



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:01 PM UTC

PDB ID : 3OZJ / pdb_00003ozj
Title : Crystal structure of human retinoic X receptor alpha complexed with bigelovin and coactivator SRC-1
Authors : Zhang, H.; Li, L.; Chen, L.; Hu, L.; Shen, X.
Deposited on : 2010-09-25
Resolution : 2.10 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

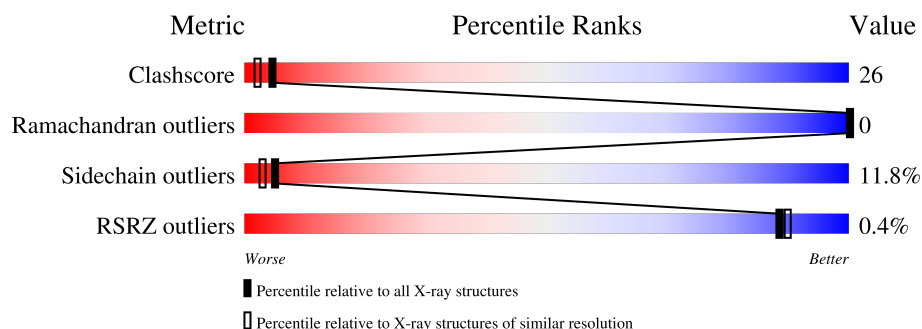
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	238	26% 42% 20% 10%
1	C	238	26% 41% 22% 10%
2	B	11	27% 55% 9% 9%
2	D	11	45% 27% 27%

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
3	BGV	A	1	-	-	X	-
3	BGV	C	1	-	-	X	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 3692 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.

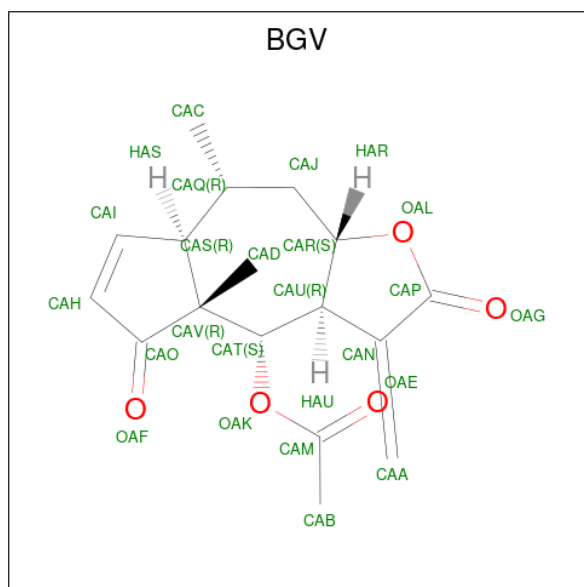
- Molecule 1 is a protein called Retinoic acid receptor RXR-alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	215	Total	C	N	O	S	0	0	0
			1697	1088	291	308	10			
1	C	215	Total	C	N	O	S	6	2	0
			1711	1098	295	308	10			

- Molecule 2 is a protein called SRC-1, peptide of Nuclear receptor coactivator 2.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	10	Total	C	N	O	0	0	0
			89	57	19	13			
2	D	11	Total	C	N	O	0	0	0
			98	63	21	14			

- Molecule 3 is (3aR,4S,4aR,7aR,8R,9aS)-4a,8-dimethyl-3-methylidene-2,5-dioxo-2,3,3a,4,4a,5,7a,8,9,9a-decahydroazuleno[6,5-b]furan-4-yl acetate (CCD ID: BGV) (formula: C₁₇H₂₀O₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			22	17	5		
3	C	1	Total	C	O	0	0
			22	17	5		

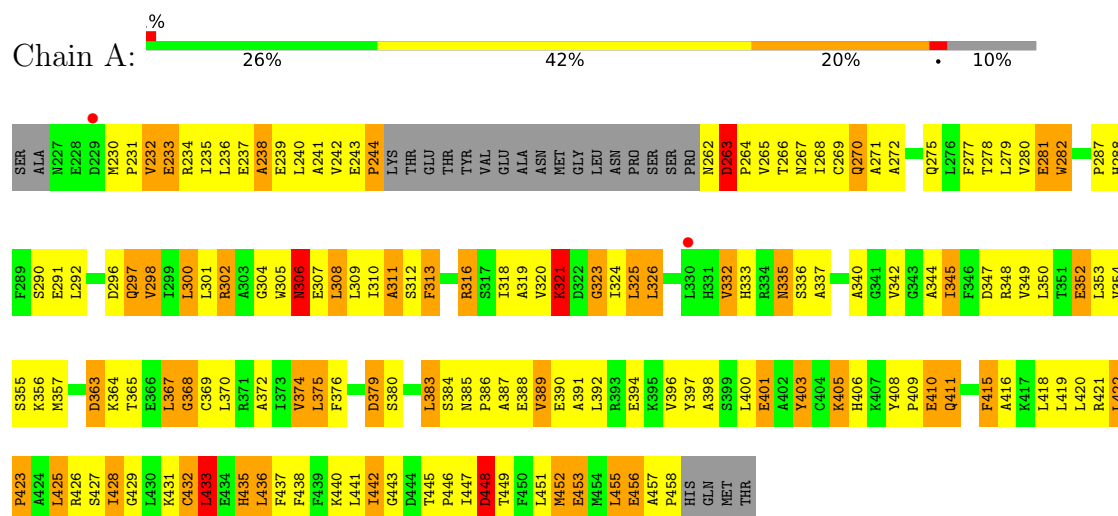
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	26	Total	O	0	0
			26	26		
4	B	1	Total	O	0	0
			1	1		
4	C	25	Total	O	0	0
			25	25		
4	D	1	Total	O	0	0
			1	1		

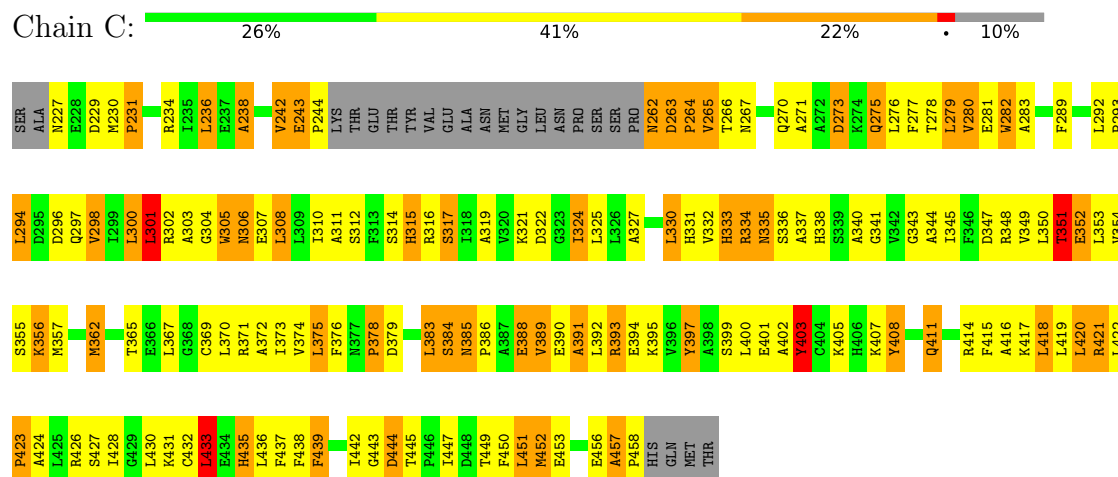
3 Residue-property plots

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: Retinoic acid receptor RXR-alpha



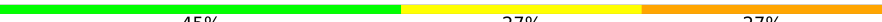
• Molecule 1: Retinoic acid receptor RXR-alpha



• Molecule 2: SRC-1, peptide of Nuclear receptor coactivator 2



- Molecule 2: SRC-1, peptide of Nuclear receptor coactivator 2

Chain D:  45% 27% 27%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	65.40Å 66.59Å 111.73Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.29 – 2.10 33.29 – 2.10	Depositor EDS
% Data completeness (in resolution range)	88.5 (33.29-2.10) 86.7 (33.29-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.08 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, R_{free}	0.245 , (Not available) 0.239 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	24.1	Xtriage
Anisotropy	0.078	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 43.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	0.080 for k,h,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	3692	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.47% 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: BGV

