



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 02:02 AM UTC

PDB ID : 6XSR / pdb_00006xsr
Title : Crystal structure of GluA2 AMPA receptor in complex with trans-4-butylcyclohexane carboxylic acid (4-BCCA) inhibitor
Authors : Yelshanskaya, M.V.; Singh, A.K.; Sobolevsky, A.I.
Deposited on : 2020-07-16
Resolution : 4.25 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

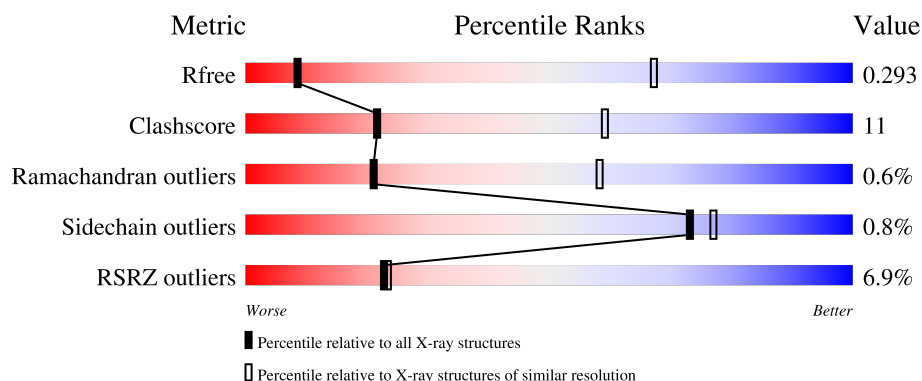
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.25 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	1029 (4.62-3.90)
Clashscore	190562	1074 (4.62-3.90)
Ramachandran outliers	187476	1001 (4.62-3.88)
Sidechain outliers	187428	1021 (4.66-3.86)
RSRZ outliers	180081	1026 (4.62-3.90)

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	808	5% 72% 23% 5%
1	B	808	9% 71% 24% • •
1	C	808	4% 70% 25% •
1	D	808	8% 77% 17% • •

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
2	NAG	B	901	-	-	X	-
3	V8G	A	902	-	-	X	-
3	V8G	C	902	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 23775 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 Glutamate receptor 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	770	Total	C	N	O	S	0	0	0
			5912	3793	984	1108	27			
1	B	772	Total	C	N	O	S	0	0	0
			5954	3815	987	1124	28			
1	C	774	Total	C	N	O	S	0	0	0
			5918	3796	985	1111	26			
1	D	772	Total	C	N	O	S	0	0	0
			5909	3788	985	1110	26			

There are 44 discrepancies between the modelled and reference sequences:

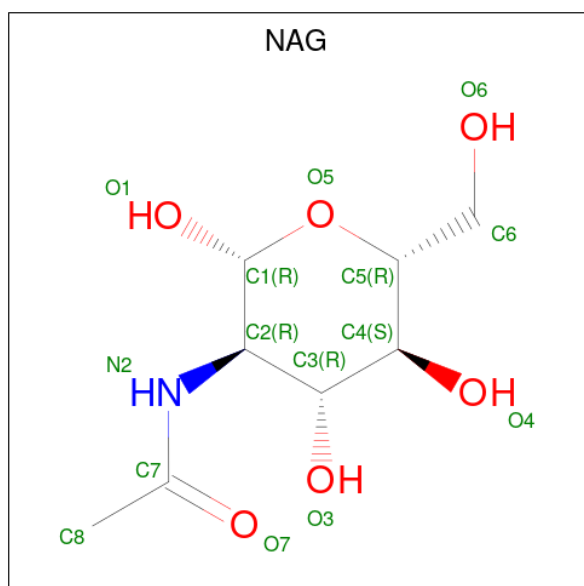
Chain	Residue	Modelled	Actual	Comment	Reference
A	241	GLU	ASN	conflict	UNP P19491
A	382	LEU	VAL	conflict	UNP P19491
A	?	-	LEU	deletion	UNP P19491
A	?	-	THR	deletion	UNP P19491
A	?	-	GLU	deletion	UNP P19491
A	?	-	LEU	deletion	UNP P19491
A	?	-	PRO	deletion	UNP P19491
A	?	-	SER	deletion	UNP P19491
A	384	GLU	GLY	conflict	UNP P19491
A	385	ASP	ASN	conflict	UNP P19491
A	392	GLN	ASN	conflict	UNP P19491
B	241	GLU	ASN	conflict	UNP P19491
B	382	LEU	VAL	conflict	UNP P19491
B	?	-	LEU	deletion	UNP P19491
B	?	-	THR	deletion	UNP P19491
B	?	-	GLU	deletion	UNP P19491
B	?	-	LEU	deletion	UNP P19491
B	?	-	PRO	deletion	UNP P19491
B	?	-	SER	deletion	UNP P19491
B	384	GLU	GLY	conflict	UNP P19491
B	385	ASP	ASN	conflict	UNP P19491

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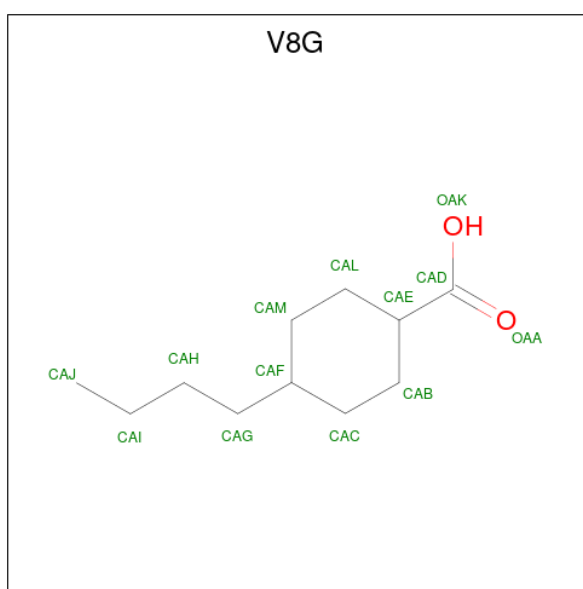
Chain	Residue	Modelled	Actual	Comment	Reference
B	392	GLN	ASN	conflict	UNP P19491
C	241	GLU	ASN	conflict	UNP P19491
C	382	LEU	VAL	conflict	UNP P19491
C	?	-	LEU	deletion	UNP P19491
C	?	-	THR	deletion	UNP P19491
C	?	-	GLU	deletion	UNP P19491
C	?	-	LEU	deletion	UNP P19491
C	?	-	PRO	deletion	UNP P19491
C	?	-	SER	deletion	UNP P19491
C	384	GLU	GLY	conflict	UNP P19491
C	385	ASP	ASN	conflict	UNP P19491
C	392	GLN	ASN	conflict	UNP P19491
D	241	GLU	ASN	conflict	UNP P19491
D	382	LEU	VAL	conflict	UNP P19491
D	?	-	LEU	deletion	UNP P19491
D	?	-	THR	deletion	UNP P19491
D	?	-	GLU	deletion	UNP P19491
D	?	-	LEU	deletion	UNP P19491
D	?	-	PRO	deletion	UNP P19491
D	?	-	SER	deletion	UNP P19491
D	384	GLU	GLY	conflict	UNP P19491
D	385	ASP	ASN	conflict	UNP P19491
D	392	GLN	ASN	conflict	UNP P19491

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	D	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 3 is trans-4-butylcyclohexane-1-carboxylic acid (CCD ID: V8G) (formula: $C_{11}H_{20}O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			13	11	2		
3	C	1	Total	C	O	0	0
			13	11	2		

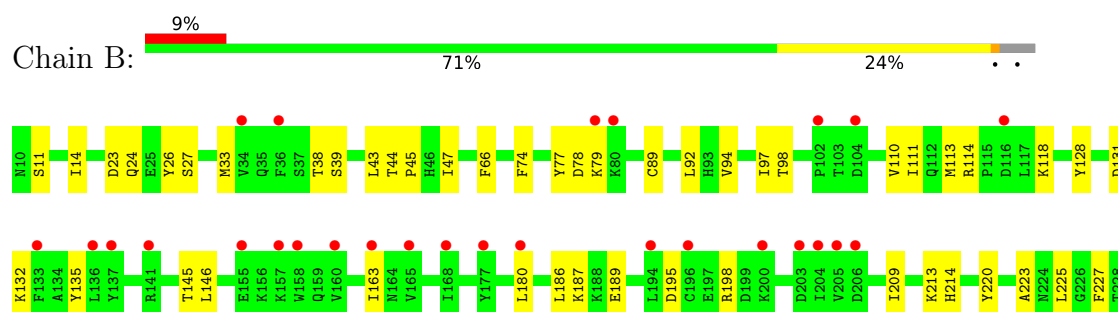
3 Residue-property plots [i](#)

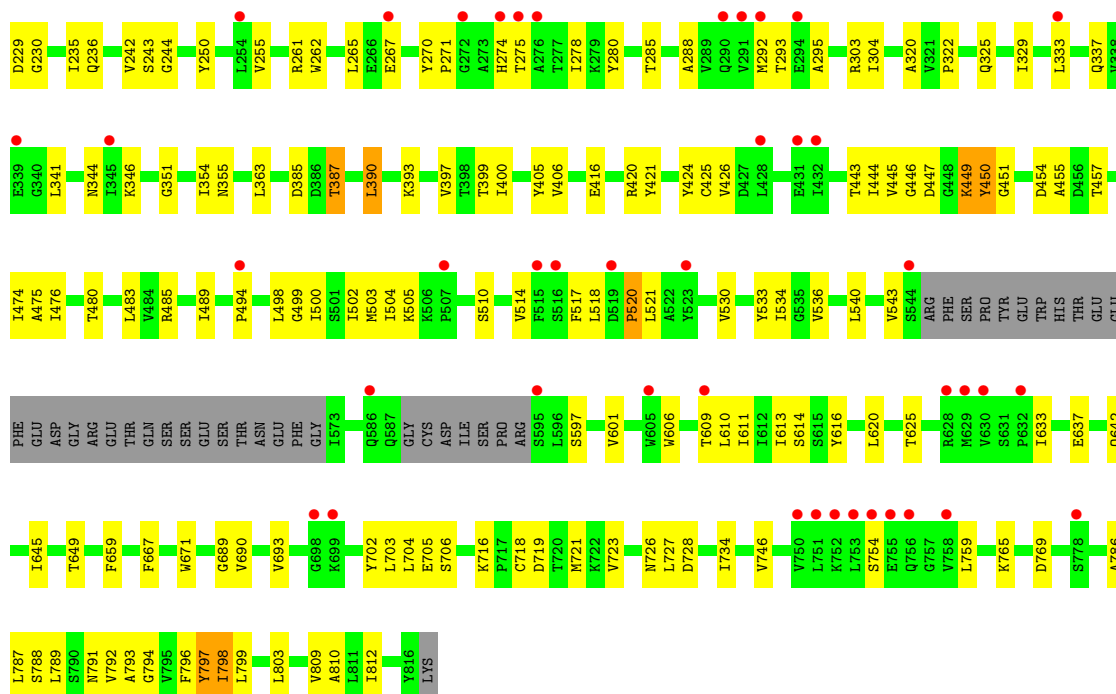
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Glutamate receptor 2

