



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 26, 2026 – 02:08 AM EDT

PDB ID : 8QW6 / pdb_00008qw6
Title : Crystal Structure of compound 3 in complex with KRAS G12V C118S GDP and pVHL:ElonginC:ElonginB
Authors : Zollman, D.; Farnaby, W.; Ciulli, A.
Deposited on : 2023-10-18
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

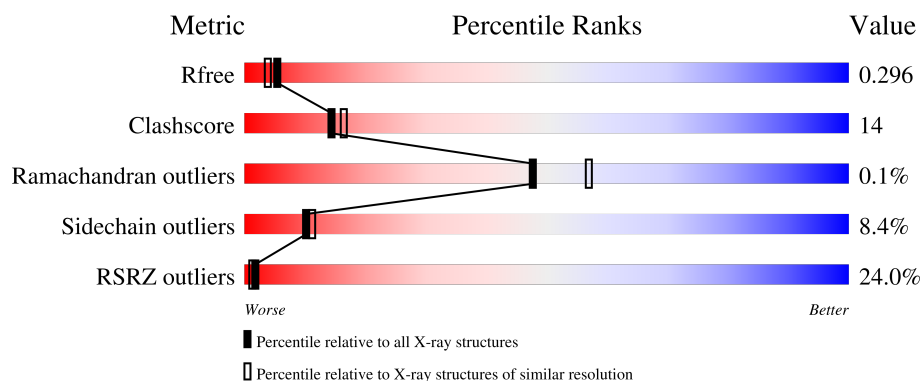
1 Overall quality at a glance

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.



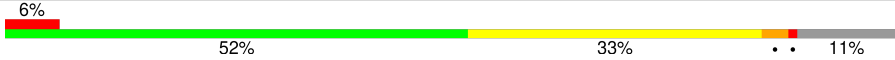
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	D	104	
1	H	104	
2	C	97	
2	G	97	
3	B	162	

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Mol	Chain	Length	Quality of chain
3	F	162	
4	A	170	
4	E	170	

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 7996 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 Elongin-B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	104	Total	C	N	O	S	0	0	0
			819	517	137	160	5			
1	D	103	Total	C	N	O	S	0	0	0
			795	503	134	153	5			

- Molecule 2 is a protein called Elongin-C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	86	Total	C	N	O	S	0	0	0
			681	440	107	128	6			
2	C	86	Total	C	N	O	S	0	0	0
			667	432	103	126	6			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	16	MET	-	initiating methionine	UNP Q15369
C	16	MET	-	initiating methionine	UNP Q15369

- Molecule 3 is a protein called von Hippel-Lindau disease tumor suppressor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	144	Total	C	N	O	S	0	0	0
			1165	741	210	212	2			
3	B	146	Total	C	N	O	S	0	0	0
			1196	759	221	214	2			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	52	GLY	-	expression tag	UNP P40337
F	53	SER	-	expression tag	UNP P40337

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Chain	Residue	Modelled	Actual	Comment	Reference
B	52	GLY	-	expression tag	UNP P40337
B	53	SER	-	expression tag	UNP P40337

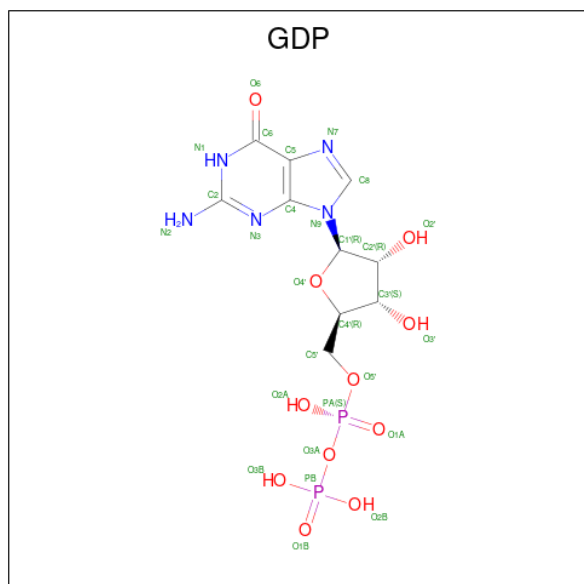
- Molecule 4 is a protein called GTPase KRas.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	155	Total	C	N	O	S	0	0	0
			1158	726	199	228	5			
4	A	163	Total	C	N	O	S	0	0	0
			1271	795	218	253	5			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	0	GLY	-	expression tag	UNP P01116
E	12	VAL	GLY	engineered mutation	UNP P01116
E	118	SER	CYS	engineered mutation	UNP P01116
A	0	GLY	-	expression tag	UNP P01116
A	12	VAL	GLY	engineered mutation	UNP P01116
A	118	SER	CYS	engineered mutation	UNP P01116

- Molecule 5 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



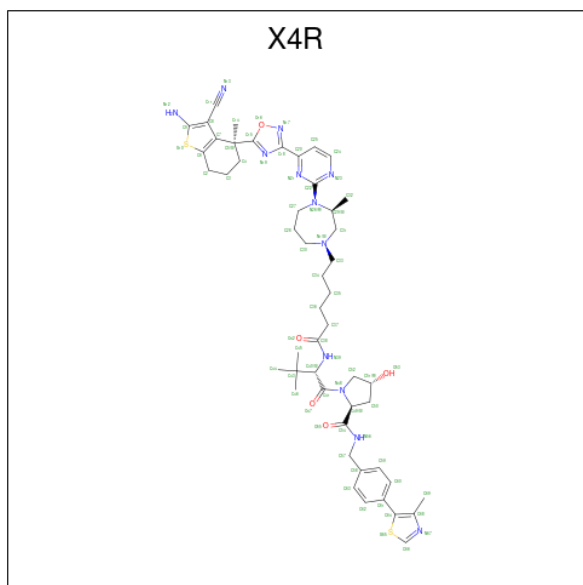
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	E	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

- Molecule 6 is (2S,4R)-1-[(2S)-2-[6-[(3S)-4-[4-[5-[(4S)-2-azanyl-3-cyano-4-methyl-6,7-dihydro-5H-1-benzothiophen-4-yl]-1,2,4-oxadiazol-3-yl]pyrimidin-2-yl]-3-methyl-1,4-diazepan-1-yl]hexanoylamino]-3,3-dimethyl-butanoyl]-N-[[4-(4-methyl-1,3-thiazol-5-yl)phenyl]methyl]-4-oxidanyl-pyrrolidine-2-carboxamide (CCD ID: X4R) (formula: C₅₀H₆₄N₁₂O₅S₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	E	1	Total	C	N	O	S	0	0
			69	50	12	5	2		
6	A	1	Total	C	N	O	S	0	0
			69	50	12	5	2		

- Molecule 7 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	E	1	Total	Mg	0	0
			1	1		
7	A	1	Total	Mg	0	0
			1	1		

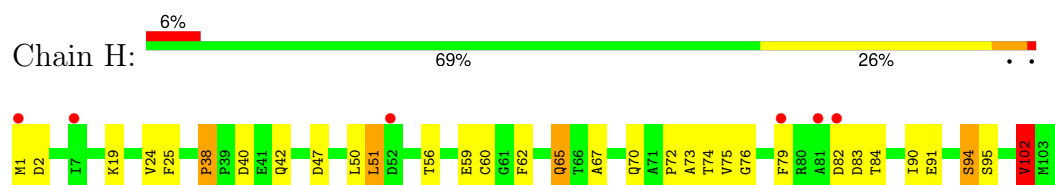
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	H	3	Total 3	O 3	0	0
8	G	7	Total 7	O 7	0	0
8	F	16	Total 16	O 16	0	0
8	E	3	Total 3	O 3	0	0
8	C	4	Total 4	O 4	0	0
8	B	11	Total 11	O 11	0	0
8	A	4	Total 4	O 4	0	0

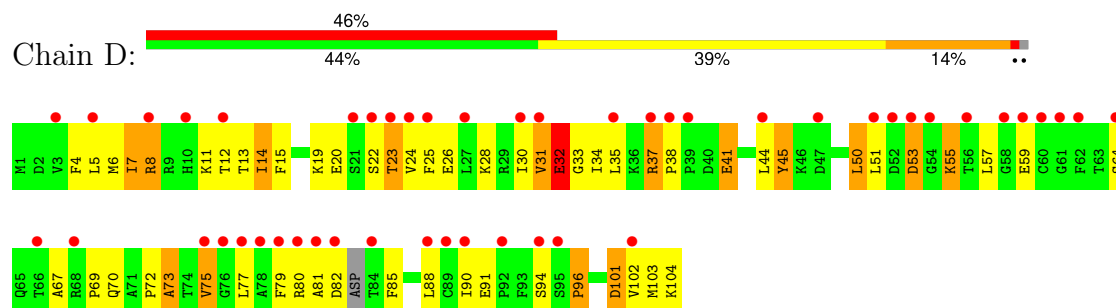
3 Residue-property plots [i](#)

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.

