



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 10:14 AM UTC

PDB ID : 3FYG / pdb_00003fyg
Title : CRYSTAL STRUCTURE OF TETRADECA-(3-FLUOROTYROSYL)-GLUTATHIONE S-TRANSFERASE
Authors : Xiao, G.; Parsons, J.F.; Armstrong, R.N.; Gilliland, G.L.
Deposited on : 1997-08-07
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

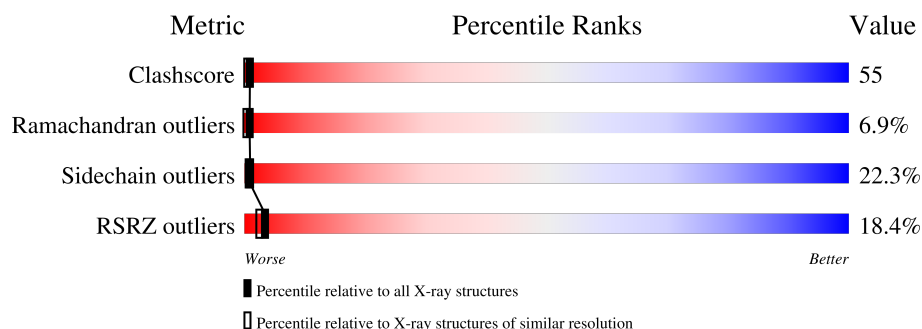
1 Overall quality at a glance

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	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	YOF	A	6	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4173 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 MU CLASS TETRADECA-(3-FLUOROTYROSYL)-GLUTATHIONE S-TRANSFERASE OF ISOENZYME.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	217	Total	C	F	N	O	S	0	1	0
			1836	1181	14	303	327	11			
1	B	217	Total	C	F	N	O	S	0	1	0
			1836	1181	14	303	327	11			

There are 26 discrepancies between the modelled and reference sequences:

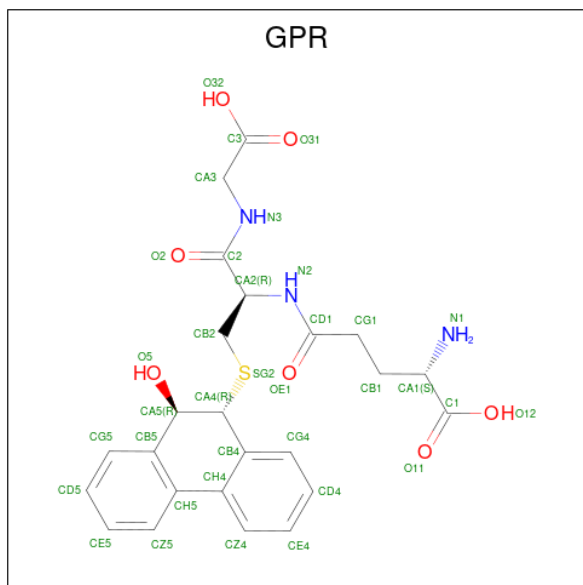
Chain	Residue	Modelled	Actual	Comment	Reference
A	6	YOF	TYR	engineered mutation	UNP P04905
A	22	YOF	TYR	engineered mutation	UNP P04905
A	27	YOF	TYR	engineered mutation	UNP P04905
A	32	YOF	TYR	engineered mutation	UNP P04905
A	40	YOF	TYR	engineered mutation	UNP P04905
A	61	YOF	TYR	engineered mutation	UNP P04905
A	78	YOF	TYR	engineered mutation	UNP P04905
A	137	YOF	TYR	engineered mutation	UNP P04905
A	154	YOF	TYR	engineered mutation	UNP P04905
A	160	YOF	TYR	engineered mutation	UNP P04905
A	166	YOF	TYR	engineered mutation	UNP P04905
A	196	YOF	TYR	engineered mutation	UNP P04905
A	202	YOF	TYR	engineered mutation	UNP P04905
B	6	YOF	TYR	engineered mutation	UNP P04905
B	22	YOF	TYR	engineered mutation	UNP P04905
B	27	YOF	TYR	engineered mutation	UNP P04905
B	32	YOF	TYR	engineered mutation	UNP P04905
B	40	YOF	TYR	engineered mutation	UNP P04905
B	61	YOF	TYR	engineered mutation	UNP P04905
B	78	YOF	TYR	engineered mutation	UNP P04905
B	137	YOF	TYR	engineered mutation	UNP P04905
B	154	YOF	TYR	engineered mutation	UNP P04905
B	160	YOF	TYR	engineered mutation	UNP P04905
B	166	YOF	TYR	engineered mutation	UNP P04905

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	196	YOF	TYR	engineered mutation	UNP P04905
B	202	YOF	TYR	engineered mutation	UNP P04905

- Molecule 2 is (9R,10R)-9-(S-GLUTATHIONYL)-10-HYDROXY-9,10-DIHYDROPHENANTHRENE (CCD ID: GPR) (formula: $C_{24}H_{27}N_3O_7S$).



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

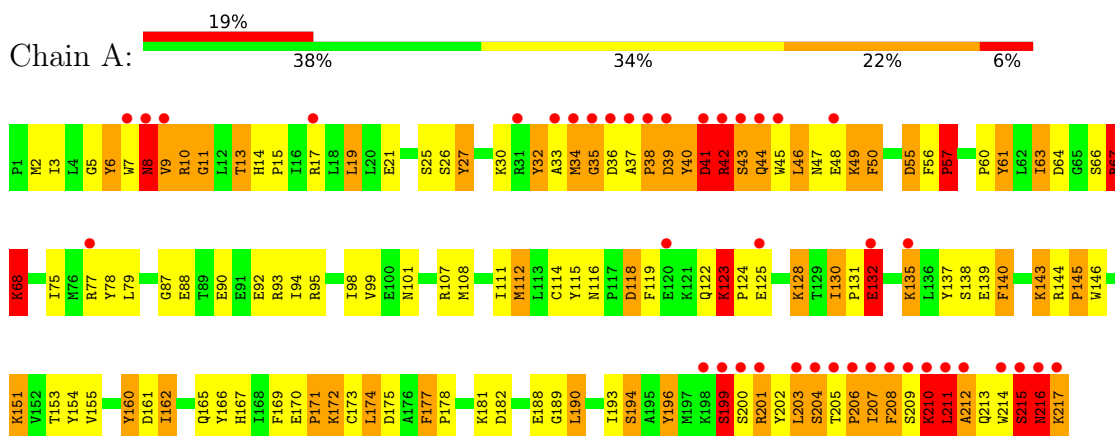
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	210	Total O 210 210	0	0
3	B	221	Total O 221 221	0	0

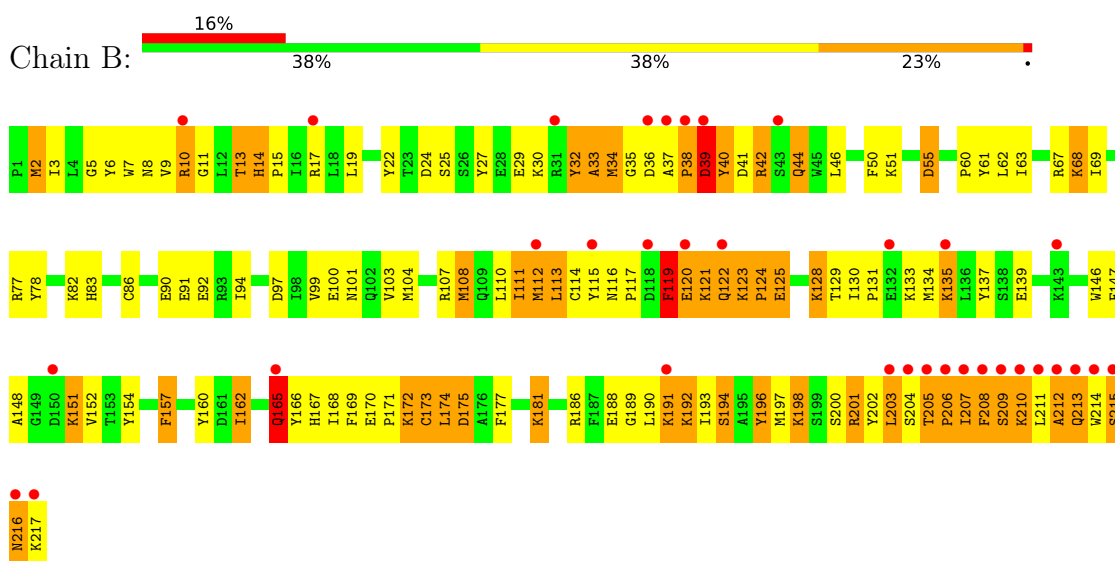
3 Residue-property plots

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: MU CLASS TETRADECA-(3-FLUOROTYROSYL)-GLUTATHIONE S-TRANSFERASE OF ISOENZYME



- Molecule 1: MU CLASS TETRADECA-(3-FLUOROTYROSYL)-GLUTATHIONE S-TRANSFERASE OF ISOENZYME



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	85.43Å 88.42Å 57.26Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.20 20.00 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.9 (20.00-2.20) 96.7 (20.00-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.33 (at 2.20Å)	Xtriage
Refinement program	TNT 5E	Depositor
R, R_{free}	0.170 , (Not available) 0.269 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	23.8	Xtriage
Anisotropy	0.281	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 184.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.011 for k,h,-l	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	4173	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.66% 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: YOF, 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	1.23	2/1685 (0.1%)	1.70	19/2242 (0.8%)
1	B	1.19	3/1685 (0.2%)	1.66	15/2242 (0.7%)
All	All	1.21	5/3370 (0.1%)	1.68	34/4484 (0.8%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	198	LYS	CD-CE	7.44	1.74	1.52
1	A	132	GLU	CD-OE2	5.63	1.36	1.25
1	B	198	LYS	CE-NZ	5.59	1.66	1.49
1	A	42	ARG	NE-CZ	5.35	1.39	1.33
1	B	198	LYS	CG-CD	5.29	1.68	1.52

