



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 2, 2025 – 01:09 pm BST

PDB ID : 9RCR / pdb\_00009rcr  
Title : 1,2-propanediol dehydratase with 0.1 % 1,2-propanediol additive  
Authors : Kalnins, G.; Estere, M.  
Deposited on : 2025-05-29  
Resolution : 2.80 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](mailto: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>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0rc1  
Mogul : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 2.0rc1  
EDS : 3.0  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.003 (Gargrove)  
Density-Fitness : 1.0.11  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.43.1

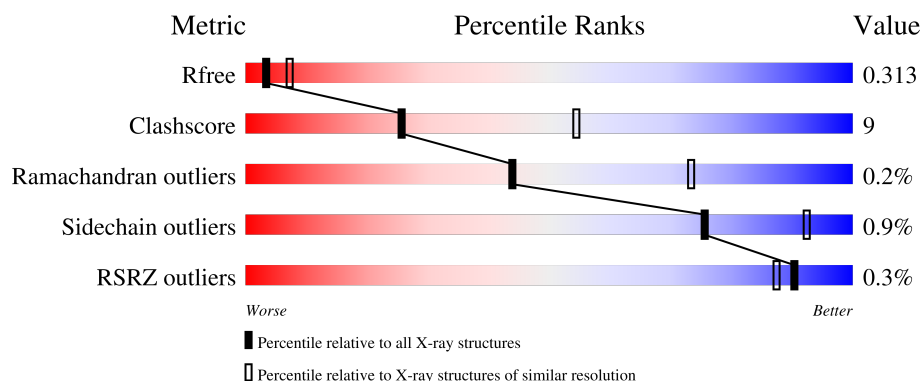
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*





The reported resolution of this entry is 2.80 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))
$R_{free}$	164625	3657 (2.80-2.80)
Clashscore	180529	4123 (2.80-2.80)
Ramachandran outliers	177936	4071 (2.80-2.80)
Sidechain outliers	177891	4073 (2.80-2.80)
RSRZ outliers	164620	3659 (2.80-2.80)

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  $\geq 3$ , 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	816	 80% 17% •
1	B	816	 77% 20% •
1	C	816	 71% 25% ••
1	D	816	 75% 22% •

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	PGR	A	801	-	-	X	-
2	PGR	B	801	-	-	X	-

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 25148 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 Glycyl radical protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	792	Total	C	N	O	S	0	0	0
			6246	3942	1087	1186	31			
1	B	792	Total	C	N	O	S	0	1	0
			6252	3946	1087	1188	31			
1	C	792	Total	C	N	O	S	0	0	0
			6246	3942	1087	1186	31			
1	D	794	Total	C	N	O	S	0	0	0
			6258	3949	1089	1188	32			