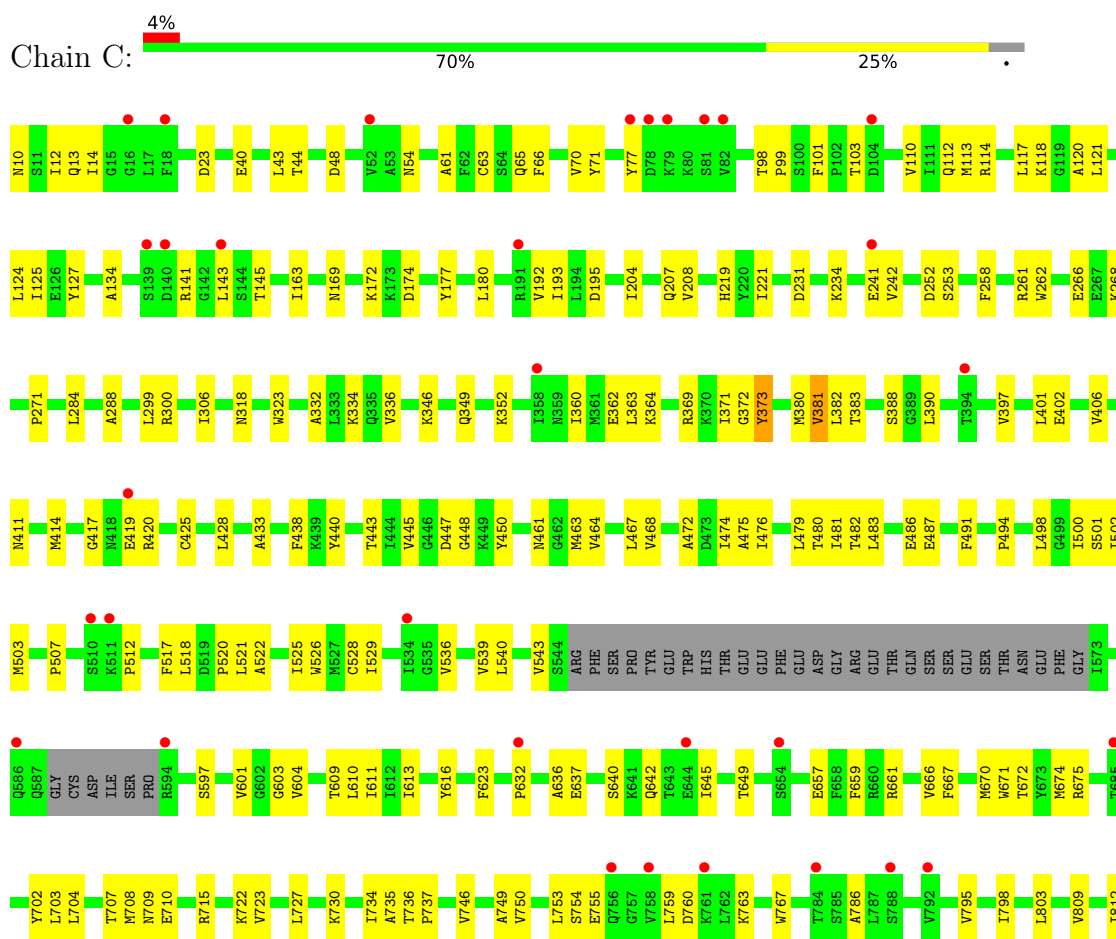


• Molecule 1: Glutamate receptor 2



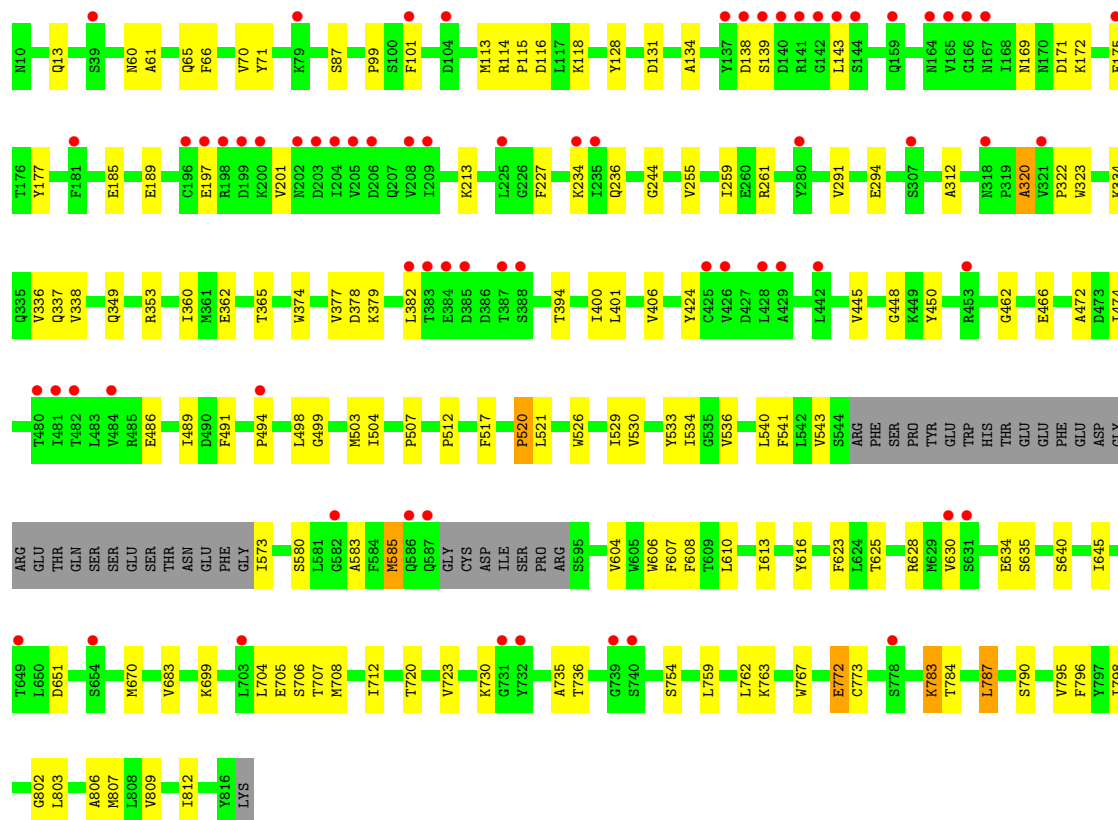
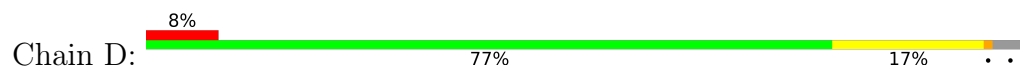


• Molecule 1: Glutamate receptor 2





• Molecule 1: Glutamate receptor 2



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	92.79Å 110.40Å 600.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.91 – 4.25 48.91 – 4.25	Depositor EDS
% Data completeness (in resolution range)	99.7 (48.91-4.25) 99.5 (48.91-4.25)	Depositor EDS
R_{merge}	0.45	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.89 (at 4.29Å)	Xtriage
Refinement program	PHENIX (1.16_3549)	Depositor
R, R_{free}	0.260 , 0.296 0.268 , 0.293	Depositor DCC
R_{free} test set	2226 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	217.9	Xtriage
Anisotropy	0.169	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 207.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	23775	wwPDB-VP
Average B, all atoms (Å ²)	259.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.30% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: V8G, NAG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.20	0/6031	0.36	0/8167
1	B	0.25	3/6073 (0.0%)	0.41	1/8221 (0.0%)
1	C	0.15	0/6037	0.32	0/8180
1	D	0.25	0/6028	0.41	1/8165 (0.0%)
All	All	0.22	3/24169 (0.0%)	0.38	2/32733 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	450	TYR	CA-C	7.00	1.61	1.52
1	B	449	LYS	C-N	6.30	1.42	1.33
1	B	450	TYR	N-CA	6.08	1.53	1.46

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	450	TYR	N-CA-C	9.27	124.82	109.06
1	D	628	ARG	N-CA-C	-5.08	104.63	111.54

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	449	LYS	Mainchain

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	5912	0	5783	143	0
1	B	5954	0	5844	161	1
1	C	5918	0	5758	145	1
1	D	5909	0	5755	111	0
2	A	14	0	13	2	0
2	B	14	0	13	15	0
2	C	14	0	13	0	0
2	D	14	0	13	1	0
3	A	13	0	0	12	0
3	C	13	0	0	9	0
All	All	23775	0	23192	509	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 11.