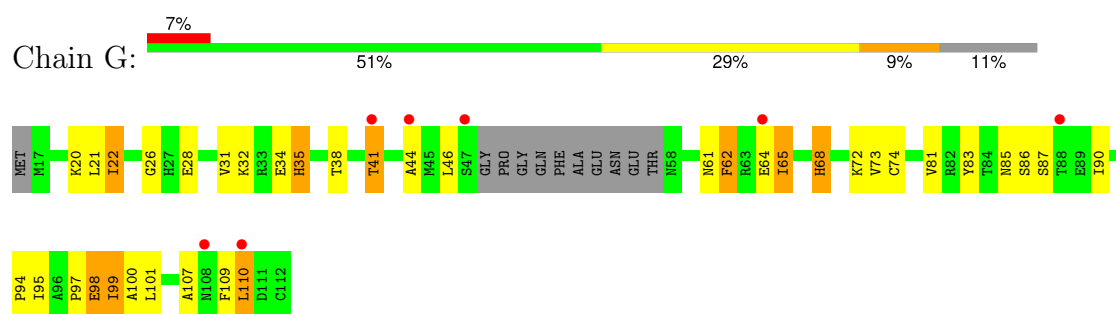
• Molecule 1: Elongin-B



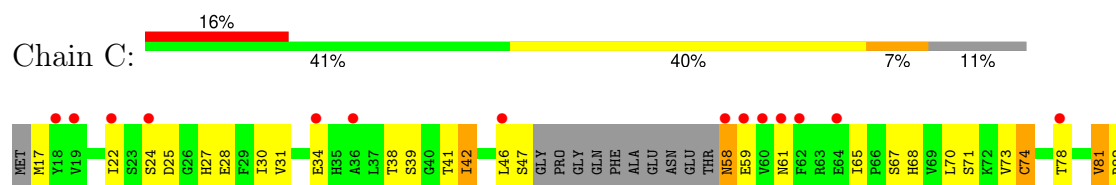
• Molecule 1: Elongin-B



• Molecule 2: Elongin-C

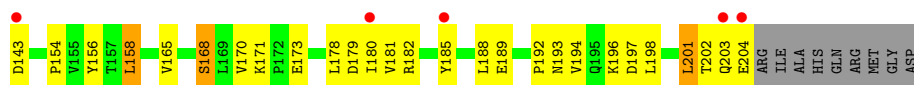


• Molecule 2: Elongin-C





- Molecule 3: von Hippel-Lindau disease tumor suppressor

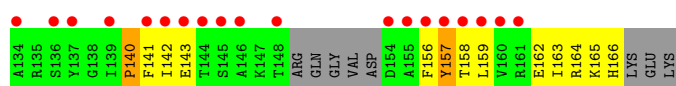
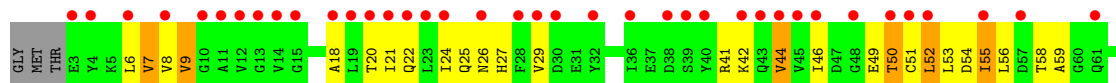


- Molecule 3: von Hippel-Lindau disease tumor suppressor

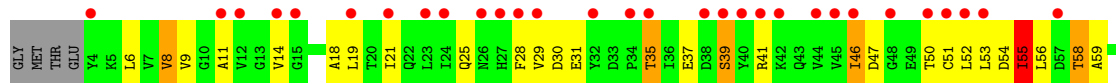


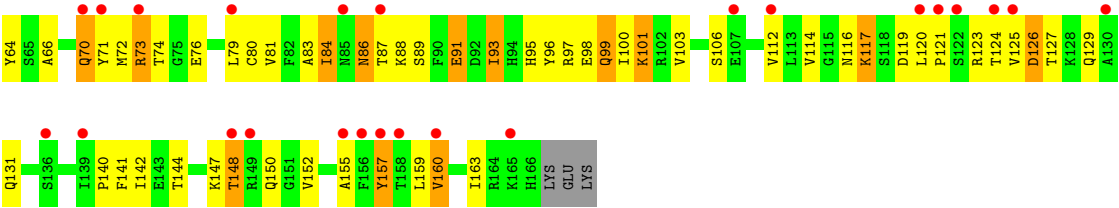
GLY
ASP

- Molecule 4: GTPase KRas



- Molecule 4: GTPase KRas





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	70.21Å 72.30Å 80.79Å 112.25° 100.61° 100.57°	Depositor
Resolution (Å)	46.37 – 2.20 46.37 – 2.20	Depositor EDS
% Data completeness (in resolution range)	55.5 (46.37-2.20) 55.6 (46.37-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.28 (at 2.20Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487, PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.255 , 0.295 0.257 , 0.296	Depositor DCC
R_{free} test set	2000 reflections (2.83%)	wwPDB-VP
Wilson B-factor (Å ²)	43.0	Xtriage
Anisotropy	0.034	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 38.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	7996	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.50% 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: MG, GDP, X4R

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	D	1.71	11/810 (1.4%)	1.47	9/1093 (0.8%)
1	H	1.81	22/835 (2.6%)	1.34	3/1128 (0.3%)
2	C	1.82	18/681 (2.6%)	1.36	7/922 (0.8%)
2	G	1.76	19/695 (2.7%)	1.29	3/938 (0.3%)
3	B	1.38	12/1227 (1.0%)	1.35	6/1674 (0.4%)
3	F	1.80	28/1196 (2.3%)	1.36	5/1634 (0.3%)
4	A	1.62	25/1292 (1.9%)	1.40	7/1749 (0.4%)
4	E	1.47	16/1174 (1.4%)	1.50	13/1587 (0.8%)
All	All	1.66	151/7910 (1.9%)	1.39	53/10725 (0.5%)

All (151) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	96	GLN	C-O	-9.14	1.14	1.24
3	F	179	ASP	C-O	-8.74	1.14	1.23
2	G	100	ALA	C-O	-8.55	1.14	1.24
2	G	62	PHE	C-O	-8.47	1.14	1.24
4	A	76	GLU	CA-C	-8.31	1.41	1.52
2	C	109	PHE	C-O	-8.09	1.14	1.24
3	F	158	LEU	C-O	-8.03	1.14	1.24
3	F	65	SER	C-O	-7.92	1.14	1.23
3	F	66	VAL	C-O	-7.90	1.14	1.24
1	H	72	PRO	C-O	-7.89	1.13	1.23
2	C	94	PRO	C-O	-7.83	1.15	1.23
3	B	201	LEU	C-O	-7.78	1.15	1.24
4	E	71	TYR	C-O	-7.75	1.15	1.24
3	F	67	ASN	C-O	-7.60	1.15	1.23
2	G	94	PRO	C-O	-7.55	1.15	1.23
4	E	70	GLN	C-O	-7.53	1.14	1.24
4	A	157	TYR	CA-C	-7.48	1.43	1.52
4	A	55	ILE	C-O	-7.46	1.16	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	99	GLN	C-O	-7.42	1.14	1.24
4	A	74	THR	C-O	-7.41	1.15	1.24
3	B	194	VAL	C-O	-7.39	1.15	1.24
3	F	95	PRO	C-O	-7.38	1.13	1.23
4	E	67	MET	C-O	-7.32	1.15	1.24
1	H	91	GLU	C-O	-7.30	1.14	1.24
2	G	99	ILE	C-O	-7.17	1.14	1.24
2	C	82	ARG	C-O	-7.09	1.14	1.24
3	B	102	PRO	C-O	-6.88	1.19	1.25
2	C	106	ALA	C-O	-6.87	1.16	1.24
1	D	64	SER	C-O	-6.83	1.15	1.24
2	C	71	SER	C-O	-6.82	1.16	1.24
3	F	127	GLY	C-O	-6.80	1.16	1.23
3	F	168	SER	C-O	-6.77	1.16	1.24
2	C	42	ILE	C-O	-6.76	1.17	1.24
4	A	160	VAL	C-O	-6.73	1.15	1.24
1	H	25	PHE	C-O	-6.70	1.16	1.24
4	A	71	TYR	CA-C	-6.65	1.44	1.52
3	B	195	GLN	C-O	-6.64	1.16	1.24
2	G	22	ILE	C-O	-6.61	1.17	1.24
3	B	184	LEU	C-O	-6.56	1.15	1.24
2	C	107	ALA	C-O	-6.55	1.16	1.24
3	F	130	VAL	C-O	-6.55	1.17	1.24
2	G	68	HIS	C-O	-6.54	1.15	1.24
3	F	102	PRO	C-O	-6.53	1.19	1.24
2	C	102	GLU	C-O	-6.52	1.15	1.24
1	H	47	ASP	C-O	-6.50	1.18	1.24
2	C	81	VAL	C-O	-6.49	1.16	1.24
4	E	8	VAL	C-O	-6.44	1.15	1.24
4	E	66	ALA	C-O	-6.40	1.16	1.24
3	F	194	VAL	C-O	-6.39	1.16	1.24
4	A	91	GLU	C-O	-6.30	1.16	1.24
3	B	182	ARG	C-O	-6.28	1.16	1.24
2	C	73	VAL	C-O	-6.25	1.16	1.24
1	H	51	LEU	C-O	-6.25	1.16	1.23
2	C	65	ILE	C-O	-6.24	1.16	1.24
2	C	97	PRO	C-O	-6.23	1.16	1.24
1	H	82	ASP	C-O	-6.20	1.18	1.24
1	H	67	ALA	C-O	-6.08	1.15	1.23
1	H	102	VAL	C-O	-6.08	1.16	1.24
4	A	35	THR	C-O	-6.07	1.18	1.24
4	E	7	VAL	C-O	-6.06	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	59	ALA	C-O	-6.05	1.16	1.23
3	F	131	ASN	C-O	-6.02	1.16	1.23
4	A	71	TYR	C-O	-6.00	1.17	1.24
4	A	64	TYR	C-O	-5.99	1.15	1.23
2	C	105	MET	C-O	-5.99	1.17	1.24
3	F	171	LYS	C-O	-5.98	1.16	1.23
4	A	101	LYS	C-O	-5.97	1.16	1.24
2	G	95	ILE	C-O	-5.94	1.17	1.24
3	F	123	GLY	C-O	-5.92	1.16	1.23
3	B	152	THR	C-O	-5.91	1.16	1.23
1	H	70	GLN	C-O	-5.90	1.15	1.24
2	G	97	PRO	C-O	-5.90	1.16	1.24
4	E	114	VAL	CA-C	-5.88	1.45	1.52
4	A	101	LYS	N-CA	-5.88	1.39	1.46
3	F	158	LEU	CA-C	-5.86	1.45	1.52
1	H	84	THR	C-O	-5.85	1.16	1.23
4	E	56	LEU	C-O	-5.84	1.16	1.24
2	C	74	CYS	C-O	-5.84	1.17	1.24
2	C	100	ALA	C-O	-5.82	1.17	1.24
3	F	88	TRP	C-O	-5.82	1.17	1.24
2	C	108	ASN	C-O	-5.80	1.17	1.24
4	A	157	TYR	C-O	-5.78	1.17	1.24
3	F	89	LEU	C-O	-5.74	1.17	1.24
2	G	73	VAL	C-O	-5.73	1.16	1.24
2	G	35	HIS	C-O	-5.73	1.16	1.24
3	F	189	GLU	C-O	-5.71	1.16	1.24
2	G	98	GLU	C-O	-5.71	1.16	1.24
4	A	131	GLN	C-O	-5.67	1.17	1.24
1	H	50	LEU	C-O	-5.66	1.17	1.23
3	F	64	ARG	C-O	-5.65	1.16	1.23
4	E	50	THR	CA-C	-5.65	1.45	1.52
3	F	76	PHE	C-O	-5.63	1.17	1.24
2	G	61	ASN	C-O	-5.62	1.17	1.23
1	H	90	ILE	C-O	-5.61	1.18	1.24
2	G	22	ILE	N-CA	-5.59	1.39	1.46
2	G	64	GLU	C-O	-5.59	1.16	1.24
4	A	18	ALA	C-O	-5.59	1.17	1.24
1	H	62	PHE	C-O	-5.58	1.17	1.24
4	A	8	VAL	C-O	-5.56	1.17	1.24
2	G	65	ILE	C-O	-5.56	1.17	1.24
3	F	202	THR	C-N	-5.55	1.26	1.33
2	G	34	GLU	C-O	-5.54	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	96	PRO	C-O	-5.51	1.18	1.24
3	B	151	ILE	N-CA	-5.49	1.40	1.46
2	C	39	SER	C-O	-5.49	1.17	1.24
4	E	55	ILE	C-O	-5.48	1.18	1.24
3	B	151	ILE	C-O	-5.48	1.17	1.23
3	F	198	LEU	C-O	-5.47	1.17	1.24
4	E	75	GLY	C-O	-5.45	1.16	1.23
4	E	77	GLY	C-O	-5.45	1.18	1.24
2	G	26	GLY	C-O	-5.45	1.16	1.24
4	A	59	ALA	C-O	-5.43	1.17	1.23
4	E	69	ASP	C-O	-5.42	1.17	1.24
1	D	38	PRO	CA-C	-5.41	1.47	1.52
1	D	72	PRO	C-O	-5.38	1.17	1.23
4	A	73	ARG	C-O	-5.38	1.17	1.24
4	E	114	VAL	C-O	-5.38	1.18	1.24
3	F	129	LEU	C-O	-5.38	1.17	1.23
1	H	24	VAL	C-O	-5.37	1.17	1.24
3	F	91	PHE	C-O	-5.36	1.17	1.24
3	F	143	ASP	C-O	-5.35	1.16	1.23
1	H	50	LEU	N-CA	-5.35	1.39	1.46
3	B	181	VAL	CA-CB	-5.33	1.49	1.54
4	A	58	THR	C-O	-5.32	1.17	1.23
1	D	73	ALA	CA-C	-5.30	1.46	1.52
3	B	149	ALA	CA-CB	-5.30	1.45	1.53
1	H	74	THR	C-O	-5.29	1.17	1.24
4	A	39	SER	C-O	-5.23	1.17	1.23
1	D	19	LYS	C-O	-5.23	1.17	1.23
1	H	76	GLY	C-O	-5.22	1.16	1.23
1	D	37	ARG	CA-C	-5.22	1.48	1.52
1	H	90	ILE	CA-CB	-5.21	1.47	1.54
4	A	103	VAL	C-O	-5.21	1.17	1.24
1	H	65	GLN	C-O	-5.20	1.17	1.24
1	D	73	ALA	N-CA	-5.19	1.39	1.46
2	G	72	LYS	C-O	-5.18	1.18	1.24
1	H	73	ALA	N-CA	-5.17	1.39	1.46
1	H	94	SER	C-O	-5.16	1.17	1.23
3	F	201	LEU	C-O	-5.16	1.18	1.24
1	D	90	ILE	C-O	-5.14	1.18	1.24
4	A	91	GLU	CA-C	-5.11	1.46	1.52
3	B	61	PRO	CA-C	-5.11	1.46	1.52
1	D	70	GLN	C-O	-5.11	1.17	1.24
2	C	96	ALA	C-O	-5.09	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	32	GLU	C-N	-5.09	1.26	1.33
4	A	18	ALA	N-CA	-5.08	1.40	1.46
2	G	32	LYS	C-O	-5.05	1.16	1.23
3	F	87	VAL	N-CA	-5.05	1.40	1.46
4	E	69	ASP	CA-C	-5.02	1.46	1.52
4	A	88	LYS	C-O	-5.01	1.17	1.24
1	H	73	ALA	C-O	-5.00	1.17	1.23

