



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:56 PM GMT

PDB ID : 1MTC
Title : GLUTATHIONE TRANSFERASE MUTANT Y115F
Authors : Ladner, J.E.; Xiao, G.; Armstrong, R.N.; Gilliland, G.L.
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
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

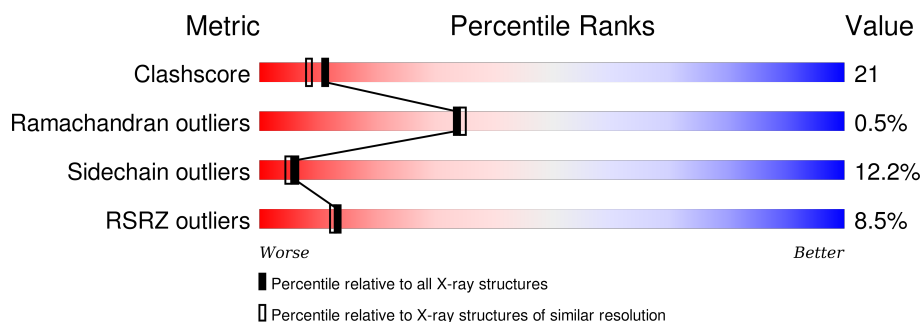
1 Overall quality at a glance

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	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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.

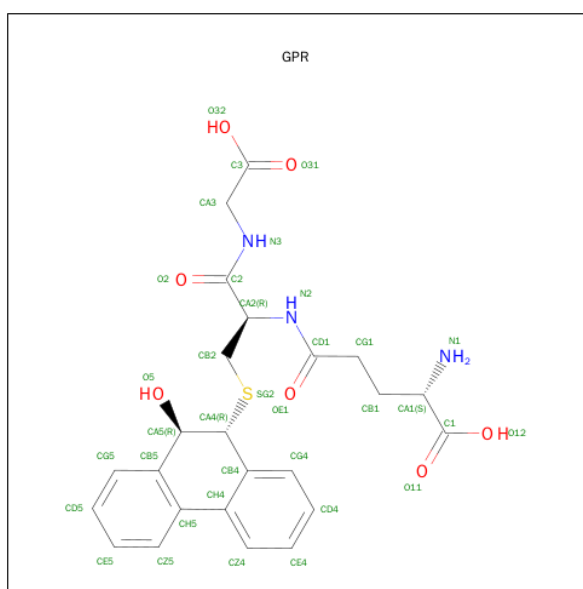
- Molecule 1 is a protein called Glutathione S-transferase YB1.

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	UNP P04905
B	115	PHE	TYR	ENGINEERED	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		

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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		

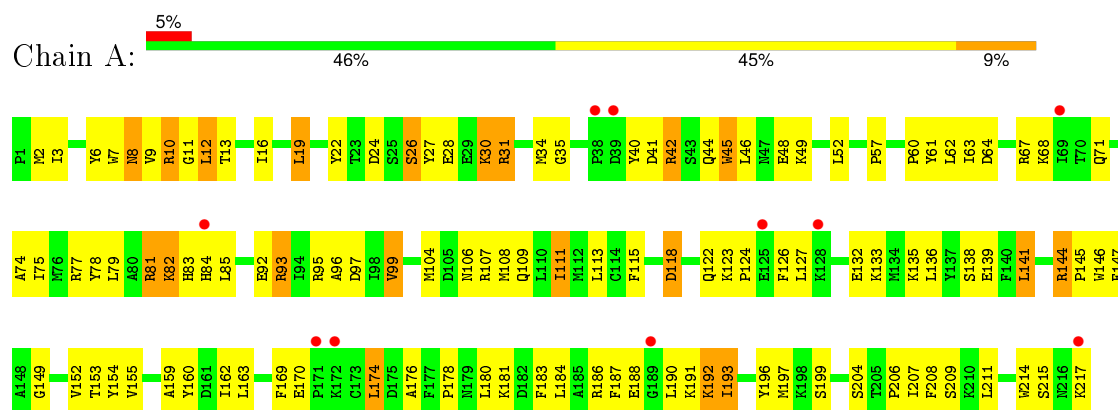
- Molecule 3 is water.

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 [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($\text{RSRZ} > 2$). 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



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 19.29 – 2.20	Depositor EDS
% Data completeness (in resolution range)	94.6 (10.00-2.20) 94.6 (19.29-2.20)	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) 0.203 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	16.6	Xtriage
Anisotropy	1.161	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.42 , 109.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 21987 reflections	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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.60	0/1865	1.85	42/2513 (1.7%)
1	B	0.58	0/1865	1.73	35/2513 (1.4%)
All	All	0.59	0/3730	1.79	77/5026 (1.5%)

There are no bond length outliers.

