



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 20, 2020 – 06:20 PM BST

PDB ID : 5FWG
Title : TETRA-(5-FLUOROTRYPTOPHANYL)-GLUTATHIONE TRANSFERASE
Authors : Parsons, J.F.; Xiao, G.; Armstrong, R.N.; Gilliland, G.L.
Deposited on : 1997-11-08
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

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

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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	:	2.13.1
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)	:	2.13.1

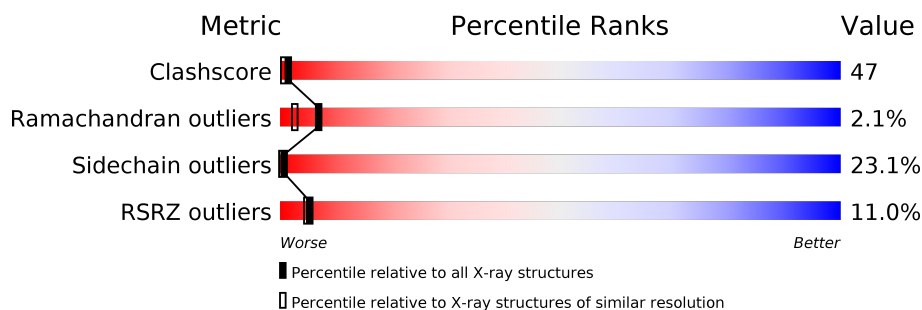
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (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 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

There are 3 unique types of molecules in this entry. The entry contains 4085 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.

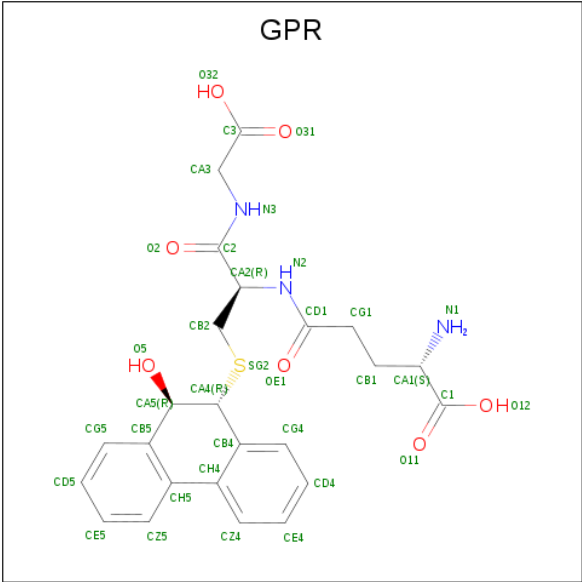
- Molecule 1 is a protein called TETRA-(5-FLUOROTRYPTOPHANYL)-GLUTATHIONE TRANSFERASE MU CLASS.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	217	Total	C	F	N	O	S	0	0	0
			1822	1177	4	303	327	11			
1	B	217	Total	C	F	N	O	S	0	0	0
			1822	1177	4	303	327	11			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	7	FTR	TRP	CONFLICT	UNP P04905
A	45	FTR	TRP	CONFLICT	UNP P04905
A	146	FTR	TRP	CONFLICT	UNP P04905
A	214	FTR	TRP	CONFLICT	UNP P04905
B	7	FTR	TRP	CONFLICT	UNP P04905
B	45	FTR	TRP	CONFLICT	UNP P04905
B	146	FTR	TRP	CONFLICT	UNP P04905
B	214	FTR	TRP	CONFLICT	UNP P04905

- Molecule 2 is (9R,10R)-9-(S-GLUTATHIONYL)-10-HYDROXY-9,10-DIHYDROPHENANTHRENE (three-letter code: GPR) (formula: C₂₄H₂₇N₃O₇S).



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

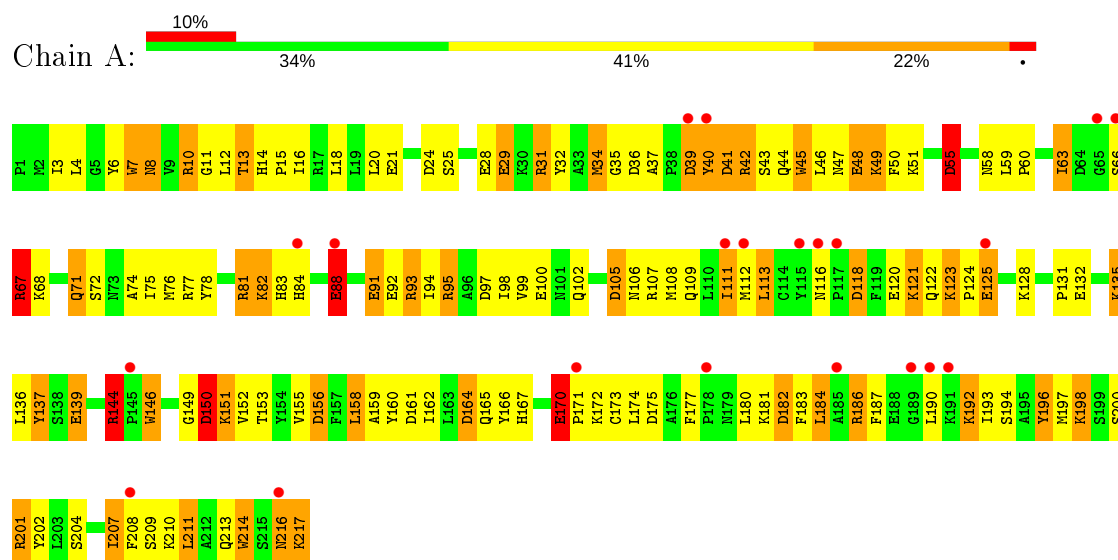
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	167	Total	O	0	0
			167	167		
3	B	204	Total	O	0	0
			204	204		

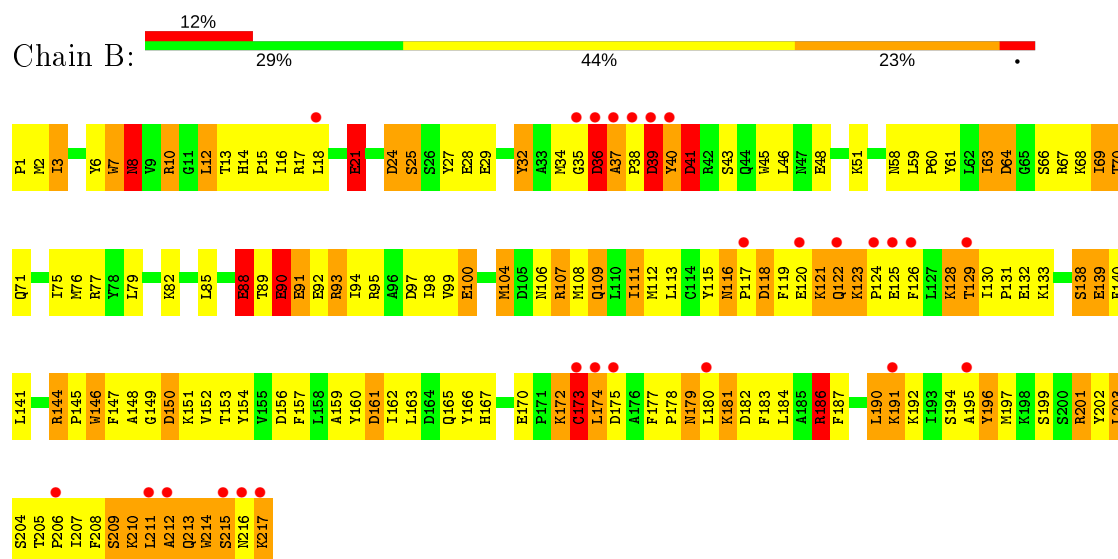
3 Residue-property plots

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: TETRA-(5-FLUOROTRYPTOPHANYL)-GLUTATHIONE TRANSFERASE MU CLASS



- Molecule 1: TETRA-(5-FLUOROTRYPTOPHANYL)-GLUTATHIONE TRANSFERASE MU CLASS



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	86.94Å 68.75Å 80.54Å 90.00° 105.08° 90.00°	Depositor
Resolution (Å)	65.00 – 2.00 22.11 – 2.00	Depositor EDS
% Data completeness (in resolution range)	90.0 (65.00-2.00) 93.8 (22.11-2.00)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.54 (at 1.99Å)	Xtriage
Refinement program	TNT 5E, X-PLOR	Depositor
R, R_{free}	0.180 , (Not available) 0.186 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	16.4	Xtriage
Anisotropy	0.752	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 114.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4085	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.30% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: FTR, 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	1.16	10/1799 (0.6%)	1.82	40/2411 (1.7%)
1	B	1.19	11/1799 (0.6%)	1.77	35/2411 (1.5%)
All	All	1.17	21/3598 (0.6%)	1.80	75/4822 (1.6%)