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	2.42	84/1731 (4.9%)	1.72	44/2342 (1.9%)
1	C	2.45	101/1753 (5.8%)	1.67	35/2372 (1.5%)
2	B	2.02	4/90 (4.4%)	1.51	1/119 (0.8%)
2	D	1.93	2/99 (2.0%)	1.72	3/130 (2.3%)
All	All	2.41	191/3673 (5.2%)	1.69	83/4963 (1.7%)

All (191) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	338[A]	HIS	N-CA	-10.54	1.33	1.46
1	C	338[B]	HIS	N-CA	-10.54	1.33	1.46
1	A	422	LEU	C-O	-8.84	1.16	1.24
1	A	323	GLY	C-O	-8.77	1.15	1.23
1	A	432	CYS	C-O	-8.56	1.14	1.24
1	C	428	ILE	C-O	-8.26	1.14	1.24
1	A	302	ARG	C-O	-8.26	1.14	1.24
1	C	279	LEU	C-O	-8.04	1.14	1.24
1	A	425	LEU	C-O	-7.86	1.15	1.24
1	A	389	VAL	C-O	-7.85	1.15	1.24
1	A	313	PHE	C-O	-7.84	1.15	1.24
1	C	282	TRP	C-O	-7.79	1.15	1.24
1	A	308	LEU	C-O	-7.73	1.15	1.24
1	A	349	VAL	C-O	-7.59	1.15	1.24
1	C	451	LEU	C-O	-7.56	1.15	1.24
1	C	263	ASP	C-O	-7.28	1.18	1.24
1	A	336	SER	C-O	-7.27	1.15	1.24
1	A	306	ASN	C-O	-7.25	1.15	1.24
1	C	283	ALA	CA-CB	-7.23	1.41	1.53
1	C	334	ARG	C-O	-7.22	1.15	1.24
1	C	452	MET	C-O	-7.01	1.15	1.24
1	A	309	LEU	C-O	-6.99	1.16	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	415	PHE	C-O	-6.96	1.16	1.24
1	C	370	LEU	C-O	-6.95	1.15	1.24
1	C	372	ALA	CA-CB	-6.89	1.42	1.53
1	C	385	ASN	C-O	-6.86	1.18	1.24
1	C	340	ALA	C-O	-6.85	1.14	1.24
1	C	311	ALA	CA-CB	-6.84	1.42	1.53
1	C	350	LEU	C-O	-6.84	1.16	1.24
1	C	426	ARG	C-O	-6.69	1.16	1.24
1	A	230	MET	C-O	-6.68	1.19	1.25
1	C	292	LEU	C-O	-6.68	1.15	1.24
1	C	405	LYS	C-O	-6.67	1.16	1.24
1	A	271	ALA	C-O	-6.52	1.16	1.24
1	A	271	ALA	CA-C	-6.51	1.44	1.52
1	C	335	ASN	C-O	-6.50	1.16	1.24
1	A	401	GLU	C-O	-6.50	1.16	1.24
1	A	429	GLY	C-O	-6.45	1.16	1.23
1	C	331[A]	HIS	CA-C	-6.43	1.44	1.52
1	C	331[B]	HIS	CA-C	-6.43	1.44	1.52
1	A	318	ILE	CA-CB	6.42	1.62	1.54
1	C	281	GLU	C-O	-6.40	1.16	1.24
1	C	453	GLU	C-O	-6.31	1.16	1.24
1	A	324	ILE	C-O	-6.31	1.15	1.23
1	C	375	LEU	C-O	-6.29	1.16	1.24
1	C	319	ALA	C-O	-6.28	1.16	1.24
1	C	294	LEU	C-O	-6.28	1.16	1.24
1	A	436	LEU	C-O	-6.25	1.16	1.24
1	C	343	GLY	C-O	-6.23	1.15	1.23
1	A	298	VAL	C-O	-6.20	1.17	1.24
2	B	6	HIS	C-O	-6.20	1.17	1.24
1	C	238	ALA	C-O	-6.20	1.16	1.24
1	C	423	PRO	C-O	-6.19	1.16	1.24
1	A	374	VAL	C-O	-6.18	1.17	1.24
1	A	241	ALA	CA-CB	-6.17	1.43	1.53
1	C	264	PRO	CA-C	-6.16	1.43	1.52
1	C	341	GLY	C-O	-6.16	1.16	1.24
1	A	354	VAL	C-O	-6.16	1.17	1.24
1	C	354	VAL	C-O	-6.16	1.17	1.24
1	A	232	VAL	C-O	-6.15	1.16	1.24
1	C	437	PHE	C-O	-6.14	1.17	1.24
1	C	379	ASP	CA-C	-6.14	1.44	1.52
1	C	273	ASP	C-O	-6.06	1.17	1.24
1	C	388	GLU	C-O	-6.04	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	411	GLN	C-O	-6.01	1.17	1.24
1	A	428	ILE	C-O	-6.00	1.17	1.24
1	A	431	LYS	C-O	-6.00	1.17	1.24
1	A	435	HIS	C-O	-6.00	1.17	1.24
1	C	340	ALA	CA-CB	-5.99	1.44	1.53
1	A	270	GLN	C-O	-5.97	1.17	1.24
1	A	423	PRO	C-O	-5.96	1.16	1.24
1	A	440	LYS	C-O	-5.93	1.17	1.24
2	D	3	LYS	C-O	-5.92	1.17	1.24
1	A	271	ALA	CA-CB	-5.92	1.44	1.53
1	C	306	ASN	C-O	-5.91	1.17	1.24
1	C	419	LEU	C-O	-5.90	1.16	1.24
1	C	344	ALA	CA-CB	-5.90	1.44	1.53
1	A	340	ALA	C-O	-5.89	1.16	1.24
1	C	315	HIS	C-O	-5.88	1.16	1.24
1	A	345	ILE	C-O	-5.88	1.17	1.24
1	A	337	ALA	C-O	-5.85	1.17	1.24
1	A	357	MET	C-O	-5.84	1.17	1.24
1	A	311	ALA	CA-CB	-5.83	1.43	1.53
1	C	310	ILE	C-O	-5.83	1.17	1.24
1	A	279	LEU	C-O	-5.83	1.17	1.24
1	C	337	ALA	C-O	-5.82	1.17	1.24
1	A	375	LEU	C-O	-5.82	1.17	1.24
1	C	314	SER	C-O	-5.81	1.17	1.24
1	A	238	ALA	CA-CB	-5.80	1.43	1.53
2	D	10	GLN	C-O	-5.77	1.16	1.24
1	C	333	HIS	C-O	-5.75	1.16	1.23
1	C	308	LEU	C-O	-5.75	1.17	1.24
1	C	402	ALA	C-O	-5.74	1.17	1.24
1	A	452	MET	C-O	-5.73	1.17	1.24
1	C	289	PHE	C-O	-5.73	1.17	1.24
1	C	378	PRO	C-O	-5.72	1.17	1.24
1	A	326	LEU	C-O	-5.71	1.16	1.23
1	A	369	CYS	C-O	-5.67	1.17	1.24
1	C	330	LEU	C-O	-5.66	1.16	1.23
1	A	426	ARG	C-O	-5.64	1.17	1.24
1	C	430	LEU	C-O	-5.64	1.17	1.24
1	C	391	ALA	C-O	-5.64	1.17	1.24
1	C	392	LEU	C-O	-5.64	1.17	1.24
1	A	406	HIS	CA-C	-5.62	1.47	1.53
1	C	399	SER	C-O	-5.61	1.17	1.24
1	A	282	TRP	C-O	-5.60	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	437	PHE	C-O	-5.60	1.17	1.24
1	C	362	MET	C-O	-5.58	1.17	1.23
1	A	297	GLN	C-O	-5.57	1.17	1.24
1	C	300	LEU	C-O	-5.56	1.17	1.24
1	C	427	SER	C-O	-5.56	1.17	1.24
1	C	421	ARG	C-O	-5.55	1.16	1.24
1	A	316	ARG	C-O	-5.54	1.17	1.24
1	A	277	PHE	C-O	-5.54	1.17	1.24
1	C	355	SER	C-O	-5.54	1.17	1.24
1	C	388	GLU	N-CA	-5.53	1.39	1.46
2	B	5	LEU	C-O	-5.52	1.17	1.24
1	A	433	LEU	C-O	-5.49	1.17	1.24
1	C	278	THR	C-O	-5.49	1.17	1.24
1	C	374	VAL	C-O	-5.49	1.18	1.24
1	A	332	VAL	C-O	-5.49	1.17	1.24
1	C	311	ALA	C-O	-5.49	1.16	1.24
1	C	433	LEU	C-O	-5.49	1.17	1.24
1	A	319	ALA	C-O	-5.47	1.17	1.24
1	A	416	ALA	CA-CB	-5.46	1.44	1.53
1	C	338[A]	HIS	C-O	-5.46	1.17	1.24
1	C	338[B]	HIS	C-O	-5.46	1.17	1.24
1	C	439	PHE	C-O	-5.46	1.17	1.24
1	A	405	LYS	C-O	-5.42	1.17	1.24
1	A	272	ALA	C-O	-5.42	1.17	1.24
1	A	335	ASN	C-O	-5.40	1.17	1.24
1	C	390	GLU	C-O	-5.39	1.17	1.24
1	C	400	LEU	C-O	-5.38	1.17	1.24
1	C	357	MET	CA-C	-5.37	1.46	1.52
1	C	374	VAL	CA-CB	5.36	1.60	1.54
1	C	351	THR	C-O	-5.36	1.17	1.24
1	C	403	TYR	C-O	-5.35	1.17	1.24
1	C	271	ALA	C-O	-5.34	1.17	1.24
1	A	321	LYS	C-O	-5.33	1.18	1.24
1	C	312	SER	C-O	-5.33	1.18	1.24
1	A	367	LEU	C-O	-5.31	1.18	1.24
1	A	233	GLU	C-O	-5.30	1.18	1.24
1	A	387	ALA	C-O	-5.30	1.17	1.24
1	A	368	GLY	C-O	-5.30	1.17	1.23
1	C	280	VAL	C-O	-5.30	1.18	1.24
1	C	435	HIS	C-O	-5.30	1.18	1.24
1	C	307	GLU	C-O	-5.28	1.18	1.24
1	C	365	THR	N-CA	-5.28	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	379	ASP	C-O	-5.27	1.17	1.24
1	A	307	GLU	C-O	-5.27	1.18	1.24
1	A	347	ASP	C-O	-5.26	1.18	1.24
1	C	303	ALA	CA-CB	-5.26	1.44	1.53
1	A	453	GLU	C-O	-5.25	1.18	1.24
1	C	424	ALA	CA-CB	-5.25	1.44	1.53
1	C	408	TYR	C-O	-5.24	1.18	1.24
1	C	305	TRP	C-O	-5.24	1.18	1.24
1	C	322	ASP	C-O	-5.23	1.18	1.24
1	A	421	ARG	C-O	-5.22	1.17	1.24
1	A	356	LYS	C-O	-5.22	1.18	1.24
1	A	269	CYS	C-O	-5.22	1.17	1.24
1	A	300	LEU	C-O	-5.22	1.18	1.24
1	A	275	GLN	C-O	-5.22	1.17	1.24
1	C	231	PRO	C-O	-5.21	1.17	1.24
1	A	280	VAL	C-O	-5.21	1.18	1.24
1	A	353	LEU	C-O	-5.19	1.17	1.24
1	C	265	VAL	C-O	-5.19	1.18	1.24
1	C	357	MET	C-O	-5.19	1.18	1.24
1	C	420	LEU	C-O	-5.19	1.17	1.24
1	A	398	ALA	C-O	-5.18	1.17	1.23
1	A	394	GLU	C-O	-5.17	1.18	1.24
1	C	298	VAL	C-O	-5.17	1.18	1.24
1	A	305	TRP	C-O	-5.17	1.18	1.24
1	A	408	TYR	C-O	-5.16	1.18	1.24
2	B	3	LYS	C-O	-5.15	1.18	1.24
1	C	317	SER	C-O	-5.15	1.17	1.24
1	A	364	LYS	C-O	-5.12	1.18	1.24
1	C	263	ASP	CA-C	-5.12	1.46	1.52
1	C	327	ALA	C-O	-5.12	1.17	1.24
2	B	8	LEU	C-O	-5.09	1.17	1.24
1	A	321	LYS	N-CA	-5.08	1.40	1.46
1	C	386	PRO	C-O	-5.08	1.17	1.24
1	A	406	HIS	C-O	-5.07	1.18	1.23
1	C	304	GLY	C-O	-5.06	1.17	1.23
1	C	353	LEU	C-O	-5.05	1.17	1.23
1	C	383	LEU	C-O	-5.05	1.17	1.24
1	C	393	ARG	C-O	-5.05	1.18	1.24
1	C	384	SER	C-O	-5.04	1.18	1.24
1	A	427	SER	CA-C	-5.04	1.46	1.52
1	A	312	SER	C-O	-5.02	1.18	1.24
1	C	267	ASN	C-O	-5.02	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	391	ALA	C-O	-5.00	1.18	1.24