All (77) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	67	ARG	NE-CZ-NH2	-15.75	112.43	120.30
1	A	61	TYR	CB-CG-CD1	13.70	129.22	121.00
1	A	144	ARG	NE-CZ-NH1	12.07	126.34	120.30
1	A	67	ARG	CD-NE-CZ	11.85	140.19	123.60
1	A	67	ARG	NE-CZ-NH2	-11.42	114.59	120.30
1	A	31	ARG	NE-CZ-NH2	-11.32	114.64	120.30
1	B	186	ARG	CD-NE-CZ	11.16	139.23	123.60
1	A	144	ARG	NE-CZ-NH2	-10.07	115.26	120.30
1	B	61	TYR	CB-CG-CD1	9.54	126.72	121.00
1	A	42	ARG	NE-CZ-NH1	9.07	124.83	120.30
1	A	196	TYR	CB-CG-CD1	8.98	126.39	121.00
1	A	22	TYR	CB-CG-CD2	-8.88	115.67	121.00
1	A	81	ARG	CD-NE-CZ	-8.85	111.21	123.60
1	A	160	TYR	CB-CG-CD1	8.67	126.20	121.00
1	A	77	ARG	NE-CZ-NH1	8.42	124.51	120.30
1	A	107	ARG	NE-CZ-NH2	-8.41	116.10	120.30
1	A	78	TYR	CB-CG-CD1	-7.99	116.21	121.00
1	A	10	ARG	NE-CZ-NH2	-7.88	116.36	120.30
1	A	144	ARG	CD-NE-CZ	7.74	134.43	123.60
1	B	144	ARG	NE-CZ-NH2	-7.72	116.44	120.30
1	B	115	PHE	CB-CG-CD1	7.72	126.20	120.80
1	A	26	SER	N-CA-CB	7.52	121.78	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	10	ARG	NE-CZ-NH1	-7.51	116.54	120.30
1	A	154	TYR	CB-CG-CD2	-7.17	116.69	121.00
1	B	42	ARG	NE-CZ-NH2	7.08	123.84	120.30
1	B	95	ARG	NE-CZ-NH1	-6.93	116.84	120.30
1	A	61	TYR	CG-CD1-CE1	6.92	126.84	121.30
1	B	100	GLU	OE1-CD-OE2	-6.88	115.04	123.30
1	B	67	ARG	NE-CZ-NH1	6.85	123.73	120.30
1	A	154	TYR	CB-CG-CD1	6.75	125.05	121.00
1	A	42	ARG	CD-NE-CZ	6.67	132.94	123.60
1	B	42	ARG	NE-CZ-NH1	-6.58	117.01	120.30
1	A	31	ARG	CD-NE-CZ	6.46	132.65	123.60
1	A	84	HIS	CA-CB-CG	-6.44	102.65	113.60
1	A	64	ASP	CB-CG-OD2	6.35	124.02	118.30
1	B	92	GLU	OE1-CD-OE2	-6.27	115.78	123.30
1	B	97	ASP	CB-CG-OD1	6.17	123.85	118.30
1	A	196	TYR	CB-CG-CD2	-6.15	117.31	121.00
1	B	10	ARG	NE-CZ-NH2	6.13	123.37	120.30
1	B	61	TYR	CA-CB-CG	6.00	124.80	113.40
1	A	93	ARG	NE-CZ-NH1	-6.00	117.30	120.30
1	B	65	GLY	CA-C-O	5.98	131.37	120.60
1	A	61	TYR	CB-CG-CD2	-5.95	117.43	121.00
1	B	137	TYR	CB-CG-CD2	-5.93	117.44	121.00
1	B	77	ARG	NE-CZ-NH1	5.81	123.20	120.30
1	B	64	ASP	CB-CG-OD2	-5.80	113.08	118.30
1	A	45	TRP	CA-C-O	5.80	132.28	120.10
1	B	91	GLU	OE1-CD-OE2	5.76	130.21	123.30
1	A	92	GLU	O-C-N	5.74	131.89	122.70
1	A	77	ARG	CD-NE-CZ	5.71	131.59	123.60
1	A	183	PHE	CB-CG-CD2	5.67	124.77	120.80
1	A	115	PHE	O-C-N	-5.62	113.71	122.70
1	B	27	TYR	CG-CD2-CE2	5.55	125.74	121.30
1	B	156	ASP	CB-CG-OD1	5.55	123.29	118.30
1	A	193	ILE	O-C-N	-5.53	113.86	122.70
1	A	183	PHE	CB-CG-CD1	-5.48	116.97	120.80
1	B	160	TYR	CB-CG-CD2	-5.42	117.75	121.00
1	B	169	PHE	O-C-N	5.42	131.37	122.70
1	B	213	GLN	C-N-CA	5.41	135.21	121.70
1	A	10	ARG	NH1-CZ-NH2	5.40	125.34	119.40
1	B	40	TYR	CB-CG-CD2	5.40	124.24	121.00
1	A	97	ASP	O-C-N	-5.38	114.08	122.70
1	A	147	PHE	C-N-CA	-5.34	108.34	121.70
1	B	95	ARG	NH1-CZ-NH2	5.29	125.22	119.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	131	PRO	C-N-CA	-5.26	108.54	121.70
1	B	160	TYR	CB-CG-CD1	5.22	124.14	121.00
1	B	113	LEU	O-C-N	-5.19	114.39	122.70
1	B	115	PHE	CA-CB-CG	5.19	126.36	113.90
1	B	144	ARG	NE-CZ-NH1	5.18	122.89	120.30
1	A	31	ARG	NE-CZ-NH1	5.16	122.88	120.30
1	B	206	PRO	O-C-N	5.14	130.92	122.70
1	A	22	TYR	CB-CG-CD1	5.09	124.06	121.00
1	A	99	VAL	O-C-N	5.08	130.84	122.70
1	B	70	THR	N-CA-CB	5.07	119.93	110.30
1	A	169	PHE	CB-CG-CD1	-5.05	117.27	120.80
1	A	107	ARG	NE-CZ-NH1	5.04	122.82	120.30
1	B	105	ASP	CB-CG-OD2	5.01	122.81	118.30