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	21	GLU	CD-OE2	11.32	1.38	1.25
1	A	139	GLU	CD-OE2	7.84	1.34	1.25
1	A	120	GLU	CD-OE2	7.63	1.34	1.25
1	A	170	GLU	CD-OE2	7.53	1.33	1.25
1	A	132	GLU	CD-OE2	7.17	1.33	1.25
1	B	132	GLU	CD-OE2	6.99	1.33	1.25
1	A	29	GLU	CD-OE2	6.97	1.33	1.25
1	A	125	GLU	CD-OE2	6.87	1.33	1.25
1	A	88	GLU	CD-OE2	6.57	1.32	1.25
1	B	91	GLU	CD-OE2	6.27	1.32	1.25
1	A	48	GLU	CD-OE2	6.24	1.32	1.25
1	A	28	GLU	CD-OE2	6.21	1.32	1.25
1	B	28	GLU	CD-OE2	6.07	1.32	1.25
1	B	48	GLU	CD-OE2	6.05	1.32	1.25
1	B	125	GLU	CD-OE2	6.04	1.32	1.25
1	B	29	GLU	CD-OE2	5.73	1.31	1.25
1	A	91	GLU	CD-OE2	5.60	1.31	1.25
1	B	88	GLU	CD-OE2	5.59	1.31	1.25
1	B	90	GLU	CD-OE2	5.41	1.31	1.25
1	B	21	GLU	CB-CG	5.33	1.62	1.52
1	B	120	GLU	CD-OE2	5.24	1.31	1.25

All (75) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	55	ASP	CB-CG-OD2	-16.68	103.29	118.30
1	B	17	ARG	NE-CZ-NH2	-13.60	113.50	120.30
1	B	17	ARG	NE-CZ-NH1	12.55	126.57	120.30
1	A	55	ASP	CB-CG-OD1	12.53	129.57	118.30
1	A	144	ARG	NE-CZ-NH1	11.01	125.80	120.30
1	B	118	ASP	CB-CG-OD2	-10.75	108.63	118.30
1	A	144	ARG	NE-CZ-NH2	-10.03	115.29	120.30
1	A	36	ASP	CB-CG-OD2	-9.72	109.56	118.30
1	A	67	ARG	NE-CZ-NH1	9.70	125.15	120.30
1	B	24	ASP	CB-CG-OD2	-9.28	109.95	118.30
1	A	156	ASP	CB-CG-OD1	8.86	126.27	118.30
1	A	36	ASP	CB-CG-OD1	8.81	126.23	118.30
1	A	97	ASP	CB-CG-OD1	8.72	126.15	118.30
1	B	182	ASP	CB-CG-OD2	-8.63	110.54	118.30
1	B	8	ASN	N-CA-CB	-8.62	95.09	110.60
1	B	10	ARG	NE-CZ-NH1	8.60	124.60	120.30
1	A	10	ARG	NE-CZ-NH2	-8.57	116.01	120.30
1	A	156	ASP	CB-CG-OD2	-8.54	110.62	118.30
1	A	95	ARG	NE-CZ-NH1	8.48	124.54	120.30
1	B	24	ASP	CB-CG-OD1	8.38	125.84	118.30
1	B	118	ASP	CB-CG-OD1	8.15	125.63	118.30
1	B	97	ASP	CB-CG-OD1	8.08	125.57	118.30
1	A	97	ASP	CB-CG-OD2	-7.83	111.25	118.30
1	A	81	ARG	NE-CZ-NH1	7.71	124.15	120.30
1	A	39	ASP	CB-CG-OD2	-7.67	111.39	118.30
1	B	39	ASP	CB-CG-OD2	-7.34	111.69	118.30
1	A	67	ARG	CD-NE-CZ	7.34	133.87	123.60
1	A	201	ARG	NE-CZ-NH1	-7.33	116.64	120.30
1	A	105	ASP	CB-CG-OD1	7.27	124.84	118.30
1	A	95	ARG	NE-CZ-NH2	-6.95	116.82	120.30
1	A	182	ASP	CB-CG-OD2	-6.79	112.19	118.30
1	A	39	ASP	CB-CG-OD1	6.77	124.39	118.30
1	A	93	ARG	NE-CZ-NH1	6.76	123.68	120.30
1	A	182	ASP	CB-CG-OD1	6.75	124.38	118.30
1	A	150	ASP	CB-CG-OD2	-6.74	112.23	118.30
1	A	24	ASP	CB-CG-OD1	6.65	124.29	118.30
1	B	107	ARG	NE-CZ-NH2	-6.54	117.03	120.30
1	B	37	ALA	C-N-CD	-6.50	106.31	120.60
1	B	70	THR	N-CA-CB	6.47	122.60	110.30
1	B	41	ASP	CB-CG-OD2	-6.46	112.49	118.30
1	B	21	GLU	CB-CG-CD	6.31	131.24	114.20
1	A	24	ASP	CB-CG-OD2	-6.30	112.63	118.30
1	B	25	SER	N-CA-CB	6.26	119.89	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	175	ASP	CB-CG-OD1	6.22	123.90	118.30
1	B	150	ASP	CB-CG-OD1	6.17	123.85	118.30
1	A	105	ASP	CB-CG-OD2	-6.12	112.80	118.30
1	A	95	ARG	CD-NE-CZ	6.09	132.13	123.60
1	B	182	ASP	CB-CG-OD1	6.07	123.76	118.30
1	A	47	ASN	N-CA-CB	6.02	121.43	110.60
1	A	31	ARG	NE-CZ-NH1	5.98	123.29	120.30
1	B	150	ASP	CB-CG-OD2	-5.98	112.92	118.30
1	B	64	ASP	CB-CG-OD2	-5.94	112.95	118.30
1	B	186	ARG	NE-CZ-NH2	-5.89	117.35	120.30
1	A	137	TYR	N-CA-CB	5.68	120.83	110.60
1	A	175	ASP	CB-CG-OD2	-5.65	113.21	118.30
1	B	139	GLU	N-CA-CB	5.51	120.52	110.60
1	A	13	THR	CA-CB-CG2	-5.50	104.69	112.40
1	A	166	TYR	CB-CG-CD2	-5.50	117.70	121.00
1	A	144	ARG	CD-NE-CZ	5.48	131.27	123.60
1	B	36	ASP	CB-CG-OD2	-5.48	113.37	118.30
1	B	32	TYR	CB-CG-CD1	-5.44	117.74	121.00
1	A	67	ARG	CG-CD-NE	5.42	123.18	111.80
1	B	161	ASP	CB-CG-OD1	5.35	123.12	118.30
1	B	97	ASP	CB-CG-OD2	-5.32	113.52	118.30
1	B	186	ARG	NE-CZ-NH1	5.31	122.95	120.30
1	B	154	TYR	CB-CG-CD1	-5.30	117.82	121.00
1	A	40	TYR	CA-CB-CG	-5.29	103.36	113.40
1	B	85	LEU	CA-CB-CG	-5.22	103.29	115.30
1	A	118	ASP	CB-CG-OD2	-5.16	113.66	118.30
1	A	196	TYR	CB-CG-CD2	-5.15	117.91	121.00
1	B	107	ARG	NH1-CZ-NH2	5.15	125.06	119.40
1	B	196	TYR	CB-CG-CD2	-5.08	117.95	121.00
1	B	100	GLU	CG-CD-OE2	-5.05	108.19	118.30
1	B	156	ASP	CB-CG-OD2	-5.03	113.78	118.30
1	B	41	ASP	CA-CB-CG	-5.00	102.39	113.40

There are no chirality outliers.

There are no planarity outliers.

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	1822	0	1799	167	0
1	B	1822	0	1799	182	0
2	A	35	0	25	6	0
2	B	35	0	25	7	0
3	A	167	0	0	18	0
3	B	204	0	0	12	1
All	All	4085	0	3648	346	1

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 47.