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	55	ASP	CA-C-N	-8.15	111.57	123.30
1	A	55	ASP	C-N-CA	-8.15	111.57	123.30
1	A	57	PRO	N-CA-CB	7.68	111.31	103.25
1	B	191	LYS	N-CA-C	7.28	119.85	111.11
1	A	41	ASP	CA-CB-CG	7.00	119.60	112.60
1	A	145	PRO	CB-CA-C	-6.57	102.70	112.55
1	B	55	ASP	CA-CB-CG	-6.51	106.09	112.60
1	A	67	ARG	N-CA-C	6.46	118.46	109.15
1	A	118	ASP	CA-CB-CG	-6.37	106.23	112.60
1	B	69	ILE	N-CA-C	6.36	117.02	108.11
1	B	147	PHE	N-CA-C	6.29	118.94	111.33
1	A	55	ASP	CB-CA-C	6.16	120.50	110.95
1	A	68	LYS	CB-CA-C	6.14	119.89	110.62
1	B	165	GLN	CB-CA-C	5.98	121.47	110.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	33	ALA	CA-C-N	-5.81	114.00	122.19
1	B	33	ALA	C-N-CA	-5.81	114.00	122.19
1	A	56	PHE	CA-CB-CG	5.75	119.55	113.80
1	B	157	PHE	CA-CB-CG	-5.68	108.12	113.80
1	B	212	ALA	N-CA-C	5.68	117.62	110.24
1	B	14	HIS	CA-CB-CG	-5.66	108.14	113.80
1	B	181	LYS	N-CA-C	-5.60	105.17	112.23
1	A	101	ASN	CA-CB-CG	-5.51	107.09	112.60
1	A	130	ILE	CA-C-O	5.47	122.86	118.71
1	A	75	ILE	O-C-N	5.30	127.11	121.91
1	A	216	ASN	CA-CB-CG	5.29	117.89	112.60
1	A	55	ASP	O-C-N	-5.26	116.34	122.03
1	B	213	GLN	N-CA-C	-5.25	103.52	111.56
1	A	140	PHE	N-CA-C	-5.25	105.56	111.28
1	B	208	PHE	CA-CB-CG	5.21	119.01	113.80
1	A	206	PRO	N-CA-CB	5.18	108.30	102.60
1	A	50	PHE	CA-CB-CG	-5.17	108.63	113.80
1	B	129	THR	N-CA-C	5.02	119.40	113.28
1	B	119	PHE	CA-CB-CG	5.01	118.81	113.80
1	A	215	SER	N-CA-CB	5.01	118.95	110.49

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	1836	0	1776	222	0
1	B	1836	0	1778	181	0
2	A	35	0	25	2	0
2	B	35	0	25	6	0
3	A	210	0	0	11	1
3	B	221	0	0	23	0
All	All	4173	0	3604	403	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 55.