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	70	0
1	B	1816	0	1805	81	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	152	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 (152) 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	1.50	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2:MET:HE3	1:A:62:LEU:HD11	1.56	0.88
1:A:63:ILE:HD12	1:A:68:LYS:HD3	1.62	0.81
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:A:108:MET:HE1	2:A:5218:GPR:HD5	1.68	0.74
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: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:H	1:A:8:ASN:HD22	1.48	0.62
1:A:138:SER:HA	1:A:180:LEU:HD21	1.82	0.61
1:B:8:ASN:H	1:B:8:ASN:HD22	1.48	0.61
1:A:184:LEU:O	1:A:188:GLU:HB2	2.01	0.60
1:B:145:PRO:HB2	1:B:146:TRP:CD1	2.36	0.60
1:B:50:PHE:CE1	1:B:57:PRO:HG2	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
1:B:172:LYS:NZ	1:B:172:LYS:HB3	2.19	0.57
1:B:6:TYR:O	1:B:31:ARG:HA	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:34:MET:HE2	1:A:40:TYR:HB3	1.88	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:N	1:B:8:ASN:HD22	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:A:108:MET:CE	2:A:5218:GPR:HD5	2.39	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:208:PHE:H	1:B:215:SER:HB3	1.76	0.51
1:B:151:LYS:CD	1:B:152:VAL:H	2.23	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:B:107:ARG:HG2	1:B:111:ILE:HD11	1.93	0.50
1:A:190:LEU:HB2	1:A:193:ILE:HG12	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:B:114:CYS:HG	1:B:119:PHE:HE1	1.60	0.48
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:B:114:CYS:SG	1:B:214:TRP:HB3	2.53	0.48
1:A:118:ASP:O	1:A:122:GLN:HB2	2.13	0.48
1:B:35:GLY:HA3	1:B:41:ASP:HB3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:96:ALA:HB1	1:A:155:VAL:HG11	1.95	0.48
1:B:213:GLN:HE21	1:B:213:GLN:N	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:188:GLU:HG2	1:A:197:MET:SD	2.54	0.47
1:A:113:LEU:CD1	1:A:122:GLN:HB3	2.45	0.47
1:B:10:ARG:HB3	1:B:207:ILE:HA	1.97	0.47
1:A:42:ARG:O	1:A:46:LEU:HG	2.15	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:A:2:MET:CE	1:A:62:LEU:HD21	2.45	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:19:LEU:HD22	1:B:23:THR:CG2	2.45	0.46
1:A:34:MET:CE	1:A:40:TYR:HB3	2.46	0.46
1:B:77:ARG:NE	1:B:100:GLU:OE1	2.49	0.46
1:B:112:MET:N	1:B:112:MET:HE2	2.30	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:HB2	1:A:82:LYS:HE2	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: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:151:LYS:HA	1:B:151:LYS:HD3	1.62	0.44
1:B:132:GLU:O	1:B:136:LEU:HG	2.18	0.44
1:B:172:LYS:NZ	1:B:175:ASP:OD2	2.50	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:B:178:PRO:HG2	3:B:453:HOH:O	2.18	0.43
1:A:9:VAL:HG12	1:A:206:PRO:HG2	2.00	0.43
1:A:176:ALA:C	1:A:178:PRO:HD3	2.38	0.43
1:A:35:GLY:HA3	1:A:41:ASP:HB3	2.00	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:B:115:PHE:CD1	1:B:212:ALA:HB2	2.55	0.42
1:A:104:MET:O	1:A:108:MET:HG2	2.19	0.42
1:B:8:ASN:HB3	1:B:31:ARG:HB3	2.01	0.42
1:A:81:ARG:HH11	1:A:81:ARG:HD3	1.59	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: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: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:HE3	1:B:143:LYS:HB3	1.91	0.41
1:A:30:LYS:HZ3	1:A:30:LYS:HG2	1.46	0.41
1:A:19:LEU:HD13	1:A:79:LEU:HB2	2.03	0.41
1:A:3:ILE:HG12	1:A:28:GLU:CG	2.46	0.41
1:B:75:ILE:O	1:B:78:TYR:HB3	2.21	0.41
1:A:40:TYR:CE2	1:A:211:LEU:HD13	2.56	0.40
1:B:2:MET:HE3	3:B:355:HOH:O	2.22	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%)	209 (97%)	6 (3%)	0	100	100
1	B	215/217 (99%)	201 (94%)	12 (6%)	2 (1%)	21	19
All	All	430/434 (99%)	410 (95%)	18 (4%)	2 (0%)	34	35