All (509) 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:355:ASN:HD21	2:B:901:NAG:C1	1.06	1.60
1:A:355:ASN:HD21	2:A:901:NAG:C1	1.03	1.58
3:A:902:V8G:CAI	1:D:610:LEU:HD12	1.47	1.45
1:B:355:ASN:ND2	2:B:901:NAG:C1	1.73	1.44
1:A:355:ASN:ND2	2:A:901:NAG:C1	1.88	1.35
3:A:902:V8G:CAI	1:D:610:LEU:CD1	2.32	1.07
1:B:337:GLN:NE2	2:B:901:NAG:O7	1.87	1.07
3:A:902:V8G:CAJ	1:D:610:LEU:HD12	1.83	1.07
3:A:902:V8G:CAJ	1:D:610:LEU:CD1	2.36	1.04
1:B:451:GLY:HA3	1:B:485:ARG:HH21	1.19	1.04
1:A:613:ILE:HG22	3:A:902:V8G:CAB	1.94	0.96
1:B:344:ASN:ND2	2:B:901:NAG:O5	1.97	0.96
1:A:525:ILE:O	1:A:529:ILE:HG22	1.65	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:449:LYS:HB3	1:A:462:GLY:HA2	1.45	0.96
1:B:610:LEU:HD23	3:C:902:V8G:CAL	1.97	0.94
1:B:610:LEU:CD2	3:C:902:V8G:CAL	2.50	0.89
1:C:539:VAL:HG21	1:D:803:LEU:HB3	1.58	0.85
1:A:521:LEU:HD13	1:A:616:TYR:HD1	1.44	0.81
1:B:344:ASN:HD21	2:B:901:NAG:H2	1.44	0.81
1:B:346:LYS:HG3	1:B:354:ILE:HG13	1.64	0.79
1:C:613:ILE:HG22	3:C:902:V8G:CAM	2.13	0.78
1:A:525:ILE:HG13	1:B:789:LEU:HD12	1.66	0.78
1:C:318:ASN:HB2	1:D:60:ASN:HD21	1.51	0.76
1:B:498:LEU:HD12	1:B:705:GLU:HB2	1.68	0.76
1:A:611:ILE:HG12	1:B:517:PHE:HE1	1.50	0.75
1:B:344:ASN:ND2	2:B:901:NAG:C1	2.50	0.75
1:A:516:SER:HA	1:A:519:ASP:HB2	1.69	0.73
1:B:451:GLY:HA3	1:B:485:ARG:NH2	2.01	0.72
1:A:103:THR:O	1:A:352:LYS:NZ	2.23	0.72
1:B:649:THR:HG22	1:B:703:LEU:HB2	1.72	0.71
1:D:337:GLN:NE2	2:D:901:NAG:O7	2.21	0.71
1:A:358:ILE:HD12	1:A:374:TRP:HE1	1.54	0.71
1:C:402:GLU:OE1	1:C:450:TYR:OH	2.08	0.71
1:A:642:GLN:HE22	1:A:645:ILE:HB	1.55	0.71
1:B:614:SER:HB2	3:C:902:V8G:OAK	1.91	0.70
1:C:616:TYR:CD1	3:C:902:V8G:OAA	2.43	0.70
1:B:610:LEU:HD12	1:B:613:ILE:HD11	1.73	0.70
1:C:498:LEU:HB3	1:C:707:THR:HG23	1.72	0.69
1:C:360:ILE:HB	1:C:372:GLY:HA3	1.74	0.69
1:C:12:ILE:HG23	1:C:71:TYR:HD2	1.58	0.69
1:A:411:ASN:HB2	1:A:414:MET:HE2	1.75	0.69
1:C:642:GLN:HE22	1:C:645:ILE:HB	1.57	0.69
1:B:494:PRO:HG3	1:C:494:PRO:HG3	1.75	0.69
1:B:611:ILE:HG21	1:C:795:VAL:HG21	1.74	0.69
1:C:498:LEU:HG	1:C:730:LYS:HG3	1.75	0.68
1:D:645:ILE:HG12	1:D:699:LYS:HA	1.76	0.68
1:D:377:VAL:HG23	1:D:378:ASP:H	1.58	0.68
1:A:659:PHE:HB3	1:A:671:TRP:HB2	1.74	0.68
1:C:177:TYR:HB3	1:C:207:GLN:HG2	1.76	0.68
1:C:521:LEU:CD2	3:C:902:V8G:CAJ	2.72	0.68
1:C:640:SER:HB3	1:C:670:MET:HG2	1.75	0.68
1:A:529:ILE:HG13	3:A:902:V8G:OAA	1.94	0.67
1:B:267:GLU:HB2	1:B:274:HIS:HB2	1.76	0.67
1:B:483:LEU:N	1:C:755:GLU:OE2	2.27	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:157:LYS:HD2	1:B:187:LYS:HE3	1.77	0.67
1:A:714:GLN:HA	1:A:773:CYS:HB2	1.76	0.67
1:C:603:GLY:HA2	1:D:585:MET:HA	1.77	0.66
1:C:649:THR:HG22	1:C:703:LEU:HB2	1.76	0.66
1:C:474:ILE:HG13	1:C:736:THR:HG22	1.75	0.66
1:A:611:ILE:HG12	1:B:517:PHE:CE1	2.30	0.66
1:D:334:LYS:NZ	1:D:349:GLN:O	2.26	0.66
1:D:498:LEU:HD12	1:D:705:GLU:HB2	1.78	0.66
1:C:71:TYR:HA	1:C:323:TRP:HH2	1.61	0.65
1:D:498:LEU:HG	1:D:730:LYS:HG3	1.77	0.65
1:B:344:ASN:HD22	2:B:901:NAG:C5	2.09	0.65
1:C:411:ASN:HB2	1:C:414:MET:HE2	1.77	0.65
1:C:371:ILE:HA	1:C:382:LEU:HD22	1.79	0.65
1:D:294:GLU:HG3	1:D:338:VAL:HG11	1.78	0.65
1:C:143:LEU:HG	1:D:143:LEU:HD11	1.79	0.65
1:A:124:LEU:HD13	1:A:360:ILE:HD13	1.79	0.65
1:A:374:TRP:HB2	1:A:379:LYS:HE3	1.79	0.65
1:C:754:SER:HB2	1:C:759:LEU:HD12	1.77	0.65
1:C:10:ASN:HB3	1:C:300:ARG:HH22	1.62	0.64
1:D:101:PHE:HA	1:D:114:ARG:HD2	1.78	0.64
1:B:642:GLN:HE22	1:B:645:ILE:HB	1.63	0.64
1:B:521:LEU:HD13	1:B:616:TYR:HD1	1.61	0.64
1:B:344:ASN:ND2	2:B:901:NAG:H2	2.13	0.63
1:C:521:LEU:HD13	1:C:616:TYR:HD2	1.63	0.63
1:D:185:GLU:OE1	1:D:213:LYS:NZ	2.27	0.63
1:B:145:THR:OG1	1:B:195:ASP:OD2	2.17	0.62
1:B:235:ILE:HD12	1:B:242:VAL:HG21	1.80	0.62
3:A:902:V8G:CAJ	1:D:610:LEU:HD13	2.27	0.62
1:B:536:VAL:HG22	1:C:803:LEU:HD21	1.79	0.62
1:B:236:GLN:HG3	1:B:363:LEU:HD11	1.81	0.62
1:C:134:ALA:HB3	1:C:192:VAL:HG22	1.81	0.62
1:D:498:LEU:HB3	1:D:707:THR:HG23	1.82	0.62
1:A:299:LEU:HD13	1:A:306:ILE:HG21	1.81	0.62
1:D:634:GLU:HA	1:D:723:VAL:HB	1.81	0.62
1:A:33:MET:HE1	1:A:43:LEU:HB2	1.82	0.62
1:C:417:GLY:O	1:C:420:ARG:NE	2.33	0.62
1:C:475:ALA:HB3	1:C:735:ALA:HB3	1.80	0.62
1:B:734:ILE:HG21	1:B:746:VAL:HG11	1.80	0.61
1:B:355:ASN:CG	2:B:901:NAG:C1	2.68	0.61
1:B:400:ILE:HG21	1:B:450:TYR:HE2	1.65	0.61
1:B:754:SER:HB2	1:B:759:LEU:HD12	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:299:LEU:HD13	1:C:306:ILE:HG21	1.83	0.61
1:C:540:LEU:HA	1:C:543:VAL:HG22	1.80	0.61
1:D:754:SER:HB2	1:D:759:LEU:HD12	1.82	0.61
1:A:121:LEU:HD21	1:A:193:ILE:HG21	1.82	0.60
1:B:236:GLN:HA	1:B:363:LEU:HD21	1.83	0.60
1:A:209:ILE:HA	1:A:214:HIS:CD2	2.36	0.60
1:A:613:ILE:HB	3:A:902:V8G:CAJ	2.31	0.60
1:A:649:THR:HG22	1:A:703:LEU:HB2	1.83	0.59
1:C:501:SER:N	1:C:704:LEU:O	2.31	0.59
1:C:48:ASP:OD1	1:C:65:GLN:NE2	2.35	0.58
1:B:611:ILE:HD12	1:C:517:PHE:HE1	1.69	0.58
1:A:185:GLU:OE1	1:A:213:LYS:NZ	2.31	0.58
1:B:229:ASP:OD2	1:B:280:TYR:N	2.36	0.58
1:C:174:ASP:OD1	1:C:207:GLN:NE2	2.36	0.58
1:B:503:MET:HE1	1:B:690:VAL:HG22	1.86	0.58
1:D:466:GLU:O	1:D:472:ALA:N	2.36	0.58
1:B:304:ILE:HD12	1:B:304:ILE:O	2.03	0.58
1:B:667:PHE:HE1	1:B:727:LEU:HD13	1.69	0.57
1:A:198:ARG:HD3	1:A:279:LYS:HD2	1.85	0.57
1:B:344:ASN:ND2	2:B:901:NAG:C2	2.67	0.57
1:B:502:ILE:HB	1:B:723:VAL:HG23	1.87	0.57
1:D:115:PRO:HA	1:D:353:ARG:HB2	1.85	0.57
1:B:213:LYS:O	1:B:220:TYR:OH	2.21	0.57
1:D:134:ALA:HB2	1:D:189:GLU:HG2	1.86	0.57
1:D:540:LEU:HA	1:D:543:VAL:HG22	1.87	0.57
1:C:14:ILE:HD13	1:C:43:LEU:HD23	1.87	0.56
1:C:521:LEU:HD23	3:C:902:V8G:CAJ	2.35	0.56
1:C:13:GLN:HA	1:C:44:THR:HB	1.87	0.56
1:C:242:VAL:HB	1:C:363:LEU:HB3	1.87	0.56
1:C:362:GLU:HG3	1:C:371:ILE:HG21	1.87	0.56
1:B:518:LEU:H	1:B:518:LEU:HD23	1.71	0.56
1:D:143:LEU:H	1:D:143:LEU:HD23	1.71	0.56
1:C:502:ILE:O	1:C:709:ASN:ND2	2.32	0.56
1:C:518:LEU:O	1:C:526:TRP:NE1	2.39	0.56
1:B:43:LEU:HD21	1:B:293:THR:HG22	1.88	0.56
1:B:499:GLY:HA3	1:B:726:ASN:HB3	1.86	0.55
1:A:809:VAL:HG13	1:A:812:ILE:HD11	1.88	0.55
1:B:480:THR:O	1:B:485:ARG:NH1	2.39	0.55
1:C:382:LEU:HG	1:C:383:THR:N	2.22	0.55
1:C:702:TYR:CE2	1:C:704:LEU:HB3	2.42	0.55
1:A:101:PHE:HA	1:A:114:ARG:HD2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:141:ARG:NH2	1:C:195:ASP:OD1	2.40	0.54
1:A:613:ILE:CG2	3:A:902:V8G:CAB	2.78	0.54
1:B:614:SER:CB	3:C:902:V8G:OAK	2.55	0.54
1:D:606:TRP:C	1:D:610:LEU:HD23	2.32	0.54
1:C:623:PHE:HE1	1:D:784:THR:HA	1.72	0.54
1:A:120:ALA:HA	1:A:379:LYS:NZ	2.23	0.54
1:B:787:LEU:HG	1:B:788:SER:N	2.21	0.54
1:A:498:LEU:HB3	1:A:707:THR:HG23	1.90	0.54
1:D:640:SER:HB3	1:D:670:MET:HG2	1.90	0.54
1:C:23:ASP:HB3	1:C:271:PRO:HG2	1.90	0.53
1:C:373:TYR:HB3	1:C:381:VAL:O	2.08	0.53
1:D:169:ASN:ND2	1:D:171:ASP:OD1	2.41	0.53
1:A:494:PRO:HG3	1:D:494:PRO:HG3	1.90	0.53
1:C:522:ALA:H	1:D:787:LEU:HD12	1.73	0.53
1:B:198:ARG:HE	1:B:230:GLY:HA2	1.73	0.53
1:A:622:ALA:HA	1:B:625:THR:HG22	1.91	0.53
1:B:500:ILE:HB	1:B:727:LEU:HB2	1.89	0.53
1:C:117:LEU:HD12	1:C:120:ALA:HB3	1.90	0.53
1:B:132:LYS:NZ	1:B:189:GLU:OE2	2.40	0.53
1:C:710:GLU:HG3	1:C:722:LYS:HD2	1.91	0.53
1:D:607:PHE:HA	1:D:610:LEU:HD23	1.91	0.53
1:A:135:TYR:CE2	1:A:137:TYR:HB3	2.44	0.53
1:A:521:LEU:HB3	1:A:526:TRP:NE1	2.23	0.53
1:A:517:PHE:CE1	1:A:795:VAL:HG22	2.44	0.53
1:A:803:LEU:HD11	1:D:536:VAL:HG22	1.91	0.53
1:B:416:GLU:HA	1:B:420:ARG:HD3	1.89	0.53
1:A:521:LEU:HD12	1:B:787:LEU:HD22	1.91	0.52
1:B:344:ASN:HD21	2:B:901:NAG:C2	2.18	0.52
1:D:541:PHE:CZ	1:D:573:ILE:HA	2.44	0.52
1:A:13:GLN:HG2	1:A:70:VAL:HG12	1.90	0.52
1:B:765:LYS:HA	1:B:769:ASP:HB2	1.91	0.52
1:C:522:ALA:HB3	1:C:525:ILE:HD13	1.90	0.52