There are 120 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-22	MET	-	initiating methionine	UNP A0AAN5KVK2
A	-21	GLY	-	expression tag	UNP A0AAN5KVK2
A	-20	SER	-	expression tag	UNP A0AAN5KVK2
A	-19	SER	-	expression tag	UNP A0AAN5KVK2
A	-18	HIS	-	expression tag	UNP A0AAN5KVK2
A	-17	HIS	-	expression tag	UNP A0AAN5KVK2
A	-16	HIS	-	expression tag	UNP A0AAN5KVK2
A	-15	HIS	-	expression tag	UNP A0AAN5KVK2
A	-14	HIS	-	expression tag	UNP A0AAN5KVK2
A	-13	HIS	-	expression tag	UNP A0AAN5KVK2
A	-12	SER	-	expression tag	UNP A0AAN5KVK2
A	-11	GLN	-	expression tag	UNP A0AAN5KVK2
A	-10	ASP	-	expression tag	UNP A0AAN5KVK2
A	-9	HIS	-	expression tag	UNP A0AAN5KVK2
A	-8	GLU	-	expression tag	UNP A0AAN5KVK2
A	-7	ASN	-	expression tag	UNP A0AAN5KVK2
A	-6	LEU	-	expression tag	UNP A0AAN5KVK2
A	-5	TYR	-	expression tag	UNP A0AAN5KVK2
A	-4	PHE	-	expression tag	UNP A0AAN5KVK2
A	-3	GLN	-	expression tag	UNP A0AAN5KVK2
A	-2	GLY	-	expression tag	UNP A0AAN5KVK2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	SER	-	expression tag	UNP A0AAN5KVK2
A	0	MET	-	expression tag	UNP A0AAN5KVK2
A	1	GLY	-	expression tag	UNP A0AAN5KVK2
A	162	ILE	VAL	conflict	UNP A0AAN5KVK2
A	589	ARG	-	linker	UNP A0AAN5KVK2
A	590	SER	-	linker	UNP A0AAN5KVK2
A	591	GLY	-	linker	UNP A0AAN5KVK2
A	592	ASN	-	linker	UNP A0AAN5KVK2
A	593	PRO	-	linker	UNP A0AAN5KVK2
B	-22	MET	-	initiating methionine	UNP A0AAN5KVK2
B	-21	GLY	-	expression tag	UNP A0AAN5KVK2
B	-20	SER	-	expression tag	UNP A0AAN5KVK2
B	-19	SER	-	expression tag	UNP A0AAN5KVK2
B	-18	HIS	-	expression tag	UNP A0AAN5KVK2
B	-17	HIS	-	expression tag	UNP A0AAN5KVK2
B	-16	HIS	-	expression tag	UNP A0AAN5KVK2
B	-15	HIS	-	expression tag	UNP A0AAN5KVK2
B	-14	HIS	-	expression tag	UNP A0AAN5KVK2
B	-13	HIS	-	expression tag	UNP A0AAN5KVK2
B	-12	SER	-	expression tag	UNP A0AAN5KVK2
B	-11	GLN	-	expression tag	UNP A0AAN5KVK2
B	-10	ASP	-	expression tag	UNP A0AAN5KVK2
B	-9	HIS	-	expression tag	UNP A0AAN5KVK2
B	-8	GLU	-	expression tag	UNP A0AAN5KVK2
B	-7	ASN	-	expression tag	UNP A0AAN5KVK2
B	-6	LEU	-	expression tag	UNP A0AAN5KVK2
B	-5	TYR	-	expression tag	UNP A0AAN5KVK2
B	-4	PHE	-	expression tag	UNP A0AAN5KVK2
B	-3	GLN	-	expression tag	UNP A0AAN5KVK2
B	-2	GLY	-	expression tag	UNP A0AAN5KVK2
B	-1	SER	-	expression tag	UNP A0AAN5KVK2
B	0	MET	-	expression tag	UNP A0AAN5KVK2
B	1	GLY	-	expression tag	UNP A0AAN5KVK2
B	162	ILE	VAL	conflict	UNP A0AAN5KVK2
B	589	ARG	-	linker	UNP A0AAN5KVK2
B	590	SER	-	linker	UNP A0AAN5KVK2
B	591	GLY	-	linker	UNP A0AAN5KVK2
B	592	ASN	-	linker	UNP A0AAN5KVK2
B	593	PRO	-	linker	UNP A0AAN5KVK2
C	-22	MET	-	initiating methionine	UNP A0AAN5KVK2
C	-21	GLY	-	expression tag	UNP A0AAN5KVK2
C	-20	SER	-	expression tag	UNP A0AAN5KVK2