All (346) 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:67:ARG:HG3	1:B:69:ILE:HD11	1.41	1.02
1:B:116:ASN:ND2	1:B:118:ASP:H	1.57	1.01
1:A:32:TYR:HD1	1:A:44:GLN:HG2	1.25	0.99
1:A:216:ASN:HD22	1:A:217:LYS:N	1.63	0.96
1:A:150:ASP:N	1:A:151:LYS:HE2	1.81	0.96
1:B:201:ARG:HG2	1:B:201:ARG:HH11	1.28	0.96
1:A:150:ASP:H	1:A:151:LYS:HE2	1.29	0.95
1:A:211:LEU:H	1:A:211:LEU:HD12	1.31	0.92
1:B:116:ASN:HD22	1:B:118:ASP:H	1.07	0.92
1:A:122:GLN:HE22	1:A:125:GLU:HG3	1.36	0.90
1:A:11:GLY:HA2	2:A:218:GPR:HZ5	1.53	0.88
1:B:15:PRO:HB2	1:B:76:MET:CE	2.04	0.87
1:B:123:LYS:HB3	1:B:124:PRO:HD3	1.56	0.87
1:B:21:GLU:HG3	1:B:196:TYR:HB2	1.58	0.85
1:A:91:GLU:HG2	1:B:67:ARG:HH22	1.44	0.81
1:A:7:FTR:HH2	1:A:42:ARG:HG2	1.63	0.81
1:B:95:ARG:O	1:B:99:VAL:HG23	1.82	0.80
1:A:108:MET:HA	1:A:111:ILE:CG1	2.14	0.78
1:A:21:GLU:HG3	1:A:196:TYR:CG	2.18	0.78
1:A:111:ILE:HG23	1:A:208:PHE:CE1	2.18	0.77
1:B:15:PRO:HB2	1:B:76:MET:HE1	1.67	0.77
1:B:124:PRO:O	1:B:128:LYS:HG3	1.86	0.76
1:B:67:ARG:HG3	1:B:69:ILE:CD1	2.14	0.76
1:B:21:GLU:HG2	3:B:824:HOH:O	1.86	0.76
1:B:214:FTR:CE3	1:B:215:SER:HB2	2.15	0.76
1:B:67:ARG:CG	1:B:69:ILE:HD11	2.15	0.75
1:A:32:TYR:CD1	1:A:44:GLN:HG2	2.17	0.74
1:A:40:TYR:CE1	1:A:211:LEU:HG	2.22	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:128:LYS:NZ	1:B:128:LYS:HB2	2.03	0.74
1:B:159:ALA:O	1:B:163:LEU:HD13	1.87	0.74
1:B:106:ASN:HA	1:B:109:GLN:OE1	1.89	0.73
1:A:40:TYR:CD1	1:A:211:LEU:HG	2.22	0.73
1:A:160:TYR:HD1	1:A:184:LEU:HD12	1.54	0.72
1:A:93:ARG:HD3	3:A:623:HOH:O	1.89	0.72
1:A:211:LEU:HD12	1:A:211:LEU:N	2.04	0.72
1:B:116:ASN:HD22	1:B:118:ASP:N	1.84	0.72
1:B:12:LEU:H	1:B:12:LEU:HD23	1.54	0.72
1:A:192:LYS:HE2	3:A:543:HOH:O	1.88	0.71
1:A:10:ARG:NH2	1:A:164:ASP:OD1	2.22	0.71
1:A:150:ASP:HB2	1:A:151:LYS:CE	2.21	0.71
1:B:14:HIS:CD2	1:B:18:LEU:HD11	2.25	0.70
1:B:177:PHE:O	1:B:180:LEU:HB2	1.90	0.70
1:B:91:GLU:O	1:B:95:ARG:HG3	1.92	0.70
1:A:144:ARG:HG2	1:A:149:GLY:HA2	1.74	0.70
1:B:201:ARG:N	1:B:201:ARG:HD3	2.07	0.70
1:B:113:LEU:HD22	1:B:126:PHE:CD2	2.28	0.69
1:A:160:TYR:CD1	1:A:184:LEU:HD12	2.27	0.69
1:B:170:GLU:HB3	1:B:173:CYS:HB3	1.75	0.69
1:A:187:PHE:O	1:A:190:LEU:HD12	1.91	0.69
1:B:126:PHE:HA	1:B:129:THR:HG23	1.75	0.68
1:B:128:LYS:HD3	3:B:741:HOH:O	1.94	0.68
2:B:218:GPR:HA4	3:B:682:HOH:O	1.93	0.68
1:A:94:ILE:O	1:A:98:ILE:HG13	1.93	0.68
1:B:21:GLU:OE2	1:B:192:LYS:HB3	1.93	0.68
1:B:201:ARG:H	1:B:201:ARG:HD3	1.57	0.68
1:B:61:TYR:HD1	1:B:63:ILE:HD13	1.59	0.68
1:B:104:MET:HE1	1:B:108:MET:SD	2.35	0.67
1:B:186:ARG:HG3	3:B:723:HOH:O	1.94	0.67
1:B:95:ARG:NH1	1:B:147:PHE:O	2.29	0.66
1:B:201:ARG:HG2	1:B:201:ARG:NH1	2.07	0.66
1:A:113:LEU:HD13	1:A:122:GLN:HG3	1.78	0.66
1:A:150:ASP:H	1:A:151:LYS:CE	2.08	0.66
1:B:15:PRO:HB2	1:B:76:MET:HE3	1.76	0.66
1:A:81:ARG:CZ	1:B:93:ARG:HG2	2.26	0.66
1:B:82:LYS:HG3	3:B:868:HOH:O	1.96	0.65
2:B:218:GPR:HA2	3:B:682:HOH:O	1.96	0.65
1:B:123:LYS:HB3	1:B:124:PRO:CD	2.27	0.65
1:B:68:LYS:C	1:B:69:ILE:HD13	2.17	0.65
1:A:21:GLU:HG3	1:A:196:TYR:CD2	2.31	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:170:GLU:HG3	1:B:173:CYS:HB3	1.78	0.65
1:B:175:ASP:OD1	1:B:181:LYS:HE3	1.97	0.65
1:A:108:MET:O	1:A:112:MET:HG3	1.96	0.65
1:B:104:MET:HE3	1:B:107:ARG:HB3	1.79	0.64
1:B:174:LEU:O	1:B:175:ASP:C	2.35	0.64
1:A:217:LYS:OXT	1:A:217:LYS:HG3	1.98	0.64
1:B:88:GLU:OE1	1:B:151:LYS:NZ	2.30	0.64
1:A:67:ARG:NH1	1:A:78:TYR:OH	2.30	0.63
1:A:151:LYS:H	1:A:151:LYS:HE2	1.64	0.63
1:B:16:ILE:HG13	1:B:76:MET:CE	2.29	0.63
1:A:216:ASN:HD22	1:A:217:LYS:H	1.47	0.63
1:B:108:MET:HA	1:B:108:MET:HE3	1.80	0.62
1:B:107:ARG:O	1:B:111:ILE:HG22	1.99	0.62
1:B:138:SER:OG	1:B:179:ASN:ND2	2.29	0.62
1:A:81:ARG:NE	1:B:90:GLU:OE2	2.29	0.62
1:B:37:ALA:HB3	3:B:790:HOH:O	1.99	0.62
1:A:8:ASN:HB3	1:A:32:TYR:O	1.99	0.62
1:A:121:LYS:HE2	1:A:121:LYS:H	1.63	0.62
1:A:194:SER:O	1:A:198:LYS:HD3	2.00	0.62
1:A:7:FTR:CH2	1:A:42:ARG:HG2	2.29	0.62
1:B:108:MET:HA	1:B:108:MET:CE	2.30	0.61
1:A:106:ASN:ND2	1:A:137:TYR:OH	2.29	0.61
1:A:146:FTR:CE2	1:A:152:VAL:HG22	2.30	0.61
1:A:71:GLN:O	1:A:74:ALA:HB3	1.99	0.61
1:B:144:ARG:HG2	1:B:149:GLY:HA2	1.83	0.60
1:A:186:ARG:HG3	1:A:186:ARG:HH11	1.66	0.60
1:A:7:FTR:HH2	1:A:42:ARG:CG	2.31	0.60
1:B:161:ASP:O	1:B:165:GLN:HG3	2.01	0.60
1:A:116:ASN:OD1	1:A:118:ASP:N	2.29	0.60
1:A:135:LYS:HE3	1:A:136:LEU:CD2	2.31	0.60
1:A:202:TYR:CE2	1:A:204:SER:HB2	2.37	0.60
1:B:109:GLN:HG3	1:B:133:LYS:NZ	2.17	0.59
1:A:150:ASP:CB	1:A:151:LYS:HD3	2.32	0.59
1:A:88:GLU:N	1:A:92:GLU:OE1	2.30	0.59
1:B:1:PRO:HB2	1:B:27:TYR:HA	1.85	0.59
1:A:13:THR:O	1:A:14:HIS:C	2.39	0.59
1:A:58:ASN:OD1	2:A:218:GPR:N3	2.36	0.59
1:A:83:HIS:O	1:A:84:HIS:ND1	2.36	0.59
1:B:145:PRO:HB2	1:B:146:FTR:CD1	2.33	0.59
1:B:82:LYS:HE2	3:B:628:HOH:O	2.03	0.59
1:A:125:GLU:HG3	3:A:814:HOH:O	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:88:GLU:HB2	1:A:92:GLU:OE1	2.02	0.58
1:B:35:GLY:O	1:B:40:TYR:HA	2.02	0.58
1:A:150:ASP:CA	1:A:151:LYS:HE2	2.34	0.58
1:B:61:TYR:CD1	1:B:63:ILE:HD13	2.38	0.58