1:D:521:LEU:HB2	1:D:526:TRP:CE2	2.45	0.52
1:A:525:ILE:HD11	1:B:789:LEU:HB2	1.92	0.52
1:B:23:ASP:HB3	1:B:271:PRO:HG2	1.91	0.52
1:B:799:LEU:O	1:B:803:LEU:N	2.40	0.52
1:B:250:TYR:OH	1:B:278:ILE:N	2.36	0.52
1:C:61:ALA:O	1:C:65:GLN:HG2	2.10	0.52
1:A:586:GLN:HA	1:D:606:TRP:CD2	2.46	0.51
1:D:255:VAL:O	1:D:259:ILE:N	2.35	0.51
1:A:131:ASP:N	1:A:131:ASP:OD1	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:131:ASP:OD1	1:B:132:LYS:N	2.43	0.51
1:D:71:TYR:HA	1:D:323:TRP:HH2	1.75	0.51
1:A:110:VAL:O	1:A:351:GLY:HA3	2.09	0.51
1:C:101:PHE:HA	1:C:114:ARG:HD2	1.92	0.51
1:B:26:TYR:HE2	1:B:47:ILE:HG12	1.75	0.51
1:C:99:PRO:HB3	1:C:284:LEU:HB2	1.93	0.51
1:C:112:GLN:HE22	1:C:352:LYS:HD3	1.75	0.51
1:B:540:LEU:HA	1:B:543:VAL:HG22	1.93	0.51
1:A:89:CYS:SG	1:A:96:PHE:HB2	2.51	0.50
1:A:134:ALA:HB3	1:A:192:VAL:HG13	1.91	0.50
1:A:543:VAL:HG12	1:B:810:ALA:HB2	1.91	0.50
1:B:474:ILE:HG12	1:B:475:ALA:H	1.76	0.50
1:A:169:ASN:ND2	1:A:171:ASP:OD1	2.44	0.50
1:B:195:ASP:HA	1:B:223:ALA:HB3	1.94	0.50
1:A:607:PHE:HA	1:A:610:LEU:HB3	1.93	0.50
1:A:613:ILE:HB	3:A:902:V8G:CAI	2.41	0.50
1:A:539:VAL:HG21	1:B:803:LEU:HB3	1.94	0.50
1:A:231:ASP:HB3	1:A:234:LYS:HE2	1.93	0.50
1:B:118:LYS:HB3	1:B:145:THR:HG22	1.93	0.50
1:D:291:VAL:HA	1:D:336:VAL:HG11	1.94	0.50
1:D:450:TYR:HA	1:D:462:GLY:HA3	1.92	0.50
1:D:66:PHE:CE2	1:D:312:ALA:HB1	2.47	0.50
1:A:96:PHE:O	1:A:111:ILE:N	2.37	0.50
1:B:702:TYR:CE2	1:B:704:LEU:HB3	2.47	0.50
1:C:397:VAL:O	1:C:443:THR:OG1	2.24	0.50
1:B:97:ILE:HD11	1:B:333:LEU:HD22	1.94	0.49
1:B:346:LYS:HE3	1:B:355:ASN:HD22	1.77	0.49
1:B:346:LYS:HZ1	2:B:901:NAG:H82	1.76	0.49
1:B:610:LEU:HD21	3:C:902:V8G:CAL	2.38	0.49
1:A:532:ALA:HB2	1:B:796:PHE:CE1	2.47	0.49
1:C:604:VAL:HG21	1:D:802:GLY:HA3	1.94	0.49
1:C:609:THR:O	1:C:613:ILE:HG23	2.13	0.49
1:A:297:ARG:HG2	1:A:301:LYS:HE3	1.94	0.49
1:C:110:VAL:HG12	1:C:112:GLN:HG3	1.93	0.49
1:A:96:PHE:CE2	1:A:98:THR:HB	2.47	0.49
1:C:193:ILE:HG12	1:C:221:ILE:HB	1.93	0.49
1:B:597:SER:HB2	1:C:809:VAL:HG12	1.94	0.49
1:A:493:LYS:HG3	1:A:751:LEU:HD21	1.93	0.49
1:A:530:VAL:HA	1:A:533:TYR:HB3	1.94	0.49
1:B:227:PHE:CD1	1:B:244:GLY:HA3	2.48	0.49
1:B:728:ASP:HA	1:C:760:ASP:OD2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:507:PRO:HG2	1:D:630:VAL:HA	1.95	0.49
1:D:61:ALA:O	1:D:65:GLN:HG2	2.13	0.49
1:A:242:VAL:HB	1:A:363:LEU:HB3	1.93	0.49
1:C:611:ILE:HG21	1:D:517:PHE:HE1	1.77	0.49
1:A:358:ILE:HB	1:A:374:TRP:CD1	2.47	0.49
1:B:809:VAL:O	1:B:812:ILE:HG12	2.12	0.49
1:A:125:ILE:HG23	1:A:130:TRP:HB2	1.95	0.49
1:C:450:TYR:HA	1:C:463:MET:HE2	1.94	0.49
1:A:255:VAL:O	1:A:259:ILE:HG12	2.13	0.48
1:B:503:MET:HA	1:B:721:MET:O	2.13	0.48
1:C:54:ASN:OD1	1:D:87:SER:OG	2.30	0.48
1:D:763:LYS:O	1:D:767:TRP:HB2	2.13	0.48
1:B:128:TYR:OH	1:B:243:SER:OG	2.19	0.48
1:C:476:ILE:HG12	1:C:734:ILE:HG23	1.94	0.48
1:C:636:ALA:CB	1:C:727:LEU:HD21	2.44	0.48
1:B:38:THR:OG1	1:B:39:SER:N	2.47	0.48
1:D:360:ILE:HD11	1:D:374:TRP:HB2	1.96	0.48
1:A:480:THR:O	1:A:485:ARG:NH1	2.46	0.48
1:A:521:LEU:HA	1:B:787:LEU:HD22	1.96	0.48
1:A:799:LEU:HA	1:D:604:VAL:HG12	1.95	0.48
1:B:476:ILE:HG22	1:B:734:ILE:HG23	1.94	0.48
1:C:666:VAL:O	1:C:670:MET:HG3	2.14	0.48
1:C:543:VAL:HG11	1:D:806:ALA:HB1	1.95	0.48
1:D:651:ASP:HB2	1:D:683:VAL:O	2.14	0.48
1:C:657:GLU:HB3	1:C:661:ARG:HH12	1.78	0.48
1:D:131:ASP:N	1:D:131:ASP:OD1	2.43	0.48
1:D:504:ILE:HD11	1:D:723:VAL:HG11	1.94	0.48
1:A:120:ALA:HB2	1:A:374:TRP:NE1	2.28	0.48
1:C:163:ILE:HG21	1:C:180:LEU:HD13	1.94	0.48
1:B:791:ASN:O	1:B:791:ASN:ND2	2.46	0.48
1:C:500:ILE:HB	1:C:727:LEU:HB2	1.96	0.48
1:B:14:ILE:O	1:B:45:PRO:HA	2.14	0.47
1:C:517:PHE:CE1	1:C:795:VAL:HG22	2.49	0.47
1:A:611:ILE:HD11	1:B:616:TYR:CZ	2.49	0.47
1:A:543:VAL:HA	1:B:810:ALA:HB1	1.96	0.47
1:B:346:LYS:NZ	2:B:901:NAG:H82	2.29	0.47
1:D:382:LEU:H	1:D:382:LEU:HD23	1.78	0.47
1:D:499:GLY:O	1:D:706:SER:N	2.48	0.47
1:A:449:LYS:CB	1:A:462:GLY:HA2	2.32	0.47
1:A:637:GLU:H	1:A:637:GLU:CD	2.23	0.47
1:B:337:GLN:HE22	2:B:901:NAG:C7	2.24	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:252:ASP:OD1	1:C:253:SER:N	2.47	0.47
1:C:334:LYS:NZ	1:C:349:GLN:O	2.35	0.47
1:C:749:ALA:O	1:C:753:LEU:HG	2.14	0.47
1:A:255:VAL:HG22	1:A:341:LEU:HA	1.95	0.47
3:A:902:V8G:CAM	1:D:610:LEU:HG	2.45	0.47
1:C:318:ASN:HB2	1:D:60:ASN:ND2	2.25	0.47
1:A:196:CYS:HB3	1:A:200:LYS:HB2	1.96	0.47
1:A:520:PRO:HG3	1:A:620:LEU:HD13	1.96	0.47
1:B:209:ILE:HG23	1:B:214:HIS:NE2	2.30	0.47
1:B:261:ARG:O	1:B:265:LEU:HG	2.15	0.47
1:B:504:ILE:HD13	1:B:633:ILE:HD12	1.95	0.47
1:C:125:ILE:HG12	1:C:193:ILE:HD11	1.97	0.47
1:C:597:SER:O	1:C:601:VAL:HG23	2.14	0.47
1:D:172:LYS:NZ	1:D:175:GLU:OE1	2.47	0.47
1:B:97:ILE:HG12	1:B:111:ILE:HB	1.96	0.47
1:D:503:MET:HG3	1:D:720:THR:HB	1.96	0.47
1:A:137:TYR:HA	1:A:195:ASP:HB3	1.96	0.47
1:B:514:VAL:HG23	1:B:794:GLY:HA2	1.96	0.47
1:B:262:TRP:HD1	1:B:275:THR:O	1.98	0.47
1:C:401:LEU:HD23	1:C:406:VAL:HG12	1.97	0.47
1:A:71:TYR:HA	1:A:323:TRP:HH2	1.79	0.46
1:A:157:LYS:HD3	1:B:186:LEU:HB3	1.98	0.46
1:B:135:TYR:CD1	1:B:146:LEU:HD13	2.50	0.46
1:A:291:VAL:HA	1:A:336:VAL:HG11	1.96	0.46
1:A:684:ARG:HG2	1:A:685:THR:HG23	1.96	0.46
1:B:74:PHE:HA	1:B:97:ILE:O	2.14	0.46
1:D:772:GLU:H	1:D:772:GLU:HG2	1.49	0.46
1:B:77:TYR:CE2	1:B:98:THR:HG21	2.50	0.46
1:B:255:VAL:HG22	1:B:341:LEU:HD22	1.98	0.46
1:C:518:LEU:HD23	1:C:518:LEU:H	1.80	0.46
1:B:454:ASP:HB3	1:B:457:THR:HB	1.97	0.46
1:C:657:GLU:HB3	1:C:661:ARG:NH1	2.30	0.46
1:D:580:SER:HA	1:D:583:ALA:HB3	1.98	0.46
1:B:27:SER:HB3	1:B:270:TYR:HB3	1.97	0.46
1:B:499:GLY:O	1:B:706:SER:N	2.49	0.46
1:C:118:LYS:HG2	1:C:145:THR:HG22	1.97	0.46
1:C:481:ILE:HA	1:C:491:PHE:CE2	2.50	0.46
1:D:489:ILE:HD13	1:D:735:ALA:HB1	1.98	0.46
1:D:517:PHE:O	1:D:520:PRO:HD2	2.16	0.46
1:A:221:ILE:HG12	1:A:243:SER:HB2	1.98	0.46
1:A:227:PHE:CD1	1:A:244:GLY:HA3	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:613:ILE:HG22	3:A:902:V8G:CAI	2.46	0.46
1:C:521:LEU:HD13	1:C:616:TYR:CD2	2.47	0.46
1:A:525:ILE:O	1:A:529:ILE:CG2	2.52	0.46
1:A:529:ILE:O	1:A:529:ILE:HG12	2.10	0.46
1:A:619:ASN:CG	1:B:787:LEU:HB2	2.41	0.46
1:C:438:PHE:CE1	1:C:440:TYR:HB3	2.50	0.46
1:A:785:SER:HA	1:D:623:PHE:CZ	2.51	0.46
1:B:295:ALA:HB2	1:B:333:LEU:HD23	1.97	0.46
1:B:444:ILE:HG22	1:B:446:GLY:H	1.79	0.46
1:C:397:VAL:HG13	1:C:474:ILE:HG23	1.97	0.46
1:A:213:LYS:O	1:A:220:TYR:OH	2.33	0.46
1:A:344:ASN:O	1:A:353:ARG:NH2	2.49	0.46
1:C:169:ASN:HD21	1:C:172:LYS:HD3	1.81	0.46
1:C:231:ASP:HB3	1:C:234:LYS:HE2	1.98	0.46
1:C:447:ASP:OD1	1:C:447:ASP:N	2.49	0.46
1:C:479:LEU:HD23	1:C:735:ALA:HB2	1.97	0.46
1:B:400:ILE:HG21	1:B:450:TYR:CE2	2.47	0.45
1:C:177:TYR:CB	1:C:207:GLN:HG2	2.46	0.45
1:D:227:PHE:CD1	1:D:244:GLY:HA3	2.51	0.45
1:A:499:GLY:O	1:A:706:SER:N	2.49	0.45
1:D:400:ILE:HG21	1:D:450:TYR:CE2	2.51	0.45
1:A:308:ARG:NE	1:A:312:ALA:HB2	2.31	0.45
1:A:375:SER:N	1:A:378:ASP:O	2.48	0.45
1:A:500:ILE:HD13	1:A:655:THR:HG23	1.98	0.45
1:C:483:LEU:O	1:C:487:GLU:HG3	2.17	0.45
1:C:536:VAL:HG22	1:D:803:LEU:HD21	1.97	0.45
1:D:401:LEU:HD23	1:D:406:VAL:HG12	1.98	0.45
1:D:424:TYR:CE1	1:D:762:LEU:HB3	2.51	0.45
1:B:520:PRO:HG3	1:B:620:LEU:HD13	1.99	0.45
1:C:124:LEU:HD13	1:C:360:ILE:HD13	1.97	0.45
1:C:464:VAL:O	1:C:468:VAL:HG23	2.17	0.45
1:C:502:ILE:HB	1:C:723:VAL:HG23	1.99	0.45
1:C:809:VAL:HA	1:C:812:ILE:HG12	1.99	0.45
1:D:474:ILE:HG13	1:D:736:THR:HG22	1.98	0.45
1:A:540:LEU:HG	1:A:601:VAL:HG11	1.99	0.45
1:B:261:ARG:HD2	1:B:261:ARG:HA	1.70	0.45
1:B:530:VAL:O	1:B:534:ILE:HG12	2.16	0.45
1:C:671:TRP:HA	1:C:674:MET:HE2	1.98	0.45
1:B:793:ALA:O	1:B:797:TYR:N	2.46	0.45
1:C:369:ARG:HD2	1:C:388:SER:H	1.82	0.45