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	156	PHE	N-CA-C	-8.21	103.40	113.50
1	D	30	ILE	N-CA-C	8.05	119.78	111.00
1	D	38	PRO	CB-CA-C	-7.65	101.59	110.92
2	C	94	PRO	CA-C-O	-7.50	112.48	121.48
1	D	31	VAL	O-C-N	7.34	130.43	122.06
4	A	131	GLN	N-CA-C	-7.20	103.52	111.36
4	E	81	VAL	N-CA-C	7.08	118.77	108.58
4	E	88	LYS	N-CA-C	-6.98	103.67	111.28
3	F	127	GLY	N-CA-C	6.66	122.09	111.64
3	F	90	ASN	N-CA-C	6.60	118.38	110.19
4	E	76	GLU	CA-C-N	6.51	129.87	121.27
4	E	76	GLU	C-N-CA	6.51	129.87	121.27
3	B	69	ARG	N-CA-C	-6.43	104.62	113.56
4	E	85	ASN	N-CA-C	-6.32	104.32	111.14
1	D	59	GLU	N-CA-C	-6.31	105.07	112.89
4	A	29	VAL	CB-CA-C	-6.22	104.52	111.23
1	D	53	ASP	N-CA-C	-6.19	104.54	111.28
4	A	71	TYR	N-CA-C	-6.04	104.61	111.14
2	C	38	THR	N-CA-C	-6.02	105.90	113.18
4	E	140	PRO	CB-CA-C	-5.98	101.69	111.56
4	A	25	GLN	N-CA-C	5.95	119.51	112.72
4	E	55	ILE	N-CA-C	5.93	116.67	108.84
1	H	38	PRO	N-CA-C	5.87	117.86	110.70
1	H	83	ASP	N-CA-C	5.82	117.70	111.36
3	F	170	VAL	N-CA-C	5.76	116.42	108.12
4	E	50	THR	CA-C-N	-5.71	112.55	122.37
4	E	50	THR	C-N-CA	-5.71	112.55	122.37
3	B	131	ASN	CB-CA-C	5.60	119.97	111.80
2	G	85	ASN	CB-CA-C	5.54	119.17	111.63
1	D	88	LEU	N-CA-C	5.52	118.24	109.96
3	B	146	PRO	N-CA-C	5.49	119.86	111.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	38	PRO	N-CA-C	5.44	117.34	110.70
4	A	152	VAL	N-CA-C	5.43	115.88	110.23
2	G	41	THR	CB-CA-C	5.41	119.77	110.79
3	B	148	PHE	N-CA-C	5.40	118.04	109.24
3	F	91	PHE	N-CA-C	5.38	118.64	111.75
1	H	75	VAL	CB-CA-C	-5.38	103.71	111.19
4	E	157	TYR	N-CA-C	-5.31	105.61	111.71
1	D	8	ARG	N-CA-CB	-5.30	101.65	111.13
4	A	148	THR	CB-CA-C	-5.30	100.48	110.01
2	C	65	ILE	N-CA-C	5.27	120.27	108.88
4	A	163	ILE	CB-CA-C	-5.25	104.97	112.22
1	D	45	TYR	N-CA-C	5.25	118.00	109.24
3	F	194	VAL	CB-CA-C	-5.23	105.08	112.14
2	C	78	THR	CB-CA-C	5.23	119.09	110.88
4	E	9	VAL	N-CA-C	5.22	115.24	108.35
3	B	70	GLU	CB-CA-C	5.21	115.65	110.33
2	G	38	THR	N-CA-C	-5.17	106.24	112.54
4	E	64	TYR	CB-CA-C	5.15	120.33	111.68
3	B	182	ARG	N-CA-C	5.07	118.57	112.38
2	C	22	ILE	N-CA-C	5.03	115.21	108.17
2	C	59	GLU	CA-C-N	-5.01	116.64	123.10
2	C	59	GLU	C-N-CA	-5.01	116.64	123.10

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	D	795	0	782	42	0
1	H	819	0	813	8	0
2	C	667	0	651	22	0
2	G	681	0	677	19	0
3	B	1196	0	1195	34	0
3	F	1165	0	1150	19	0
4	A	1271	0	1210	47	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	E	1158	0	1070	38	0
5	A	28	0	12	0	0
5	E	28	0	12	0	0
6	A	69	0	0	2	0
6	E	69	0	0	3	0
7	A	1	0	0	0	0
7	E	1	0	0	0	0
8	A	4	0	0	1	0
8	B	11	0	0	0	0
8	C	4	0	0	0	0
8	E	3	0	0	0	0
8	F	16	0	0	0	0
8	G	7	0	0	0	0
8	H	3	0	0	0	0
All	All	7996	0	7572	218	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 14.