1:A:186:ARG:HH11	1:A:186:ARG:CG	2.17	0.57
1:A:207:ILE:HD11	1:A:214:FTR:CH2	2.34	0.57
1:B:130:ILE:HB	1:B:131:PRO:HD3	1.86	0.57
1:A:49:LYS:HE2	3:A:630:HOH:O	2.05	0.57
1:A:128:LYS:O	1:A:131:PRO:HD2	2.04	0.57
1:B:184:LEU:O	1:B:187:PHE:N	2.38	0.57
1:A:193:ILE:O	1:A:197:MET:HG3	2.03	0.57
1:B:212:ALA:HB3	1:B:216:ASN:HB3	1.86	0.57
1:B:106:ASN:OD1	1:B:109:GLN:OE1	2.22	0.57
1:B:108:MET:HA	1:B:111:ILE:CG2	2.34	0.57
1:A:150:ASP:HB2	1:A:151:LYS:HD3	1.88	0.56
1:B:197:MET:HG2	1:B:202:TYR:CZ	2.41	0.56
1:B:181:LYS:HE2	3:B:670:HOH:O	2.06	0.56
1:B:2:MET:HE1	3:B:628:HOH:O	2.05	0.56
1:A:16:ILE:HG22	1:A:20:LEU:HD12	1.86	0.56
1:B:141:LEU:O	1:B:144:ARG:HB2	2.06	0.56
1:B:163:LEU:N	1:B:163:LEU:HD12	2.19	0.56
1:A:112:MET:HG2	3:A:615:HOH:O	2.06	0.55
1:B:170:GLU:O	1:B:173:CYS:HB3	2.06	0.55
1:A:68:LYS:NZ	3:A:830:HOH:O	2.39	0.55
1:A:55:ASP:HB2	3:A:848:HOH:O	2.05	0.55
1:A:3:ILE:HG22	1:A:4:LEU:N	2.20	0.55
1:B:116:ASN:C	1:B:116:ASN:HD22	2.10	0.55
1:A:108:MET:HA	1:A:111:ILE:HD11	1.88	0.55
1:B:187:PHE:HA	1:B:190:LEU:HD22	1.87	0.55
1:B:187:PHE:O	1:B:190:LEU:HD22	2.06	0.55
1:A:151:LYS:CE	1:A:151:LYS:H	2.20	0.54
1:A:161:ASP:O	1:A:165:GLN:HG3	2.06	0.54
1:A:16:ILE:HD13	1:A:76:MET:SD	2.46	0.54
1:A:209:SER:HB3	2:A:218:GPR:HE4	1.88	0.54
1:B:12:LEU:N	1:B:12:LEU:HD23	2.19	0.54
1:A:150:ASP:HB2	1:A:151:LYS:HE2	1.89	0.54
1:A:216:ASN:HD22	1:A:216:ASN:C	2.10	0.54
1:A:78:TYR:CE2	1:A:82:LYS:HE2	2.42	0.54
1:B:119:PHE:O	1:B:123:LYS:HB2	2.07	0.54
1:B:121:LYS:HD2	1:B:122:GLN:OE1	2.07	0.54
1:A:10:ARG:HB3	1:A:207:ILE:HA	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:151:LYS:HG3	1:B:152:VAL:O	2.07	0.53
1:B:170:GLU:CB	1:B:173:CYS:HB3	2.38	0.53
1:B:71:GLN:O	1:B:75:ILE:HG13	2.08	0.53
1:B:10:ARG:HB3	1:B:207:ILE:HA	1.89	0.53
1:B:12:LEU:H	1:B:12:LEU:CD2	2.21	0.53
1:B:130:ILE:N	1:B:131:PRO:HD2	2.22	0.53
1:B:122:GLN:O	1:B:123:LYS:HB2	2.09	0.53
1:B:170:GLU:CG	1:B:173:CYS:HB3	2.39	0.53
1:A:207:ILE:HD11	1:A:214:FTR:CZ3	2.39	0.53
1:A:135:LYS:CE	1:A:136:LEU:HG	2.39	0.53
1:A:67:ARG:NH1	1:A:78:TYR:CE1	2.77	0.53
1:A:108:MET:HA	1:A:111:ILE:CD1	2.39	0.53
1:A:45:FTR:CE2	1:A:49:LYS:HG3	2.39	0.53
1:B:113:LEU:HD22	1:B:126:PHE:CG	2.44	0.53
1:B:214:FTR:CZ3	1:B:215:SER:HB2	2.38	0.53
1:B:8:ASN:OD1	1:B:8:ASN:N	2.26	0.53
1:B:183:PHE:O	1:B:184:LEU:C	2.41	0.52
1:A:18:LEU:HD13	1:A:187:PHE:CZ	2.44	0.52
1:B:206:PRO:HB3	1:B:217:LYS:N	2.24	0.52
1:A:14:HIS:HB3	1:A:15:PRO:HD3	1.92	0.52
1:A:88:GLU:HA	1:A:88:GLU:OE1	2.10	0.52
1:B:34:MET:HB3	1:B:41:ASP:O	2.09	0.52
1:B:8:ASN:OD1	1:B:32:TYR:O	2.27	0.52
1:B:128:LYS:HZ3	1:B:128:LYS:HB2	1.74	0.52
1:A:39:ASP:HA	3:A:593:HOH:O	2.10	0.52
1:A:94:ILE:HD13	1:B:67:ARG:HD2	1.91	0.52
1:A:211:LEU:H	1:A:211:LEU:CD1	2.15	0.51
1:A:49:LYS:HD3	1:A:50:PHE:CE1	2.45	0.51
1:A:123:LYS:O	1:A:124:PRO:C	2.47	0.51
1:A:11:GLY:CA	2:A:218:GPR:HZ5	2.33	0.51
1:A:21:GLU:HG3	1:A:196:TYR:CD1	2.45	0.51
1:B:145:PRO:HG2	1:B:150:ASP:HA	1.91	0.51
1:A:150:ASP:HB2	1:A:151:LYS:CD	2.39	0.51
1:B:162:ILE:HD11	1:B:166:TYR:HE2	1.74	0.51
1:B:157:PHE:CD1	1:B:157:PHE:N	2.78	0.51
1:B:39:ASP:N	1:B:39:ASP:OD1	2.31	0.51
2:A:218:GPR:HB12	3:A:779:HOH:O	2.11	0.50
1:A:91:GLU:OE2	1:B:67:ARG:NH1	2.42	0.50
1:B:16:ILE:HG13	1:B:76:MET:HE1	1.93	0.50
1:B:199:SER:HB2	1:B:201:ARG:HE	1.76	0.50
1:A:144:ARG:HG2	1:A:149:GLY:CA	2.40	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:118:ASP:OD2	1:B:122:GLN:OE1	2.29	0.50
1:A:151:LYS:N	1:A:151:LYS:HE2	2.27	0.50
1:B:7:FTR:HB2	1:B:8:ASN:OD1	2.12	0.50
1:B:211:LEU:O	1:B:212:ALA:O	2.29	0.50
1:A:34:MET:SD	1:A:211:LEU:HD11	2.52	0.50
1:B:126:PHE:CA	1:B:129:THR:HG23	2.39	0.50
1:A:20:LEU:HD23	1:A:25:SER:CB	2.42	0.49
1:B:201:ARG:CG	1:B:201:ARG:HH11	2.11	0.49
1:A:35:GLY:O	1:A:40:TYR:HA	2.13	0.49
1:B:116:ASN:ND2	1:B:118:ASP:N	2.41	0.49
1:B:13:THR:HG23	1:B:16:ILE:HD12	1.95	0.49
1:B:95:ARG:HH11	1:B:148:ALA:C	2.15	0.49
1:A:92:GLU:OE2	1:A:151:LYS:HE3	2.13	0.49
1:B:108:MET:HA	1:B:111:ILE:HG22	1.94	0.49
1:B:113:LEU:HD11	1:B:122:GLN:O	2.13	0.49
1:A:122:GLN:HE22	1:A:125:GLU:CG	2.14	0.49
1:B:108:MET:HE3	1:B:108:MET:CA	2.43	0.49
1:B:39:ASP:C	1:B:40:TYR:HD1	2.16	0.49
1:A:167:HIS:NE2	1:A:171:PRO:O	2.45	0.49
1:A:108:MET:HA	1:A:111:ILE:HG13	1.91	0.49
1:A:10:ARG:HH22	1:A:164:ASP:CG	2.10	0.48
1:B:7:FTR:HE3	1:B:8:ASN:OD1	2.12	0.48
1:A:125:GLU:O	1:A:125:GLU:OE1	2.31	0.48
1:B:208:PHE:CD2	1:B:215:SER:HB3	2.48	0.48
1:B:130:ILE:HG21	1:B:173:CYS:HB2	1.95	0.48
1:A:144:ARG:CG	1:A:149:GLY:HA2	2.43	0.48
1:B:115:TYR:O	1:B:117:PRO:HD3	2.12	0.48
1:B:6:TYR:CG	1:B:7:FTR:N	2.82	0.48
1:B:109:GLN:HG3	1:B:133:LYS:HZ3	1.79	0.48
1:A:93:ARG:NH1	3:A:623:HOH:O	2.35	0.48
1:B:130:ILE:N	1:B:131:PRO:CD	2.77	0.48
1:B:13:THR:O	1:B:13:THR:HG22	2.14	0.47
1:B:99:VAL:O	1:B:100:GLU:C	2.53	0.47
1:B:2:MET:HG2	1:B:64:ASP:HA	1.95	0.47
1:A:6:TYR:CG	1:A:7:FTR:N	2.82	0.47
1:B:128:LYS:HE2	1:B:128:LYS:HB3	1.67	0.47
1:B:151:LYS:HG2	1:B:153:THR:CG2	2.45	0.47
1:B:2:MET:CE	1:B:82:LYS:NZ	2.78	0.47