1:A:127:TYR:CG	1:A:380:MET:HE2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:397:VAL:HG13	1:A:474:ILE:HG23	1.99	0.45
1:B:113:MET:HG3	1:B:288:ALA:HB2	1.98	0.45
1:D:503:MET:HE3	1:D:704:LEU:HD21	1.98	0.45
1:A:485:ARG:O	1:A:489:ILE:HG13	2.17	0.45
1:B:114:ARG:HD2	1:B:280:TYR:HE2	1.82	0.45
1:C:438:PHE:CD1	1:C:440:TYR:HB3	2.52	0.45
1:B:789:LEU:HG	1:B:792:VAL:HB	1.98	0.44
1:C:121:LEU:O	1:C:125:ILE:HG13	2.17	0.44
1:C:299:LEU:HD13	1:C:306:ILE:HD13	1.98	0.44
1:D:512:PRO:HB2	1:D:790:SER:CB	2.47	0.44
1:A:671:TRP:CZ2	1:A:675:ARG:HD3	2.53	0.44
1:B:689:GLY:O	1:B:693:VAL:HG23	2.17	0.44
1:C:332:ALA:O	1:C:336:VAL:HG23	2.18	0.44
1:D:517:PHE:CE1	1:D:795:VAL:HG22	2.53	0.44
1:D:809:VAL:HA	1:D:812:ILE:HG12	1.98	0.44
1:C:467:LEU:HD22	1:C:737:PRO:HG3	1.99	0.44
1:B:485:ARG:O	1:B:489:ILE:HG13	2.18	0.44
1:D:13:GLN:HG3	1:D:70:VAL:HG12	2.00	0.44
1:A:177:TYR:CD2	1:A:207:GLN:HG3	2.53	0.44
1:B:33:MET:SD	1:B:45:PRO:HG3	2.58	0.44
1:B:242:VAL:O	1:B:363:LEU:N	2.51	0.44
1:A:117:LEU:HD12	1:A:120:ALA:HB3	2.00	0.43
1:B:517:PHE:HB2	1:B:791:ASN:ND2	2.32	0.43
1:B:606:TRP:HA	1:B:609:THR:HG22	2.00	0.43
1:D:197:GLU:O	1:D:201:VAL:HG23	2.18	0.43
1:A:70:VAL:O	1:A:308:ARG:NH1	2.51	0.43
1:B:421:TYR:O	1:B:426:VAL:HG11	2.18	0.43
1:C:63:CYS:HA	1:C:66:PHE:HB3	2.00	0.43
1:C:103:THR:O	1:C:352:LYS:NZ	2.51	0.43
1:D:66:PHE:CZ	1:D:312:ALA:HB1	2.53	0.43
1:D:795:VAL:O	1:D:798:ILE:HG22	2.18	0.43
1:A:261:ARG:O	1:A:265:LEU:HG	2.18	0.43
1:A:521:LEU:HA	1:B:787:LEU:CD2	2.47	0.43
1:A:639:LEU:HD21	1:A:647:TYR:CD2	2.54	0.43
1:C:258:PHE:O	1:C:262:TRP:N	2.51	0.43
1:A:122:LEU:HD23	1:A:122:LEU:HA	1.90	0.43
1:A:211:ILE:HG13	1:A:213:LYS:HG3	1.99	0.43
1:A:521:LEU:HD12	1:B:787:LEU:CD2	2.48	0.43
1:B:320:ALA:O	1:B:322:PRO:HD3	2.18	0.43
1:B:716:LYS:HA	1:B:718:CYS:N	2.34	0.43
1:C:529:ILE:HA	1:D:796:PHE:CZ	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:113:MET:HE3	1:A:113:MET:HB3	1.89	0.43
1:C:364:LYS:HG3	1:C:369:ARG:NH2	2.33	0.43
1:A:702:TYR:HE2	1:A:704:LEU:HD13	1.84	0.43
1:C:204:ILE:O	1:C:208:VAL:HG23	2.19	0.43
1:D:606:TRP:CE3	1:D:610:LEU:HD21	2.54	0.43
1:A:522:ALA:H	1:B:787:LEU:HD23	1.83	0.43
1:C:503:MET:HE3	1:C:704:LEU:HD21	2.00	0.43
1:A:288:ALA:O	1:A:292:MET:HG3	2.19	0.43
1:A:705:GLU:CD	1:A:705:GLU:H	2.27	0.43
1:A:710:GLU:O	1:A:714:GLN:HG2	2.19	0.43
1:B:514:VAL:HG21	1:B:797:TYR:CD2	2.53	0.43
1:B:637:GLU:H	1:B:637:GLU:CD	2.26	0.43
1:D:234:LYS:H	1:D:234:LYS:HG2	1.63	0.43
1:A:391:GLU:HA	1:A:393:LYS:HE2	2.01	0.43
1:A:445:VAL:HG22	1:A:446:GLY:H	1.84	0.43
1:C:667:PHE:HE1	1:C:727:LEU:HD13	1.83	0.43
1:D:530:VAL:O	1:D:534:ILE:HG12	2.19	0.43
1:B:225:LEU:HB2	1:B:280:TYR:CD2	2.54	0.42
1:B:454:ASP:OD1	1:B:455:ALA:N	2.46	0.42
1:D:169:ASN:OD1	1:D:169:ASN:N	2.47	0.42
1:A:153:ALA:HA	1:A:158:TRP:HB2	2.01	0.42
1:B:719:ASP:OD1	1:B:719:ASP:N	2.53	0.42
1:C:13:GLN:HG2	1:C:70:VAL:HG12	2.01	0.42
1:D:606:TRP:O	1:D:610:LEU:HD23	2.20	0.42
1:D:708:MET:O	1:D:712:ILE:HG12	2.18	0.42
1:D:783:LYS:HB2	1:D:783:LYS:HE3	1.43	0.42
1:A:299:LEU:HD13	1:A:306:ILE:HD13	2.01	0.42
1:A:543:VAL:HG21	1:A:601:VAL:HG21	2.00	0.42
1:A:623:PHE:HZ	1:B:786:ALA:HA	1.83	0.42
1:B:337:GLN:NE2	2:B:901:NAG:C7	2.75	0.42
1:C:445:VAL:HG22	1:C:448:GLY:H	1.85	0.42
1:C:610:LEU:HD21	1:D:613:ILE:HG22	2.00	0.42
1:C:704:LEU:HD12	1:C:708:MET:HB3	2.00	0.42
1:D:128:TYR:OH	1:D:362:GLU:OE2	2.29	0.42
1:D:138:ASP:OD1	1:D:139:SER:N	2.53	0.42
1:D:533:TYR:CD1	1:D:533:TYR:C	2.97	0.42
1:D:606:TRP:CD2	1:D:610:LEU:HD21	2.54	0.42
1:A:215:VAL:HA	1:A:238:GLY:O	2.19	0.42
1:A:795:VAL:HG12	1:D:608:PHE:HD1	1.85	0.42
1:B:89:CYS:HB3	1:B:94:VAL:O	2.19	0.42
1:C:659:PHE:CE2	1:C:667:PHE:HD1	2.38	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:74:PHE:CZ	1:A:285:THR:HG23	2.54	0.42
1:B:74:PHE:CZ	1:B:285:THR:HG23	2.54	0.42
1:B:387:THR:O	1:B:390:LEU:HB2	2.19	0.42
1:A:61:ALA:O	1:A:65:GLN:HG2	2.20	0.42
1:B:77:TYR:HE2	1:B:98:THR:HG21	1.85	0.42
1:B:606:TRP:O	1:B:610:LEU:HB2	2.20	0.42
1:D:261:ARG:HD2	1:D:261:ARG:HA	1.82	0.42
1:B:11:SER:OG	1:B:44:THR:OG1	2.37	0.42
1:B:405:TYR:HA	1:B:424:TYR:HB3	2.00	0.42
1:C:10:ASN:ND2	1:C:40:GLU:O	2.44	0.42
1:D:116:ASP:OD1	1:D:118:LYS:HE3	2.20	0.42
1:D:521:LEU:HD13	1:D:616:TYR:HD1	1.84	0.42
1:A:489:ILE:HD13	1:A:735:ALA:HB1	2.02	0.42
1:D:787:LEU:HD22	1:D:787:LEU:HA	1.77	0.42
1:A:412:HIS:CE1	1:A:413:GLU:HG3	2.55	0.42
1:A:174:ASP:O	1:A:178:ARG:HG3	2.20	0.42
1:A:504:ILE:HG22	1:A:701:ALA:HB2	2.02	0.42
1:C:763:LYS:O	1:C:767:TRP:HB2	2.20	0.42
1:D:236:GLN:NE2	1:D:365:THR:O	2.41	0.42
1:D:645:ILE:HG23	1:D:699:LYS:C	2.45	0.42
1:A:358:ILE:HB	1:A:374:TRP:NE1	2.34	0.41
1:B:97:ILE:HD12	1:B:292:MET:HE3	2.01	0.41
1:C:127:TYR:HB2	1:C:380:MET:HE3	2.01	0.41
1:C:425:CYS:HA	1:C:428:LEU:HB3	2.02	0.41
1:D:803:LEU:O	1:D:807:MET:HG2	2.20	0.41
1:A:454:ASP:OD1	1:A:455:ALA:N	2.53	0.41
1:A:535:GLY:O	1:A:538:VAL:HG12	2.20	0.41
1:B:406:VAL:HG23	1:B:425:CYS:HB2	2.02	0.41
1:D:541:PHE:HD1	1:D:541:PHE:O	2.04	0.41
1:A:16:GLY:HA2	1:A:74:PHE:O	2.20	0.41
1:B:325:GLN:O	1:B:329:ILE:HG13	2.21	0.41
1:C:77:TYR:HE2	1:C:98:THR:HG21	1.85	0.41
1:C:219:HIS:ND1	1:C:241:GLU:O	2.52	0.41
1:C:486:GLU:OE2	1:C:491:PHE:HB2	2.19	0.41
1:C:521:LEU:HA	1:D:787:LEU:HG	2.03	0.41
1:A:642:GLN:NE2	1:A:645:ILE:HB	2.30	0.41
1:B:110:VAL:O	1:B:351:GLY:HA3	2.20	0.41
1:C:419:GLU:N	1:C:419:GLU:OE1	2.54	0.41
1:C:715:ARG:HD3	1:C:715:ARG:HA	1.89	0.41
1:C:746:VAL:O	1:C:750:VAL:HG23	2.20	0.41
1:D:486:GLU:OE1	1:D:491:PHE:HB2	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:728:ASP:OD2	1:A:730:LYS:HE3	2.20	0.41
1:B:66:PHE:CE2	1:B:92:LEU:HD13	2.56	0.41
1:B:78:ASP:OD1	1:B:79:LYS:N	2.54	0.41
1:B:288:ALA:O	1:B:292:MET:HG3	2.20	0.41
1:B:597:SER:O	1:B:601:VAL:HG23	2.21	0.41
1:C:447:ASP:OD2	1:C:461:ASN:HB2	2.20	0.41
1:A:294:GLU:HG3	1:A:338:VAL:HG11	2.02	0.41
1:A:607:PHE:HD1	1:A:610:LEU:HD23	1.86	0.41
1:B:24:GLN:HG3	1:B:262:TRP:HZ2	1.86	0.41
1:B:163:ILE:HG21	1:B:180:LEU:HD13	2.01	0.41
1:B:637:GLU:OE1	1:B:637:GLU:N	2.47	0.41
1:C:113:MET:HE3	1:C:288:ALA:HA	2.03	0.41
1:C:261:ARG:HA	1:C:261:ARG:HD2	1.91	0.41
1:C:433:ALA:HA	1:C:438:PHE:CE2	2.56	0.41
1:C:529:ILE:HA	1:D:796:PHE:CE2	2.55	0.41
1:D:177:TYR:HD1	1:D:177:TYR:HA	1.77	0.41
1:A:409:LYS:HG2	1:A:422:GLU:CD	2.46	0.41
1:B:791:ASN:HD22	1:B:791:ASN:C	2.28	0.41
1:C:672:THR:HG22	1:C:675:ARG:NH2	2.36	0.41
1:D:99:PRO:HA	1:D:113:MET:HB2	2.03	0.41
1:C:795:VAL:O	1:C:798:ILE:HG22	2.20	0.41
1:A:299:LEU:HD21	1:A:332:ALA:HB2	2.02	0.41
1:B:390:LEU:HD13	1:B:390:LEU:HA	1.78	0.41
1:B:397:VAL:O	1:B:443:THR:OG1	2.27	0.41
1:C:480:THR:O	1:C:482:THR:HG23	2.21	0.41
1:D:504:ILE:O	1:D:720:THR:HA	2.21	0.41
1:A:119:GLY:O	1:A:379:LYS:NZ	2.48	0.41
1:A:609:THR:O	1:A:613:ILE:HG23	2.21	0.41
1:B:399:THR:HG21	1:B:406:VAL:HG21	2.03	0.41
1:A:395:VAL:N	1:A:439:LYS:O	2.53	0.40
1:A:536:VAL:HG22	1:B:803:LEU:HD21	2.03	0.40
1:B:611:ILE:HD12	1:C:517:PHE:CE1	2.51	0.40
1:D:171:ASP:OD1	1:D:172:LYS:N	2.53	0.40
1:D:445:VAL:HG13	1:D:448:GLY:HA2	2.02	0.40
1:A:380:MET:HE3	1:A:380:MET:HB3	1.89	0.40
1:A:796:PHE:HZ	1:D:529:ILE:HA	1.87	0.40
1:C:23:ASP:HB3	1:C:271:PRO:CG	2.50	0.40
1:C:467:LEU:HD23	1:C:472:ALA:HB3	2.03	0.40
1:C:525:ILE:HA	1:C:528:CYS:HB3	2.03	0.40
1:A:74:PHE:HA	1:A:97:ILE:O	2.22	0.40
1:B:659:PHE:HB3	1:B:671:TRP:HB2	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:266:GLU:HG2	1:C:268:LYS:H	1.86	0.40
1:D:320:ALA:O	1:D:322:PRO:HD3	2.21	0.40
1:B:796:PHE:C	1:B:798:ILE:H	2.29	0.40
1:C:637:GLU:O	1:C:640:SER:OG	2.36	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)
1:B:303:ARG:NH2	1:C:346:LYS:NZ[3_545]	1.53	0.67