All (403) 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:198:LYS:CE	1:B:198:LYS:CD	1.74	1.57
1:A:2:MET:HE1	1:A:25:SER:HB3	1.29	1.11
1:B:10:ARG:HD3	1:B:207:ILE:HG13	1.34	1.06
1:A:143:LYS:H	1:A:143:LYS:HD2	1.22	1.03
1:B:11:GLY:H	1:B:207:ILE:HA	1.20	1.03
1:B:33:ALA:H	1:B:44:GLN:NE2	1.56	1.02
1:A:8:ASN:HD21	1:A:33:ALA:HA	1.22	1.01
1:A:207:ILE:HD12	1:A:207:ILE:H	1.29	0.98
1:B:40:YOF:HE2	1:B:210:LYS:HB2	1.40	0.98
1:A:35:GLY:HA3	1:A:41:ASP:HB3	1.43	0.97
1:B:207:ILE:HG22	2:B:218:GPR:HE5	1.47	0.97
1:A:14:HIS:HB3	1:A:15:PRO:HD3	1.48	0.95
1:B:10:ARG:HG2	1:B:207:ILE:HA	1.48	0.94
1:A:207:ILE:HD13	1:A:208:PHE:CZ	2.03	0.93
1:B:114:CYS:HA	1:B:119:PHE:CE1	2.04	0.92
1:A:208:PHE:CD1	1:A:215:SER:HB3	2.04	0.92
1:B:103:VAL:HG13	1:B:162:ILE:HG13	1.49	0.92
1:A:10:ARG:HH11	1:A:207:ILE:HG13	1.34	0.92
1:A:170:GLU:HG3	1:A:173:CYS:HB3	1.50	0.92
1:B:165:GLN:HB2	1:B:207:ILE:HD11	1.53	0.90
1:A:2:MET:CE	1:A:25:SER:HB3	2.02	0.90
1:A:45:TRP:CZ2	1:A:49:LYS:HD2	2.09	0.88
1:B:114:CYS:HA	1:B:119:PHE:HE1	1.40	0.85
1:B:201:ARG:HH11	1:B:201:ARG:HG2	1.42	0.83
1:A:143:LYS:HD2	1:A:143:LYS:N	1.94	0.82
2:B:218:GPR:HB21	2:B:218:GPR:CG4	2.09	0.81
1:B:63:ILE:HG12	1:B:68:LYS:HG3	1.62	0.81
1:B:10:ARG:HG2	1:B:207:ILE:CA	2.10	0.80
1:A:7:TRP:CH2	1:A:42:ARG:HB3	2.16	0.78
1:A:208:PHE:HB2	1:A:212:ALA:HB2	1.63	0.78
1:B:146:TRP:CE2	1:B:152:VAL:HG22	2.18	0.78
1:A:208:PHE:CE1	1:A:215:SER:HB3	2.20	0.77
1:A:33:ALA:HB3	1:A:44:GLN:OE1	1.86	0.76
1:A:63:ILE:HG13	1:A:68:LYS:HB3	1.69	0.75
1:A:181:LYS:HD2	3:A:713:HOH:O	1.87	0.74
1:B:216:ASN:HD22	1:B:216:ASN:H	1.33	0.74
1:A:135:LYS:HD3	1:A:177:PHE:CE2	2.23	0.74
1:A:208:PHE:HD1	1:A:215:SER:HB3	1.51	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:10:ARG:NH1	1:A:207:ILE:HG13	2.02	0.73
1:A:6:YOF:CD1	1:A:7:TRP:H	2.02	0.73
1:A:13:THR:HG21	1:A:17:ARG:NH1	2.05	0.72
1:B:125:GLU:O	1:B:128:LYS:HB2	1.89	0.72
1:B:32:YOF:HA	1:B:44:GLN:HE21	1.54	0.72
1:A:42:ARG:O	1:A:46:LEU:HG	1.90	0.71
1:A:35:GLY:O	1:A:40:YOF:HA	1.91	0.71
1:A:10:ARG:HH12	1:A:165:GLN:HB3	1.54	0.70
1:B:104:MET:SD	1:B:108:MET:HE2	2.31	0.70
1:B:33:ALA:H	1:B:44:GLN:HE21	1.39	0.70
1:A:6:YOF:CD2	1:A:13:THR:HB	2.21	0.70
1:A:35:GLY:HA3	1:A:41:ASP:CB	2.20	0.70
1:B:205:THR:HG23	1:B:206:PRO:CB	2.21	0.70
1:B:11:GLY:HA2	1:B:207:ILE:CG2	2.21	0.70
1:A:189:GLY:O	1:A:190:LEU:C	2.30	0.70
1:A:190:LEU:HB2	1:A:193:ILE:CG1	2.21	0.70
1:A:10:ARG:HG2	1:A:11:GLY:N	2.06	0.69
1:B:10:ARG:CD	1:B:207:ILE:HG13	2.18	0.69
1:B:36:ASP:O	1:B:40:YOF:N	2.26	0.69
1:B:24:ASP:OD1	1:B:192:LYS:HE2	1.93	0.68
1:B:14:HIS:HB3	1:B:15:PRO:HD3	1.75	0.68
1:B:165:GLN:CD	1:B:207:ILE:HD13	2.19	0.68
1:A:43:SER:O	1:A:44:GLN:C	2.34	0.68
1:A:124:PRO:O	1:A:128:LYS:HD3	1.92	0.68
1:B:121:LYS:O	1:B:124:PRO:HD2	1.93	0.67
1:B:35:GLY:HA3	1:B:41:ASP:HB3	1.76	0.67
1:B:40:YOF:CE2	1:B:210:LYS:HB2	2.20	0.67
1:B:211:LEU:HD12	1:B:211:LEU:H	1.59	0.67
1:A:64:ASP:O	1:A:67:ARG:HB2	1.94	0.67
1:B:51:LYS:HD3	3:B:739:HOH:O	1.94	0.67
1:A:87:GLY:O	1:A:93:ARG:NH1	2.27	0.67
2:B:218:GPR:N1	3:B:804:HOH:O	2.27	0.67
1:A:63:ILE:CG1	1:A:68:LYS:HB3	2.25	0.67
1:A:115:TYR:CE2	1:A:211:LEU:HB2	2.30	0.66
1:A:2:MET:HE1	1:A:25:SER:CB	2.16	0.66
1:A:44:GLN:O	1:A:45:TRP:C	2.37	0.66
1:A:211:LEU:HD12	1:A:211:LEU:N	2.10	0.66
1:B:13:THR:HG23	1:B:17:ARG:HG3	1.75	0.66
1:A:43:SER:O	1:A:46:LEU:N	2.28	0.66
1:A:207:ILE:HB	1:A:208:PHE:CD2	2.31	0.66
1:B:205:THR:HG23	1:B:206:PRO:CA	2.25	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:17:ARG:NH2	1:B:29:GLU:OE1	2.28	0.65
1:A:8:ASN:ND2	1:A:32:YOF:O	2.28	0.65
1:A:35:GLY:HA3	1:A:41:ASP:N	2.12	0.65
1:A:38:PRO:O	1:A:40:YOF:N	2.30	0.65
1:B:103:VAL:CG1	1:B:162:ILE:HG13	2.25	0.65
1:B:205:THR:OG1	1:B:206:PRO:HA	1.96	0.65
1:A:88:GLU:O	1:A:93:ARG:NH2	2.30	0.65
1:A:119:PHE:CZ	1:A:214:TRP:HB2	2.32	0.65
1:A:151:LYS:HE2	1:A:153:THR:HG22	1.78	0.65
1:B:11:GLY:HA2	1:B:207:ILE:HG22	1.78	0.65
1:B:77:ARG:NE	3:B:614:HOH:O	2.26	0.65
1:A:34:MET:CE	1:A:42:ARG:HD3	2.27	0.65
1:A:107:ARG:HD2	1:A:108:MET:CE	2.26	0.65
1:A:7:TRP:HH2	1:A:42:ARG:HB3	1.63	0.64
1:A:108:MET:HE2	1:A:108:MET:N	2.11	0.64
1:B:38:PRO:CG	1:B:39:ASP:H	2.10	0.64
1:A:209:SER:O	1:A:216:ASN:HA	1.96	0.64
1:B:37:ALA:HB2	1:B:40:YOF:CZ	2.27	0.64
1:B:193:ILE:O	1:B:197:MET:HG3	1.97	0.64
1:A:212:ALA:O	1:A:216:ASN:HB3	1.97	0.64
1:A:170:GLU:CG	1:A:173:CYS:HB3	2.27	0.64
1:A:34:MET:O	1:A:34:MET:HG3	1.97	0.64
1:A:115:TYR:HE2	1:A:211:LEU:HB2	1.63	0.63
1:B:83:HIS:HB3	3:B:774:HOH:O	1.98	0.63
1:B:128:LYS:NZ	3:B:622:HOH:O	2.31	0.63
1:A:43:SER:O	1:A:47:ASN:N	2.30	0.63
1:B:11:GLY:N	1:B:207:ILE:HA	2.04	0.63
1:B:203:LEU:O	1:B:204:SER:C	2.42	0.63
1:A:10:ARG:O	1:A:13:THR:HG22	1.99	0.62
1:B:209:SER:O	1:B:216:ASN:HA	1.99	0.62
1:A:44:GLN:HG3	1:A:45:TRP:H	1.65	0.62
1:A:34:MET:HG3	1:A:210:LYS:HD2	1.82	0.61
1:A:190:LEU:HB2	1:A:193:ILE:HG12	1.82	0.61
1:A:35:GLY:HA3	1:A:41:ASP:H	1.64	0.61
1:B:10:ARG:HD2	1:B:204:SER:O	2.00	0.61
1:A:34:MET:HE1	1:A:42:ARG:HD3	1.81	0.61
1:A:172:LYS:HG3	1:A:175:ASP:OD2	2.00	0.61
1:A:7:TRP:CZ2	1:A:42:ARG:HD2	2.35	0.61
1:B:113:LEU:HD21	1:B:119:PHE:CE1	2.36	0.61
1:B:34:MET:HE2	1:B:42:ARG:HD2	1.82	0.61
1:A:3:ILE:HD12	1:A:3:ILE:N	2.16	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:GLY:CA	1:A:41:ASP:HB3	2.27	0.60
1:B:205:THR:HG23	1:B:206:PRO:N	2.16	0.60
1:A:165:GLN:CD	1:A:207:ILE:HG12	2.26	0.60
1:B:11:GLY:HA2	2:B:218:GPR:HE5	1.82	0.60
1:A:143:LYS:NZ	3:A:907:HOH:O	2.34	0.60
1:A:114:CYS:O	1:A:213:GLN:N	2.26	0.60
1:A:138:SER:OG	1:A:177:PHE:HB3	2.02	0.60
1:A:10:ARG:HB3	1:A:206:PRO:O	2.02	0.59
1:A:135:LYS:HD3	1:A:177:PHE:CZ	2.38	0.59
1:A:207:ILE:HB	1:A:208:PHE:CE2	2.38	0.59
1:A:217:LYS:N	3:A:857:HOH:O	2.32	0.59
1:B:103:VAL:HG13	1:B:162:ILE:CG1	2.29	0.59
1:A:7:TRP:O	1:A:9:VAL:N	2.35	0.58
1:A:42:ARG:O	1:A:43:SER:C	2.46	0.58
1:B:34:MET:SD	1:B:211:LEU:HD11	2.43	0.58
1:A:49:LYS:HG2	1:A:50:PHE:CE2	2.38	0.58
1:A:95:ARG:O	1:A:99:VAL:HG23	2.04	0.58
1:B:123:LYS:O	1:B:123:LYS:HG2	2.03	0.58
1:A:203:LEU:HB2	3:A:785:HOH:O	2.04	0.58
1:B:116:ASN:O	1:B:119:PHE:N	2.37	0.58
1:A:2:MET:HE3	1:A:27:YOF:HB2	1.86	0.58
1:A:7:TRP:HB3	1:A:9:VAL:HG13	1.85	0.58
1:B:165:GLN:HB2	1:B:207:ILE:CD1	2.31	0.58
1:A:201:ARG:HH11	1:A:201:ARG:CG	2.17	0.57
1:A:10:ARG:HD3	1:A:207:ILE:HG13	1.85	0.57
1:B:116:ASN:O	1:B:117:PRO:C	2.45	0.57
1:A:46:LEU:HB3	3:A:827:HOH:O	2.03	0.57
1:A:207:ILE:HD12	1:A:207:ILE:N	2.10	0.57
1:A:207:ILE:H	1:A:207:ILE:CD1	2.04	0.57
1:A:36:ASP:O	1:A:39:ASP:HB2	2.04	0.57
1:B:207:ILE:HG12	3:B:550:HOH:O	2.05	0.56
1:A:10:ARG:HH21	1:A:14:HIS:CD2	2.23	0.56
1:A:161:ASP:O	1:A:165:GLN:HG2	2.05	0.56
1:A:48:GLU:O	1:A:50:PHE:N	2.38	0.56
1:B:131:PRO:HA	3:B:611:HOH:O	2.04	0.56
1:B:135:LYS:HD3	1:B:177:PHE:HE1	1.69	0.56
1:B:10:ARG:NH1	1:B:207:ILE:HD11	2.20	0.56
1:A:116:ASN:O	1:A:213:GLN:HG3	2.06	0.56
1:B:135:LYS:O	1:B:139:GLU:HG3	2.06	0.56
1:B:201:ARG:HG2	3:B:564:HOH:O	2.05	0.56
1:A:199:SER:HB2	1:A:201:ARG:HH12	1.70	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:211:LEU:HD12	1:B:211:LEU:N	2.19	0.56
1:B:216:ASN:H	1:B:216:ASN:ND2	2.04	0.56
1:A:9:VAL:HG23	1:A:10:ARG:N	2.19	0.56
1:B:119:PHE:O	1:B:121:LYS:N	2.39	0.56
1:B:213:GLN:NE2	3:B:744:HOH:O	2.38	0.55
1:A:190:LEU:O	1:A:193:ILE:N	2.36	0.55
1:B:30:LYS:NZ	3:B:875:HOH:O	2.39	0.55
1:A:194:SER:HA	3:A:937:HOH:O	2.06	0.55
1:B:63:ILE:HG12	1:B:68:LYS:CG	2.35	0.55
1:B:8:ASN:H	1:B:8:ASN:ND2	2.03	0.55
1:B:17:ARG:NH2	1:B:29:GLU:HG2	2.21	0.55
1:A:10:ARG:HH11	1:A:207:ILE:CG1	2.14	0.55
1:B:205:THR:CB	1:B:206:PRO:HA	2.35	0.55
1:B:50:PHE:C	1:B:51:LYS:HD2	2.32	0.55
1:A:48:GLU:O	1:A:49:LYS:C	2.49	0.54
1:B:119:PHE:CD1	1:B:213:GLN:HB2	2.42	0.54
1:A:210:LYS:O	1:A:211:LEU:C	2.50	0.54
1:B:207:ILE:HG21	3:B:825:HOH:O	2.06	0.54
1:A:116:ASN:OD1	1:A:118:ASP:N	2.35	0.54
1:B:174:LEU:C	1:B:181:LYS:HE3	2.32	0.54
1:A:165:GLN:HE22	1:A:207:ILE:HG21	1.72	0.54
1:A:39:ASP:O	1:A:40:YOF:C	2.55	0.53
1:B:191:LYS:HA	3:B:836:HOH:O	2.08	0.53
1:B:205:THR:HG23	1:B:206:PRO:HB3	1.89	0.53
1:B:37:ALA:HA	1:B:38:PRO:C	2.34	0.53
1:A:174:LEU:HB3	1:A:181:LYS:HE2	1.90	0.53
1:A:206:PRO:HG2	1:A:208:PHE:O	2.09	0.53
1:B:2:MET:HG2	3:B:879:HOH:O	2.07	0.53
1:B:7:TRP:HH2	1:B:42:ARG:HB3	1.73	0.53
1:B:17:ARG:HH12	1:B:29:GLU:CD	2.16	0.53
1:B:111:ILE:HD13	1:B:111:ILE:N	2.24	0.53
1:B:201:ARG:HH11	1:B:201:ARG:CG	2.16	0.53
1:B:216:ASN:HD22	1:B:216:ASN:N	2.02	0.53
1:A:6:YOF:CG	1:A:7:TRP:H	2.22	0.52
1:B:11:GLY:HA2	1:B:207:ILE:HG23	1.89	0.52
1:A:14:HIS:HB3	1:A:15:PRO:CD	2.29	0.52
1:A:167:HIS:O	1:A:171:PRO:HA	2.09	0.52
1:A:175:ASP:HA	1:A:181:LYS:HE3	1.92	0.52
1:B:8:ASN:H	1:B:8:ASN:HD22	1.57	0.52
1:B:39:ASP:O	1:B:40:YOF:HB3	2.09	0.52