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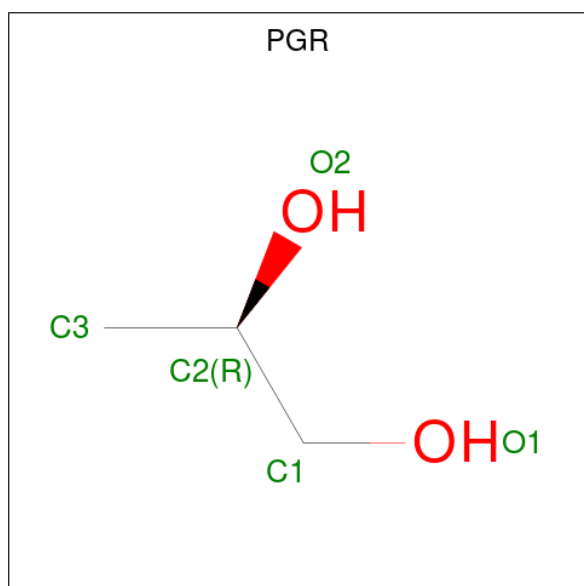
Chain	Residue	Modelled	Actual	Comment	Reference
C	-19	SER	-	expression tag	UNP A0AAN5KVK2
C	-18	HIS	-	expression tag	UNP A0AAN5KVK2
C	-17	HIS	-	expression tag	UNP A0AAN5KVK2
C	-16	HIS	-	expression tag	UNP A0AAN5KVK2
C	-15	HIS	-	expression tag	UNP A0AAN5KVK2
C	-14	HIS	-	expression tag	UNP A0AAN5KVK2
C	-13	HIS	-	expression tag	UNP A0AAN5KVK2
C	-12	SER	-	expression tag	UNP A0AAN5KVK2
C	-11	GLN	-	expression tag	UNP A0AAN5KVK2
C	-10	ASP	-	expression tag	UNP A0AAN5KVK2
C	-9	HIS	-	expression tag	UNP A0AAN5KVK2
C	-8	GLU	-	expression tag	UNP A0AAN5KVK2
C	-7	ASN	-	expression tag	UNP A0AAN5KVK2
C	-6	LEU	-	expression tag	UNP A0AAN5KVK2
C	-5	TYR	-	expression tag	UNP A0AAN5KVK2
C	-4	PHE	-	expression tag	UNP A0AAN5KVK2
C	-3	GLN	-	expression tag	UNP A0AAN5KVK2
C	-2	GLY	-	expression tag	UNP A0AAN5KVK2
C	-1	SER	-	expression tag	UNP A0AAN5KVK2
C	0	MET	-	expression tag	UNP A0AAN5KVK2
C	1	GLY	-	expression tag	UNP A0AAN5KVK2
C	162	ILE	VAL	conflict	UNP A0AAN5KVK2
C	589	ARG	-	linker	UNP A0AAN5KVK2
C	590	SER	-	linker	UNP A0AAN5KVK2
C	591	GLY	-	linker	UNP A0AAN5KVK2
C	592	ASN	-	linker	UNP A0AAN5KVK2
C	593	PRO	-	linker	UNP A0AAN5KVK2
D	-22	MET	-	initiating methionine	UNP A0AAN5KVK2
D	-21	GLY	-	expression tag	UNP A0AAN5KVK2
D	-20	SER	-	expression tag	UNP A0AAN5KVK2
D	-19	SER	-	expression tag	UNP A0AAN5KVK2
D	-18	HIS	-	expression tag	UNP A0AAN5KVK2
D	-17	HIS	-	expression tag	UNP A0AAN5KVK2
D	-16	HIS	-	expression tag	UNP A0AAN5KVK2
D	-15	HIS	-	expression tag	UNP A0AAN5KVK2
D	-14	HIS	-	expression tag	UNP A0AAN5KVK2
D	-13	HIS	-	expression tag	UNP A0AAN5KVK2
D	-12	SER	-	expression tag	UNP A0AAN5KVK2
D	-11	GLN	-	expression tag	UNP A0AAN5KVK2
D	-10	ASP	-	expression tag	UNP A0AAN5KVK2
D	-9	HIS	-	expression tag	UNP A0AAN5KVK2
D	-8	GLU	-	expression tag	UNP A0AAN5KVK2

