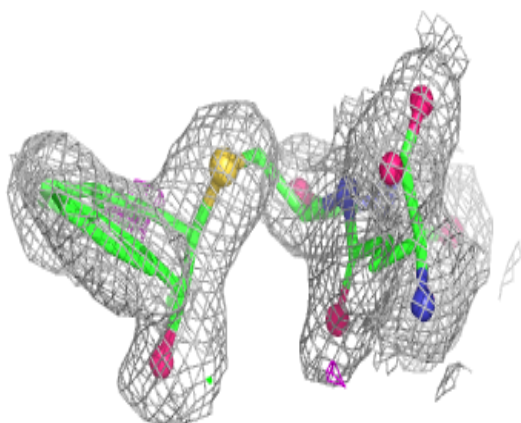
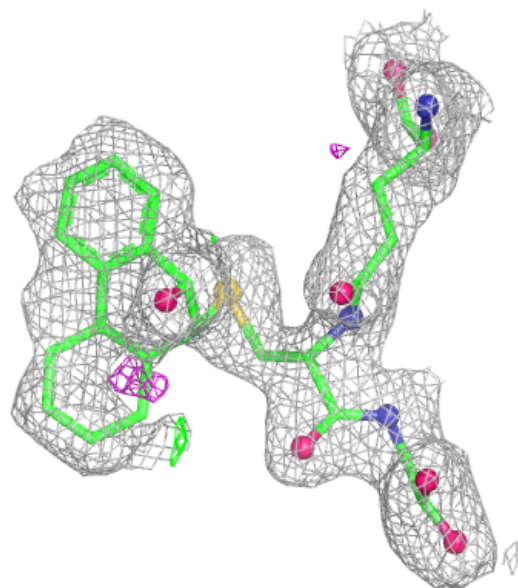
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	GPR	B	6218	35/35	0.93	0.09	12,27,42,43	0
2	GPR	A	5218	35/35	0.94	0.10	15,27,67,72	0

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

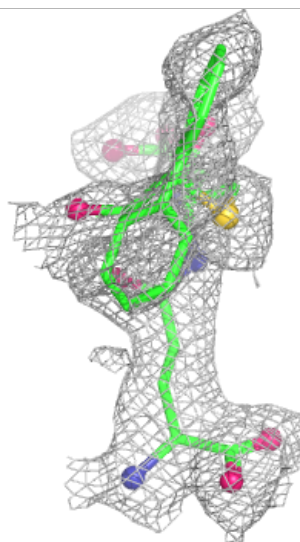
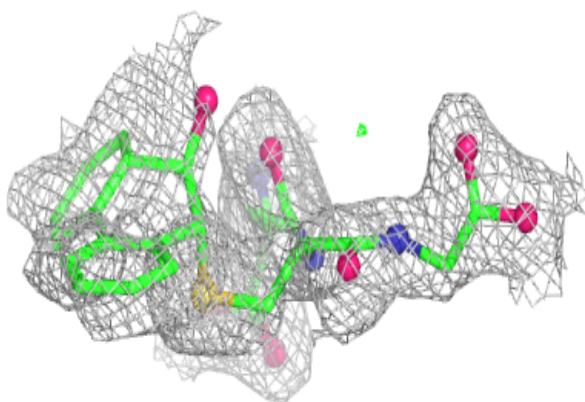
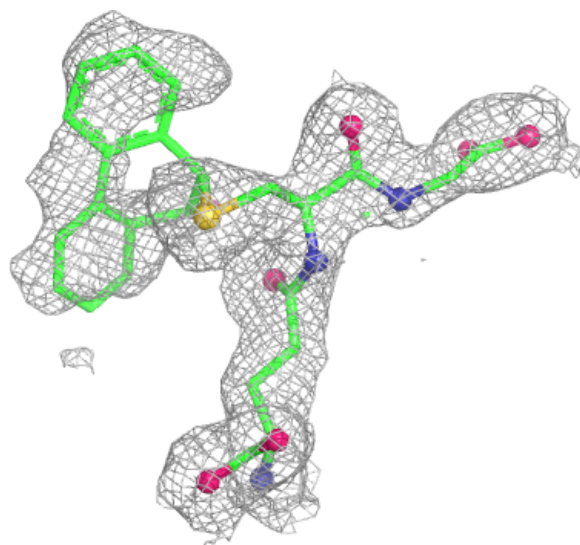
Electron density around GPR B 6218:

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 GPR A 5218:

$2mF_o-DF_c$ (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.