All (83) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	408	TYR	CA-C-N	10.16	129.82	119.56
1	C	408	TYR	C-N-CA	10.16	129.82	119.56
1	C	457	ALA	N-CA-C	8.96	122.44	110.08
2	D	2	HIS	N-CA-C	8.18	121.24	111.02
1	C	449	THR	N-CA-C	8.18	120.19	111.28
1	C	308	LEU	N-CA-C	8.13	120.05	111.03
1	C	337	ALA	CA-C-N	8.13	131.83	120.29
1	C	337	ALA	C-N-CA	8.13	131.83	120.29
1	A	301	LEU	N-CA-C	7.76	119.82	111.36
1	A	443	GLY	N-CA-C	7.45	126.03	115.30
1	A	296	ASP	N-CA-C	7.34	119.36	111.36
1	A	263	ASP	N-CA-C	-7.15	99.31	109.24
1	A	336	SER	N-CA-C	-6.89	103.77	111.28
1	A	384	SER	N-CA-C	6.86	118.76	111.28
1	A	344	ALA	N-CA-C	6.84	118.39	111.07
1	C	319	ALA	N-CA-C	6.79	118.47	111.14
1	C	337	ALA	N-CA-C	6.71	118.67	111.36
1	A	307	GLU	N-CA-C	6.62	118.50	111.28
1	A	263	ASP	CA-C-N	6.61	126.55	119.28
1	A	263	ASP	C-N-CA	6.61	126.55	119.28
2	D	3	LYS	N-CA-C	6.61	118.36	111.03
1	A	411	GLN	CA-C-N	6.60	126.04	118.85
1	A	411	GLN	C-N-CA	6.60	126.04	118.85
1	A	324	ILE	N-CA-C	6.57	119.29	109.17
1	C	372	ALA	N-CA-C	6.55	118.50	111.36
1	C	270	GLN	N-CA-C	-6.38	104.32	111.28
1	A	298	VAL	N-CA-C	6.33	116.48	110.53
1	A	306	ASN	CA-C-N	6.28	128.69	120.28
1	A	306	ASN	C-N-CA	6.28	128.69	120.28
1	A	455	LEU	N-CA-C	-6.23	106.36	112.97
1	C	273	ASP	N-CA-C	-6.04	104.60	111.07
1	C	300	LEU	N-CA-C	6.00	117.82	111.28
1	A	350	LEU	N-CA-C	5.88	117.49	111.14
1	A	277	PHE	N-CA-C	5.87	117.48	111.14
1	A	441	LEU	N-CA-C	5.87	117.47	111.14
1	A	272	ALA	N-CA-C	5.86	118.45	111.71
1	C	389	VAL	CB-CA-C	-5.86	104.23	112.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	369	CYS	N-CA-C	5.85	117.74	111.36
2	B	4	ILE	N-CA-C	5.82	116.60	110.72
1	C	301	LEU	N-CA-C	5.78	117.66	111.36
1	A	386	PRO	CA-C-N	5.72	128.41	120.29
1	A	386	PRO	C-N-CA	5.72	128.41	120.29
1	C	243	GLU	N-CA-C	5.72	117.71	109.48
1	C	397	TYR	N-CA-C	5.67	120.33	113.41
1	C	242	VAL	CA-C-N	5.67	128.35	120.65
1	C	242	VAL	C-N-CA	5.67	128.35	120.65
1	A	309	LEU	N-CA-C	5.66	117.26	111.14
2	D	10	GLN	N-CA-C	-5.65	98.77	110.80
1	A	408	TYR	CA-C-N	5.61	125.23	119.56
1	A	408	TYR	C-N-CA	5.61	125.23	119.56
1	A	390	GLU	N-CA-C	-5.61	104.58	111.75
1	C	306	ASN	N-CA-C	5.59	117.18	111.14
1	C	352	GLU	N-CA-C	5.56	117.42	111.36
1	C	379	ASP	N-CA-C	-5.51	106.23	113.17
1	A	426	ARG	CA-C-N	5.50	128.11	120.29
1	A	426	ARG	C-N-CA	5.50	128.11	120.29
1	C	354	VAL	N-CA-C	5.47	116.85	110.62
1	A	332	VAL	N-CA-C	5.43	115.36	106.72
1	C	330	LEU	CA-C-N	5.36	130.97	122.94
1	C	330	LEU	C-N-CA	5.36	130.97	122.94
1	C	428	ILE	N-CA-C	5.34	116.06	110.62
1	A	238	ALA	N-CA-C	-5.33	106.85	113.19
1	A	241	ALA	N-CA-C	5.30	117.14	111.36
1	A	352	GLU	N-CA-C	5.29	117.96	111.82
1	A	271	ALA	N-CA-C	-5.18	105.64	111.28
1	A	410	GLU	N-CA-C	-5.17	106.74	113.16
1	C	443	GLY	CA-C-N	5.17	127.64	120.29
1	C	443	GLY	C-N-CA	5.17	127.64	120.29
1	A	363	ASP	N-CA-C	5.15	118.06	110.59
1	C	298	VAL	N-CA-C	5.15	115.87	110.62
1	C	349	VAL	CB-CA-C	-5.14	105.39	111.97
1	C	418	LEU	N-CA-C	5.11	116.93	111.36
1	A	448	ASP	N-CA-C	5.08	117.36	110.35
1	A	353	LEU	N-CA-C	5.08	119.22	112.72
1	C	267	ASN	N-CA-C	5.07	116.62	111.14
1	A	449	THR	N-CA-C	5.06	116.48	111.07
1	A	313	PHE	N-CA-C	5.06	116.60	111.14
1	A	275	GLN	N-CA-C	5.04	117.67	111.82
1	C	384	SER	N-CA-C	5.04	116.47	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	452	MET	N-CA-C	-5.04	105.30	111.75
1	A	403	TYR	CA-C-N	5.03	127.02	120.28
1	A	403	TYR	C-N-CA	5.03	127.02	120.28
1	A	333	HIS	N-CA-C	5.02	117.57	110.50