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-7	ASN	-	expression tag	UNP A0AAN5KVK2
D	-6	LEU	-	expression tag	UNP A0AAN5KVK2
D	-5	TYR	-	expression tag	UNP A0AAN5KVK2
D	-4	PHE	-	expression tag	UNP A0AAN5KVK2
D	-3	GLN	-	expression tag	UNP A0AAN5KVK2
D	-2	GLY	-	expression tag	UNP A0AAN5KVK2
D	-1	SER	-	expression tag	UNP A0AAN5KVK2
D	0	MET	-	expression tag	UNP A0AAN5KVK2
D	1	GLY	-	expression tag	UNP A0AAN5KVK2
D	162	ILE	VAL	conflict	UNP A0AAN5KVK2
D	589	ARG	-	linker	UNP A0AAN5KVK2
D	590	SER	-	linker	UNP A0AAN5KVK2
D	591	GLY	-	linker	UNP A0AAN5KVK2
D	592	ASN	-	linker	UNP A0AAN5KVK2
D	593	PRO	-	linker	UNP A0AAN5KVK2

- Molecule 2 is R-1,2-PROPANEDIOL (CCD ID: PGR) (formula:  $C_3H_8O_2$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			5	3	2		
2	B	1	Total	C	O	0	0
			5	3	2		
2	C	1	Total	C	O	0	0
			5	3	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	D	1	Total	C	O	0	0
			5	3	2		

- Molecule 3 is water.

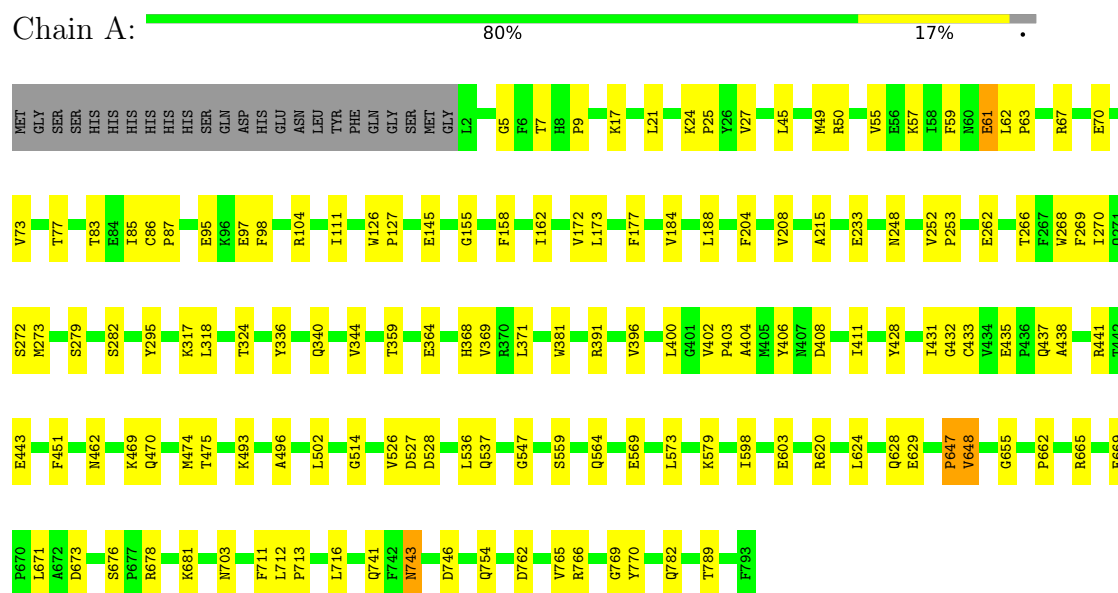
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	42	Total	O	0	0
			42	42		
3	B	34	Total	O	0	0
			34	34		
3	C	28	Total	O	0	0
			28	28		
3	D	22	Total	O	0	0
			22	22		