1:A:119:PHE:CZ	1:A:123:LYS:HD2	2.45	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:208:PHE:O	1:A:215:SER:O	2.27	0.52
1:B:202:YOF:CZ	1:B:204:SER:HA	2.40	0.52
1:A:7:TRP:C	1:A:9:VAL:H	2.18	0.52
1:B:189:GLY:O	1:B:190:LEU:C	2.50	0.52
1:B:212:ALA:HB3	1:B:216:ASN:HA	1.92	0.52
1:A:135:LYS:HD3	1:A:177:PHE:HE2	1.74	0.52
1:B:7:TRP:CH2	1:B:42:ARG:HB3	2.45	0.52
1:A:112:MET:CE	1:B:112:MET:HE3	2.40	0.52
1:A:11:GLY:HA2	1:A:207:ILE:HG22	1.91	0.51
1:A:45:TRP:HE1	2:A:218:GPR:C3	2.23	0.51
1:B:114:CYS:O	1:B:213:GLN:HG2	2.10	0.51
1:B:196:YOF:HA	3:B:718:HOH:O	2.09	0.51
1:A:160:YOF:OH	1:A:188:GLU:OE2	2.28	0.51
1:A:36:ASP:CG	1:A:37:ALA:H	2.18	0.51
1:B:17:ARG:HH22	1:B:29:GLU:CD	2.18	0.51
1:A:209:SER:O	1:A:212:ALA:HB3	2.10	0.51
1:B:211:LEU:H	1:B:211:LEU:CD1	2.24	0.51
1:A:36:ASP:O	1:A:38:PRO:O	2.29	0.51
1:A:49:LYS:HE3	1:A:57:PRO:HB2	1.93	0.51
1:B:213:GLN:HA	1:B:213:GLN:OE1	2.11	0.51
1:A:36:ASP:C	1:A:38:PRO:O	2.53	0.50
1:A:122:GLN:O	1:A:125:GLU:HB2	2.10	0.50
1:A:45:TRP:CE2	1:A:49:LYS:HB2	2.47	0.50
1:A:63:ILE:HG12	1:A:68:LYS:HD3	1.93	0.50
1:B:11:GLY:CA	1:B:207:ILE:HG23	2.42	0.50
1:A:208:PHE:CE1	1:A:214:TRP:CZ3	2.99	0.50
1:B:122:GLN:C	1:B:124:PRO:HD2	2.37	0.50
1:A:6:YOF:CE2	1:A:9:VAL:HG22	2.42	0.50
1:A:45:TRP:O	1:A:49:LYS:N	2.35	0.50
1:A:190:LEU:HB2	1:A:193:ILE:HG13	1.92	0.50
1:A:49:LYS:HE2	1:A:50:PHE:CZ	2.47	0.50
1:A:165:GLN:HE22	1:A:207:ILE:CG2	2.24	0.50
1:A:11:GLY:HA2	1:A:207:ILE:CG2	2.42	0.50
1:B:38:PRO:HG2	1:B:39:ASP:H	1.76	0.50
1:A:170:GLU:O	1:A:172:LYS:N	2.45	0.50
1:A:208:PHE:CE1	1:A:214:TRP:CE3	3.00	0.50
1:B:33:ALA:N	1:B:44:GLN:NE2	2.41	0.49
1:B:175:ASP:HA	1:B:181:LYS:NZ	2.27	0.49
1:A:49:LYS:HG2	1:A:50:PHE:CD2	2.48	0.49
1:A:94:ILE:O	1:A:98:ILE:HG13	2.12	0.49
1:B:216:ASN:O	1:B:217:LYS:HG2	2.12	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:214:TRP:HA	3:B:868:HOH:O	2.13	0.49
1:A:199:SER:OG	1:A:201:ARG:NH1	2.45	0.49
1:B:151:LYS:O	1:B:151:LYS:HG2	2.03	0.49
1:A:17:ARG:O	1:A:21:GLU:HG2	2.12	0.49
1:A:205:THR:HG23	1:A:206:PRO:HB3	1.95	0.49
1:A:77:ARG:HG2	1:A:77:ARG:HH11	1.78	0.49
1:A:199:SER:CB	1:A:201:ARG:HH12	2.25	0.49
1:B:86:CYS:HB3	3:B:632:HOH:O	2.12	0.49
1:A:131:PRO:CB	1:A:135:LYS:HZ1	2.26	0.49
1:A:201:ARG:HH11	1:A:201:ARG:HG2	1.77	0.48
1:B:13:THR:O	1:B:14:HIS:C	2.55	0.48
1:B:107:ARG:CA	1:B:162:ILE:HD11	2.43	0.48
1:A:201:ARG:CG	1:A:201:ARG:NH1	2.76	0.48
1:B:32:YOF:HD2	1:B:44:GLN:HG3	1.95	0.48
1:A:77:ARG:HG2	1:A:77:ARG:NH1	2.29	0.48
1:B:35:GLY:N	1:B:41:ASP:O	2.38	0.48
1:A:153:THR:OG1	1:A:155:VAL:HG22	2.14	0.48
1:B:170:GLU:HG3	1:B:173:CYS:HB3	1.95	0.48
1:A:6:YOF:HD2	1:A:13:THR:HB	1.95	0.47
1:A:130:ILE:N	1:A:131:PRO:HD2	2.28	0.47
1:A:55:ASP:OD1	3:A:645:HOH:O	2.20	0.47
1:A:177:PHE:N	1:A:178:PRO:HD3	2.29	0.47
1:A:208:PHE:CZ	1:A:214:TRP:HZ3	2.32	0.47
1:B:38:PRO:CD	1:B:39:ASP:H	2.28	0.47
1:B:194:SER:O	1:B:198:LYS:HG3	2.14	0.47
1:A:208:PHE:HB2	1:A:212:ALA:CB	2.38	0.47
1:A:209:SER:O	1:A:210:LYS:O	2.32	0.47
1:B:34:MET:CE	1:B:42:ARG:HD2	2.44	0.47
1:A:35:GLY:HA3	1:A:41:ASP:CA	2.45	0.47
1:B:107:ARG:HA	1:B:162:ILE:HD11	1.96	0.47
1:A:208:PHE:CZ	1:A:214:TRP:CZ3	3.01	0.47
1:B:33:ALA:N	1:B:44:GLN:HE21	2.11	0.47
1:A:6:YOF:CE2	1:A:13:THR:HB	2.44	0.47
1:A:37:ALA:HA	1:A:40:YOF:CZ	2.45	0.47
1:A:206:PRO:HB3	1:A:215:SER:OG	2.15	0.47
1:A:10:ARG:HD2	1:A:204:SER:O	2.15	0.46
1:B:92:GLU:HG2	1:B:148:ALA:O	2.15	0.46
1:A:19:LEU:HD12	1:A:79:LEU:HB2	1.96	0.46
1:A:151:LYS:O	1:A:151:LYS:HG2	2.14	0.46
1:B:119:PHE:O	1:B:122:GLN:N	2.48	0.46
1:B:197:MET:O	1:B:202:YOF:HD2	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:146:TRP:CH2	1:B:186:ARG:HG2	2.51	0.46
1:B:207:ILE:HG23	3:B:550:HOH:O	2.15	0.46
1:B:210:LYS:NZ	3:B:936:HOH:O	2.48	0.46
1:B:210:LYS:O	1:B:216:ASN:HB2	2.16	0.46
1:A:112:MET:HE2	1:B:112:MET:HE3	1.97	0.46
1:B:11:GLY:H	1:B:207:ILE:CA	2.09	0.46
1:A:203:LEU:HD23	1:A:203:LEU:HA	1.73	0.46
1:A:208:PHE:HZ	1:A:214:TRP:HZ3	1.63	0.46
1:B:110:LEU:O	1:B:111:ILE:C	2.59	0.46
1:B:123:LYS:N	1:B:124:PRO:CD	2.79	0.46
1:B:113:LEU:CD2	1:B:119:PHE:CE1	2.99	0.46
1:B:133:LYS:NZ	3:B:633:HOH:O	2.31	0.46
1:A:2:MET:HA	1:A:63:ILE:O	2.16	0.45
1:A:205:THR:HA	1:A:206:PRO:HA	1.73	0.45
1:B:188:GLU:HG2	1:B:197:MET:HE1	1.97	0.45
1:A:6:YOF:HD1	1:A:6:YOF:HA	1.73	0.45
1:B:5:GLY:O	1:B:60:PRO:HA	2.16	0.45
1:B:146:TRP:CD2	1:B:152:VAL:HG22	2.50	0.45
1:B:167:HIS:HA	1:B:173:CYS:SG	2.56	0.45
1:A:21:GLU:HG3	1:A:196:YOF:CD2	2.46	0.45
1:A:199:SER:CB	1:A:201:ARG:NH1	2.79	0.45
1:A:216:ASN:N	3:A:857:HOH:O	2.49	0.45
1:B:191:LYS:NZ	3:B:706:HOH:O	2.50	0.45
1:A:123:LYS:HB3	1:A:124:PRO:HD3	1.98	0.45
1:A:40:YOF:HE2	1:A:210:LYS:HB2	1.99	0.45
1:A:99:VAL:CG2	1:A:140:PHE:CE2	3.00	0.45
1:B:13:THR:HG21	1:B:17:ARG:HE	1.82	0.44
1:B:17:ARG:NH2	1:B:29:GLU:CG	2.80	0.44
1:A:6:YOF:CG	1:A:7:TRP:N	2.80	0.44
1:A:205:THR:HG23	1:A:206:PRO:CA	2.47	0.44
1:B:17:ARG:NH1	3:B:683:HOH:O	2.49	0.44
1:A:123:LYS:HB3	1:A:124:PRO:CD	2.48	0.44
1:B:39:ASP:HB3	1:B:41:ASP:H	1.82	0.44
1:A:7:TRP:HH2	1:A:42:ARG:CB	2.29	0.44
1:A:145:PRO:HB2	1:A:146:TRP:CD1	2.53	0.44
1:B:90:GLU:O	1:B:94:ILE:HG13	2.18	0.44
1:B:206:PRO:O	1:B:207:ILE:C	2.59	0.44
1:A:178:PRO:O	1:A:182:ASP:OD2	2.36	0.44
1:A:213:GLN:OE1	1:A:213:GLN:HA	2.17	0.44
1:B:113:LEU:O	1:B:119:PHE:HD1	2.01	0.44
1:A:130:ILE:N	1:A:131:PRO:CD	2.81	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:77:ARG:NH2	1:B:100:GLU:OE1	2.51	0.43
1:B:190:LEU:HB2	1:B:193:ILE:HG13	2.00	0.43
1:A:34:MET:HE3	1:A:34:MET:HB2	1.88	0.43
1:A:7:TRP:C	1:A:9:VAL:N	2.77	0.43
1:A:19:LEU:CD1	1:A:79:LEU:HB2	2.49	0.43
1:B:146:TRP:CZ2	1:B:152:VAL:HG22	2.53	0.43
1:A:99:VAL:HG22	1:A:140:PHE:CE2	2.54	0.43
1:A:45:TRP:HZ2	1:A:49:LYS:HD2	1.76	0.43
1:A:207:ILE:HD13	1:A:208:PHE:CE2	2.48	0.43
1:A:90:GLU:HA	1:A:90:GLU:OE1	2.18	0.43
1:A:162:ILE:HD13	1:A:162:ILE:HA	1.72	0.43
1:B:13:THR:CG2	1:B:17:ARG:HD2	2.48	0.43
1:B:90:GLU:OE1	1:B:90:GLU:HA	2.19	0.43
2:B:218:GPR:HB21	2:B:218:GPR:HG4	1.98	0.43
1:B:17:ARG:HH22	1:B:29:GLU:CG	2.32	0.43
1:A:112:MET:CE	1:B:112:MET:CE	2.97	0.42
1:B:115:TYR:HE2	1:B:211:LEU:HB2	1.83	0.42
1:B:116:ASN:HA	1:B:117:PRO:HD2	1.84	0.42
1:A:132:GLU:HG2	3:A:689:HOH:O	2.18	0.42
1:A:135:LYS:HB2	1:A:135:LYS:HE2	1.67	0.42
1:B:120:GLU:OE1	1:B:120:GLU:O	2.38	0.42
1:B:135:LYS:HB2	1:B:135:LYS:NZ	2.35	0.42
1:A:210:LYS:O	1:A:212:ALA:N	2.52	0.42
1:B:113:LEU:HD23	1:B:114:CYS:SG	2.59	0.42
1:A:37:ALA:HA	1:A:38:PRO:O	2.19	0.42
1:A:107:ARG:HD2	1:A:108:MET:HE1	1.98	0.42
1:B:34:MET:SD	1:B:211:LEU:CD1	3.08	0.42
1:A:7:TRP:HA	1:A:7:TRP:CE3	2.55	0.42
1:A:13:THR:HG22	1:A:14:HIS:N	2.34	0.42
1:A:107:ARG:HD2	1:A:108:MET:HE3	2.02	0.42
1:A:199:SER:HB2	1:A:201:ARG:NH1	2.35	0.42
1:B:2:MET:CE	1:B:25:SER:HB3	2.50	0.42
1:B:169:PHE:HD1	1:B:214:TRP:CE3	2.37	0.42
1:B:201:ARG:CG	1:B:201:ARG:NH1	2.80	0.42
1:A:49:LYS:HG3	1:A:57:PRO:CB	2.50	0.42
1:A:211:LEU:O	1:A:212:ALA:C	2.63	0.42
1:A:36:ASP:CG	1:A:37:ALA:N	2.78	0.41
2:A:218:GPR:C3	3:A:704:HOH:O	2.68	0.41
1:B:13:THR:CG2	1:B:17:ARG:CD	2.98	0.41
1:A:14:HIS:HD2	1:A:161:ASP:OD1	2.02	0.41
1:B:10:ARG:HH21	1:B:14:HIS:CE1	2.39	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:YOF:CD1	1:A:61:YOF:C	2.97	0.41
1:A:63:ILE:HA	1:A:67:ARG:O	2.21	0.41
1:B:9:VAL:HB	1:B:206:PRO:O	2.20	0.41
1:B:3:ILE:O	1:B:62:LEU:HA	2.19	0.41
1:B:107:ARG:HB2	1:B:162:ILE:HD11	2.01	0.41
1:B:113:LEU:HG	1:B:119:PHE:CE1	2.54	0.41
1:B:7:TRP:HE3	1:B:32:YOF:O	2.03	0.41
1:B:50:PHE:HB2	3:B:739:HOH:O	2.20	0.41
1:B:114:CYS:O	1:B:213:GLN:N	2.43	0.41
1:B:38:PRO:CG	1:B:39:ASP:N	2.79	0.41
1:B:22:YOF:O	1:B:192:LYS:HD3	2.21	0.41
1:A:36:ASP:O	1:A:38:PRO:C	2.63	0.41
1:A:88:GLU:N	1:A:92:GLU:OE1	2.38	0.41
1:A:115:TYR:HE2	1:A:211:LEU:HD13	1.86	0.41
1:A:123:LYS:HE2	1:A:169:PHE:CZ	2.56	0.41
1:B:130:ILE:O	1:B:134:MET:HG2	2.21	0.41
1:B:172:LYS:C	1:B:174:LEU:N	2.79	0.41
1:B:202:YOF:OH	1:B:204:SER:HA	2.21	0.41
1:B:209:SER:HB2	1:B:210:LYS:H	1.49	0.41
1:A:5:GLY:O	1:A:60:PRO:HA	2.20	0.40
1:A:13:THR:CG2	1:A:14:HIS:N	2.79	0.40
1:A:37:ALA:HA	1:A:38:PRO:HA	1.70	0.40
1:A:112:MET:HE2	1:B:112:MET:CE	2.52	0.40
1:B:97:ASP:O	1:B:101:ASN:ND2	2.31	0.40
1:A:10:ARG:O	1:A:11:GLY:C	2.64	0.40
1:A:42:ARG:NH2	3:A:910:HOH:O	2.53	0.40
1:A:167:HIS:HB2	1:A:174:LEU:HD22	2.03	0.40
1:A:170:GLU:HG3	1:A:173:CYS:CB	2.36	0.40
1:A:205:THR:HG23	1:A:206:PRO:CB	2.51	0.40
1:A:209:SER:HB2	1:A:210:LYS:H	1.70	0.40
1:B:207:ILE:O	2:B:218:GPR:HZ5	2.21	0.40
1:A:34:MET:HG3	1:A:210:LYS:CD	2.50	0.40
1:B:99:VAL:O	1:B:100:GLU:C	2.62	0.40
1:B:217:LYS:HE2	3:B:828:HOH:O	2.21	0.40
1:A:210:LYS:O	1:A:216:ASN:HB2	2.21	0.40
1:B:107:ARG:CB	1:B:162:ILE:HD11	2.51	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:A:649:HOH:O	3:A:649:HOH:O[2_655]	1.90	0.30