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	1697	0	1727	93	0
1	C	1711	0	1741	87	0
2	B	89	0	95	2	0
2	D	98	0	111	4	0
3	A	22	0	20	24	0
3	C	22	0	20	14	0
4	A	26	0	0	1	0
4	B	1	0	0	0	0
4	C	25	0	0	0	0
4	D	1	0	0	0	0
All	All	3692	0	3714	191	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 26.

All (191) 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:C:439:PHE:CE2	3:C:1:BGV:HAC	1.70	1.26
1:A:304:GLY:O	1:A:308:LEU:HD12	1.53	1.08
1:C:439:PHE:HE2	3:C:1:BGV:CAC	1.68	1.06
1:C:231:PRO:HB2	1:C:234:ARG:HG3	1.39	1.02
3:A:1:BGV:HAR	3:A:1:BGV:HADB	1.35	1.01
1:A:320:VAL:CG2	1:A:323:GLY:O	2.11	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:320:VAL:HG21	1:A:323:GLY:O	1.64	0.97
1:A:392:LEU:O	1:A:396:VAL:HG23	1.64	0.97
1:C:439:PHE:HE2	3:C:1:BGV:HAC	0.78	0.93
1:A:264:PRO:HA	1:A:267:ASN:HD22	1.34	0.91
1:C:273:ASP:OD1	1:C:450:PHE:HB3	1.75	0.87
3:A:1:BGV:HADB	3:A:1:BGV:CAR	2.04	0.87
1:A:268:ILE:CG2	3:A:1:BGV:HADB	2.09	0.83
1:C:439:PHE:CE2	3:C:1:BGV:CAC	2.52	0.83
1:C:333:HIS:CD2	1:C:335:ASN:H	1.98	0.82
1:C:407:LYS:HG2	1:C:408:TYR:CE1	2.14	0.81
1:A:268:ILE:HG21	3:A:1:BGV:HADB	1.60	0.81
1:A:316:ARG:HD2	1:A:325:LEU:O	1.81	0.81
1:C:302:ARG:HH12	1:C:458:PRO:HG3	1.46	0.81
1:A:436:LEU:HG	3:A:1:BGV:HACB	1.62	0.80
1:C:238:ALA:O	1:C:242:VAL:HG22	1.82	0.80
1:C:436:LEU:HD23	3:C:1:BGV:HACB	1.64	0.79
3:A:1:BGV:CAR	3:A:1:BGV:CAD	2.60	0.79
1:C:391:ALA:HA	1:C:394:GLU:OE1	1.83	0.79
1:A:321:LYS:HA	1:A:321:LYS:HE3	1.65	0.79
1:C:416:ALA:O	1:C:420:LEU:HD12	1.82	0.79
1:C:436:LEU:HD21	3:C:1:BGV:HAJ	1.64	0.79
1:C:347:ASP:O	1:C:351:THR:HG23	1.84	0.77
1:C:333:HIS:HD2	1:C:335:ASN:H	1.33	0.77
1:A:380:SER:HB2	1:A:383:LEU:HD22	1.67	0.77
1:C:373:ILE:O	1:C:393:ARG:NH2	2.18	0.76
1:A:320:VAL:HG23	1:A:323:GLY:O	1.84	0.76
1:C:273:ASP:OD1	1:C:450:PHE:CB	2.33	0.76
1:A:436:LEU:HG	3:A:1:BGV:CAC	2.15	0.76
1:A:238:ALA:O	1:A:282:TRP:HD1	1.70	0.75
1:C:333:HIS:CD2	1:C:334:ARG:N	2.55	0.75
1:C:236:LEU:CD2	1:C:236:LEU:O	2.36	0.74
1:C:348:ARG:O	1:C:352:GLU:HB2	1.88	0.73
1:A:435:HIS:O	1:A:438:PHE:N	2.21	0.73
1:C:376:PHE:O	1:C:378:PRO:HD3	1.88	0.72
1:C:432:CYS:SG	3:C:1:BGV:CAN	2.78	0.72
1:C:435:HIS:HB3	3:C:1:BGV:HAI	1.71	0.71
1:A:313:PHE:HE2	3:A:1:BGV:HAA	1.56	0.71
1:A:268:ILE:HG21	3:A:1:BGV:CAD	2.20	0.70
1:A:239:GLU:OE2	1:A:282:TRP:NE1	2.25	0.69
1:C:333:HIS:HD2	1:C:334:ARG:N	1.91	0.69
1:A:438:PHE:O	1:A:442:ILE:HG22	1.92	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:447:ILE:HG23	1:A:451:LEU:HD23	1.74	0.68
1:C:306:ASN:ND2	1:C:433:LEU:HG	2.09	0.68
1:A:304:GLY:C	1:A:308:LEU:HD12	2.19	0.67
1:C:444:ASP:OD1	1:C:445:THR:N	2.27	0.67
1:C:447:ILE:HG23	1:C:451:LEU:HD23	1.76	0.67
1:A:436:LEU:HD13	1:A:455:LEU:HD21	1.78	0.66
1:C:316:ARG:HG2	1:C:316:ARG:O	1.94	0.66
1:A:457:ALA:O	1:A:458:PRO:C	2.39	0.66
1:C:436:LEU:CD2	3:C:1:BGV:HACB	2.26	0.66
1:A:436:LEU:CG	3:A:1:BGV:HACB	2.26	0.65
1:C:452:MET:O	1:C:456:GLU:HG3	1.97	0.65
1:C:236:LEU:O	1:C:236:LEU:HD22	1.98	0.64
1:C:236:LEU:O	1:C:236:LEU:HD23	1.97	0.64
1:A:313:PHE:CE2	3:A:1:BGV:HAA	2.32	0.64
1:C:431:LYS:HE3	1:C:435:HIS:CE1	2.34	0.63
1:A:240:LEU:O	1:A:243:GLU:HG2	2.01	0.61
2:B:3:LYS:HB3	2:B:7:ARG:NH1	2.15	0.61
1:C:403:TYR:CD2	1:C:403:TYR:C	2.79	0.60
1:A:298:VAL:O	1:A:302:ARG:HG3	2.00	0.60
1:A:264:PRO:C	1:A:266:THR:H	2.09	0.60
3:A:1:BGV:HAR	3:A:1:BGV:CAD	2.16	0.59
2:D:10:GLN:O	2:D:11:ASP:HB3	2.03	0.59
1:C:302:ARG:NH2	1:C:456:GLU:O	2.36	0.59
1:A:348:ARG:O	1:A:352:GLU:HB2	2.03	0.58
1:C:394:GLU:HA	1:C:397:TYR:CE2	2.38	0.58
1:A:281:GLU:HA	1:A:281:GLU:OE2	2.03	0.58
1:A:238:ALA:O	1:A:282:TRP:CD1	2.55	0.57
1:C:373:ILE:HD11	1:C:397:TYR:HB3	1.86	0.57
1:A:306:ASN:OD1	1:A:433:LEU:HG	2.05	0.56
1:C:306:ASN:HD21	1:C:433:LEU:HG	1.69	0.56
1:A:264:PRO:C	1:A:266:THR:N	2.63	0.56
1:A:448:ASP:O	1:A:452:MET:HB2	2.05	0.56
1:C:276:LEU:HD21	1:C:305:TRP:HE3	1.72	0.55
1:C:302:ARG:NH1	1:C:458:PRO:HG3	2.20	0.55
1:C:333:HIS:CD2	1:C:334:ARG:H	2.23	0.55
1:A:268:ILE:HG22	3:A:1:BGV:HADB	1.85	0.55
1:C:275:GLN:OE1	1:C:275:GLN:HA	2.06	0.54
1:C:296:ASP:OD2	1:C:384:SER:OG	2.22	0.54
1:A:335:ASN:N	1:A:335:ASN:OD1	2.39	0.54
1:A:410:GLU:HG2	1:A:411:GLN:HG3	1.90	0.54
1:C:438:PHE:O	1:C:442:ILE:HG12	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:300:LEU:HD13	1:A:375:LEU:O	2.07	0.53
1:A:432:CYS:O	3:A:1:BGV:HACA	2.08	0.53
1:A:401:GLU:HG2	1:A:405:LYS:HD3	1.90	0.53
1:C:393:ARG:O	1:C:397:TYR:CD2	2.62	0.53
1:C:231:PRO:CB	1:C:234:ARG:HG3	2.27	0.53
1:C:391:ALA:O	1:C:394:GLU:HB2	2.08	0.53
1:C:300:LEU:HD22	1:C:375:LEU:O	2.08	0.53
1:A:379:ASP:CG	1:C:421:ARG:HH22	2.18	0.52
1:C:435:HIS:CB	3:C:1:BGV:HAI	2.40	0.52