All (218) 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:D:101:ASP:HA	1:D:104:LYS:HG3	1.30	1.13
4:E:27:HIS:O	4:E:27:HIS:ND1	2.07	0.86
3:F:165:VAL:O	3:F:168:SER:HB3	1.79	0.82
3:F:75:ILE:HG12	3:F:108:ARG:HG2	1.60	0.82
3:F:182:ARG:HA	3:F:185:TYR:CD2	2.16	0.81
4:A:112:VAL:HG12	4:A:140:PRO:HG2	1.62	0.81
4:A:66:ALA:O	4:A:70:GLN:HG2	1.81	0.79
4:E:162:GLU:N	4:E:162:GLU:OE1	2.15	0.78
4:E:44:VAL:O	4:E:51:CYS:HB2	1.84	0.78
4:E:58:THR:HG22	4:E:72:MET:HE1	1.66	0.78
1:D:7:ILE:HG12	1:D:14:ILE:CG2	2.13	0.77
2:G:41:THR:HG21	2:G:109:PHE:O	1.87	0.74
4:E:42:LYS:O	4:E:52:LEU:HA	1.90	0.72
4:A:28:PHE:CD2	4:A:147:LYS:HA	2.25	0.71
4:A:41:ARG:HA	4:A:53:LEU:O	1.91	0.70
4:A:58:THR:HG21	4:A:72:MET:HE1	1.73	0.69
4:A:19:LEU:HD21	4:A:114:VAL:HG11	1.73	0.69
2:C:31:VAL:HG11	2:C:74:CYS:SG	2.32	0.69
1:D:7:ILE:HG22	1:D:75:VAL:HB	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:25:PHE:N	1:D:53:ASP:O	2.27	0.68
4:E:41:ARG:HG2	4:E:54:ASP:OD1	1.93	0.68
2:C:83:TYR:HB3	2:C:90:ILE:HG12	1.76	0.68
2:C:58:ASN:N	2:C:58:ASN:HD22	1.91	0.68
1:D:96:PRO:HB3	2:C:68:HIS:CD2	2.28	0.67
4:A:39:SER:HB3	4:A:56:LEU:HA	1.76	0.67
3:F:154:PRO:HG2	3:F:156:TYR:CE1	2.31	0.65
4:A:70:GLN:NE2	8:A:301:HOH:O	2.28	0.65
2:G:41:THR:OG1	2:G:110:LEU:HA	1.99	0.62
4:A:46:ILE:HD12	4:A:157:TYR:HB3	1.80	0.62
4:A:148:THR:O	4:A:148:THR:HG22	2.00	0.62
4:A:86:ASN:HD21	4:A:89:SER:HB3	1.64	0.61
3:F:192:PRO:HA	3:F:196:LYS:HE3	1.82	0.61
4:E:49:GLU:HG2	4:E:50:THR:H	1.65	0.61
1:D:102:VAL:HG13	3:B:174:ASN:HB3	1.81	0.61
3:B:171:LYS:HB2	3:B:174:ASN:ND2	2.16	0.61
4:A:37:GLU:HG3	4:A:58:THR:HA	1.82	0.60
1:D:101:ASP:HA	1:D:104:LYS:CG	2.20	0.60
2:C:103:LEU:HD21	3:B:158:LEU:HD11	1.84	0.60
3:F:72:SER:OG	3:F:141:ASN:ND2	2.36	0.59
3:B:118:LEU:HD13	3:B:120:ARG:HD3	1.84	0.59
2:G:35:HIS:CD2	2:G:81:VAL:HG21	2.38	0.58
4:A:81:VAL:HG12	4:A:114:VAL:HB	1.85	0.58
2:C:46:LEU:O	2:C:47:SER:C	2.43	0.58
4:E:21:ILE:HG21	4:E:29:VAL:HG23	1.84	0.58
4:A:41:ARG:HB3	4:A:52:LEU:HD11	1.84	0.58
4:E:85:ASN:OD1	4:E:117:LYS:HE3	2.04	0.58
1:D:8:ARG:HG3	1:D:13:THR:OG1	2.04	0.58
4:E:9:VAL:HG21	6:E:202:X4R:C4	2.35	0.57
1:H:42:GLN:HG2	1:H:79:PHE:HE1	1.70	0.57
3:B:174:ASN:OD1	3:B:177:ARG:NH1	2.36	0.57
1:D:5:LEU:HD23	1:D:73:ALA:HB3	1.87	0.57
1:D:7:ILE:HG12	1:D:14:ILE:HG22	1.85	0.56
4:E:7:VAL:HG12	4:E:7:VAL:O	2.04	0.56
3:B:115:HIS:O	3:B:138:PRO:HD2	2.05	0.56
4:E:25:GLN:HB3	4:E:27:HIS:CD2	2.41	0.56
2:G:86:SER:HB3	2:G:90:ILE:HD11	1.88	0.56
3:B:136:PHE:CE1	3:B:138:PRO:HD3	2.42	0.55
4:E:109:VAL:O	4:E:110:PRO:C	2.50	0.55
4:A:35:THR:O	4:A:35:THR:HG22	2.06	0.55
3:F:112:TYR:HB2	3:F:115:HIS:CE1	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E:202:X4R:C11	6:E:202:X4R:C14	2.85	0.54
2:C:41:THR:HG22	2:C:41:THR:O	2.06	0.54
3:F:182:ARG:HA	3:F:185:TYR:HD2	1.69	0.54
4:A:112:VAL:HG12	4:A:140:PRO:CG	2.37	0.54
1:D:14:ILE:HG23	1:D:14:ILE:O	2.07	0.54
3:B:60:ARG:HG2	3:B:60:ARG:HH11	1.72	0.54
4:E:112:VAL:HG22	4:E:140:PRO:HD2	1.89	0.54
1:D:77:LEU:HD21	1:D:79:PHE:CZ	2.43	0.54
1:D:7:ILE:HA	1:D:75:VAL:O	2.08	0.53
4:A:119:ASP:OD1	4:A:120:LEU:N	2.40	0.53
4:A:72:MET:HE2	6:A:202:X4R:C14	2.39	0.53
4:E:84:ILE:HD12	4:E:84:ILE:C	2.33	0.53
4:E:142:ILE:O	4:E:143:GLU:C	2.51	0.53
1:H:38:PRO:HB2	1:H:40:ASP:OD1	2.09	0.53
4:A:80:CYS:HB3	4:A:93:ILE:HD12	1.90	0.53
2:G:107:ALA:HB2	3:F:158:LEU:HG	1.90	0.52
3:B:90:ASN:OD1	3:B:94:GLU:HG2	2.09	0.52
4:E:22:GLN:O	4:E:26:ASN:HA	2.10	0.52
4:A:97:ARG:O	4:A:101:LYS:HG3	2.09	0.52
4:E:41:ARG:HA	4:E:53:LEU:O	2.08	0.52
4:A:142:ILE:HG21	4:A:155:ALA:HB2	1.91	0.52
1:D:28:LYS:HE2	1:D:44:LEU:HG	1.91	0.52
1:D:45:TYR:CZ	1:D:50:LEU:HD12	2.44	0.52
1:D:102:VAL:HG12	3:B:170:VAL:HG13	1.92	0.52
2:C:27:HIS:HB2	2:C:67:SER:OG	2.10	0.52
4:A:87:THR:O	4:A:91:GLU:HG3	2.09	0.51
1:D:31:VAL:HG12	1:D:35:LEU:HB2	1.93	0.51
1:D:32:GLU:HG2	1:D:33:GLY:N	2.26	0.51
4:E:157:TYR:O	4:E:158:THR:C	2.52	0.50
4:A:79:LEU:HG	4:A:159:LEU:HD22	1.93	0.50
1:H:56:THR:HG22	1:H:59:GLU:CD	2.36	0.50
4:E:96:TYR:CE1	6:E:202:X4R:C18	2.94	0.50
2:C:25:ASP:OD1	2:C:67:SER:OG	2.28	0.50
3:B:154:PRO:HG2	3:B:156:TYR:CE1	2.47	0.50
4:A:6:LEU:HD13	4:A:159:LEU:HD23	1.93	0.50
1:D:37:ARG:NH2	1:D:80:ARG:O	2.44	0.50
2:C:42:ILE:O	2:C:42:ILE:HG22	2.11	0.49
3:B:142:VAL:O	3:B:145:GLN:HG2	2.11	0.49
4:A:86:ASN:HD21	4:A:89:SER:CB	2.24	0.49
3:B:113:ARG:HD3	3:B:140:LEU:HG	1.93	0.49
1:D:6:MET:HE3	1:D:15:PHE:CE2	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:1:MET:HE2	1:H:1:MET:HA	1.94	0.49
1:D:23:THR:HA	1:D:55:LYS:O	2.13	0.49
3:F:192:PRO:HA	3:F:196:LYS:CE	2.43	0.49
1:D:28:LYS:HE2	1:D:44:LEU:CG	2.42	0.49
3:F:193:ASN:OD1	3:F:196:LYS:HG2	2.13	0.49
1:D:34:ILE:HG21	2:C:30:ILE:HG21	1.96	0.48
4:A:114:VAL:HG13	4:A:144:THR:CG2	2.44	0.48
4:E:41:ARG:HD3	4:E:52:LEU:HD21	1.95	0.48
3:B:84:VAL:HG22	3:B:128:LEU:HD13	1.94	0.47
1:H:102:VAL:HG11	3:F:178:LEU:HD23	1.97	0.47
3:B:170:VAL:HG21	3:B:178:LEU:HD11	1.95	0.47
4:A:9:VAL:O	4:A:81:VAL:HG22	2.14	0.47
3:B:161:ARG:O	3:B:165:VAL:HG12	2.15	0.47
2:C:70:LEU:HD12	2:C:70:LEU:HA	1.75	0.47
3:B:176:ARG:HA	3:B:185:TYR:CE1	2.50	0.47
1:D:8:ARG:NH2	1:D:91:GLU:O	2.48	0.47
4:A:28:PHE:CE2	4:A:147:LYS:CB	2.98	0.47
2:G:83:TYR:HB3	2:G:90:ILE:HD12	1.96	0.46
4:E:18:ALA:O	4:E:21:ILE:N	2.48	0.46
4:E:157:TYR:N	4:E:157:TYR:CD1	2.83	0.46
3:B:112:TYR:HB2	3:B:115:HIS:CE1	2.50	0.46
1:D:81:ALA:O	1:D:82:ASP:C	2.58	0.46
3:B:76:PHE:CD2	3:B:109:ILE:HG13	2.50	0.46
2:G:62:PHE:HB3	2:G:65:ILE:HD12	1.97	0.46
4:A:84:ILE:HD12	4:A:123:ARG:HA	1.98	0.46
2:G:35:HIS:NE2	2:G:81:VAL:HG11	2.31	0.46
2:C:96:ALA:HB3	2:C:99:ILE:HD13	1.98	0.46
4:A:98:GLU:HA	4:A:101:LYS:HE2	1.98	0.46
2:G:35:HIS:CD2	2:G:81:VAL:HG11	2.52	0.45
3:F:129:LEU:HG	3:F:154:PRO:HB3	1.98	0.45
3:F:84:VAL:HG22	3:F:128:LEU:CD1	2.46	0.45
1:D:4:PHE:CD1	1:D:69:PRO:HD3	2.51	0.45
3:B:128:LEU:HD23	3:B:153:LEU:HA	1.99	0.45
2:G:83:TYR:CD1	2:G:90:ILE:HD12	2.51	0.45
3:F:109:ILE:C	3:F:109:ILE:HD12	2.42	0.45
4:E:89:SER:OG	4:E:90:PHE:N	2.49	0.45
4:E:27:HIS:O	4:E:27:HIS:CG	2.67	0.45
1:D:50:LEU:HG	1:D:51:LEU:H	1.81	0.45
4:E:79:LEU:HG	4:E:159:LEU:HD22	2.00	0.44
4:E:110:PRO:HB3	4:E:163:ILE:HG12	1.99	0.44
2:C:99:ILE:HG22	2:C:99:ILE:O	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:102:PRO:HB2	3:B:105:THR:CG2	2.47	0.44
3:F:135:LEU:HD11	3:F:201:LEU:HD13	1.99	0.44
2:C:25:ASP:CG	2:C:67:SER:HG	2.26	0.44
4:E:91:GLU:O	4:E:91:GLU:HG2	2.17	0.44
1:D:11:LYS:O	2:C:28:GLU:N	2.47	0.44
1:D:101:ASP:C	1:D:103:MET:N	2.74	0.44
4:A:127:THR:HG23	4:A:141:PHE:HE2	1.83	0.44
4:A:144:THR:HA	4:A:150:GLN:O	2.18	0.44
2:G:44:ALA:C	2:G:46:LEU:N	2.76	0.44
2:C:84:THR:HG23	3:B:155:VAL:HG11	2.00	0.44
1:H:51:LEU:HD22	1:H:60:CYS:SG	2.58	0.44
2:G:31:VAL:HG11	2:G:74:CYS:SG	2.58	0.44
2:G:44:ALA:C	2:G:46:LEU:H	2.26	0.44
3:B:175:TYR:HE2	3:B:191:HIS:HE1	1.66	0.44
3:B:200:ARG:O	3:B:204:GLU:HG3	2.17	0.44
2:G:20:LYS:HD2	2:G:28:GLU:HB3	2.00	0.43
3:F:203:GLN:HG2	3:F:204:GLU:N	2.33	0.43
1:D:22:SER:O	1:D:57:LEU:HG	2.18	0.43
2:C:99:ILE:N	2:C:99:ILE:HD12	2.33	0.43
3:B:171:LYS:HB2	3:B:174:ASN:HD22	1.83	0.43
3:B:184:LEU:HD23	3:B:184:LEU:HA	1.81	0.43
2:G:98:GLU:N	2:G:98:GLU:CD	2.76	0.43
1:H:94:SER:O	2:G:68:HIS:ND1	2.52	0.43
1:D:50:LEU:HG	1:D:51:LEU:N	2.34	0.43
3:B:74:VAL:HG12	3:B:75:ILE:N	2.33	0.43
1:D:37:ARG:HG2	1:D:79:PHE:CE1	2.54	0.43
3:B:90:ASN:HD21	3:B:94:GLU:CG	2.32	0.43
3:F:130:VAL:HG21	3:F:136:PHE:HB2	2.02	0.42
4:A:126:ASP:O	4:A:129:GLN:HG2	2.19	0.42
4:A:8:VAL:HG22	4:A:79:LEU:HD13	2.01	0.42
4:E:20:THR:O	4:E:24:ILE:HG12	2.18	0.42
1:D:37:ARG:HG2	1:D:79:PHE:CD1	2.54	0.42
3:B:170:VAL:HG11	3:B:178:LEU:HD11	2.00	0.42
4:A:142:ILE:HG13	4:A:155:ALA:HA	2.02	0.42
3:B:120:ARG:NH2	3:B:197:ASP:OD2	2.49	0.42
4:E:21:ILE:O	4:E:25:GLN:N	2.44	0.42
1:D:24:VAL:HG12	1:D:28:LYS:HE3	2.02	0.42
1:D:102:VAL:HG13	3:B:174:ASN:CB	2.49	0.42
3:B:96:GLN:HA	3:B:97:PRO:HD2	1.81	0.42
4:A:11:ALA:O	4:A:14:VAL:HG22	2.20	0.42
4:E:67:MET:HE2	4:E:67:MET:HB3	1.89	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:164:ARG:O	4:E:165:LYS:C	2.63	0.41
2:G:21:LEU:HD12	2:G:21:LEU:N	2.35	0.41
4:A:55:ILE:O	4:A:55:ILE:HG22	2.20	0.41
4:E:111:MET:HG2	4:E:112:VAL:N	2.35	0.41
1:D:94:SER:HB2	2:C:68:HIS:ND1	2.35	0.41
4:A:9:VAL:HG21	4:A:100:ILE:HD11	2.01	0.41
4:A:30:ASP:OD1	4:A:30:ASP:N	2.53	0.41
4:A:96:TYR:CE1	6:A:202:X4R:C18	3.04	0.41
4:E:6:LEU:HD12	4:E:6:LEU:N	2.36	0.41
1:D:28:LYS:HE2	1:D:44:LEU:HB2	2.01	0.41
4:A:14:VAL:HG21	4:A:81:VAL:HG23	2.03	0.41
4:A:93:ILE:HD13	4:A:93:ILE:HA	1.80	0.41
2:C:24:SER:OG	2:C:25:ASP:N	2.53	0.41
2:C:42:ILE:O	2:C:42:ILE:CG2	2.69	0.41
4:A:41:ARG:HG3	4:A:54:ASP:HA	2.02	0.41
2:C:81:VAL:O	2:C:81:VAL:HG12	2.20	0.41
3:F:196:LYS:NZ	3:F:197:ASP:OD1	2.50	0.41
4:E:141:PHE:HD1	4:E:143:GLU:H	1.69	0.41
4:A:19:LEU:CD2	4:A:114:VAL:HG11	2.47	0.41
4:A:83:ALA:HB3	4:A:86:ASN:HD22	1.86	0.41
4:E:58:THR:CG2	4:E:72:MET:HE1	2.44	0.41
1:D:67:ALA:HB2	1:D:73:ALA:HB2	2.03	0.41
1:D:101:ASP:OD1	1:D:101:ASP:N	2.54	0.41
1:D:5:LEU:HD22	1:D:75:VAL:CG2	2.50	0.40
3:B:63:LEU:HD12	3:B:202:THR:OG1	2.21	0.40
1:H:19:LYS:HE3	1:H:19:LYS:HB2	1.89	0.40
2:G:22:ILE:HG12	2:G:28:GLU:HG2	2.03	0.40
1:D:41:GLU:O	1:D:85:PHE:HE1	2.04	0.40
3:B:68:SER:C	3:B:70:GLU:N	2.79	0.40
4:A:116:ASN:CG	4:A:117:LYS:H	2.29	0.40
2:G:101:LEU:HD23	2:G:101:LEU:HA	1.94	0.40
4:E:84:ILE:HG21	4:E:123:ARG:NH1	2.36	0.40
4:E:89:SER:C	4:E:91:GLU:N	2.80	0.40
4:A:95:HIS:O	4:A:99:GLN:HG2	2.21	0.40
1:D:23:THR:O	1:D:26:GLU:HB2	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	99/104 (95%)	94 (95%)	5 (5%)	0	100	100
1	H	102/104 (98%)	95 (93%)	7 (7%)	0	100	100
2	C	82/97 (84%)	78 (95%)	4 (5%)	0	100	100
2	G	82/97 (84%)	79 (96%)	3 (4%)	0	100	100
3	B	144/162 (89%)	140 (97%)	4 (3%)	0	100	100
3	F	142/162 (88%)	138 (97%)	4 (3%)	0	100	100
4	A	161/170 (95%)	150 (93%)	10 (6%)	1 (1%)	21	23
4	E	147/170 (86%)	134 (91%)	13 (9%)	0	100	100
All	All	959/1066 (90%)	908 (95%)	50 (5%)	1 (0%)	48	57