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	202/217 (93%)	176 (87%)	9 (4%)	17 (8%)	0	0
1	B	202/217 (93%)	173 (86%)	18 (9%)	11 (5%)	1	0
All	All	404/434 (93%)	349 (86%)	27 (7%)	28 (7%)	1	0

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	8	ASN
1	A	38	PRO
1	A	39	ASP
1	A	210	LYS
1	A	211	LEU
1	B	39	ASP
1	B	119	PHE
1	B	120	GLU
1	A	11	GLY
1	A	43	SER
1	A	49	LYS
1	B	124	PRO
1	B	173	CYS
1	A	35	GLY
1	A	190	LEU
1	A	212	ALA
1	A	215	SER
1	B	215	SER
1	A	44	GLN
1	A	171	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	123	LYS
1	B	55	ASP
1	B	123	LYS
1	A	199	SER
1	B	38	PRO
1	A	57	PRO
1	B	171	PRO
1	B	206	PRO

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	184/184 (100%)	143 (78%)	41 (22%)	1	1
1	B	184/184 (100%)	143 (78%)	41 (22%)	1	1
All	All	368/368 (100%)	286 (78%)	82 (22%)	1	1

All (82) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	ASN
1	A	9	VAL
1	A	10	ARG
1	A	13	THR
1	A	19	LEU
1	A	26	SER
1	A	30	LYS
1	A	34	MET
1	A	41	ASP
1	A	42	ARG
1	A	46	LEU
1	A	63	ILE
1	A	66	SER
1	A	67	ARG
1	A	68	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	111	ILE
1	A	112	MET
1	A	123	LYS
1	A	128	LYS
1	A	132	GLU
1	A	135	LYS
1	A	139	GLU
1	A	143	LYS
1	A	144	ARG
1	A	151	LYS
1	A	162	ILE
1	A	172	LYS
1	A	174	LEU
1	A	177	PHE
1	A	194	SER
1	A	199	SER
1	A	200	SER
1	A	201	ARG
1	A	203	LEU
1	A	204	SER
1	A	207	ILE
1	A	208	PHE
1	A	210	LYS
1	A	211	LEU
1	A	216	ASN
1	A	217	LYS
1	B	2	MET
1	B	10	ARG
1	B	13	THR
1	B	19	LEU
1	B	34	MET
1	B	39	ASP
1	B	42	ARG
1	B	44	GLN
1	B	46	LEU
1	B	67	ARG
1	B	68	LYS
1	B	82	LYS
1	B	91	GLU
1	B	108	MET
1	B	111	ILE
1	B	112	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	113	LEU
1	B	121	LYS
1	B	122	GLN
1	B	125	GLU
1	B	128	LYS
1	B	135	LYS
1	B	151	LYS
1	B	162	ILE
1	B	165	GLN
1	B	168	ILE
1	B	172	LYS
1	B	174	LEU
1	B	175	ASP
1	B	192	LYS
1	B	194	SER
1	B	200	SER
1	B	201	ARG
1	B	203	LEU
1	B	205	THR
1	B	207	ILE
1	B	208	PHE
1	B	209	SER
1	B	210	LYS
1	B	215	SER
1	B	216	ASN

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

Mol	Chain	Res	Type
1	A	8	ASN
1	A	14	HIS
1	A	165	GLN
1	B	8	ASN
1	B	44	GLN
1	B	179	ASN
1	B	216	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