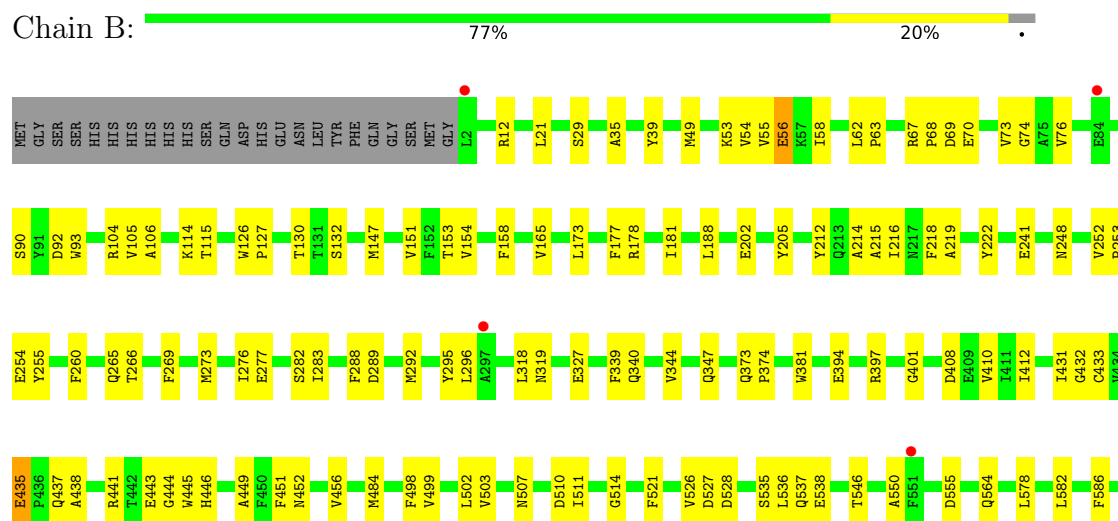
### 3 Residue-property plots

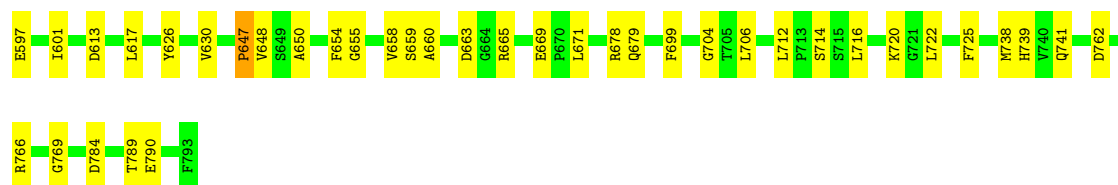
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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



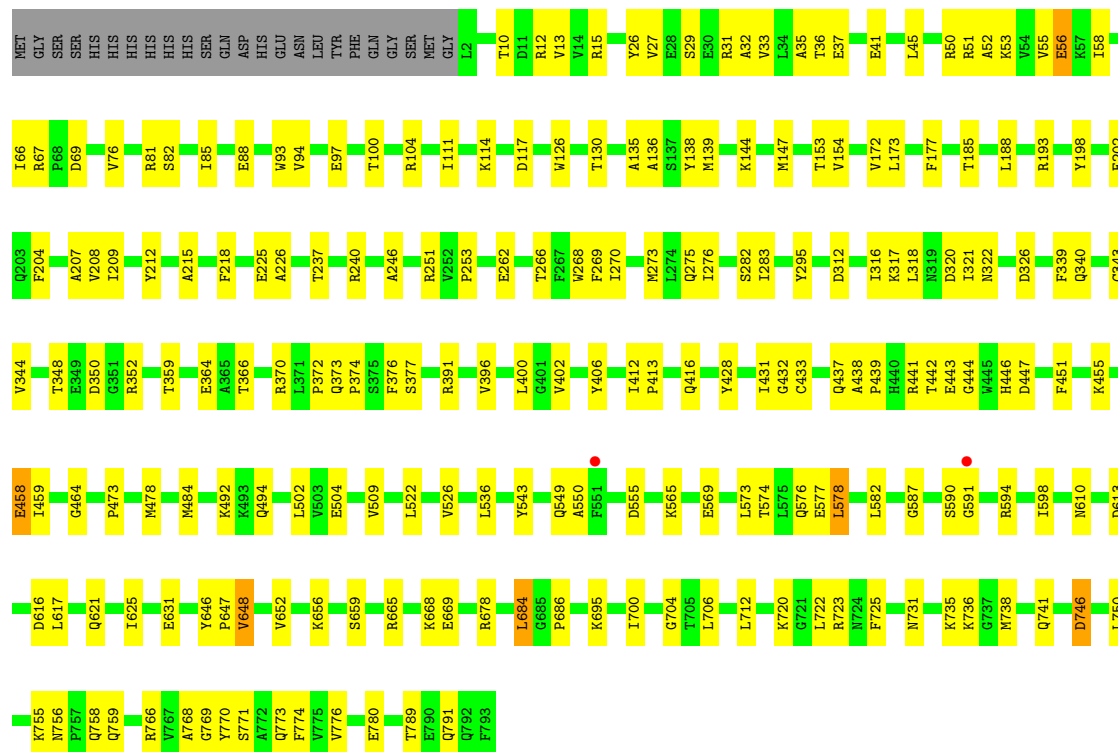
#### • Molecule 1: Glycyl radical protein