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	A	121	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	D	86/92 (94%)	75 (87%)	11 (13%)	4	4
1	H	91/92 (99%)	87 (96%)	4 (4%)	25	34
2	C	74/86 (86%)	65 (88%)	9 (12%)	5	4
2	G	77/86 (90%)	74 (96%)	3 (4%)	28	39

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	B	136/148 (92%)	129 (95%)	7 (5%)	21	27
3	F	132/148 (89%)	122 (92%)	10 (8%)	12	14
4	A	135/150 (90%)	117 (87%)	18 (13%)	4	3
4	E	115/150 (77%)	106 (92%)	9 (8%)	11	13
All	All	846/952 (89%)	775 (92%)	71 (8%)	10	11

All (71) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	2	ASP
1	H	65	GLN
1	H	95	SER
1	H	102	VAL
2	G	87	SER
2	G	99	ILE
2	G	110	LEU
3	F	66	VAL
3	F	101	LEU
3	F	116	LEU
3	F	130	VAL
3	F	133	THR
3	F	139	SER
3	F	173	GLU
3	F	180	ILE
3	F	181	VAL
3	F	188	LEU
4	E	44	VAL
4	E	46	ILE
4	E	52	LEU
4	E	55	ILE
4	E	85	ASN
4	E	87	THR
4	E	94	HIS
4	E	127	THR
4	E	166	HIS
1	D	7	ILE
1	D	12	THR
1	D	14	ILE
1	D	20	GLU
1	D	23	THR
1	D	32	GLU

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Mol	Chain	Res	Type
1	D	41	GLU
1	D	50	LEU
1	D	55	LYS
1	D	75	VAL
1	D	101	ASP
2	C	17	MET
2	C	34	GLU
2	C	58	ASN
2	C	61	ASN
2	C	85	ASN
2	C	90	ILE
2	C	92	GLU
2	C	98	GLU
2	C	102	GLU
3	B	62	VAL
3	B	66	VAL
3	B	80	SER
3	B	107	ARG
3	B	139	SER
3	B	165	VAL
3	B	180	ILE
4	A	21	ILE
4	A	31	GLU
4	A	46	ILE
4	A	47	ASP
4	A	50	THR
4	A	51	CYS
4	A	55	ILE
4	A	70	GLN
4	A	73	ARG
4	A	84	ILE
4	A	86	ASN
4	A	93	ILE
4	A	106	SER
4	A	117	LYS
4	A	124	THR
4	A	125	VAL
4	A	126	ASP
4	A	160	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
2	G	35	HIS
2	G	108	ASN
3	F	67	ASN
3	F	141	ASN
3	F	195	GLN
1	D	10	HIS
3	B	110	HIS
4	A	22	GLN
4	A	86	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 for Mogul analysis.