28 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	YOF	A	154[B]	-	12,13,14	0.94	0	10,17,19	0.95	1 (10%)
1	YOF	B	6	1	12,13,14	0.99	0	10,17,19	1.43	1 (10%)
1	YOF	A	202	1	12,13,14	0.86	0	10,17,19	1.38	1 (10%)
1	YOF	A	40	1	12,13,14	1.28	1 (8%)	10,17,19	1.22	1 (10%)
1	YOF	B	27	1	12,13,14	0.97	1 (8%)	10,17,19	1.05	1 (10%)
1	YOF	A	6	1	12,13,14	1.21	1 (8%)	10,17,19	1.96	1 (10%)
1	YOF	B	32	1	12,13,14	0.84	0	10,17,19	1.25	2 (20%)
1	YOF	B	61	1	12,13,14	0.67	0	10,17,19	1.50	1 (10%)
1	YOF	B	196	1	12,13,14	0.92	0	10,17,19	2.08	2 (20%)
1	YOF	A	154[A]	-	12,13,14	0.97	0	10,17,19	1.17	1 (10%)
1	YOF	A	22	1	12,13,14	0.71	0	10,17,19	1.06	0
1	YOF	A	27	1	12,13,14	1.17	0	10,17,19	1.06	1 (10%)
1	YOF	B	154[B]	-	12,13,14	0.87	0	10,17,19	1.25	1 (10%)
1	YOF	B	137	1	12,13,14	0.86	0	10,17,19	1.31	1 (10%)
1	YOF	B	166	1	12,13,14	1.07	0	10,17,19	1.04	1 (10%)
1	YOF	A	61	1	12,13,14	1.47	2 (16%)	10,17,19	1.60	1 (10%)
1	YOF	B	78	1	12,13,14	0.85	0	10,17,19	1.52	3 (30%)
1	YOF	A	32	1	12,13,14	0.78	0	10,17,19	1.12	1 (10%)
1	YOF	A	160	1	12,13,14	0.72	0	10,17,19	1.26	1 (10%)
1	YOF	B	154[A]	-	12,13,14	0.75	0	10,17,19	1.16	1 (10%)
1	YOF	A	196	1	12,13,14	1.18	1 (8%)	10,17,19	0.87	0
1	YOF	B	40	1	12,13,14	1.10	1 (8%)	10,17,19	1.06	1 (10%)
1	YOF	A	137	1	12,13,14	0.78	0	10,17,19	1.55	2 (20%)
1	YOF	A	78	1	12,13,14	1.00	0	10,17,19	1.55	2 (20%)
1	YOF	B	160	1	12,13,14	0.92	0	10,17,19	1.37	1 (10%)
1	YOF	B	22	1	12,13,14	0.92	0	10,17,19	1.04	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	YOF	B	202	1	12,13,14	0.83	0	10,17,19	0.85	0
1	YOF	A	166	1	12,13,14	1.06	1 (8%)	10,17,19	1.23	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	YOF	A	154[B]	-	-	0/5/6/8	0/1/1/1
1	YOF	B	6	1	-	2/5/6/8	0/1/1/1
1	YOF	A	202	1	-	0/5/6/8	0/1/1/1
1	YOF	A	40	1	-	0/5/6/8	0/1/1/1
1	YOF	B	27	1	-	0/5/6/8	0/1/1/1
1	YOF	A	6	1	-	2/5/6/8	0/1/1/1
1	YOF	B	32	1	-	0/5/6/8	0/1/1/1
1	YOF	B	61	1	-	0/5/6/8	0/1/1/1
1	YOF	B	196	1	-	2/5/6/8	0/1/1/1
1	YOF	A	154[A]	-	-	0/5/6/8	0/1/1/1
1	YOF	A	22	1	-	0/5/6/8	0/1/1/1
1	YOF	A	27	1	-	0/5/6/8	0/1/1/1
1	YOF	B	154[B]	-	-	2/5/6/8	0/1/1/1
1	YOF	B	137	1	-	0/5/6/8	0/1/1/1
1	YOF	B	166	1	-	2/5/6/8	0/1/1/1
1	YOF	A	61	1	-	0/5/6/8	0/1/1/1
1	YOF	B	78	1	-	1/5/6/8	0/1/1/1
1	YOF	A	32	1	-	0/5/6/8	0/1/1/1
1	YOF	A	160	1	-	1/5/6/8	0/1/1/1
1	YOF	B	154[A]	-	-	2/5/6/8	0/1/1/1
1	YOF	A	196	1	-	2/5/6/8	0/1/1/1
1	YOF	B	40	1	-	5/5/6/8	0/1/1/1
1	YOF	A	137	1	-	1/5/6/8	0/1/1/1
1	YOF	A	78	1	-	0/5/6/8	0/1/1/1
1	YOF	B	160	1	-	0/5/6/8	0/1/1/1
1	YOF	B	22	1	-	1/5/6/8	0/1/1/1
1	YOF	B	202	1	-	0/5/6/8	0/1/1/1
1	YOF	A	166	1	-	2/5/6/8	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	40	YOF	CZ-CE1	3.16	1.41	1.39
1	B	40	YOF	CZ-CE1	2.76	1.41	1.39
1	A	61	YOF	CE2-CD2	2.63	1.43	1.38
1	A	61	YOF	CB-CA	-2.42	1.48	1.53
1	A	6	YOF	CZ-CE1	2.33	1.41	1.39
1	A	196	YOF	CZ-CE1	2.24	1.41	1.39
1	B	27	YOF	CB-CA	2.20	1.58	1.53
1	A	166	YOF	CZ-CE1	2.20	1.41	1.39

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	6	YOF	CG-CD1-CE1	5.54	123.00	119.37
1	B	196	YOF	CD2-CE2-CZ	-4.36	116.14	120.50
1	A	202	YOF	CG-CD1-CE1	4.02	122.00	119.37
1	A	61	YOF	CD2-CE2-CZ	-3.82	116.68	120.50
1	A	78	YOF	CD2-CE2-CZ	-3.47	117.03	120.50
1	B	160	YOF	CG-CD1-CE1	3.46	121.64	119.37
1	A	137	YOF	CD2-CE2-CZ	-3.44	117.06	120.50
1	B	6	YOF	CG-CD1-CE1	3.35	121.56	119.37
1	B	61	YOF	CG-CD1-CE1	3.29	121.53	119.37
1	B	196	YOF	CG-CD1-CE1	-3.18	117.29	119.37
1	A	40	YOF	CG-CD1-CE1	3.17	121.45	119.37
1	A	154[A]	YOF	CG-CD1-CE1	3.16	121.44	119.37
1	B	154[B]	YOF	CG-CD1-CE1	3.08	121.39	119.37
1	B	137	YOF	CG-CD1-CE1	2.96	121.31	119.37
1	B	40	YOF	CG-CD1-CE1	2.87	121.25	119.37
1	B	154[A]	YOF	CG-CD1-CE1	2.82	121.22	119.37
1	B	166	YOF	CG-CD1-CE1	2.76	121.18	119.37
1	B	27	YOF	CD2-CE2-CZ	-2.57	117.93	120.50
1	B	78	YOF	CD2-CE2-CZ	-2.50	118.00	120.50
1	A	160	YOF	CD2-CE2-CZ	-2.45	118.05	120.50
1	B	78	YOF	F-CE1-CZ	2.41	122.68	118.34
1	B	78	YOF	CB-CG-CD1	-2.27	116.53	120.43
1	A	137	YOF	F-CE1-CZ	2.22	122.33	118.34
1	B	32	YOF	CD2-CE2-CZ	-2.18	118.32	120.50
1	A	32	YOF	CG-CD1-CE1	2.16	120.79	119.37
1	B	32	YOF	CG-CD1-CE1	2.13	120.77	119.37
1	A	154[B]	YOF	CG-CD1-CE1	2.12	120.76	119.37
1	A	27	YOF	F-CE1-CZ	2.11	122.13	118.34
1	A	78	YOF	F-CE1-CZ	2.09	122.10	118.34

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	166	YOF	C-CA-CB-CG
1	B	40	YOF	O-C-CA-CB
1	B	166	YOF	C-CA-CB-CG
1	B	40	YOF	N-CA-CB-CG
1	B	166	YOF	N-CA-CB-CG
1	A	6	YOF	CA-CB-CG-CD1
1	A	6	YOF	CA-CB-CG-CD2
1	B	6	YOF	CA-CB-CG-CD2
1	B	6	YOF	CA-CB-CG-CD1
1	B	40	YOF	CA-CB-CG-CD2
1	B	40	YOF	CA-CB-CG-CD1
1	A	137	YOF	C-CA-CB-CG
1	A	160	YOF	C-CA-CB-CG
1	A	166	YOF	N-CA-CB-CG
1	B	22	YOF	C-CA-CB-CG
1	B	40	YOF	C-CA-CB-CG
1	B	78	YOF	C-CA-CB-CG
1	B	154[A]	YOF	N-CA-CB-CG
1	B	154[A]	YOF	C-CA-CB-CG
1	B	154[B]	YOF	N-CA-CB-CG
1	B	154[B]	YOF	C-CA-CB-CG
1	B	196	YOF	CA-CB-CG-CD2
1	A	196	YOF	CA-CB-CG-CD1
1	B	196	YOF	CA-CB-CG-CD1
1	A	196	YOF	CA-CB-CG-CD2

There are no ring outliers.