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%)	175 (89%)	22 (11%)	7	6
1	B	197/197 (100%)	171 (87%)	26 (13%)	5	4
All	All	394/394 (100%)	346 (88%)	48 (12%)	6	5

All (48) 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	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	118	ASP
1	A	141	LEU
1	A	162	ILE

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Mol	Chain	Res	Type
1	A	170	GLU
1	A	174	LEU
1	A	191	LYS
1	A	192	LYS
1	A	199	SER
1	A	204	SER
1	A	215	SER
1	A	217	LYS
1	B	8	ASN
1	B	12	LEU
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	132	GLU
1	B	134	MET
1	B	143	LYS
1	B	151	LYS
1	B	174	LEU
1	B	205	THR
1	B	207	ILE
1	B	210	LYS
1	B	211	LEU
1	B	213	GLN
1	B	215	SER
1	B	217	LYS

Some 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	B	8	ASN
1	B	116	ASN

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Mol	Chain	Res	Type
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 carbohydrates 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	-	29,37,37	1.49	5 (17%)	35,51,51	2.42	17 (48%)
2	GPR	B	6218	-	29,37,37	1.89	7 (24%)	35,51,51	2.72	17 (48%)

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	-	-	0/21/43/43	0/3/3/3
2	GPR	B	6218	-	-	0/21/43/43	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	6218	GPR	CG1-CD1	-3.48	1.44	1.51
2	A	5218	GPR	CG1-CD1	-3.29	1.44	1.51
2	B	6218	GPR	CH5-CB5	-2.93	1.36	1.40
2	A	5218	GPR	CA2-C2	2.14	1.58	1.52
2	A	5218	GPR	CA3-N3	2.24	1.50	1.46
2	B	6218	GPR	CH4-CB4	2.47	1.44	1.40
2	B	6218	GPR	CA2-N2	2.64	1.51	1.45
2	A	5218	GPR	CZ5-CH5	2.72	1.44	1.39
2	B	6218	GPR	CA3-N3	2.87	1.51	1.46
2	B	6218	GPR	CZ5-CH5	3.19	1.45	1.39
2	A	5218	GPR	CG4-CB4	3.19	1.44	1.39
2	B	6218	GPR	CG4-CB4	4.78	1.46	1.39