1:A:113:LEU:CD1	1:A:122:GLN:HG3	2.44	0.47
1:A:186:ARG:NH1	1:A:186:ARG:CG	2.77	0.47
1:B:162:ILE:HD11	1:B:166:TYR:CE2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:11:GLY:HA2	2:A:218:GPR:CZ5	2.34	0.47
1:A:150:ASP:CB	1:A:151:LYS:HE2	2.44	0.47
1:A:170:GLU:HA	1:A:171:PRO:HD2	1.55	0.46
1:A:91:GLU:HG3	3:A:622:HOH:O	2.15	0.46
1:A:122:GLN:O	1:A:122:GLN:NE2	2.48	0.46
1:A:77:ARG:O	1:A:81:ARG:HG3	2.15	0.46
1:B:144:ARG:HG3	1:B:145:PRO:HD2	1.96	0.46
1:A:40:TYR:CG	1:A:211:LEU:HG	2.51	0.46
1:B:61:TYR:CD1	1:B:63:ILE:CD1	2.99	0.46
1:A:151:LYS:CD	1:A:151:LYS:N	2.79	0.46
1:A:40:TYR:CD2	1:A:211:LEU:CD2	2.99	0.46
1:A:3:ILE:CG2	1:A:4:LEU:N	2.79	0.46
1:B:58:ASN:OD1	2:B:218:GPR:N3	2.42	0.46
1:A:180:LEU:O	1:A:181:LYS:C	2.53	0.46
1:A:45:FTR:CZ2	1:A:49:LYS:HG3	2.45	0.46
1:B:163:LEU:CD1	1:B:163:LEU:N	2.79	0.46
1:B:88:GLU:HG2	1:B:92:GLU:OE1	2.16	0.46
1:A:105:ASP:OD1	2:B:218:GPR:N1	2.37	0.46
1:A:6:TYR:O	1:A:31:ARG:HA	2.17	0.45
1:B:12:LEU:N	1:B:12:LEU:CD2	2.78	0.45
1:A:7:FTR:NE1	1:A:59:LEU:HD12	2.32	0.45
1:B:2:MET:C	1:B:3:ILE:HD13	2.36	0.45
1:B:207:ILE:HD12	1:B:215:SER:OG	2.17	0.45
1:A:40:TYR:O	1:A:41:ASP:C	2.54	0.45
1:B:24:ASP:HB2	1:B:192:LYS:NZ	2.32	0.45
1:A:159:ALA:O	1:A:160:TYR:C	2.54	0.45
1:B:203:LEU:C	1:B:203:LEU:HD12	2.36	0.45
1:B:24:ASP:HB2	1:B:192:LYS:HZ1	1.82	0.45
1:A:67:ARG:NH1	1:A:78:TYR:CZ	2.85	0.45
1:B:177:PHE:HA	1:B:178:PRO:HD2	1.77	0.45
1:B:212:ALA:O	1:B:213:GLN:NE2	2.50	0.45
1:A:123:LYS:HB3	1:A:124:PRO:HD3	1.99	0.45
1:A:160:TYR:O	1:A:164:ASP:HB3	2.16	0.45
1:A:42:ARG:HG2	1:A:42:ARG:NH1	2.32	0.44
1:A:173:CYS:HB2	3:A:551:HOH:O	2.17	0.44
1:B:46:LEU:N	1:B:46:LEU:CD1	2.79	0.44
1:A:18:LEU:HD13	1:A:187:PHE:CE2	2.52	0.44
1:A:202:TYR:HE2	1:A:204:SER:HB2	1.81	0.44
1:A:72:SER:HB2	3:A:750:HOH:O	2.17	0.44
1:B:123:LYS:N	1:B:124:PRO:CD	2.79	0.44
1:A:106:ASN:HA	1:A:109:GLN:OE1	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:172:LYS:O	1:B:175:ASP:N	2.41	0.44
1:A:111:ILE:HG23	1:A:208:PHE:HE1	1.77	0.44
1:B:144:ARG:HE	1:B:144:ARG:HB2	1.62	0.44
1:A:102:GLN:HE21	1:A:106:ASN:HD21	1.65	0.44
1:A:217:LYS:NZ	3:A:788:HOH:O	2.48	0.44
1:B:94:ILE:O	1:B:98:ILE:HG13	2.18	0.44
1:A:162:ILE:HA	1:A:162:ILE:HD12	1.70	0.44
1:B:123:LYS:CB	1:B:124:PRO:HD3	2.39	0.44
1:B:37:ALA:HA	1:B:38:PRO:HA	1.56	0.44
1:B:144:ARG:CG	1:B:149:GLY:HA2	2.47	0.43
1:A:135:LYS:HE3	1:A:136:LEU:HD23	1.99	0.43
1:B:109:GLN:HG3	1:B:133:LYS:HZ1	1.84	0.43
1:B:187:PHE:CD1	1:B:190:LEU:HD23	2.53	0.43
1:B:194:SER:HA	1:B:197:MET:HE2	2.00	0.43
1:A:78:TYR:CZ	1:A:82:LYS:HE2	2.53	0.43
1:B:34:MET:HA	1:B:41:ASP:O	2.18	0.43
1:A:207:ILE:HG21	1:A:207:ILE:HD12	1.55	0.43
2:B:218:GPR:HA4	2:B:218:GPR:HA2	1.69	0.43
1:B:32:TYR:CD1	1:B:32:TYR:N	2.86	0.43
1:A:100:GLU:HA	1:A:158:LEU:HD23	2.00	0.43
1:A:91:GLU:O	1:A:95:ARG:HG3	2.16	0.43
1:A:14:HIS:HB2	3:A:638:HOH:O	2.18	0.43
1:B:108:MET:CA	1:B:111:ILE:HG22	2.49	0.43
1:A:186:ARG:HB2	1:A:186:ARG:NH1	2.34	0.42
1:B:12:LEU:CD2	2:B:218:GPR:SG2	3.07	0.42
1:A:108:MET:HA	1:A:111:ILE:HG12	1.97	0.42
1:B:70:THR:O	1:B:71:GLN:HB2	2.19	0.42
1:A:60:PRO:HG2	1:A:75:ILE:HD12	2.02	0.42
1:B:108:MET:CE	1:B:111:ILE:HG21	2.50	0.42
1:B:128:LYS:HG2	3:B:789:HOH:O	2.17	0.42
1:B:160:TYR:CD1	1:B:184:LEU:HD23	2.55	0.42
1:B:210:LYS:HD3	1:B:210:LYS:HA	1.79	0.42
1:B:51:LYS:HE2	3:B:605:HOH:O	2.19	0.42
1:A:201:ARG:NH1	3:A:792:HOH:O	2.51	0.42
1:B:130:ILE:O	1:B:133:LYS:N	2.51	0.42
1:B:195:ALA:O	1:B:196:TYR:C	2.57	0.42
1:A:192:LYS:HG3	3:A:543:HOH:O	2.19	0.42
1:B:104:MET:CE	1:B:108:MET:SD	3.06	0.42
1:A:121:LYS:HE2	1:A:121:LYS:N	2.33	0.42
1:A:81:ARG:NH2	1:B:90:GLU:OE2	2.53	0.42
1:B:126:PHE:O	1:B:129:THR:HG23	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:135:LYS:HE2	1:A:136:LEU:N	2.35	0.42
1:A:37:ALA:HB2	1:A:40:TYR:OH	2.20	0.42
1:B:67:ARG:HA	1:B:67:ARG:HD3	1.71	0.41
1:A:10:ARG:HD3	1:A:207:ILE:HG22	2.02	0.41
1:B:119:PHE:CZ	1:B:214:FTR:HB3	2.55	0.41
1:B:89:THR:H	1:B:92:GLU:HB2	1.85	0.41
1:A:40:TYR:CZ	1:A:211:LEU:HG	2.55	0.41
1:A:94:ILE:HD13	1:B:67:ARG:CD	2.50	0.41
1:B:116:ASN:HA	1:B:117:PRO:HD2	1.52	0.41
1:B:113:LEU:CD2	1:B:126:PHE:CD2	3.00	0.41
1:B:12:LEU:HD21	2:B:218:GPR:SG2	2.61	0.41
1:A:180:LEU:O	1:A:183:PHE:N	2.54	0.41
1:B:108:MET:O	1:B:112:MET:SD	2.79	0.41
1:B:146:FTR:CE2	1:B:152:VAL:HG22	2.51	0.41
1:B:77:ARG:HH11	1:B:77:ARG:HD3	1.63	0.41
1:A:177:PHE:O	1:A:180:LEU:N	2.53	0.41
1:A:136:LEU:HA	1:A:136:LEU:HD23	1.85	0.41
1:A:146:FTR:HD1	1:A:150:ASP:O	2.21	0.41
1:A:153:THR:OG1	1:A:155:VAL:HG22	2.21	0.41
1:A:146:FTR:HB2	1:A:156:ASP:OD2	2.21	0.41
1:A:20:LEU:CD2	1:A:25:SER:CB	2.99	0.41
1:B:167:HIS:CG	1:B:174:LEU:HD22	2.56	0.41
1:A:55:ASP:HA	3:A:590:HOH:O	2.21	0.41
1:A:20:LEU:HD23	1:A:25:SER:HB2	2.03	0.40
1:B:209:SER:O	1:B:210:LYS:C	2.59	0.40
1:A:40:TYR:CG	1:A:211:LEU:HD21	2.57	0.40
1:B:108:MET:CE	1:B:111:ILE:CG2	2.99	0.40
1:B:99:VAL:HG22	1:B:140:PHE:CE2	2.56	0.40
1:A:63:ILE:CG1	1:A:68:LYS:HD2	2.51	0.40
1:B:191:LYS:HE2	1:B:192:LYS:HE3	2.04	0.40
1:B:59:LEU:HA	1:B:60:PRO:HA	1.78	0.40