1:A:265:VAL:O	1:A:265:VAL:CG1	2.57	0.52
1:C:236:LEU:CD2	1:C:236:LEU:C	2.81	0.52
1:A:436:LEU:HD21	3:A:1:BGV:HAJ	1.92	0.52
1:C:411:GLN:HG3	1:C:414:ARG:HB2	1.91	0.52
1:A:243:GLU:O	1:A:244:PRO:C	2.53	0.51
3:C:1:BGV:HAB	3:C:1:BGV:HAAA	1.91	0.51
1:C:401:GLU:HB2	1:C:415:PHE:CZ	2.44	0.51
1:C:391:ALA:O	1:C:394:GLU:N	2.45	0.50
1:A:436:LEU:CD2	3:A:1:BGV:HACB	2.41	0.50
1:C:407:LYS:HG2	1:C:408:TYR:CZ	2.47	0.50
1:A:310:ILE:HA	1:A:313:PHE:CE2	2.47	0.50
1:C:243:GLU:O	1:C:244:PRO:C	2.52	0.50
1:C:277:PHE:CD1	1:C:450:PHE:HD1	2.29	0.50
1:A:262:ASN:CG	1:A:262:ASN:O	2.55	0.50
1:A:385:ASN:ND2	1:A:388:GLU:HB2	2.27	0.50
1:C:401:GLU:HB2	1:C:415:PHE:CE2	2.46	0.49
1:A:265:VAL:O	1:A:265:VAL:HG12	2.10	0.49
1:A:263:ASP:OD1	1:A:264:PRO:HD2	2.12	0.49
1:A:236:LEU:HD13	1:A:365:THR:OG1	2.13	0.49
1:C:298:VAL:HG21	2:D:6:HIS:NE2	2.28	0.49
1:C:432:CYS:SG	3:C:1:BGV:CAP	3.00	0.49
1:C:242:VAL:HG11	1:C:282:TRP:HB2	1.95	0.49
1:C:333:HIS:HD2	1:C:335:ASN:N	2.05	0.49
1:C:452:MET:O	1:C:456:GLU:CG	2.61	0.49
1:A:436:LEU:HG	3:A:1:BGV:HACA	1.95	0.49
3:C:1:BGV:HAAA	3:C:1:BGV:OAK	2.13	0.48
1:A:332:VAL:O	1:A:332:VAL:HG12	2.12	0.48
1:A:370:LEU:O	1:A:374:VAL:HG23	2.14	0.48
1:C:422:LEU:N	1:C:423:PRO:CD	2.76	0.48
1:A:442:ILE:HG12	1:A:442:ILE:O	2.13	0.48
1:C:442:ILE:HD13	1:C:442:ILE:N	2.29	0.48
1:A:409:PRO:HD2	1:A:410:GLU:OE1	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:237:GLU:C	1:A:239:GLU:H	2.22	0.48
1:A:428:ILE:O	1:A:432:CYS:HB2	2.12	0.48
1:C:438:PHE:CE1	1:C:442:ILE:HD11	2.48	0.48
1:C:308:LEU:HD21	1:C:371:ARG:O	2.15	0.47
1:C:263:ASP:O	1:C:264:PRO:C	2.53	0.47
1:A:290:SER:O	1:A:292:LEU:N	2.47	0.47
1:C:315:HIS:C	1:C:317:SER:H	2.22	0.47
1:A:304:GLY:O	1:A:308:LEU:CD1	2.44	0.47
1:A:435:HIS:O	1:A:436:LEU:C	2.58	0.47
1:C:277:PHE:CE1	1:C:450:PHE:HD1	2.32	0.47
1:A:310:ILE:HD13	1:A:428:ILE:HG22	1.98	0.46
1:A:400:LEU:O	1:A:403:TYR:HB3	2.15	0.46
1:A:234:ARG:NH2	4:A:27:HOH:O	2.49	0.46
1:C:457:ALA:HA	1:C:458:PRO:HD3	1.75	0.46
1:A:297:GLN:OE1	2:B:9:LEU:HD22	2.16	0.45
1:C:362:MET:HE2	1:C:418:LEU:HD23	1.99	0.45
1:A:400:LEU:HD21	1:A:418:LEU:HD13	1.98	0.45
1:A:268:ILE:CG2	3:A:1:BGV:CAD	2.85	0.45
1:C:280:VAL:HG13	1:C:301:LEU:HD11	1.98	0.45
1:A:372:ALA:O	1:A:376:PHE:CD1	2.70	0.45
1:A:287:PRO:O	1:A:288:HIS:HB2	2.18	0.44
1:C:442:ILE:HG22	1:C:444:ASP:HB3	2.00	0.44
2:D:9:LEU:HD23	2:D:9:LEU:HA	1.86	0.44
1:A:420:LEU:HD13	1:C:393:ARG:HD3	1.98	0.44
1:A:453:GLU:O	1:A:456:GLU:HB2	2.18	0.44
3:A:1:BGV:HAU	3:A:1:BGV:HAS	1.11	0.44
1:C:356:LYS:HA	1:C:356:LYS:HD3	1.59	0.44
1:A:268:ILE:CG2	3:A:1:BGV:HAR	2.48	0.44
1:A:311:ALA:HB2	1:A:425:LEU:HD11	1.98	0.44
1:A:446:PRO:C	1:A:447:ILE:HG13	2.42	0.44
1:A:268:ILE:HG22	3:A:1:BGV:HAR	1.99	0.43
1:A:268:ILE:HG12	1:A:326:LEU:HD21	1.99	0.43
1:C:362:MET:HG3	1:C:418:LEU:HD21	1.99	0.43
3:C:1:BGV:HAU	3:C:1:BGV:HAS	1.17	0.43
1:A:290:SER:O	1:A:291:GLU:C	2.60	0.43
1:A:237:GLU:C	1:A:239:GLU:N	2.76	0.43
1:C:444:ASP:OD1	1:C:444:ASP:C	2.62	0.43
1:A:268:ILE:HG21	3:A:1:BGV:HAT	2.01	0.43
1:A:367:LEU:O	1:A:368:GLY:C	2.58	0.43
1:C:317:SER:OG	1:C:324:ILE:HG22	2.19	0.43
1:C:385:ASN:OD1	1:C:385:ASN:C	2.62	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:415:PHE:O	1:A:419:LEU:HG	2.20	0.42
1:C:294:LEU:O	1:C:297:GLN:HB2	2.19	0.42
2:D:3:LYS:HE2	2:D:3:LYS:HB2	1.75	0.42
1:A:231:PRO:O	1:A:235:ILE:HG13	2.20	0.42
1:A:232:VAL:O	1:A:233:GLU:C	2.63	0.42
1:A:342:VAL:O	1:A:342:VAL:HG23	2.19	0.41
1:C:300:LEU:HD23	1:C:300:LEU:HA	1.81	0.41
1:A:290:SER:HA	1:A:297:GLN:NE2	2.35	0.41
1:C:279:LEU:O	1:C:279:LEU:HG	2.18	0.41
1:C:262:ASN:OD1	1:C:262:ASN:N	2.52	0.41
1:A:287:PRO:O	1:A:288:HIS:CB	2.68	0.41
3:A:1:BGV:HADA	3:A:1:BGV:HAQ	1.20	0.41
1:A:235:ILE:O	1:A:235:ILE:HG22	2.19	0.41
1:A:380:SER:O	1:A:383:LEU:HB2	2.21	0.41
1:A:290:SER:C	1:A:292:LEU:N	2.77	0.41
1:A:313:PHE:CE2	3:A:1:BGV:CAA	3.02	0.41
1:C:230:MET:HE2	1:C:395:LYS:HB3	2.03	0.41
1:A:422:LEU:N	1:A:423:PRO:CD	2.84	0.40
1:A:372:ALA:O	1:A:376:PHE:HD1	2.04	0.40
1:C:293:PRO:O	1:C:294:LEU:C	2.64	0.40
1:A:243:GLU:O	1:A:243:GLU:HG3	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	211/238 (89%)	204 (97%)	7 (3%)	0	100	100
1	C	213/238 (90%)	207 (97%)	6 (3%)	0	100	100
2	B	8/11 (73%)	8 (100%)	0	0	100	100
2	D	9/11 (82%)	7 (78%)	2 (22%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	441/498 (89%)	426 (97%)	15 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	185/205 (90%)	165 (89%)	20 (11%)	6	4
1	C	187/205 (91%)	162 (87%)	25 (13%)	4	2
2	B	10/11 (91%)	10 (100%)	0	100	100
2	D	11/11 (100%)	10 (91%)	1 (9%)	9	6
All	All	393/432 (91%)	347 (88%)	46 (12%)	5	3