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	$\# Z > 2$
6	X4R	E	202	-	74,76,76	1.92	15 (20%)	94,111,111	1.07	7 (7%)
6	X4R	A	202	-	74,76,76	2.04	10 (13%)	94,111,111	1.32	9 (9%)
5	GDP	A	201	7	29,30,30	0.53	0	45,47,47	0.55	0
5	GDP	E	201	-	29,30,30	0.53	0	45,47,47	0.46	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
6	X4R	E	202	-	-	3/50/94/94	0/8/8/8
6	X4R	A	202	-	-	5/50/94/94	0/8/8/8
5	GDP	A	201	7	-	0/16/32/32	0/3/3/3
5	GDP	E	201	-	-	1/16/32/32	0/3/3/3

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	202	X4R	C31-N1	-10.81	1.35	1.46
6	E	202	X4R	C31-N1	-7.44	1.38	1.46
6	E	202	X4R	C5-C7	-6.26	1.40	1.52
6	A	202	X4R	C64-S65	-5.33	1.60	1.73
6	E	202	X4R	C29-N26	-5.04	1.36	1.47
6	E	202	X4R	C5-C15	-4.73	1.42	1.51
6	A	202	X4R	C29-N26	-4.18	1.38	1.47
6	A	202	X4R	C66-S65	-4.10	1.65	1.72
6	A	202	X4R	C11-N13	-3.93	1.07	1.14
6	E	202	X4R	C64-S65	-3.88	1.63	1.73
6	A	202	X4R	C66-N67	-3.66	1.21	1.30
6	A	202	X4R	C5-C15	-3.53	1.44	1.51
6	E	202	X4R	C9-N12	-3.27	1.29	1.35
6	E	202	X4R	C8-C9	-3.11	1.35	1.39
6	E	202	X4R	C6-S10	-3.08	1.67	1.74
6	A	202	X4R	C11-C8	-2.86	1.37	1.43
6	E	202	X4R	C11-N13	-2.61	1.10	1.14
6	A	202	X4R	C9-S10	-2.38	1.69	1.73
6	A	202	X4R	C60-C61	-2.37	1.35	1.39
6	E	202	X4R	O16-N17	-2.26	1.38	1.42
6	E	202	X4R	C9-S10	-2.24	1.69	1.73
6	E	202	X4R	C52-N48	-2.13	1.44	1.47
6	E	202	X4R	C31-C29	-2.09	1.48	1.52
6	E	202	X4R	C3-C2	-2.06	1.45	1.52
6	E	202	X4R	O55-C54	-2.05	1.19	1.23

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	202	X4R	C50-C49-C54	-5.06	101.66	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	202	X4R	C4-C5-C15	-3.70	100.26	107.75
6	A	202	X4R	C66-S65-C64	3.54	90.82	88.96
6	A	202	X4R	C30-C28-C27	3.45	122.06	113.99
6	A	202	X4R	C58-C57-N56	3.41	120.26	113.07
6	A	202	X4R	C51-C50-C49	2.86	107.09	103.75
6	E	202	X4R	C14-C5-C7	-2.85	100.56	108.96
6	E	202	X4R	C43-C40-C41	2.68	116.80	113.23
6	A	202	X4R	O16-C15-N19	-2.67	113.53	115.25
6	A	202	X4R	C54-C49-N48	2.60	119.58	112.50
6	E	202	X4R	C44-C43-C40	2.25	114.33	109.71
6	A	202	X4R	O53-C51-C52	2.21	114.83	110.33
6	E	202	X4R	C58-C57-N56	2.20	117.70	113.07
6	E	202	X4R	C66-N67-C68	-2.12	108.33	110.71
6	E	202	X4R	C4-C5-C15	2.11	112.03	107.75
6	E	202	X4R	C20-C18-N17	-2.06	120.19	123.21

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	202	X4R	C58-C57-N56-C54
6	E	202	X4R	C36-C37-C38-N39
6	E	202	X4R	C36-C37-C38-O42
6	A	202	X4R	C36-C37-C38-O42
6	A	202	X4R	C36-C37-C38-N39
5	E	201	GDP	O4'-C4'-C5'-O5'
6	A	202	X4R	C33-C34-C35-C36
6	E	202	X4R	N19-C15-C5-C4
6	A	202	X4R	C49-C54-N56-C57

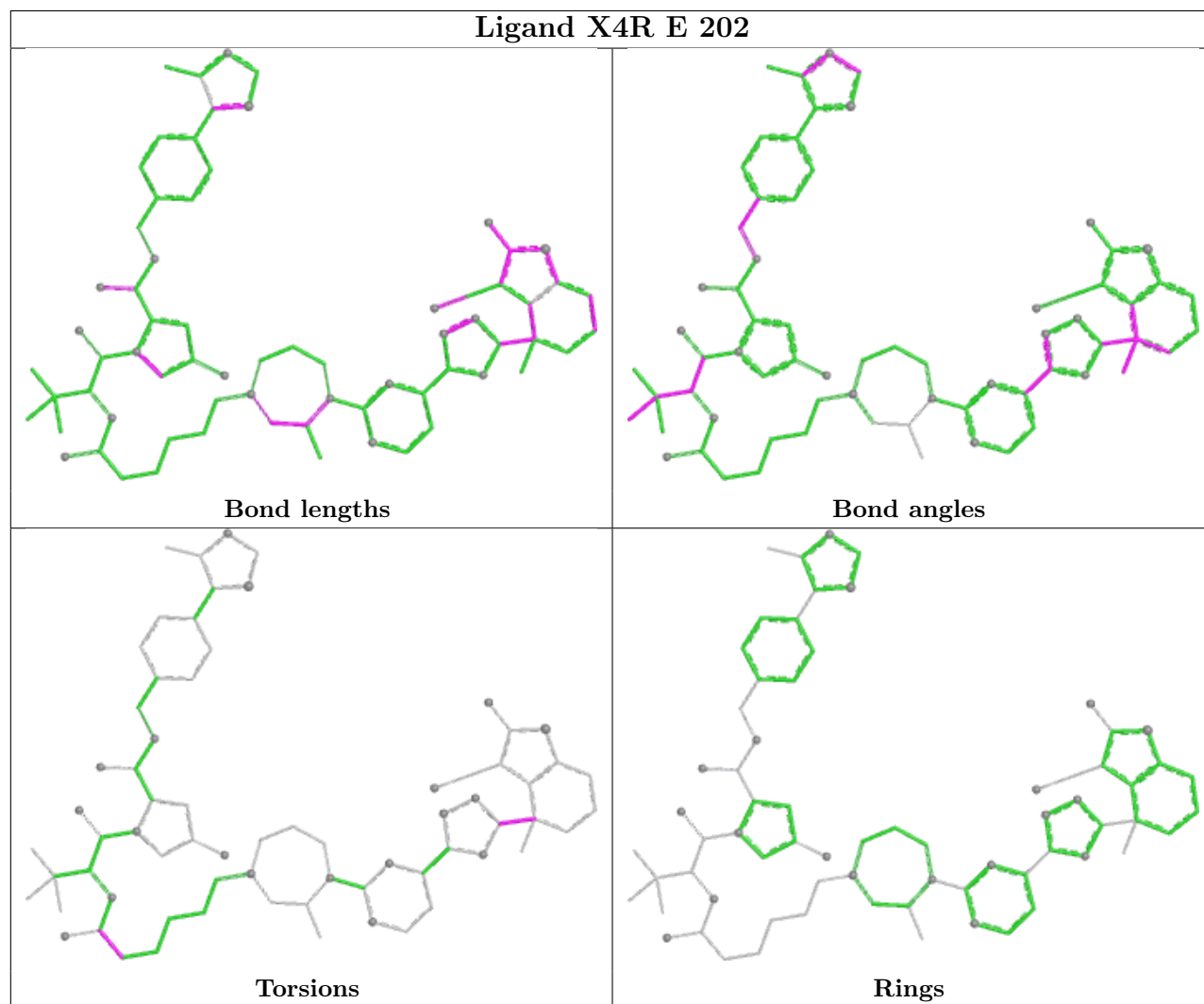
There are no ring outliers.

2 monomers are involved in 5 short contacts:

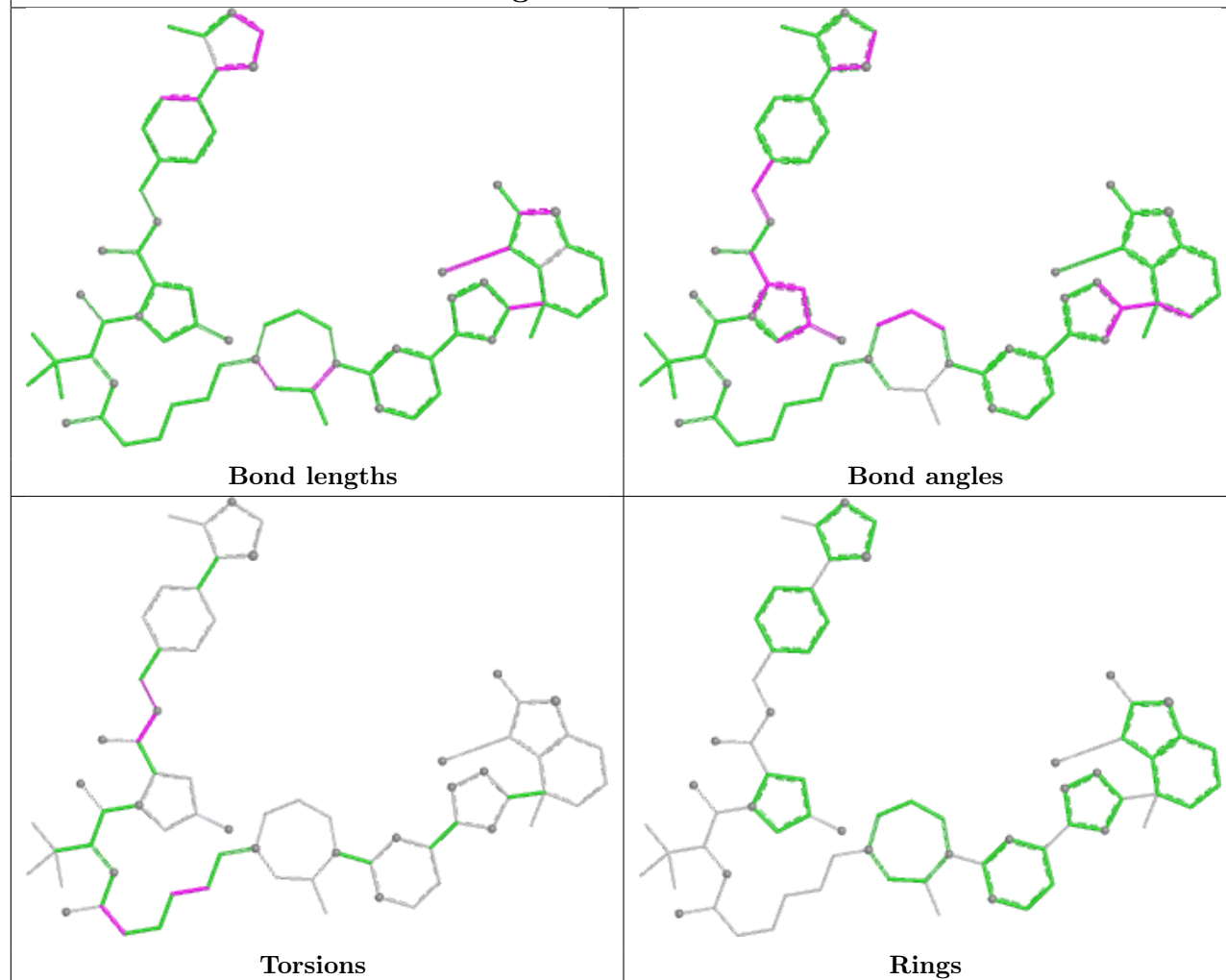
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	E	202	X4R	3	0
6	A	202	X4R	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.

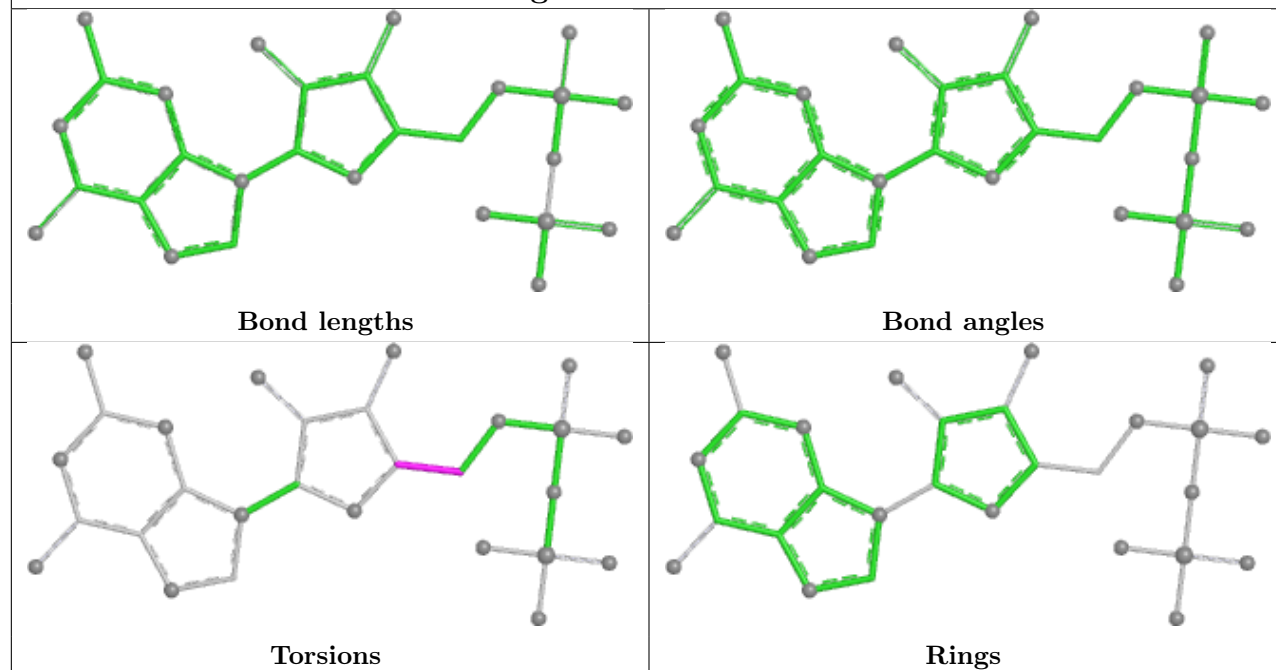
Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



Ligand X4R A 202



Ligand GDP E 201



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	D	103/104 (99%)	1.98	48 (46%) 0 0	37, 74, 90, 94	0
1	H	104/104 (100%)	0.71	6 (5%) 29 25	22, 40, 55, 66	0
2	C	86/97 (88%)	1.17	16 (18%) 3 2	25, 49, 72, 85	0
2	G	86/97 (88%)	0.59	7 (8%) 18 15	18, 33, 56, 77	0
3	B	146/162 (90%)	0.59	9 (6%) 26 23	15, 28, 52, 84	0
3	F	144/162 (88%)	0.55	9 (6%) 26 23	16, 29, 51, 81	0
4	A	163/170 (95%)	1.65	54 (33%) 1 0	22, 60, 82, 86	0
4	E	155/170 (91%)	2.38	88 (56%) 0 0	29, 72, 91, 98	0
All	All	987/1066 (92%)	1.25	237 (24%) 2 1	15, 46, 86, 98	0

All (237) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	E	86	ASN	5.9
4	E	124	THR	5.7
4	E	14	VAL	5.5
4	A	34	PRO	5.3
1	D	54	GLY	5.3
4	E	84	ILE	5.2
4	E	125	VAL	5.1
4	E	130	ALA	5.0
4	A	52	LEU	4.9
4	E	154	ASP	4.8
4	E	148	THR	4.8
1	D	76	GLY	4.6
4	E	40	TYR	4.6
4	E	155	ALA	4.5
4	A	32	TYR	4.4
4	E	94	HIS	4.4

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Mol	Chain	Res	Type	RSRZ
4	E	50	THR	4.4
4	A	39	SER	4.4
4	E	28	PHE	4.4
4	E	87	THR	4.3
4	E	121	PRO	4.3
4	E	122	SER	4.3
4	E	4	TYR	4.2
4	E	134	ALA	4.2
4	E	46	ILE	4.2
1	D	79	PHE	4.1
4	E	24	ILE	4.1
4	E	51	CYS	4.1
1	D	27	LEU	4.0
4	A	158	THR	4.0
4	E	158	THR	4.0
4	E	8	VAL	4.0
4	E	43	GLN	4.0
4	E	44	VAL	3.9
1	D	84	THR	3.9
4	E	20	THR	3.9
4	A	14	VAL	3.9
4	E	52	LEU	3.9
1	D	21	SER	3.8
4	A	87	THR	3.8
4	E	142	ILE	3.8
2	C	64	GLU	3.7
4	A	51	CYS	3.7
4	E	83	ALA	3.7
1	D	44	LEU	3.7
4	E	10	GLY	3.6
1	D	77	LEU	3.6
4	A	4	TYR	3.6
2	C	62	PHE	3.6
4	E	141	PHE	3.6
1	H	81	ALA	3.6
1	D	78	ALA	3.6
2	G	88	THR	3.5
1	D	90	ILE	3.5
1	D	75	VAL	3.5
4	E	123	ARG	3.5
4	E	157	TYR	3.5
4	A	46	ILE	3.5

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Mol	Chain	Res	Type	RSRZ
4	E	32	TYR	3.5
3	F	140	LEU	3.5
4	E	30	ASP	3.5
4	E	12	VAL	3.4
3	B	60	ARG	3.4
4	A	157	TYR	3.4
4	E	26	ASN	3.3
4	E	132	ASP	3.3
1	D	35	LEU	3.3
4	E	23	LEU	3.3
4	E	21	ILE	3.3
4	A	44	VAL	3.3
4	A	79	LEU	3.3
4	E	127	THR	3.3
4	A	120	LEU	3.2
4	A	50	THR	3.2
1	H	52	ASP	3.2
4	E	6	LEU	3.2
4	A	12	VAL	3.2
4	E	91	GLU	3.2
4	E	116	ASN	3.2
4	E	107	GLU	3.1
4	E	160	VAL	3.1
4	E	161	ARG	3.1
4	E	36	ILE	3.1
4	E	117	LYS	3.1
4	E	55	ILE	3.1
1	D	89	CYS	3.1
2	C	22	ILE	3.0
4	E	131	GLN	3.0
1	D	58	GLY	3.0
4	A	45	VAL	3.0
4	E	3	GLU	3.0
3	F	139	SER	3.0
4	A	121	PRO	3.0
3	B	178	LEU	3.0
4	E	29	VAL	3.0
2	C	87	SER	3.0
4	A	136	SER	3.0
1	H	82	ASP	3.0
1	D	12	THR	3.0
4	A	53	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
4	E	45	VAL	2.9
1	D	8	ARG	2.9
1	D	102	VAL	2.9
4	E	93	ILE	2.9
4	E	143	GLU	2.9
4	E	85	ASN	2.9
4	A	26	ASN	2.9
1	D	39	PRO	2.9
1	D	62	PHE	2.9
1	D	61	GLY	2.9
2	C	58	ASN	2.9
1	D	81	ALA	2.9
2	C	36	ALA	2.9
4	E	156	PHE	2.9
1	D	59	GLU	2.9
1	D	5	LEU	2.8
3	F	108	ARG	2.8
4	E	13	GLY	2.8
1	D	25	PHE	2.8
4	E	126	ASP	2.8
4	A	23	LEU	2.8
1	D	56	THR	2.8
4	A	124	THR	2.8
4	A	148	THR	2.8
4	A	38	ASP	2.8
1	H	79	PHE	2.8
4	E	61	GLN	2.7
4	A	35	THR	2.7
4	A	19	LEU	2.7
4	E	81	VAL	2.7
2	C	61	ASN	2.7
1	D	31	VAL	2.7
4	A	85	ASN	2.7
4	A	112	VAL	2.6
4	E	15	GLY	2.6
1	D	95	SER	2.6
2	G	64	GLU	2.6
1	D	82	ASP	2.6
4	E	144	THR	2.6
3	B	61	PRO	2.6
4	E	146	ALA	2.6
4	A	73	ARG	2.6