All (1) 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)
3:B:828:HOH:O	3:B:828:HOH:O[2_655]	1.95	0.25

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	211/217 (97%)	194 (92%)	16 (8%)	1 (0%)	29	23
1	B	211/217 (97%)	191 (90%)	12 (6%)	8 (4%)	3	1
All	All	422/434 (97%)	385 (91%)	28 (7%)	9 (2%)	7	2

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	123	LYS
1	B	191	LYS
1	B	212	ALA
1	B	8	ASN
1	B	41	ASP
1	B	213	GLN
1	B	173	CYS
1	B	36	ASP
1	A	71	GLN

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	193/193 (100%)	148 (77%)	45 (23%)	1	0
1	B	193/193 (100%)	149 (77%)	44 (23%)	1	0
All	All	386/386 (100%)	297 (77%)	89 (23%)	1	0

All (89) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	ASN
1	A	12	LEU
1	A	29	GLU
1	A	34	MET
1	A	41	ASP
1	A	42	ARG
1	A	43	SER
1	A	46	LEU
1	A	48	GLU
1	A	49	LYS
1	A	51	LYS
1	A	55	ASP
1	A	63	ILE
1	A	66	SER
1	A	67	ARG
1	A	82	LYS
1	A	88	GLU
1	A	99	VAL
1	A	107	ARG
1	A	111	ILE
1	A	113	LEU
1	A	121	LYS
1	A	123	LYS
1	A	135	LYS
1	A	139	GLU
1	A	144	ARG
1	A	150	ASP
1	A	151	LYS
1	A	158	LEU
1	A	164	ASP
1	A	170	GLU
1	A	172	LYS
1	A	174	LEU
1	A	182	ASP
1	A	184	LEU
1	A	186	ARG
1	A	192	LYS
1	A	198	LYS
1	A	200	SER
1	A	207	ILE
1	A	210	LYS
1	A	211	LEU

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Mol	Chain	Res	Type
1	A	213	GLN
1	A	216	ASN
1	A	217	LYS
1	B	3	ILE
1	B	8	ASN
1	B	12	LEU
1	B	21	GLU
1	B	25	SER
1	B	36	ASP
1	B	39	ASP
1	B	40	TYR
1	B	41	ASP
1	B	43	SER
1	B	63	ILE
1	B	66	SER
1	B	69	ILE
1	B	79	LEU
1	B	88	GLU
1	B	90	GLU
1	B	93	ARG
1	B	104	MET
1	B	109	GLN
1	B	111	ILE
1	B	116	ASN
1	B	121	LYS
1	B	122	GLN
1	B	128	LYS
1	B	129	THR
1	B	138	SER
1	B	139	GLU
1	B	144	ARG
1	B	172	LYS
1	B	173	CYS
1	B	174	LEU
1	B	179	ASN
1	B	181	LYS
1	B	186	ARG
1	B	190	LEU
1	B	201	ARG
1	B	203	LEU
1	B	204	SER
1	B	205	THR

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Mol	Chain	Res	Type
1	B	209	SER
1	B	210	LYS
1	B	211	LEU
1	B	215	SER
1	B	217	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	44	GLN
1	A	47	ASN
1	A	83	HIS
1	A	106	ASN
1	A	122	GLN
1	A	165	GLN
1	A	216	ASN
1	B	14	HIS
1	B	71	GLN
1	B	102	GLN
1	B	106	ASN
1	B	116	ASN
1	B	179	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

8 non-standard protein/DNA/RNA residues 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
1	FTR	A	214	1	14,16,17	1.03	1 (7%)	14,22,24	1.49	4 (28%)
1	FTR	B	214	1	14,16,17	1.21	1 (7%)	14,22,24	1.60	2 (14%)
1	FTR	A	146	1	14,16,17	0.99	0	14,22,24	1.92	5 (35%)
1	FTR	A	45	1	14,16,17	1.10	0	14,22,24	1.39	3 (21%)
1	FTR	A	7	1	14,16,17	1.06	0	14,22,24	1.06	1 (7%)
1	FTR	B	45	1	14,16,17	0.99	0	14,22,24	1.61	3 (21%)
1	FTR	B	7	1	14,16,17	0.93	0	14,22,24	1.39	2 (14%)
1	FTR	B	146	1	14,16,17	1.08	0	14,22,24	1.26	2 (14%)

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
1	FTR	A	214	1	-	0/4/6/8	0/2/2/2
1	FTR	B	214	1	-	0/4/6/8	0/2/2/2
1	FTR	A	146	1	-	0/4/6/8	0/2/2/2
1	FTR	A	45	1	-	1/4/6/8	0/2/2/2
1	FTR	A	7	1	-	0/4/6/8	0/2/2/2
1	FTR	B	45	1	-	0/4/6/8	0/2/2/2
1	FTR	B	7	1	-	0/4/6/8	0/2/2/2
1	FTR	B	146	1	-	0/4/6/8	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	214	FTR	CE3-CZ3	3.52	1.41	1.36
1	A	214	FTR	CZ2-CE2	-2.22	1.38	1.41

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	45	FTR	CB-CG-CD1	-4.14	122.86	127.97
1	A	146	FTR	CG-CB-CA	-3.80	108.66	114.53
1	A	146	FTR	CH2-CZ3-CE3	-3.39	119.49	123.23
1	B	214	FTR	CG-CB-CA	-3.17	109.63	114.53
1	B	214	FTR	CB-CG-CD1	-3.12	124.11	127.97
1	A	214	FTR	CH2-CZ2-CE2	-2.87	117.23	120.84
1	A	45	FTR	CH2-CZ2-CE2	-2.84	117.26	120.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	7	FTR	CB-CG-CD1	-2.76	124.56	127.97
1	A	146	FTR	CZ2-CH2-CZ3	2.69	121.81	118.74
1	B	146	FTR	CG-CB-CA	-2.64	110.44	114.53
1	A	45	FTR	CB-CA-C	-2.45	106.87	111.47
1	A	214	FTR	CH2-CZ3-CE3	-2.41	120.57	123.23
1	A	146	FTR	CZ3-CE3-CD2	2.40	120.68	118.80
1	B	45	FTR	CB-CG-CD2	2.37	129.93	126.25
1	A	214	FTR	CZ2-CH2-CZ3	2.32	121.40	118.74
1	B	45	FTR	CZ3-CE3-CD2	2.30	120.60	118.80
1	A	7	FTR	CZ3-CE3-CD2	2.28	120.59	118.80
1	A	146	FTR	CH2-CZ2-CE2	-2.23	118.03	120.84
1	A	45	FTR	CB-CG-CD1	-2.18	125.27	127.97
1	A	214	FTR	CB-CG-CD1	-2.17	125.28	127.97
1	B	146	FTR	CZ3-CE3-CD2	2.15	120.48	118.80
1	B	7	FTR	CH2-CZ2-CE2	-2.07	118.24	120.84

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	45	FTR	CA-CB-CG-CD1

There are no ring outliers.

7 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	214	FTR	2	0
1	B	214	FTR	3	0
1	A	146	FTR	3	0
1	A	45	FTR	2	0
1	A	7	FTR	5	0
1	B	7	FTR	3	0
1	B	146	FTR	2	0

5.5 Carbohydrates

There are no monosaccharides 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	218	-	29,37,37	3.14	12 (41%)	37,51,51	2.63	16 (43%)
2	GPR	B	218	-	29,37,37	1.73	8 (27%)	37,51,51	2.02	11 (29%)

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	218	-	-	3/21/43/43	0/3/3/3
2	GPR	B	218	-	-	4/21/43/43	0/3/3/3

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	218	GPR	CB2-SG2	-11.16	1.70	1.82
2	A	218	GPR	CG5-CB5	7.13	1.49	1.39
2	A	218	GPR	CH5-CH4	-4.92	1.38	1.47
2	A	218	GPR	CD5-CE5	4.25	1.49	1.38
2	A	218	GPR	CA4-SG2	-3.54	1.75	1.84
2	B	218	GPR	CG5-CB5	3.50	1.44	1.39
2	B	218	GPR	CH5-CH4	-3.39	1.41	1.47
2	A	218	GPR	O5-CA5	2.82	1.48	1.42
2	B	218	GPR	CB2-CA2	2.73	1.59	1.53
2	A	218	GPR	CB5-CA5	2.71	1.55	1.51
2	B	218	GPR	CA4-SG2	-2.70	1.77	1.84
2	A	218	GPR	CD5-CG5	2.67	1.44	1.38
2	A	218	GPR	CB2-CA2	2.60	1.59	1.53
2	B	218	GPR	CD1-N2	2.55	1.39	1.34
2	A	218	GPR	CE4-CZ4	2.36	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	218	GPR	CZ5-CH5	2.24	1.43	1.40
2	B	218	GPR	CZ5-CH5	2.22	1.43	1.40
2	A	218	GPR	CG1-CD1	-2.12	1.47	1.51
2	B	218	GPR	CB5-CA5	-2.10	1.48	1.51
2	B	218	GPR	CE4-CD4	2.05	1.43	1.38