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	764/808 (95%)	706 (92%)	54 (7%)	4 (0%)	24	62
1	B	766/808 (95%)	704 (92%)	58 (8%)	4 (0%)	24	62
1	C	768/808 (95%)	703 (92%)	58 (8%)	7 (1%)	14	49
1	D	766/808 (95%)	708 (92%)	54 (7%)	4 (0%)	24	62
All	All	3064/3232 (95%)	2821 (92%)	224 (7%)	19 (1%)	21	58

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	632	PRO
1	C	512	PRO
1	D	585	MET
1	A	507	PRO
1	B	798	ILE
1	D	320	ALA

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Mol	Chain	Res	Type
1	D	379	LYS
1	D	520	PRO
1	B	520	PRO
1	B	797	TYR
1	C	373	TYR
1	A	437	GLY
1	B	533	TYR
1	C	786	ALA
1	A	630	VAL
1	C	520	PRO
1	C	381	VAL
1	A	520	PRO
1	C	507	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	613/691 (89%)	609 (99%)	4 (1%)	76	78
1	B	625/691 (90%)	617 (99%)	8 (1%)	61	71
1	C	609/691 (88%)	608 (100%)	1 (0%)	87	85
1	D	609/691 (88%)	602 (99%)	7 (1%)	65	73
All	All	2456/2764 (89%)	2436 (99%)	20 (1%)	73	77

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	381	VAL
1	A	382	LEU
1	A	393	LYS
1	A	529	ILE
1	B	385	ASP
1	B	387	THR
1	B	390	LEU
1	B	393	LYS