12 monomers are involved in 31 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	40	YOF	5	0
1	A	6	YOF	8	0
1	B	32	YOF	3	0
1	B	196	YOF	1	0
1	A	27	YOF	1	0
1	A	61	YOF	1	0
1	A	32	YOF	1	0
1	A	160	YOF	1	0
1	A	196	YOF	1	0
1	B	40	YOF	5	0
1	B	22	YOF	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	202	YOF	3	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	-	35,37,37	3.27	7 (20%)	46,51,51	2.11	9 (19%)
2	GPR	B	218	-	35,37,37	2.42	11 (31%)	46,51,51	1.72	11 (23%)

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	-	-	5/27/43/43	0/3/3/3
2	GPR	B	218	-	-	1/27/43/43	0/3/3/3

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	218	GPR	CB2-SG2	-17.31	1.65	1.82
2	B	218	GPR	CB2-SG2	-8.78	1.73	1.82
2	B	218	GPR	CG4-CB4	4.96	1.45	1.39
2	B	218	GPR	CG5-CB5	4.48	1.45	1.39
2	B	218	GPR	CA4-SG2	-4.04	1.74	1.84
2	A	218	GPR	O5-CA5	4.01	1.50	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	218	GPR	CH5-CH4	-3.39	1.40	1.47
2	B	218	GPR	CD5-CG5	3.07	1.44	1.38
2	B	218	GPR	CA4-CA5	-2.85	1.45	1.53
2	B	218	GPR	CZ5-CH5	2.70	1.44	1.40
2	A	218	GPR	CD5-CE5	2.61	1.44	1.38
2	A	218	GPR	CD5-CG5	2.48	1.43	1.38
2	A	218	GPR	CG4-CB4	2.47	1.42	1.39
2	B	218	GPR	CB5-CA5	2.42	1.55	1.51
2	B	218	GPR	CD1-N2	2.35	1.39	1.34
2	A	218	GPR	CA4-SG2	-2.33	1.78	1.84
2	A	218	GPR	CH5-CH4	-2.12	1.43	1.47
2	B	218	GPR	O12-C1	-2.02	1.24	1.30

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	218	GPR	CB2-CA2-C2	-7.12	93.40	109.46
2	A	218	GPR	CD4-CG4-CB4	-6.53	113.17	120.99
2	A	218	GPR	CG4-CB4-CH4	4.73	125.14	119.35
2	B	218	GPR	CD4-CG4-CB4	-4.48	115.62	120.99
2	B	218	GPR	CB2-CA2-N2	-4.44	99.44	111.06
2	B	218	GPR	CB2-CA2-C2	-3.69	101.13	109.46
2	B	218	GPR	CH5-CH4-CB4	-3.38	114.80	119.64
2	A	218	GPR	CZ5-CH5-CB5	3.11	121.87	118.50
2	A	218	GPR	CG4-CB4-CA4	-2.95	112.43	119.69
2	A	218	GPR	CD5-CG5-CB5	-2.91	117.51	120.99
2	A	218	GPR	CE4-CD4-CG4	2.69	123.56	120.24
2	A	218	GPR	CA5-CA4-SG2	2.59	118.81	110.88
2	B	218	GPR	CB4-CA4-SG2	-2.55	104.39	111.02
2	B	218	GPR	CG5-CB5-CH5	-2.21	116.64	119.35
2	A	218	GPR	CA2-CB2-SG2	-2.14	105.88	113.66
2	B	218	GPR	O5-CA5-CB5	2.13	114.50	110.42
2	B	218	GPR	CZ4-CH4-CH5	2.05	125.78	121.61
2	B	218	GPR	OE1-CD1-N2	-2.02	119.53	122.95
2	B	218	GPR	CH4-CH5-CB5	-2.02	116.75	119.64
2	B	218	GPR	CB5-CA5-CA4	-2.01	105.46	110.64

There are no chirality outliers.

All (6) torsion outliers are listed below:

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

Continued on next page...

Continued from previous page...

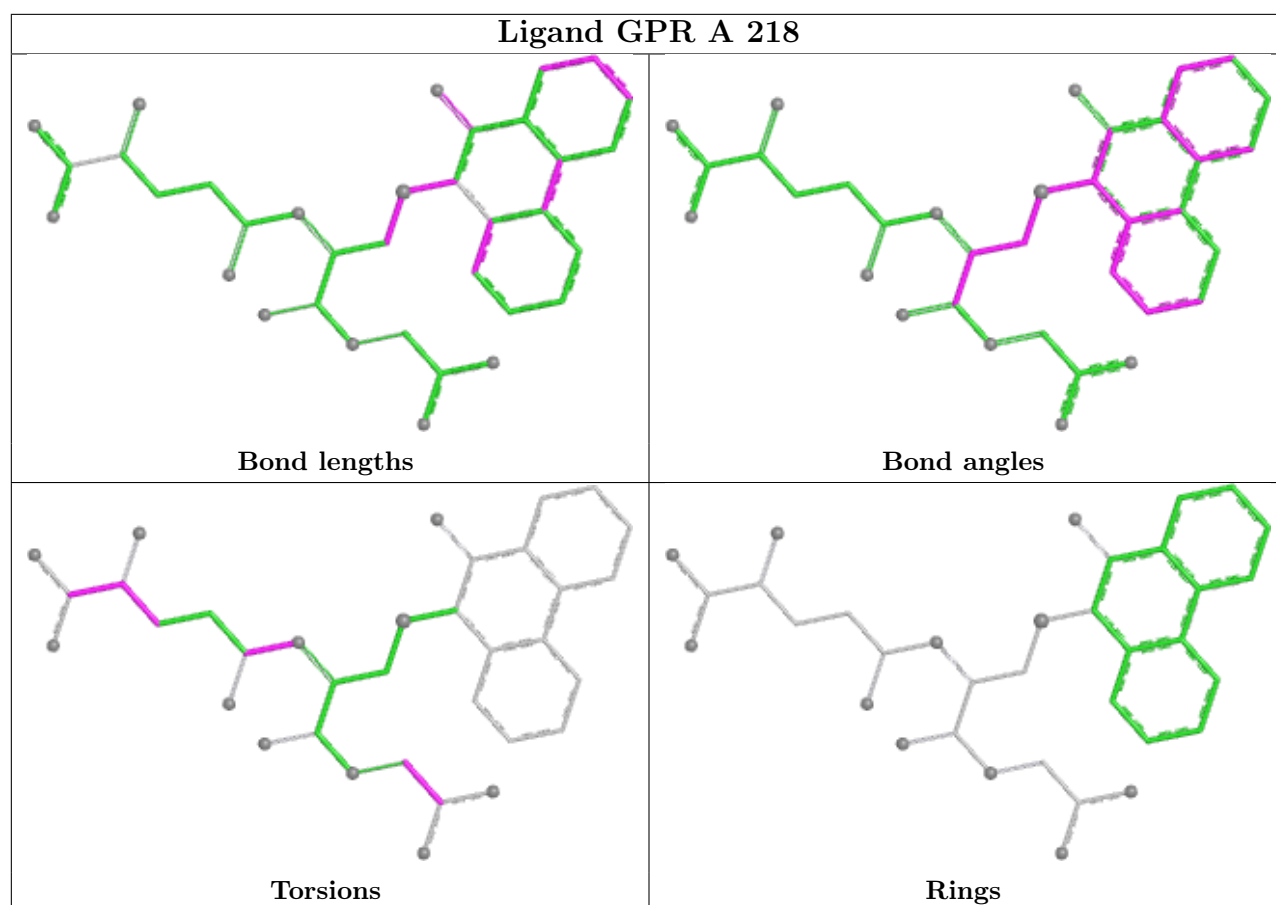
Mol	Chain	Res	Type	Atoms
2	B	218	GPR	OE1-CD1-N2-CA2
2	A	218	GPR	C1-CA1-CB1-CG1
2	A	218	GPR	OE1-CD1-N2-CA2
2	A	218	GPR	O31-C3-CA3-N3
2	A	218	GPR	O11-C1-CA1-N1

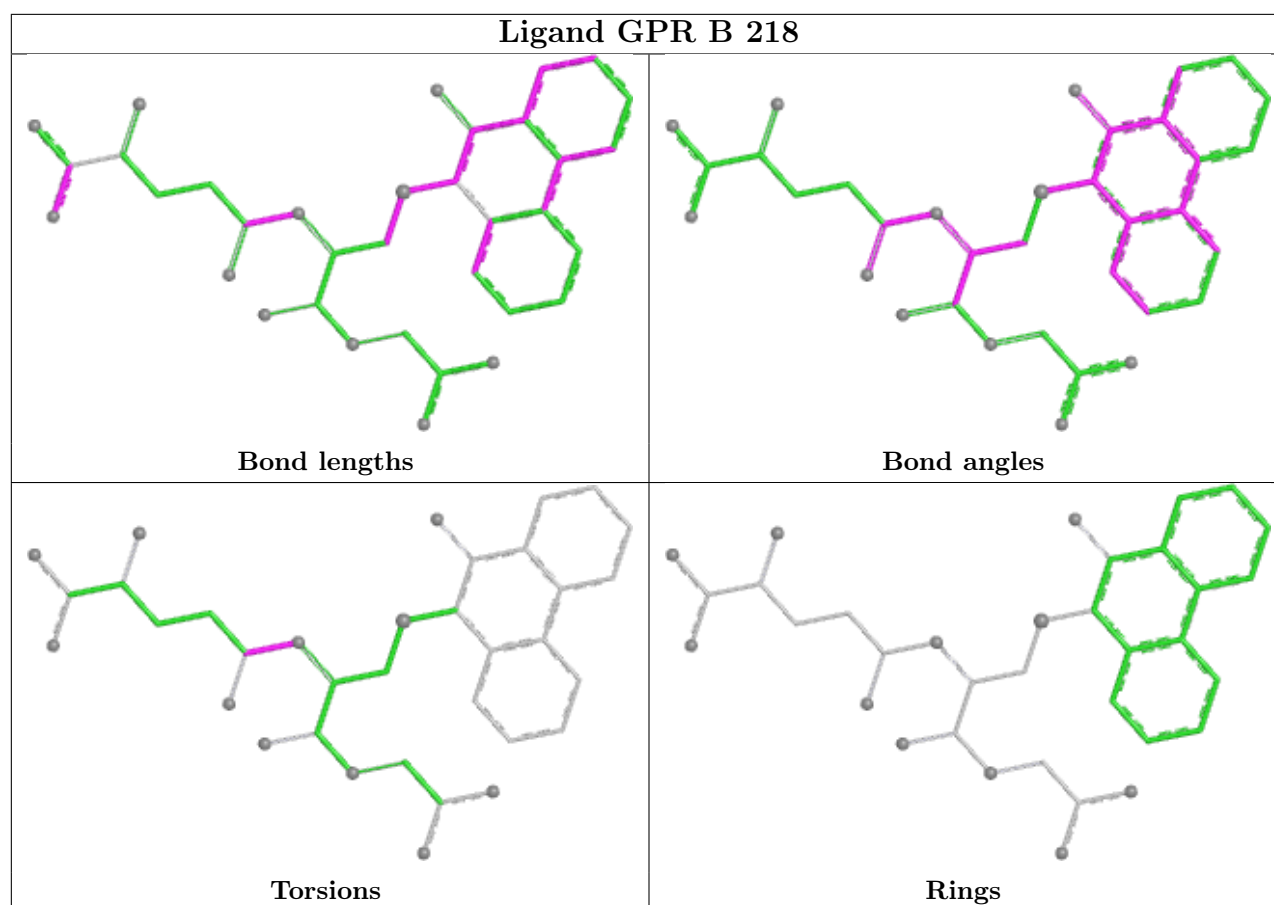
There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	218	GPR	2	0
2	B	218	GPR	6	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	204/217 (94%)	1.03	41 (20%) 3 2	12, 32, 82, 90	0
1	B	204/217 (94%)	0.79	34 (16%) 4 3	13, 30, 68, 89	0
All	All	408/434 (94%)	0.91	75 (18%) 3 2	12, 32, 78, 90	0