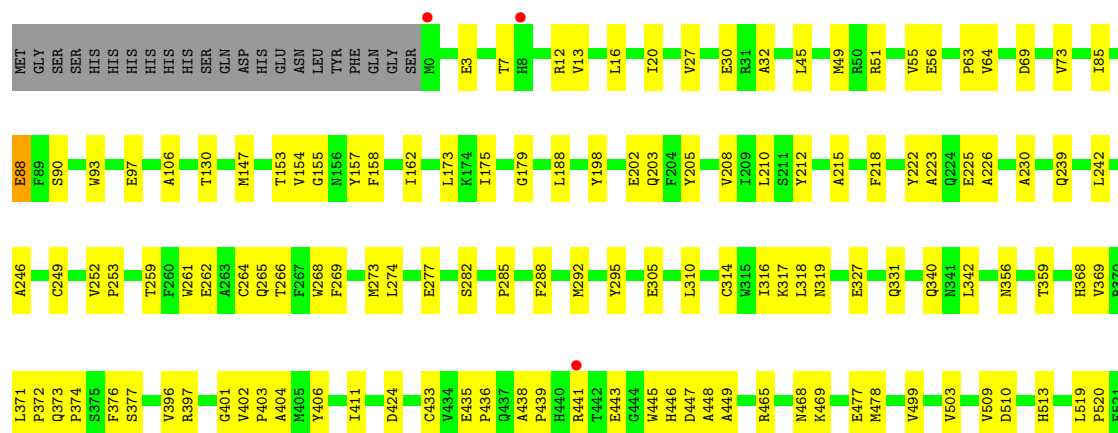
- Molecule 1: Glycyl radical protein

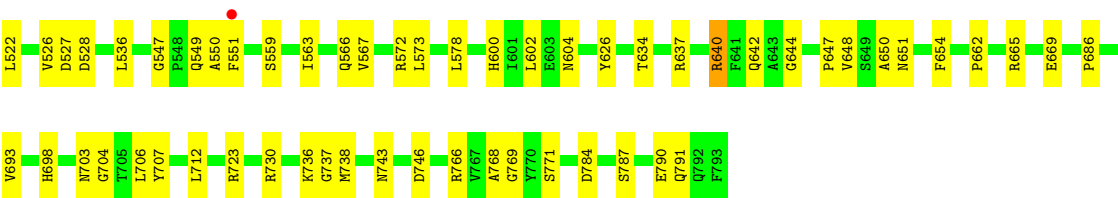
Chain C: 71% 25% . .



- Molecule 1: Glycyl radical protein

Chain D: 75% 22% .





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	80.89Å 199.97Å 118.38Å 90.00° 106.32° 90.00°	Depositor
Resolution (Å)	98.70 – 2.80 98.70 – 2.80	Depositor EDS
% Data completeness (in resolution range)	97.1 (98.70-2.80) 97.1 (98.70-2.80)	Depositor EDS
$R_{merge}$	0.86	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.86 (at 2.82Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, $R_{free}$	0.263 , 0.318 0.258 , 0.313	Depositor DCC
$R_{free}$ test set	4144 reflections (4.66%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	21.7	Xtriage
Anisotropy	0.748	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 29.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.81	EDS
Total number of atoms	25148	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.17% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: PGR