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Mol	Chain	Res	Type
1	B	445	VAL
1	B	447	ASP
1	B	505	LYS
1	B	510	SER
1	C	390	LEU
1	D	394	THR
1	D	625	THR
1	D	635	SER
1	D	772	GLU
1	D	773	CYS
1	D	783	LYS
1	D	787	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	46	HIS
1	A	355	ASN
1	B	24	GLN
1	B	344	ASN
1	B	355	ASN
1	B	642	GLN
1	C	46	HIS
1	C	274	HIS
1	C	337	GLN
1	C	344	ASN
1	D	24	GLN
1	D	60	ASN
1	D	167	ASN
1	D	344	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

6 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	V8G	A	902	-	13,13,13	0.73	0	16,16,16	1.08	1 (6%)
2	NAG	D	901	1	14,14,15	0.38	0	17,19,21	0.53	0
3	V8G	C	902	-	13,13,13	0.74	0	16,16,16	1.08	1 (6%)
2	NAG	A	901	-	14,14,15	0.51	0	17,19,21	0.51	0
2	NAG	B	901	-	14,14,15	0.36	0	17,19,21	0.54	0
2	NAG	C	901	-	14,14,15	0.31	0	17,19,21	0.61	1 (5%)

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	V8G	A	902	-	-	3/8/18/18	0/1/1/1
2	NAG	D	901	1	-	0/6/23/26	0/1/1/1
3	V8G	C	902	-	-	3/8/18/18	0/1/1/1
2	NAG	A	901	-	-	0/6/23/26	0/1/1/1
2	NAG	B	901	-	-	0/6/23/26	0/1/1/1
2	NAG	C	901	-	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	902	V8G	OAK-CAD-CAE	2.26	120.03	114.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	902	V8G	OAK-CAD-CAE	2.23	119.95	114.16
2	C	901	NAG	C1-O5-C5	2.05	114.93	112.19

There are no chirality outliers.

All (6) torsion outliers are listed below:

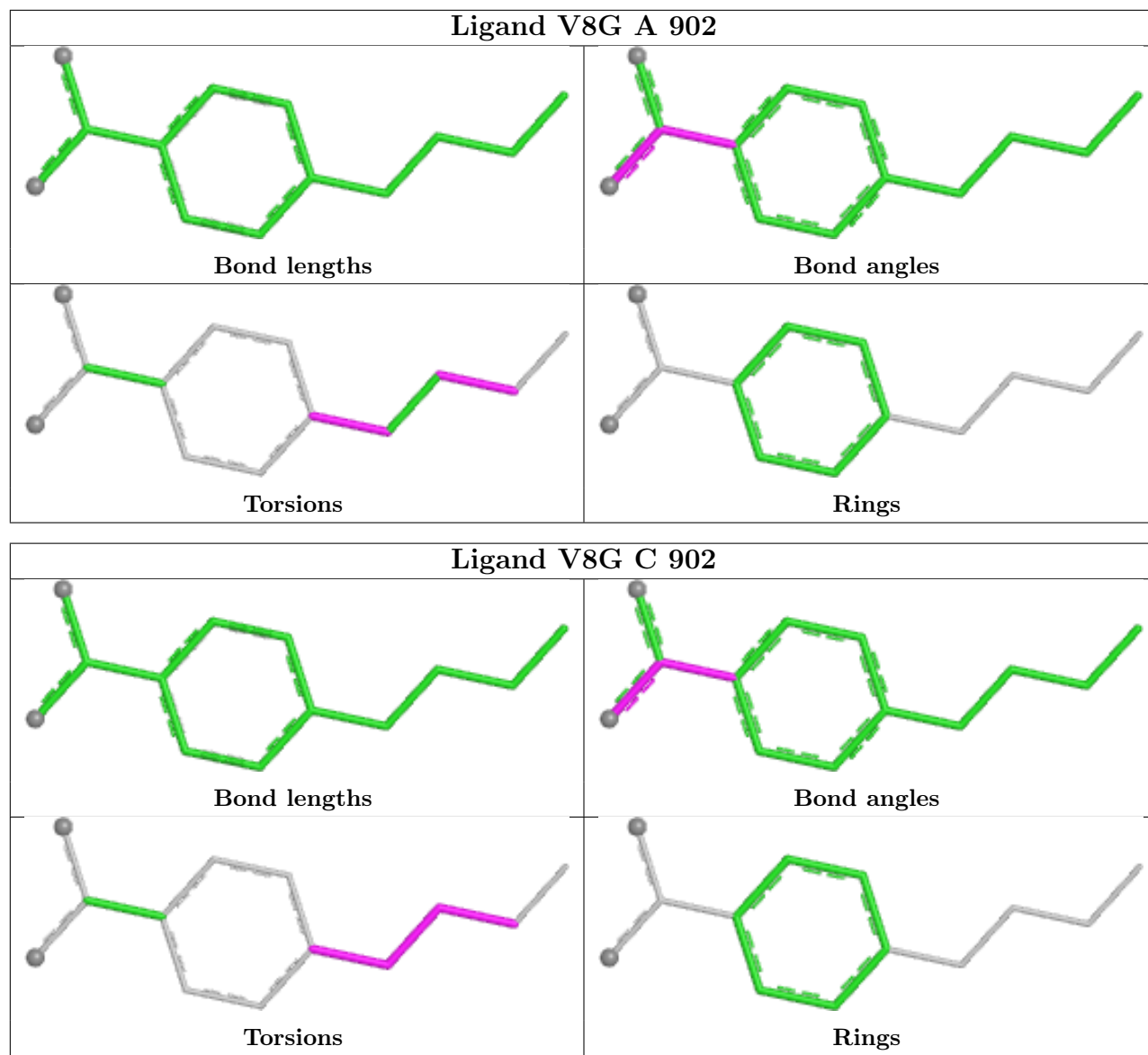
Mol	Chain	Res	Type	Atoms
3	A	902	V8G	CAC-CAF-CAG-CAH
3	C	902	V8G	CAC-CAF-CAG-CAH
3	A	902	V8G	CAG-CAH-CAI-CAJ
3	C	902	V8G	CAG-CAH-CAI-CAJ
3	A	902	V8G	CAM-CAF-CAG-CAH
3	C	902	V8G	CAF-CAG-CAH-CAI

There are no ring outliers.

5 monomers are involved in 39 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	902	V8G	12	0
2	D	901	NAG	1	0
3	C	902	V8G	9	0
2	A	901	NAG	2	0
2	B	901	NAG	15	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	770/808 (95%)	0.18	43 (5%)	30	28	159, 239, 367, 393	0
1	B	772/808 (95%)	0.38	69 (8%)	15	18	154, 222, 377, 407	0
1	C	774/808 (95%)	0.19	32 (4%)	41	35	178, 258, 368, 408	0
1	D	772/808 (95%)	0.39	68 (8%)	15	19	191, 287, 378, 395	0
All	All	3088/3232 (95%)	0.29	212 (6%)	23	23	154, 248, 374, 408	0

All (212) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	309	ARG	12.6
1	D	200	LYS	10.8
1	D	139	SER	9.8
1	D	197	GLU	7.3
1	B	630	VAL	7.2
1	B	431	GLU	6.6
1	C	79	LYS	6.4
1	D	204	ILE	6.3
1	B	165	VAL	6.3
1	C	792	VAL	6.1
1	B	756	GLN	5.9
1	D	140	ASP	5.8
1	B	755	GLU	5.6
1	C	78	ASP	5.6
1	A	45	PRO	5.6
1	B	204	ILE	5.5
1	D	280	TYR	5.4
1	A	20	ARG	5.3
1	B	750	VAL	5.2
1	B	632	PRO	5.1
1	D	142	GLY	5.1

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Mol	Chain	Res	Type	RSRZ
1	B	205	VAL	5.0
1	D	480	THR	5.0
1	B	751	LEU	4.9
1	D	167	ASN	4.8
1	D	143	LEU	4.8
1	A	11	SER	4.7
1	D	494	PRO	4.7
1	D	165	VAL	4.6
1	B	753	LEU	4.6
1	D	141	ARG	4.5
1	A	384	GLU	4.5
1	B	157	LYS	4.4
1	B	290	GLN	4.4
1	B	177	TYR	4.3
1	D	198	ARG	4.2
1	A	186	LEU	4.2
1	D	164	ASN	4.2
1	C	761	LYS	4.2
1	A	389	GLY	4.2
1	C	510	SER	4.2
1	D	203	ASP	4.2
1	D	484	VAL	4.2
1	D	199	ASP	4.1
1	A	13	GLN	4.1
1	D	205	VAL	4.1
1	D	225	LEU	4.0
1	D	79	LYS	4.0
1	A	388	SER	4.0
1	C	143	LEU	3.9
1	B	36	PHE	3.9
1	B	292	MET	3.9
1	B	754	SER	3.9
1	D	138	ASP	3.9
1	D	587	GLN	3.9
1	A	47	ILE	3.9
1	D	586	GLN	3.8
1	D	732	TYR	3.8
1	C	756	GLN	3.8
1	B	752	LYS	3.7
1	D	206	ASP	3.7
1	D	104	ASP	3.7
1	B	605	TRP	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	196	CYS	3.6
1	C	594	ARG	3.5
1	D	202	ASN	3.5
1	D	235	ILE	3.5
1	A	44	THR	3.5
1	B	494	PRO	3.5
1	B	200	LYS	3.5
1	A	310	GLY	3.4
1	D	166	GLY	3.4
1	B	515	PHE	3.4
1	B	254	LEU	3.4
1	A	654	SER	3.4
1	B	141	ARG	3.3
1	B	291	VAL	3.3
1	A	390	LEU	3.3
1	B	609	THR	3.3
1	B	428	LEU	3.3
1	B	104	ASP	3.2
1	B	507	PRO	3.2
1	A	527	MET	3.2
1	C	139	SER	3.2
1	B	168	ILE	3.2
1	A	49	ASN	3.1
1	D	630	VAL	3.1
1	B	276	ALA	3.1
1	C	788	SER	3.1
1	B	136	LEU	3.1
1	D	703	LEU	3.1
1	A	187	LYS	3.0
1	D	234	LYS	3.0
1	B	180	LEU	3.0
1	D	144	SER	3.0
1	A	787	LEU	2.9
1	C	82	VAL	2.9
1	D	739	GLY	2.9
1	A	46	HIS	2.9
1	B	272	GLY	2.9
1	D	428	LEU	2.8
1	A	526	TRP	2.8
1	D	196	CYS	2.8
1	B	698	GLY	2.8
1	C	77	TYR	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	494	PRO	2.8
1	C	394	THR	2.8
1	B	194	LEU	2.7
1	C	18	PHE	2.7
1	A	68	ARG	2.7
1	C	586	GLN	2.7
1	B	778	SER	2.7
1	B	629	MET	2.7
1	C	140	ASP	2.7
1	A	14	ILE	2.7
1	B	628	ARG	2.7
1	B	294	GLU	2.7
1	A	620	LEU	2.6
1	D	39	SER	2.6
1	D	778	SER	2.6
1	B	203	ASP	2.6
1	D	101	PHE	2.6
1	B	544	SER	2.6
1	A	42	ARG	2.6
1	D	383	THR	2.6
1	B	432	ILE	2.6
1	A	314	ASP	2.6
1	D	384	GLU	2.6
1	B	34	VAL	2.6
1	D	208	VAL	2.6
1	D	137	TYR	2.5
1	B	274	HIS	2.5
1	B	345	ILE	2.5
1	A	385	ASP	2.5
1	B	80	LYS	2.5
1	B	758	VAL	2.5
1	A	760	ASP	2.5
1	D	631	SER	2.5
1	B	116	ASP	2.5
1	B	102	PRO	2.5
1	C	654	SER	2.5
1	A	386	ASP	2.5
1	C	534	ILE	2.4
1	A	43	LEU	2.4
1	B	339	GLU	2.4
1	D	159	GLN	2.4
1	B	79	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	800	VAL	2.4
1	C	784	THR	2.4
1	B	595	SER	2.4
1	D	731	GLY	2.3
1	D	429	ALA	2.3
1	D	481	ILE	2.3
1	D	740	SER	2.3
1	D	482	THR	2.3
1	B	267	GLU	2.3
1	D	442	LEU	2.3
1	C	419	GLU	2.3
1	C	191	ARG	2.3
1	D	388	SER	2.3
1	B	206	ASP	2.3
1	B	160	VAL	2.3
1	B	586	GLN	2.3
1	C	81	SER	2.3
1	D	426	VAL	2.3
1	B	133	PHE	2.3
1	D	209	ILE	2.3
1	C	632	PRO	2.3
1	C	644	GLU	2.2
1	C	685	THR	2.2
1	B	333	LEU	2.2
1	C	241	GLU	2.2
1	A	29	PHE	2.2
1	A	50	LEU	2.2
1	B	275	THR	2.2
1	D	321	VAL	2.2
1	D	582	GLY	2.2
1	D	649	THR	2.2
1	C	358	ILE	2.2
1	C	511	LYS	2.2
1	A	792	VAL	2.2
1	A	80	LYS	2.2
1	D	307	SER	2.2
1	C	104	ASP	2.1
1	B	163	ILE	2.1
1	B	137	TYR	2.1
1	D	175	GLU	2.1
1	C	16	GLY	2.1
1	B	519	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	523	TYR	2.1
1	A	624	LEU	2.1
1	A	303	ARG	2.1
1	B	158	TRP	2.1
1	A	447	ASP	2.1
1	D	385	ASP	2.1
1	A	83	ASN	2.1
1	D	387	THR	2.1
1	A	587	GLN	2.1
1	B	699	LYS	2.1
1	A	12	ILE	2.1
1	D	181	PHE	2.1
1	D	425	CYS	2.1
1	D	382	LEU	2.1
1	B	155	GLU	2.1
1	D	654	SER	2.1
1	C	758	VAL	2.1
1	C	52	VAL	2.1
1	A	742	LEU	2.0
1	D	453	ARG	2.0
1	A	306	ILE	2.0
1	B	516	SER	2.0
1	D	318	ASN	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](#)