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	242	VAL
1	A	244	PRO
1	A	263	ASP
1	A	270	GLN
1	A	278	THR
1	A	281	GLU
1	A	306	ASN
1	A	321	LYS
1	A	325	LEU
1	A	345	ILE
1	A	355	SER
1	A	363	ASP
1	A	383	LEU
1	A	389	VAL
1	A	397	TYR
1	A	433	LEU
1	A	442	ILE

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Mol	Chain	Res	Type
1	A	445	THR
1	A	448	ASP
1	A	456	GLU
1	C	227	ASN
1	C	229	ASP
1	C	236	LEU
1	C	262	ASN
1	C	265	VAL
1	C	266	THR
1	C	275	GLN
1	C	301	LEU
1	C	321	LYS
1	C	324	ILE
1	C	325	LEU
1	C	330	LEU
1	C	332	VAL
1	C	336	SER
1	C	345	ILE
1	C	351	THR
1	C	356	LYS
1	C	367	LEU
1	C	383	LEU
1	C	388	GLU
1	C	389	VAL
1	C	403	TYR
1	C	417	LYS
1	C	433	LEU
1	C	444	ASP
2	D	2	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	262	ASN
1	A	267	ASN
1	A	275	GLN
1	A	385	ASN
1	C	227	ASN
1	C	270	GLN
1	C	288	HIS
1	C	306	ASN
1	C	333	HIS

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Mol	Chain	Res	Type
1	C	335	ASN
2	D	2	HIS

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](#)

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	$\# Z > 2$
3	BGV	A	1	-	23,24,24	3.95	13 (56%)	34,38,38	3.65	17 (50%)
3	BGV	C	1	-	23,24,24	4.90	15 (65%)	34,38,38	4.26	21 (61%)

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
3	BGV	A	1	-	-	3/4/55/55	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	BGV	C	1	-	-	2/4/55/55	0/3/3/3

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1	BGV	CAV-CAO	-12.71	1.41	1.54
3	C	1	BGV	CAV-CAS	-9.88	1.43	1.55
3	A	1	BGV	CAH-CAO	-9.37	1.28	1.46
3	C	1	BGV	CAH-CAO	-8.23	1.30	1.46
3	A	1	BGV	CAV-CAO	-7.64	1.46	1.54
3	A	1	BGV	CAV-CAS	-7.50	1.46	1.55
3	C	1	BGV	CAS-CAQ	-6.12	1.43	1.54
3	A	1	BGV	CAP-CAN	-5.83	1.37	1.48
3	C	1	BGV	CAJ-CAR	-5.62	1.41	1.51
3	A	1	BGV	OAL-CAR	-5.53	1.38	1.46
3	C	1	BGV	OAK-CAT	-5.15	1.36	1.45
3	C	1	BGV	CAP-CAN	-4.78	1.39	1.48
3	C	1	BGV	OAL-CAR	-4.65	1.39	1.46
3	C	1	BGV	CAJ-CAQ	-4.17	1.49	1.54
3	A	1	BGV	CAU-CAR	-4.04	1.48	1.54
3	C	1	BGV	CAA-CAN	3.99	1.39	1.32
3	C	1	BGV	CAU-CAR	-3.82	1.48	1.54
3	A	1	BGV	OAL-CAP	-3.80	1.29	1.36
3	C	1	BGV	OAK-CAM	-3.67	1.27	1.35
3	A	1	BGV	CAS-CAQ	-3.29	1.48	1.54
3	A	1	BGV	CAV-CAT	-2.95	1.48	1.53
3	A	1	BGV	CAJ-CAQ	-2.59	1.50	1.54
3	A	1	BGV	CAA-CAN	2.54	1.37	1.32
3	A	1	BGV	CAJ-CAR	-2.54	1.46	1.51
3	C	1	BGV	CAV-CAT	2.46	1.56	1.53
3	C	1	BGV	OAL-CAP	-2.42	1.32	1.36
3	A	1	BGV	OAK-CAM	-2.37	1.29	1.35
3	C	1	BGV	CAD-CAV	-2.16	1.50	1.54