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	218	GPR	CB2-CA2-N2	-7.93	89.56	111.00
2	A	218	GPR	CD5-CG5-CB5	-5.66	113.82	121.01
2	A	218	GPR	OE1-CD1-N2	-5.48	113.70	122.95
2	B	218	GPR	OE1-CD1-N2	-4.71	115.01	122.95
2	A	218	GPR	CZ5-CH5-CB5	4.62	123.64	118.53
2	B	218	GPR	CD4-CG4-CB4	-4.49	115.31	121.01
2	B	218	GPR	CB2-CA2-C2	-3.74	101.63	109.73
2	B	218	GPR	CZ4-CH4-CB4	3.62	122.53	118.53
2	B	218	GPR	CH5-CH4-CB4	-3.60	114.54	119.64
2	B	218	GPR	O5-CA5-CB5	-3.48	103.63	110.49
2	A	218	GPR	CD4-CG4-CB4	-3.20	116.94	121.01
2	A	218	GPR	CA2-CB2-SG2	-3.08	102.75	113.84
2	B	218	GPR	CE4-CD4-CG4	2.99	124.74	120.19
2	A	218	GPR	CG1-CD1-N2	-2.98	110.66	115.83
2	A	218	GPR	CE5-CD5-CG5	2.83	124.51	120.19
2	A	218	GPR	O5-CA5-CB5	2.80	116.01	110.49
2	B	218	GPR	CD4-CE4-CZ4	-2.77	115.97	120.19
2	A	218	GPR	CB2-CA2-C2	-2.56	104.17	109.73
2	B	218	GPR	CA2-CB2-SG2	-2.53	104.74	113.84
2	A	218	GPR	CA5-CA4-SG2	2.44	118.35	110.88
2	B	218	GPR	C3-CA3-N3	2.36	114.97	110.43
2	A	218	GPR	C3-CA3-N3	2.25	114.77	110.43
2	A	218	GPR	CH5-CH4-CB4	-2.23	116.49	119.64
2	A	218	GPR	CH4-CH5-CB5	-2.20	116.52	119.64
2	A	218	GPR	CZ4-CH4-CB4	2.17	120.93	118.53
2	B	218	GPR	CA3-N3-C2	2.12	125.39	122.34
2	A	218	GPR	OE1-CD1-CG1	2.12	125.89	122.02

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	218	GPR	N1-CA1-CB1-CG1

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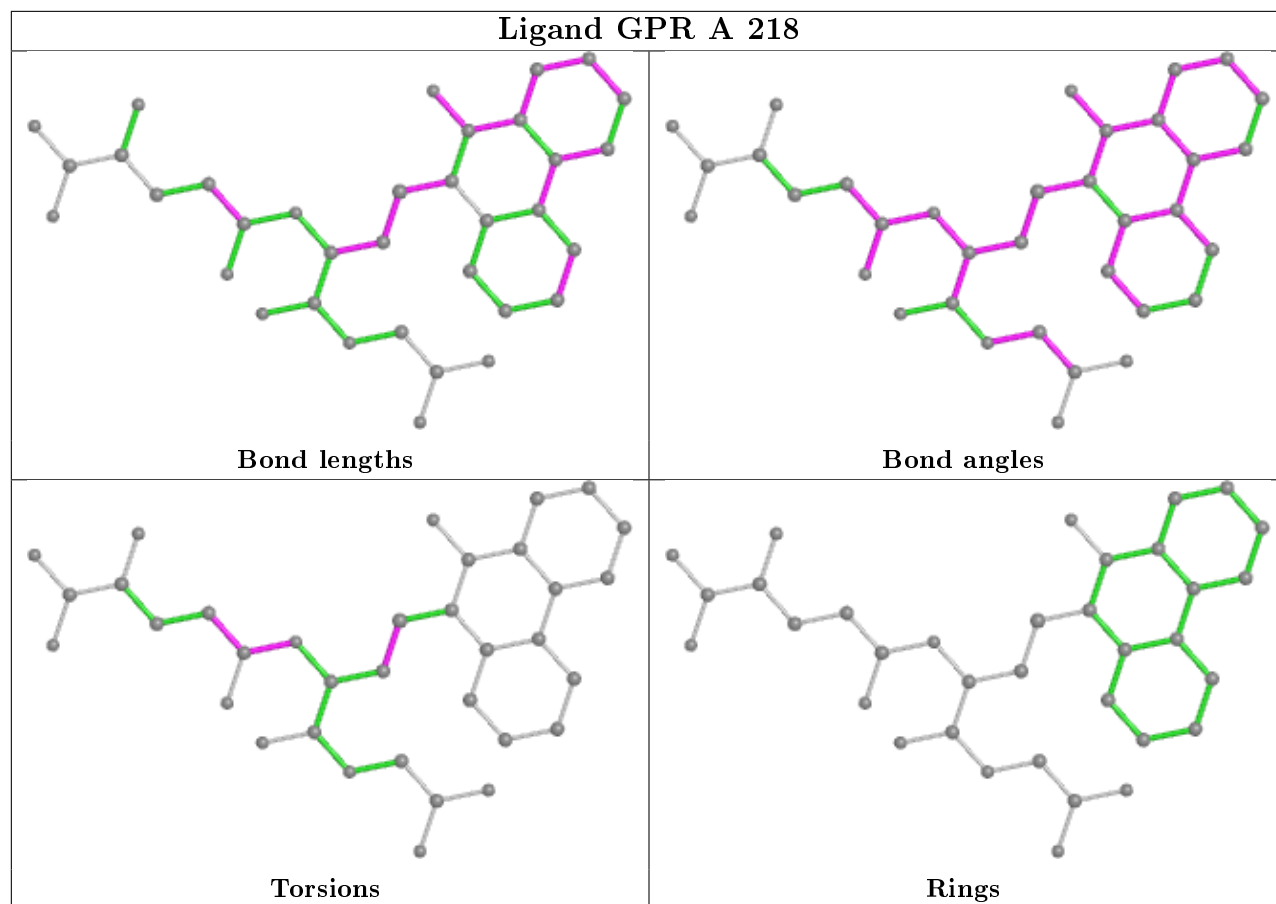
Mol	Chain	Res	Type	Atoms
2	B	218	GPR	C1-CA1-CB1-CG1
2	B	218	GPR	OE1-CD1-N2-CA2
2	A	218	GPR	OE1-CD1-CG1-CB1
2	A	218	GPR	OE1-CD1-N2-CA2
2	A	218	GPR	CA2-CB2-SG2-CA4
2	B	218	GPR	OE1-CD1-CG1-CB1

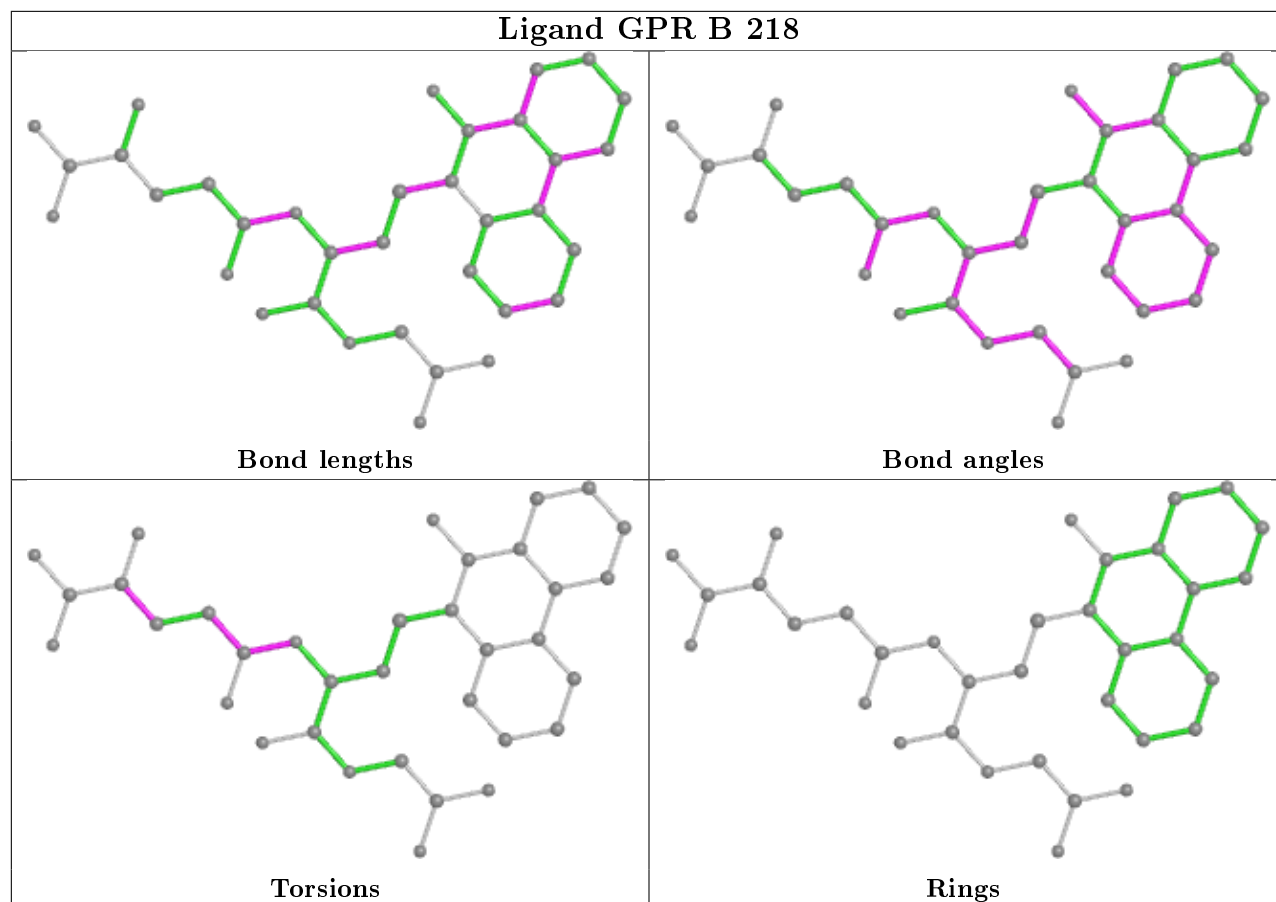
There are no ring outliers.