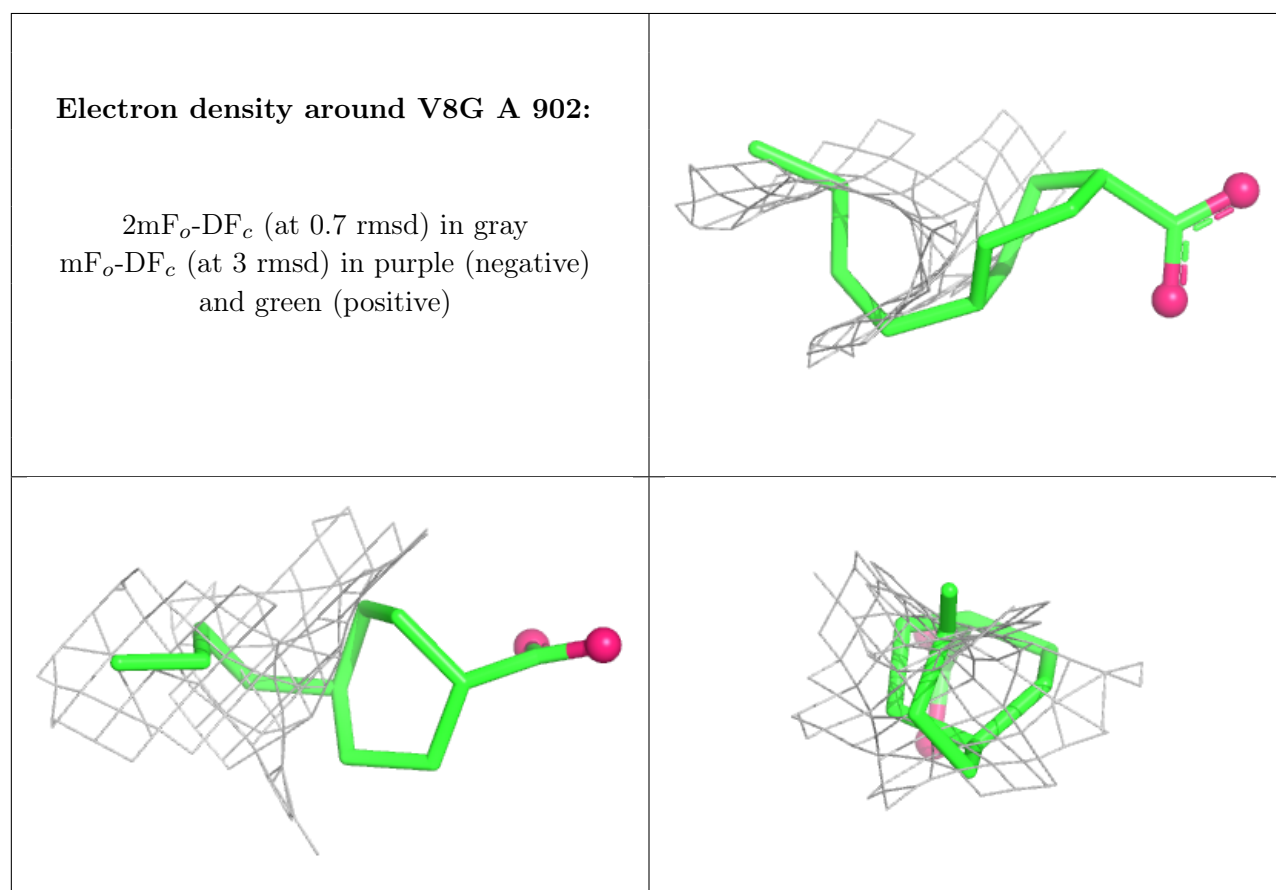
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists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

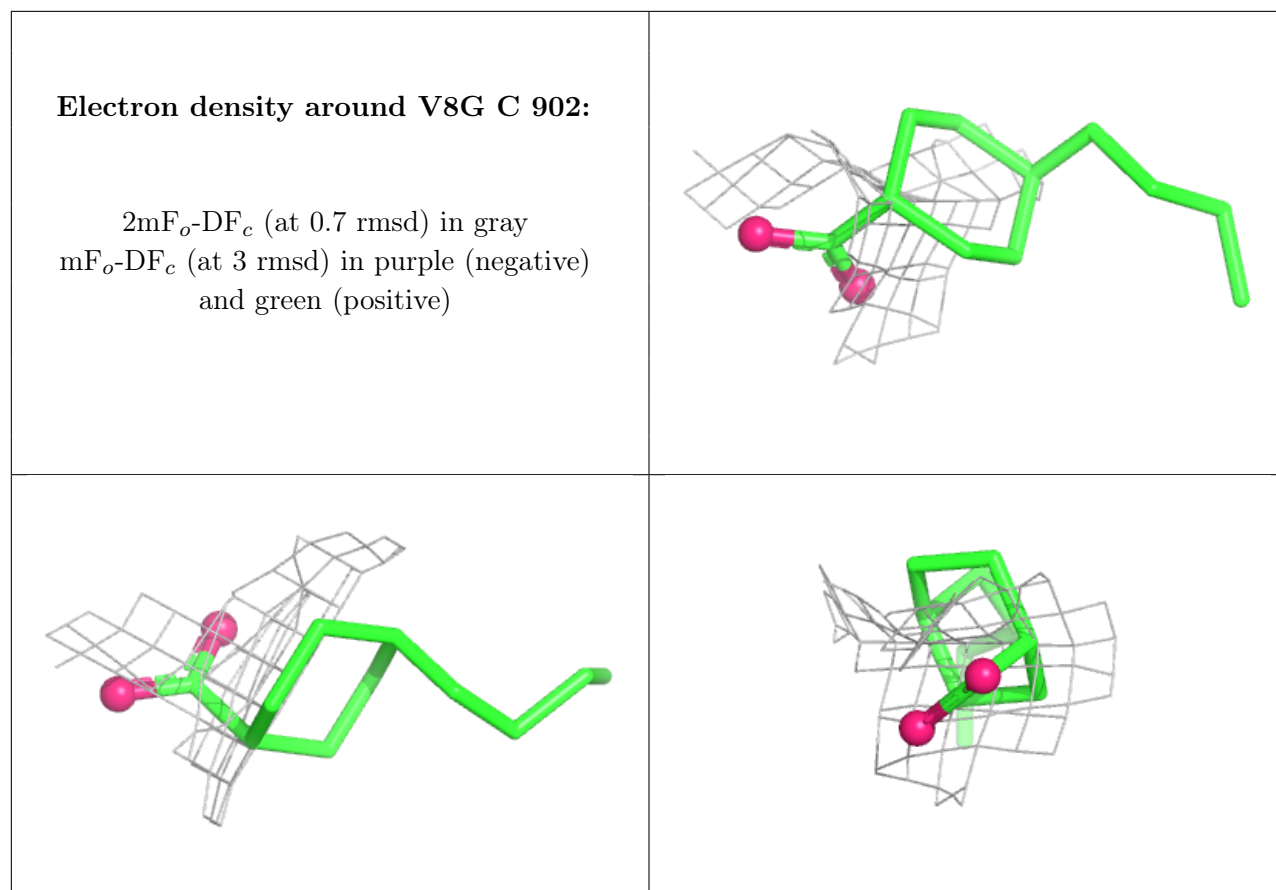
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NAG	B	901	14/15	0.56	0.15	196,196,199,200	0
2	NAG	D	901	14/15	0.60	0.16	269,269,270,272	0
2	NAG	A	901	14/15	0.70	0.17	255,255,257,262	0
2	NAG	C	901	14/15	0.78	0.18	416,416,418,424	0
3	V8G	A	902	13/13	0.86	0.12	331,331,331,331	0
3	V8G	C	902	13/13	0.92	0.11	341,341,341,341	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.





6.5 Other polymers ⓘ

There are no such residues in this entry.