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1	BGV	CAJ-CAQ-CAS	-9.48	99.91	111.00
3	C	1	BGV	CAT-OAK-CAM	-9.47	104.35	117.79
3	A	1	BGV	CAV-CAO-CAH	8.85	115.20	107.31
3	C	1	BGV	CAD-CAV-CAO	-8.68	90.31	103.97
3	C	1	BGV	CAJ-CAR-CAU	-8.38	94.46	116.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1	BGV	OAL-CAR-CAJ	-8.11	93.08	108.00
3	A	1	BGV	CAJ-CAR-CAU	-7.85	95.84	116.54
3	A	1	BGV	CAV-CAS-CAQ	-6.97	106.59	117.37
3	C	1	BGV	OAK-CAM-CAB	6.64	122.94	111.09
3	C	1	BGV	CAS-CAI-CAH	-6.11	106.14	112.71
3	A	1	BGV	CAR-CAU-CAN	-5.69	96.21	102.47
3	C	1	BGV	CAD-CAV-CAT	5.38	119.58	112.45
3	C	1	BGV	OAF-CAO-CAV	-4.96	120.40	124.77
3	A	1	BGV	CAT-OAK-CAM	4.73	124.50	117.79
3	C	1	BGV	CAU-CAN-CAA	-4.61	122.98	130.51
3	C	1	BGV	CAV-CAS-CAQ	-4.61	110.25	117.37
3	A	1	BGV	CAU-CAN-CAA	-4.55	123.08	130.51
3	A	1	BGV	OAK-CAT-CAU	4.35	117.89	105.95
3	C	1	BGV	CAR-CAU-CAN	-3.92	98.16	102.47
3	A	1	BGV	CAQ-CAS-CAI	-3.84	112.01	117.66
3	A	1	BGV	CAD-CAV-CAT	-3.74	107.50	112.45
3	A	1	BGV	OAK-CAM-CAB	3.73	117.74	111.09
3	C	1	BGV	CAV-CAO-CAH	3.61	110.53	107.31
3	A	1	BGV	OAF-CAO-CAH	-3.31	122.30	127.73
3	A	1	BGV	OAF-CAO-CAV	-3.23	121.92	124.77
3	C	1	BGV	OAK-CAT-CAU	3.16	114.62	105.95
3	C	1	BGV	CAA-CAN-CAP	2.97	126.34	122.13
3	A	1	BGV	CAA-CAN-CAP	2.94	126.30	122.13
3	C	1	BGV	CAV-CAS-CAI	2.68	104.82	102.66
3	C	1	BGV	OAL-CAR-CAJ	-2.61	103.20	108.00
3	C	1	BGV	CAC-CAQ-CAS	-2.57	107.09	112.14
3	C	1	BGV	CAQ-CAS-CAI	-2.44	114.06	117.66
3	A	1	BGV	CAU-CAN-CAP	2.32	110.62	107.32
3	C	1	BGV	OAK-CAM-OAE	-2.21	118.73	122.99
3	C	1	BGV	CAI-CAH-CAO	2.20	111.93	109.91
3	C	1	BGV	CAQ-CAJ-CAR	-2.18	109.40	115.41
3	A	1	BGV	OAL-CAP-OAG	2.04	123.96	121.27
3	A	1	BGV	CAS-CAI-CAH	-2.03	110.53	112.71

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1	BGV	CAU-CAT-OAK-CAM
3	A	1	BGV	CAB-CAM-OAK-CAT
3	C	1	BGV	CAB-CAM-OAK-CAT
3	A	1	BGV	OAE-CAM-OAK-CAT

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Mol	Chain	Res	Type	Atoms
3	C	1	BGV	OAE-CAM-OAK-CAT

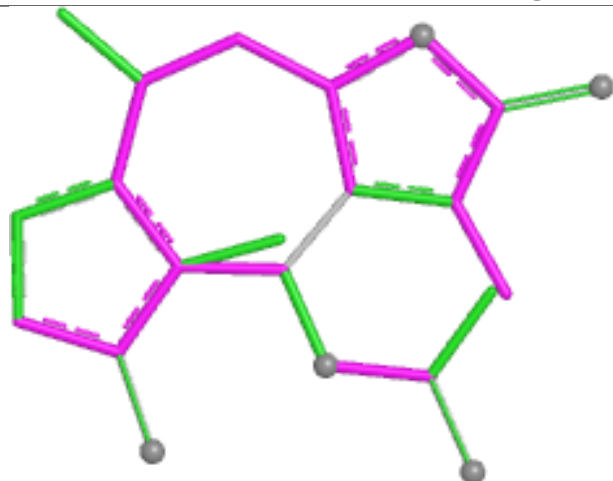
There are no ring outliers.

2 monomers are involved in 38 short contacts:

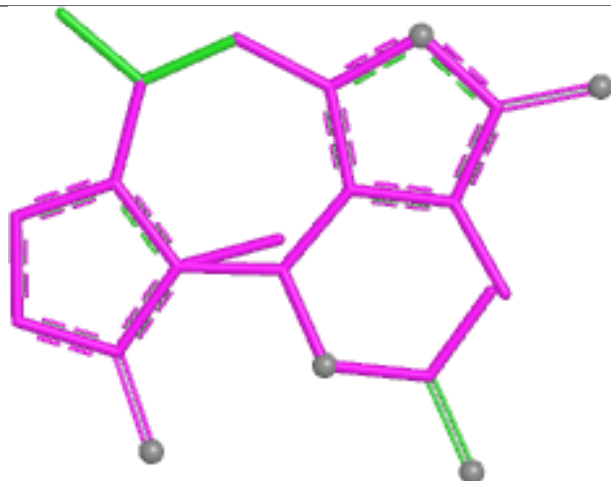
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1	BGV	24	0
3	C	1	BGV	14	0

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.