2 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	218	GPR	6	0
2	B	218	GPR	7	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	213/217 (98%)	0.86	21 (9%) 7 6	17, 30, 56, 70	0
1	B	213/217 (98%)	0.99	26 (12%) 4 3	15, 29, 59, 82	0
All	All	426/434 (98%)	0.92	47 (11%) 5 5	15, 30, 58, 82	0

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	37	ALA	6.4
1	B	124	PRO	5.3
1	B	212	ALA	5.0
1	B	122	GLN	5.0
1	B	40	TYR	4.8
1	B	191	LYS	4.8
1	B	38	PRO	4.7
1	A	112	MET	4.3
1	A	39	ASP	4.0
1	B	35	GLY	3.9
1	B	36	ASP	3.8
1	B	125	GLU	3.6
1	A	125	GLU	3.5
1	B	215	SER	3.4
1	A	84	HIS	3.2
1	B	217	LYS	3.2
1	B	39	ASP	3.0
1	A	189	GLY	2.9
1	B	18	LEU	2.9
1	B	129	THR	2.9
1	B	180	LEU	2.8
1	B	206	PRO	2.7
1	B	211	LEU	2.7
1	A	216	ASN	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	111	ILE	2.6
1	B	174	LEU	2.5
1	A	65	GLY	2.5
1	B	120	GLU	2.4
1	A	115	TYR	2.4
1	B	175	ASP	2.4
1	B	195	ALA	2.3
1	A	117	PRO	2.3
1	B	173	CYS	2.3
1	A	185	ALA	2.2
1	A	208	PHE	2.2
1	B	117	PRO	2.2
1	A	40	TYR	2.2
1	B	126	PHE	2.2
1	A	190	LEU	2.1
1	A	66	SER	2.1
1	A	171	PRO	2.1
1	A	191	LYS	2.1
1	A	178	PRO	2.1
1	B	216	ASN	2.1
1	A	116	ASN	2.0
1	A	88	GLU	2.0
1	A	145	PRO	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	FTR	B	214	15/16	0.88	0.17	15,38,60,64	0
1	FTR	A	7	15/16	0.88	0.15	17,35,80,100	0
1	FTR	A	146	15/16	0.90	0.15	16,27,74,83	0
1	FTR	A	214	15/16	0.90	0.13	23,34,100,100	0
1	FTR	B	146	15/16	0.91	0.12	15,22,33,43	0
1	FTR	B	7	15/16	0.92	0.12	12,25,71,79	0
1	FTR	B	45	15/16	0.92	0.14	14,20,38,40	0
1	FTR	A	45	15/16	0.93	0.11	12,20,30,36	0

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

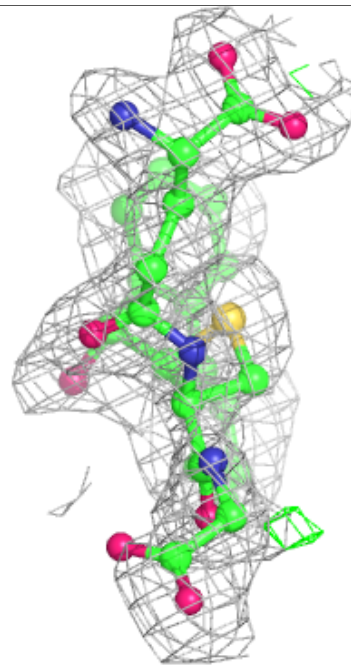
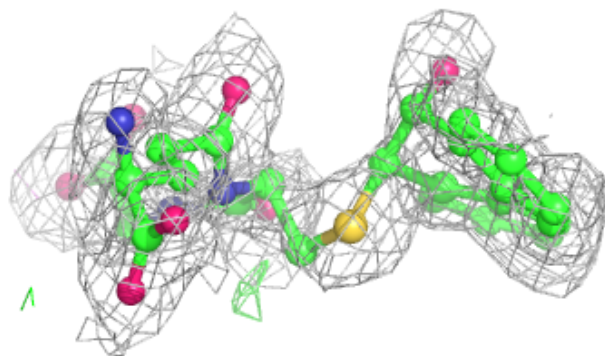
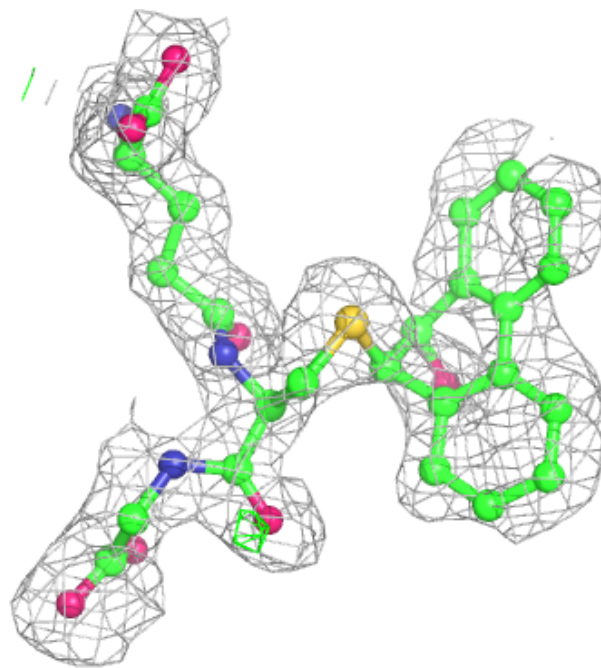
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	GPR	A	218	35/35	0.84	0.20	19,39,100,100	0
2	GPR	B	218	35/35	0.85	0.18	17,34,100,100	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.

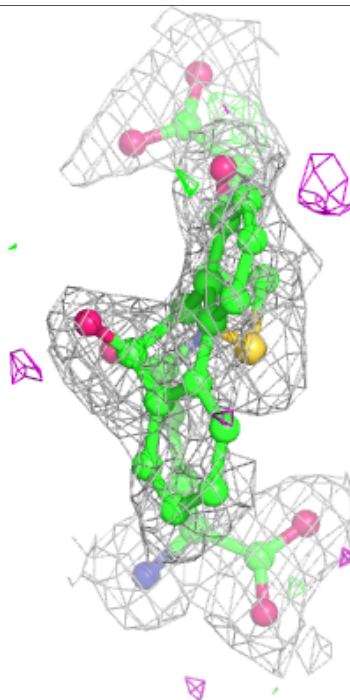
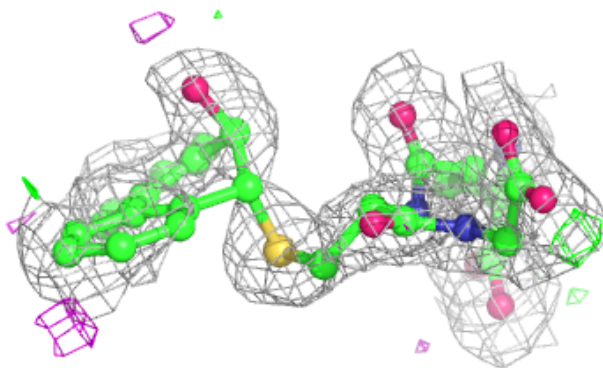
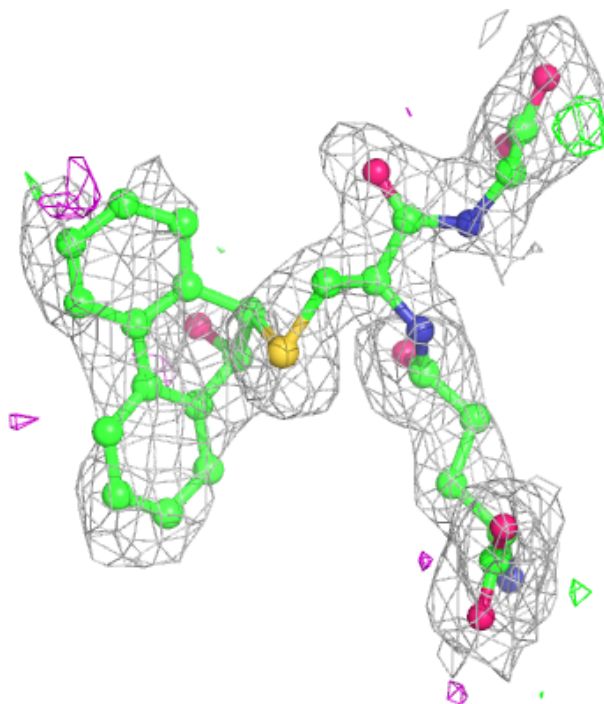
Electron density around GPR A 218:

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



Electron density around GPR B 218:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.