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	5218	GPR	CG5-CB5-CA5	-6.13	106.56	120.75
2	B	6218	GPR	CA2-N2-CD1	-5.63	107.24	121.58
2	B	6218	GPR	O2-C2-CA2	-4.84	109.65	120.36
2	B	6218	GPR	CE5-CZ5-CH5	-4.69	112.16	120.33
2	B	6218	GPR	CH5-CH4-CB4	-3.97	113.57	119.78
2	B	6218	GPR	CD5-CG5-CB5	-3.92	115.92	121.02
2	B	6218	GPR	CA3-N3-C2	-3.59	117.40	122.34
2	B	6218	GPR	CG5-CB5-CA5	-3.48	112.71	120.75
2	A	5218	GPR	CE5-CZ5-CH5	-3.47	114.29	120.33
2	A	5218	GPR	CA2-N2-CD1	-3.37	112.99	121.58
2	A	5218	GPR	CH5-CH4-CB4	-3.12	114.91	119.78
2	B	6218	GPR	CB1-CA1-N1	-3.10	101.71	110.52
2	A	5218	GPR	CD5-CG5-CB5	-2.98	117.15	121.02
2	A	5218	GPR	O2-C2-CA2	-2.94	113.85	120.36
2	A	5218	GPR	CA2-CB2-SG2	-2.82	106.27	112.97
2	A	5218	GPR	CD4-CG4-CB4	-2.79	117.39	121.02
2	B	6218	GPR	CZ5-CH5-CH4	-2.54	115.58	121.48
2	B	6218	GPR	CA2-CB2-SG2	-2.48	107.09	112.97
2	B	6218	GPR	C3-CA3-N3	-2.30	105.80	111.74
2	A	5218	GPR	O5-CA5-CB5	-2.30	105.64	110.42
2	A	5218	GPR	CB2-CA2-N2	-2.12	105.61	110.83
2	B	6218	GPR	C2-CA2-N2	-2.01	105.61	111.26
2	A	5218	GPR	CZ5-CH5-CB5	2.01	120.61	118.41
2	A	5218	GPR	CB4-CA4-CA5	2.22	114.95	109.89
2	B	6218	GPR	O2-C2-N3	2.39	127.88	123.08
2	A	5218	GPR	CG5-CB5-CH5	2.40	122.67	119.41

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Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	B	6218	GPR	CH4-CH5-CB5	2.50	123.69	119.78
2	A	5218	GPR	O2-C2-N3	2.58	128.26	123.08
2	A	5218	GPR	CB1-CG1-CD1	3.24	120.98	113.27
2	B	6218	GPR	CB1-CG1-CD1	3.34	121.21	113.27
2	A	5218	GPR	CD5-CE5-CZ5	3.58	125.43	120.19
2	B	6218	GPR	CG5-CB5-CH5	4.63	125.70	119.41
2	A	5218	GPR	O5-CA5-CA4	4.66	127.42	109.64
2	B	6218	GPR	CD5-CE5-CZ5	5.01	127.52	120.19

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	5218	GPR	5	0
2	B	6218	GPR	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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%)	0.31	10 (4%) 36 35	14, 26, 45, 53	0
1	B	217/217 (100%)	0.52	27 (12%) 5 5	13, 25, 70, 91	0
All	All	434/434 (100%)	0.42	37 (8%) 13 12	13, 26, 55, 91	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	216	ASN	6.6
1	B	217	LYS	5.6
1	B	211	LEU	5.5
1	B	214	TRP	5.4
1	B	38	PRO	4.6
1	B	40	TYR	4.2
1	B	124	PRO	4.0
1	B	122	GLN	3.7
1	B	212	ALA	3.7
1	B	36	ASP	3.7
1	B	213	GLN	3.6
1	B	118	ASP	3.5
1	B	120	GLU	3.5
1	B	121	LYS	3.5
1	B	39	ASP	3.5
1	B	117	PRO	3.3
1	B	37	ALA	3.2
1	B	125	GLU	3.0
1	B	126	PHE	3.0
1	B	115	PHE	2.9
1	A	172	LYS	2.8
1	B	119	PHE	2.8
1	A	38	PRO	2.8
1	B	205	THR	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	125	GLU	2.7
1	B	215	SER	2.7
1	A	217	LYS	2.3
1	A	128	LYS	2.3
1	B	210	LYS	2.2
1	A	69	ILE	2.2
1	A	171	PRO	2.2
1	A	39	ASP	2.1
1	A	189	GLY	2.1
1	B	116	ASN	2.1
1	B	209	SER	2.1
1	B	114	CYS	2.1
1	A	84	HIS	2.1

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
2	GPR	A	5218	35/35	0.91	0.16	1.73	15,27,67,72	0
2	GPR	B	6218	35/35	0.91	0.15	0.20	12,27,42,43	0

6.5 Other polymers [i](#)

There are no such residues in this entry.