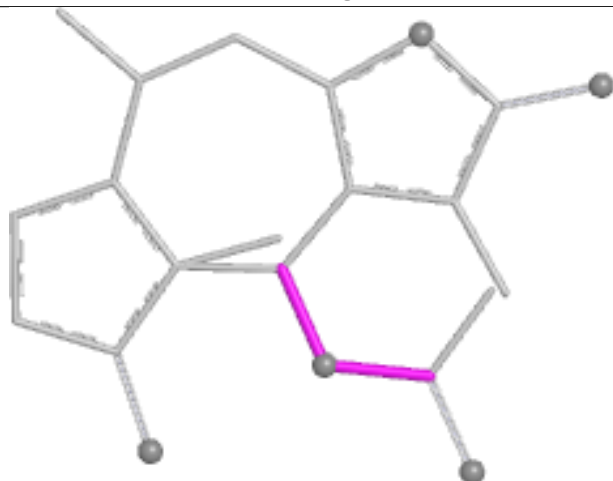
Ligand BGV A 1



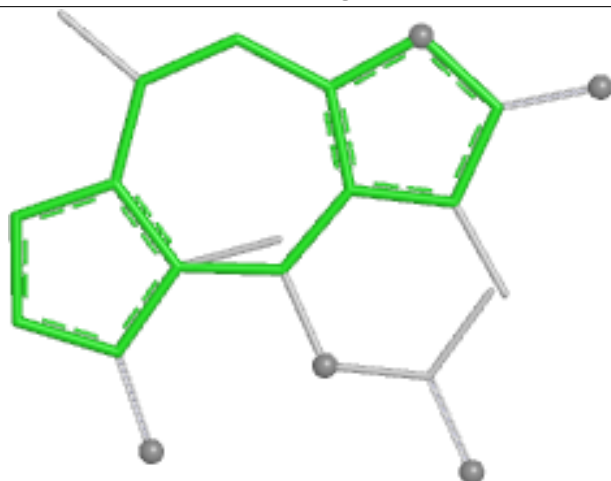
Bond lengths



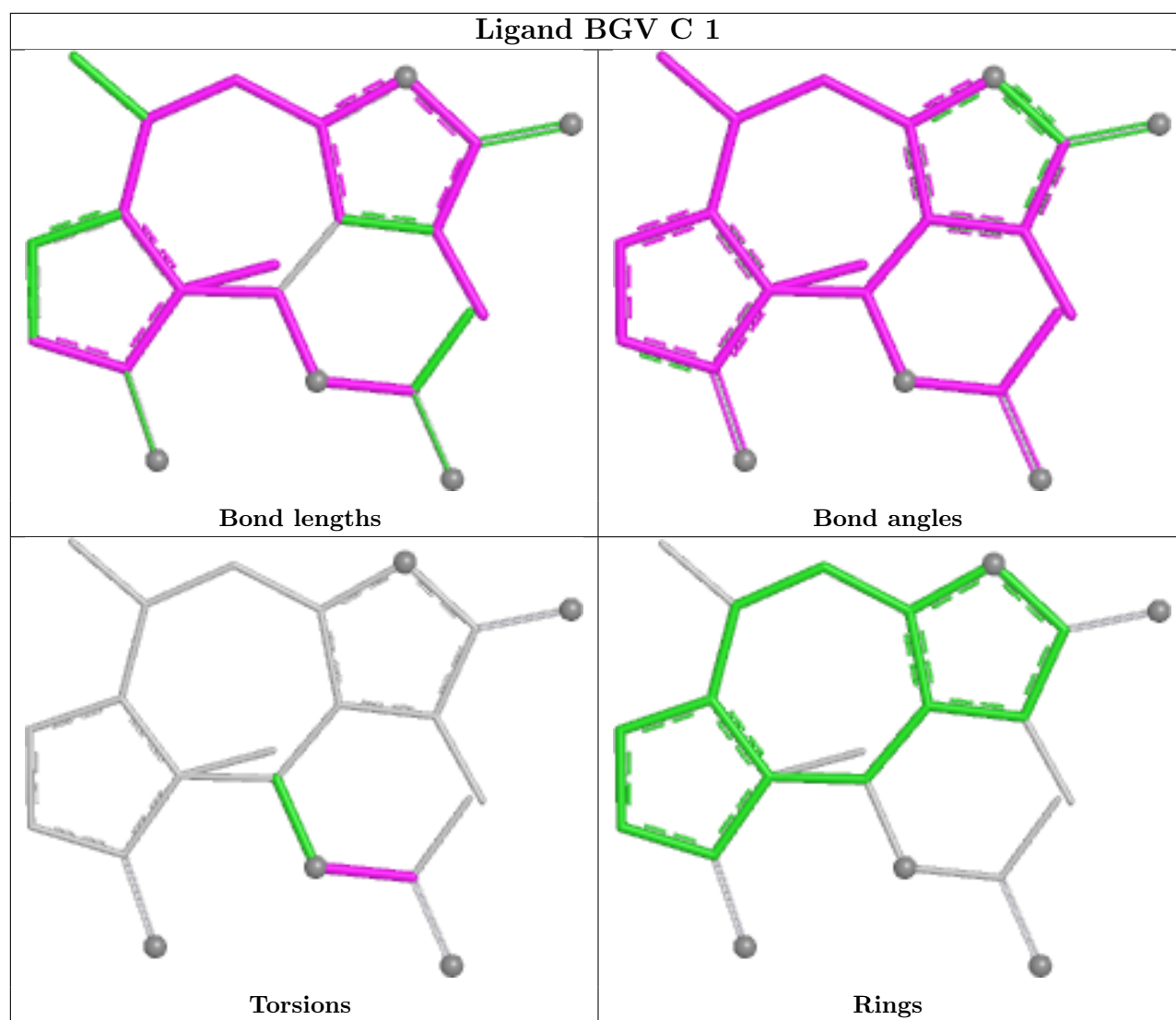
Bond angles



Torsions



Rings



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	215/238 (90%)	-0.03	2 (0%) 81 83	6, 19, 32, 45	0
1	C	215/238 (90%)	-0.06	0 100 100	6, 20, 32, 41	5 (2%)
2	B	10/11 (90%)	-0.17	0 100 100	13, 17, 23, 24	0
2	D	11/11 (100%)	0.24	0 100 100	17, 22, 27, 33	0
All	All	451/498 (90%)	-0.04	2 (0%) 88 90	6, 19, 32, 45	5 (1%)

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	229	ASP	4.4
1	A	330	LEU	2.3

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

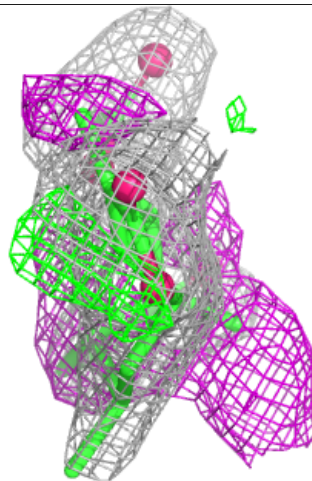
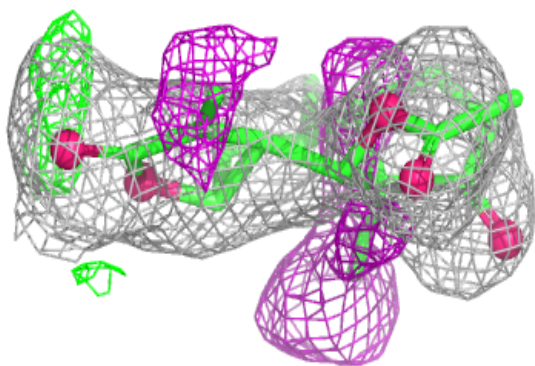
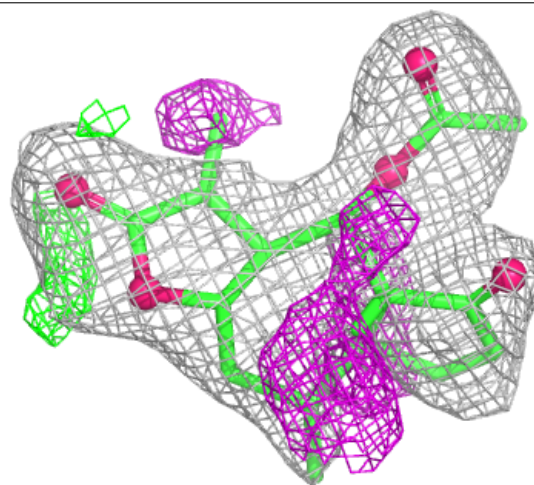
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

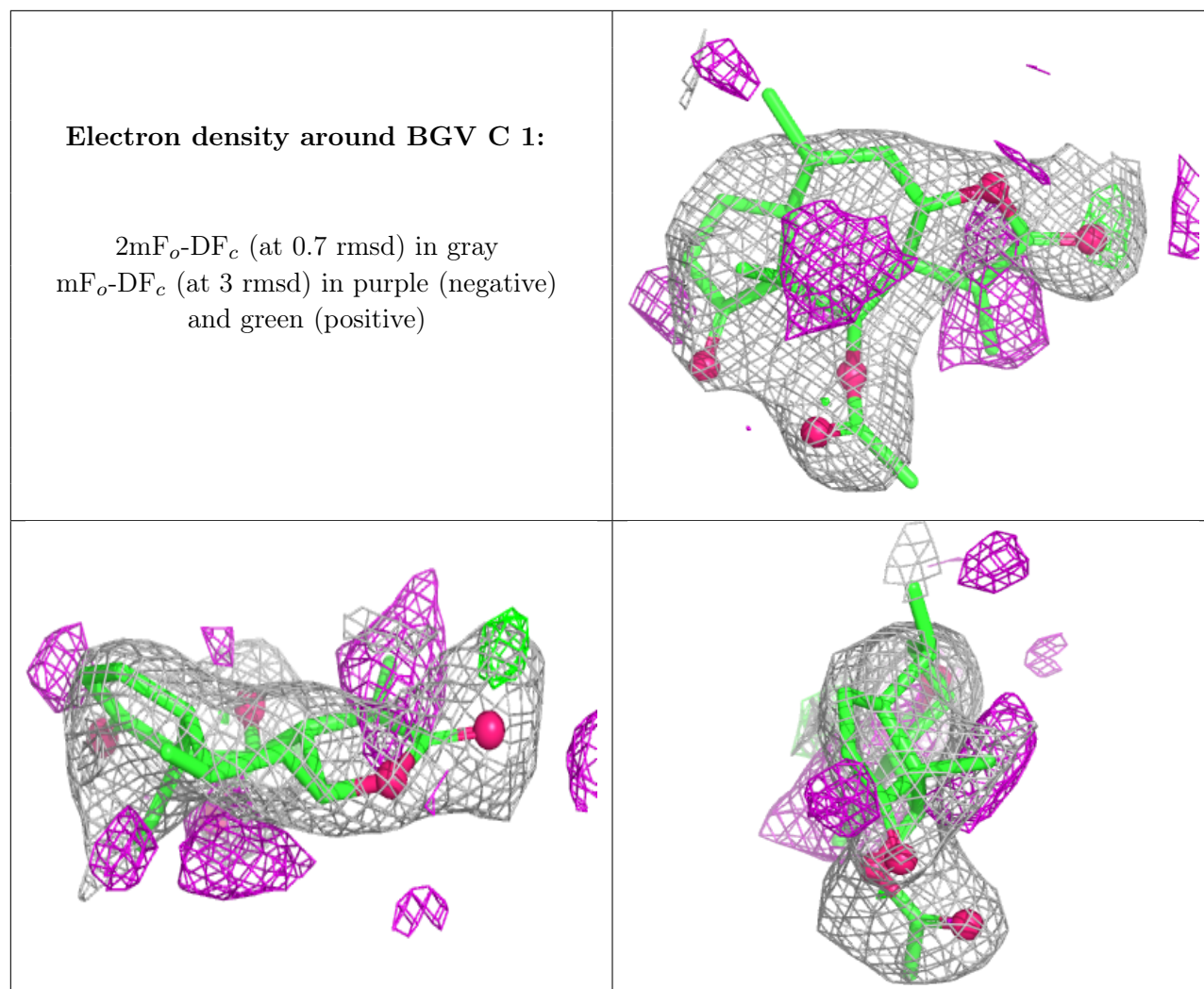
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	BGV	A	1	22/22	0.83	0.14	25,32,33,34	0
3	BGV	C	1	22/22	0.86	0.13	28,31,34,35	0

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 BGV A 1:

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.