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Mol	Chain	Res	Type	RSRZ
3	F	143	ASP	2.6
1	D	38	PRO	2.6
4	A	40	TYR	2.6
4	A	160	VAL	2.6
2	C	24	SER	2.6
4	A	24	ILE	2.6
1	D	30	ILE	2.6
4	E	139	ILE	2.6
4	A	41	ARG	2.5
4	E	90	PHE	2.5
4	E	38	ASP	2.5
4	E	133	LEU	2.5
1	D	53	ASP	2.5
3	F	61	PRO	2.5
3	F	203	GLN	2.5
4	A	48	GLY	2.5
1	D	94	SER	2.4
3	B	139	SER	2.4
4	A	28	PHE	2.4
4	E	108	ASP	2.4
1	D	80	ARG	2.4
3	B	173	GLU	2.4
1	D	64	SER	2.4
4	E	137	TYR	2.4
4	A	21	ILE	2.4
1	D	51	LEU	2.4
3	F	185	TYR	2.4
4	E	57	ASP	2.4
4	A	107	GLU	2.4
4	E	11	ALA	2.4
4	A	155	ALA	2.4
2	C	88	THR	2.4
4	E	118	SER	2.4
1	H	7	ILE	2.4
4	A	15	GLY	2.3
3	B	62	VAL	2.3
1	D	23	THR	2.3
4	A	139	ILE	2.3
1	D	3	VAL	2.3
2	C	60	VAL	2.3
1	D	52	ASP	2.3
4	A	57	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
4	E	48	GLY	2.3
1	D	37	ARG	2.3
4	E	136	SER	2.3
4	A	70	GLN	2.3
3	F	180	ILE	2.3
4	A	29	VAL	2.3
4	A	125	VAL	2.3
2	G	44	ALA	2.3
4	E	22	GLN	2.2
4	E	39	SER	2.2
3	B	138	PRO	2.2
1	D	22	SER	2.2
4	E	42	LYS	2.2
4	A	27	HIS	2.2
2	G	41	THR	2.2
2	G	47	SER	2.2
4	E	145	SER	2.2
1	D	68	ARG	2.2
2	C	46	LEU	2.2
4	E	159	LEU	2.2
4	A	149	ARG	2.2
2	C	34	GLU	2.2
1	D	66	THR	2.2
4	E	18	ALA	2.2
4	E	111	MET	2.1
1	D	10	HIS	2.1
4	E	77	GLY	2.1
4	A	122	SER	2.1
2	C	59	GLU	2.1
4	E	110	PRO	2.1
1	D	60	CYS	2.1
2	C	78	THR	2.1
4	E	19	LEU	2.1
1	D	24	VAL	2.1
4	A	156	PHE	2.1
4	A	11	ALA	2.1
4	A	130	ALA	2.1
1	H	1	MET	2.1
3	F	204	GLU	2.1
1	D	88	LEU	2.1
2	G	108	ASN	2.1
4	A	165	LYS	2.0

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Mol	Chain	Res	Type	RSRZ
4	E	89	SER	2.0
1	D	47	ASP	2.0
1	D	92	PRO	2.0
2	C	18	TYR	2.0
4	A	71	TYR	2.0
2	C	19	VAL	2.0
4	E	115	GLY	2.0
3	B	122	ALA	2.0
2	G	110	LEU	2.0
3	B	108	ARG	2.0
4	A	42	LYS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

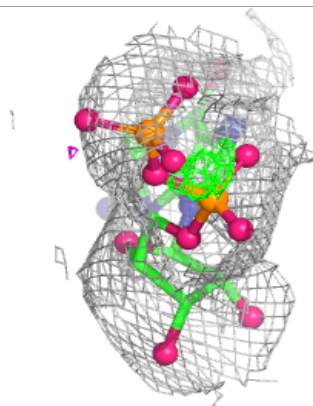
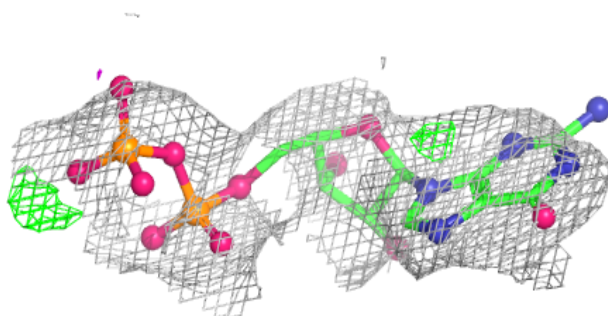
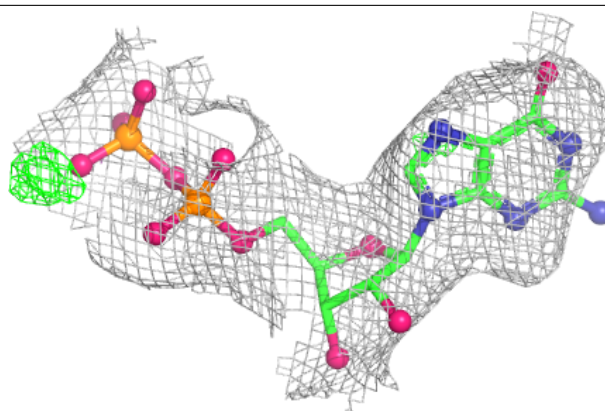
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	MG	A	203	1/1	0.69	0.34	62,62,62,62	0
5	GDP	E	201	28/28	0.83	0.14	52,75,88,91	0
7	MG	E	203	1/1	0.87	0.10	57,57,57,57	0
5	GDP	A	201	28/28	0.88	0.11	47,62,68,70	0
6	X4R	A	202	69/69	0.93	0.10	12,27,47,53	0
6	X4R	E	202	69/69	0.94	0.10	16,30,53,62	0

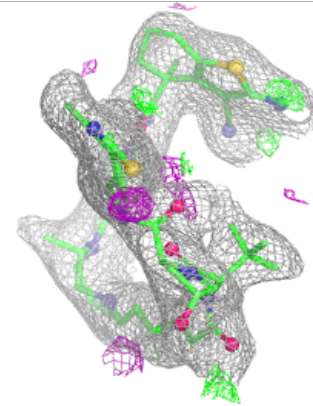
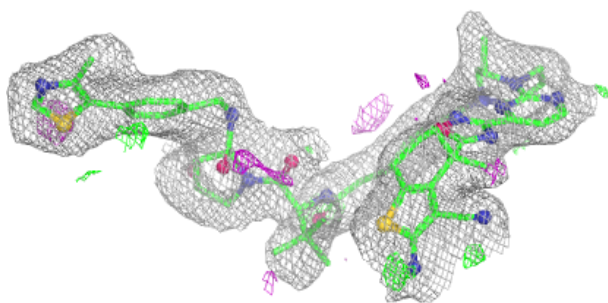
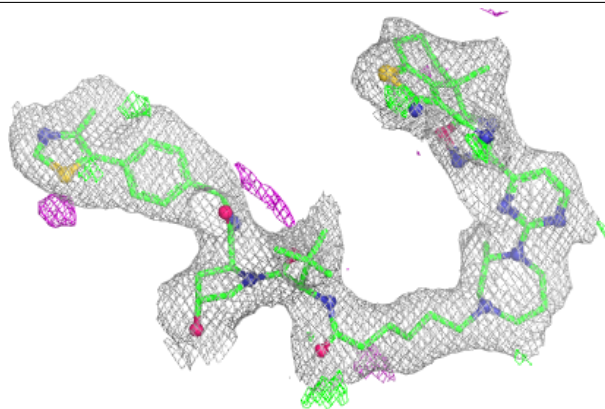
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around GDP E 201:

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

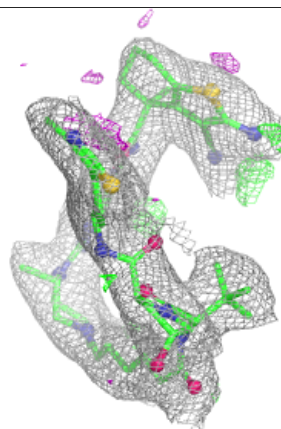
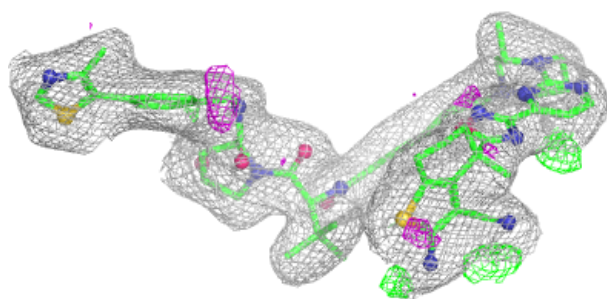
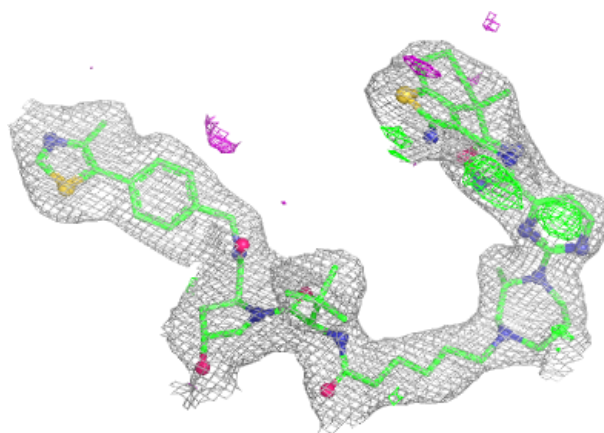
**Electron density around X4R A 202:**

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



Electron density around X4R E 202:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.