All (75) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	205	THR	11.3
1	A	209	SER	10.6
1	A	216	ASN	9.7
1	B	207	ILE	8.5
1	B	208	PHE	8.0
1	B	216	ASN	7.0
1	A	217	LYS	7.0
1	A	39	ASP	7.0
1	B	213	GLN	6.6
1	A	210	LYS	6.1
1	A	204	SER	5.7
1	A	207	ILE	5.5
1	A	36	ASP	5.5
1	B	205	THR	5.3
1	B	120	GLU	5.1
1	A	42	ARG	4.9
1	A	212	ALA	4.9
1	A	38	PRO	4.7
1	B	217	LYS	4.6
1	A	31	ARG	4.6
1	B	39	ASP	4.6
1	B	43	SER	4.5
1	A	44	GLN	4.5
1	B	203	LEU	4.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	206	PRO	4.3
1	A	211	LEU	4.2
1	B	122	GLN	4.2
1	B	215	SER	4.1
1	A	203	LEU	4.0
1	B	204	SER	3.9
1	A	37	ALA	3.9
1	A	9	VAL	3.8
1	B	209	SER	3.8
1	A	135	LYS	3.8
1	A	206	PRO	3.7
1	A	208	PHE	3.7
1	B	212	ALA	3.7
1	A	43	SER	3.7
1	B	36	ASP	3.6
1	B	165	GLN	3.4
1	A	8	ASN	3.4
1	A	199	SER	3.3
1	A	132	GLU	3.3
1	A	120	GLU	3.2
1	B	118	ASP	3.2
1	B	37	ALA	3.2
1	A	214	TRP	3.2
1	A	7	TRP	3.1
1	A	33	ALA	3.0
1	A	77	ARG	3.0
1	B	115	TYR	2.9
1	A	35	GLY	2.9
1	B	211	LEU	2.9
1	A	34	MET	2.9
1	A	201	ARG	2.8
1	B	214	TRP	2.7
1	A	17	ARG	2.7
1	B	38	PRO	2.6
1	A	41	ASP	2.5
1	B	132	GLU	2.5
1	B	17	ARG	2.3
1	B	143	LYS	2.3
1	A	125	GLU	2.3
1	A	198	LYS	2.2
1	A	48	GLU	2.2
1	B	210	LYS	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	150	ASP	2.2
1	A	215	SER	2.1
1	B	31	ARG	2.1
1	A	200	SER	2.1
1	B	135	LYS	2.1
1	B	191	LYS	2.1
1	B	112	MET	2.1
1	A	45	TRP	2.0
1	B	10	ARG	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	YOF	B	40	13/14	0.42	0.30	0,63,91,98	0
1	YOF	A	40	13/14	0.55	0.34	0,0,88,96	0
1	YOF	A	6	13/14	0.57	0.28	0,30,70,95	0
1	YOF	A	196	13/14	0.61	0.19	0,34,52,94	0
1	YOF	B	137	13/14	0.64	0.14	0,21,42,59	0
1	YOF	A	32	13/14	0.74	0.15	0,31,54,62	0
1	YOF	A	202	13/14	0.75	0.16	0,39,85,86	0
1	YOF	B	6	13/14	0.75	0.15	0,25,40,87	0
1	YOF	B	166	13/14	0.76	0.13	0,21,41,50	0
1	YOF	B	32	13/14	0.81	0.11	0,25,35,38	0
1	YOF	B	202	13/14	0.85	0.14	22,29,73,98	0
1	YOF	B	196	13/14	0.88	0.12	13,28,42,99	0
1	YOF	A	137	13/14	0.90	0.10	17,26,33,48	0
1	YOF	B	27	13/14	0.90	0.08	11,18,31,47	0
1	YOF	B	22	13/14	0.91	0.08	16,25,38,55	0
1	YOF	A	27	13/14	0.91	0.08	15,24,44,53	0
1	YOF	A	166	13/14	0.92	0.08	9,24,38,52	0
1	YOF	A	78	13/14	0.92	0.09	12,17,60,64	0
1	YOF	A	22	13/14	0.92	0.08	10,20,31,41	0
1	YOF	A	154[B]	13/14	0.93	0.09	7,17,28,31	5
1	YOF	A	61	13/14	0.93	0.08	15,22,31,31	0
1	YOF	A	154[A]	13/14	0.93	0.09	7,17,28,30	5
1	YOF	B	78	13/14	0.93	0.08	10,18,45,56	0
1	YOF	B	61	13/14	0.94	0.08	10,19,34,84	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
1	YOF	B	154[B]	13/14	0.95	0.08	12,18,33,42	5
1	YOF	B	154[A]	13/14	0.95	0.08	12,18,42,50	5
1	YOF	B	160	13/14	0.96	0.08	9,17,46,59	0
1	YOF	A	160	13/14	0.96	0.06	6,20,33,40	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

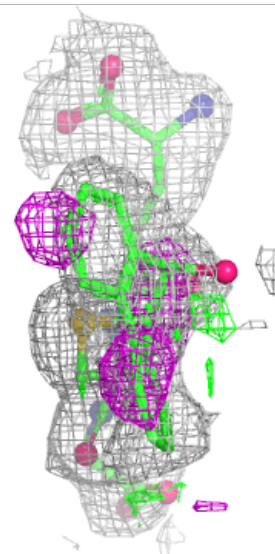
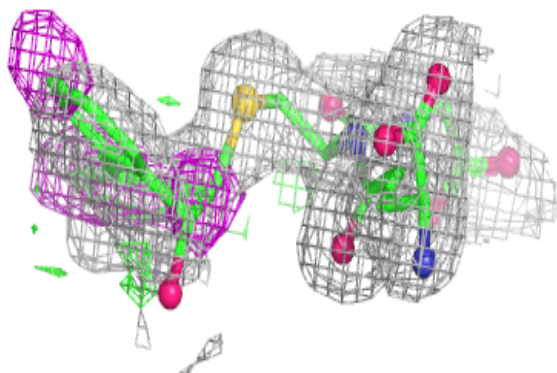
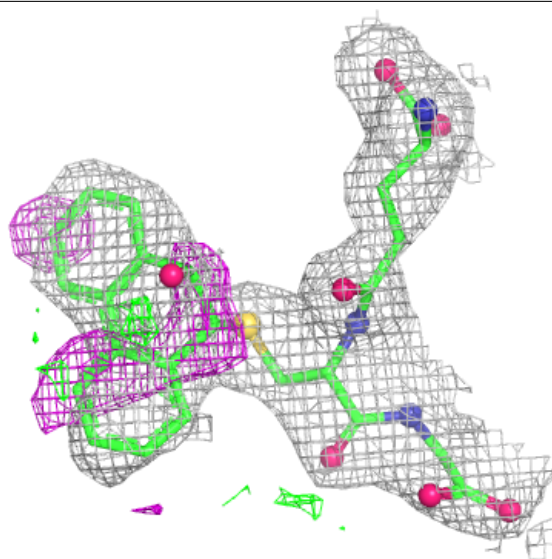
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	A	218	35/35	0.69	0.19	0,31,68,88	0
2	GPR	B	218	35/35	0.82	0.16	0,33,97,98	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.

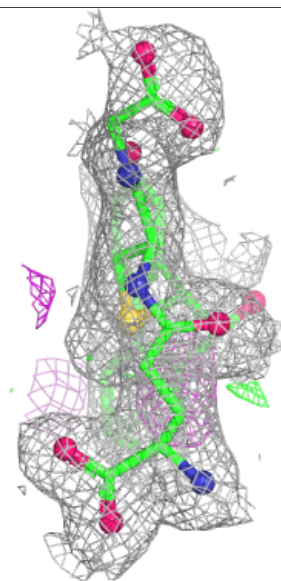
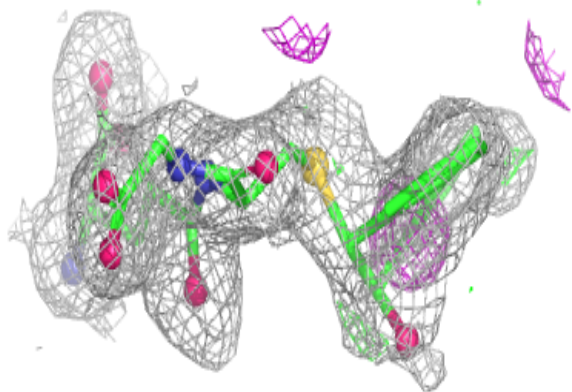
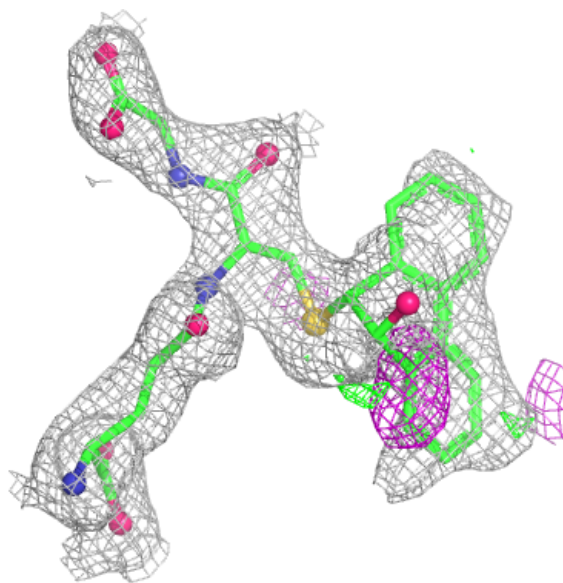
Electron density around GPR A 218:

$2mF_o-DF_c$ (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.