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	0.71	0/6385	1.01	0/8648
1	B	0.70	0/6394	1.01	0/8660
1	C	0.71	0/6385	1.02	0/8648
1	D	0.71	0/6397	1.01	1/8663 (0.0%)
All	All	0.71	0/25561	1.01	1/34619 (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	A	0	1
1	B	0	1
1	C	0	2
1	D	0	1
All	All	0	5

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	640	ARG	CB-CG-CD	5.01	122.83	111.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	647	PRO	Peptide

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Mol	Chain	Res	Type	Group
1	B	647	PRO	Peptide
1	C	550	ALA	Peptide
1	C	647	PRO	Peptide
1	D	647	PRO	Peptide

## 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	6246	0	6071	91	0
1	B	6252	0	6077	118	0
1	C	6246	0	6071	140	0
1	D	6258	0	6086	122	0
2	A	5	0	8	6	0
2	B	5	0	8	8	0
2	C	5	0	8	3	0
2	D	5	0	8	2	0
3	A	42	0	0	1	0
3	B	34	0	0	0	0
3	C	28	0	0	0	0
3	D	22	0	0	1	0
All	All	25148	0	24337	466	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 9.

All (466) 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:10:THR:HG22	1:C:12:ARG:H	1.43	0.82
1:B:451:PHE:HD2	1:B:502:LEU:HD22	1.44	0.81
1:C:458:GLU:OE2	1:C:659:SER:N	2.12	0.81
1:A:97:GLU:OE2	1:A:104:ARG:NH1	2.16	0.79
1:C:51:ARG:NH1	1:C:88:GLU:OE1	2.16	0.79
1:D:401:GLY:HA3	1:D:766:ARG:HB2	1.66	0.77
1:A:665:ARG:NH1	1:A:669:GLU:O	2.17	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:435:GLU:OE2	2:B:801:PGR:O1	2.02	0.76
1:B:401:GLY:HA3	1:B:766:ARG:HG2	1.67	0.75
1:A:282:SER:OG	2:A:801:PGR:H12	1.87	0.75
1:D:340:GLN:HG2	1:D:373:GLN:OE1	1.86	0.74
1:C:237:THR:HG22	1:C:240:ARG:HH12	1.54	0.72
1:B:665:ARG:NH1	1:B:669:GLU:O	2.23	0.71
1:B:318:LEU:O	1:B:340:GLN:NE2	2.23	0.71
1:C:364:GLU:OE2	1:C:391:ARG:NH2	2.24	0.69
1:D:665:ARG:NH1	1:D:669:GLU:O	2.24	0.69
1:D:723:ARG:HG2	1:D:723:ARG:HH11	1.57	0.69
1:A:404:ALA:HB2	1:A:766:ARG:HH21	1.58	0.68
1:A:741:GLN:HE22	1:A:769:GLY:H	1.42	0.68
1:C:188:LEU:HD11	1:C:202:GLU:HG3	1.76	0.67
1:D:369:VAL:HG12	1:D:371:LEU:HG	1.76	0.67
1:B:21:LEU:HD21	1:B:762:ASP:HB3	1.77	0.67
1:A:435:GLU:OE1	2:A:801:PGR:O1	2.12	0.67
1:C:610:ASN:HB3	1:C:684:LEU:HD23	1.75	0.67
1:B:451:PHE:CD2	1:B:502:LEU:HD22	2.30	0.67
1:C:177:PHE:CE2	1:C:253:PRO:HG2	2.30	0.66
1:C:478:MET:HE1	1:C:578:LEU:CD2	2.26	0.66
1:C:26:TYR:O	1:C:82:SER:HB3	1.95	0.65
1:B:712:LEU:HB3	1:B:790:GLU:OE2	1.97	0.65
1:A:573:LEU:HD22	1:A:598:ILE:HG12	1.77	0.65
1:A:743:ASN:HD21	1:A:765:VAL:HB	1.61	0.65
1:B:397:ARG:HD2	1:B:722:LEU:HD21	1.80	0.64
1:B:178:ARG:NH2	1:B:254:GLU:OE1	2.31	0.63
1:D:7:THR:OG1	1:D:368:HIS:NE2	2.24	0.63
1:C:348:THR:HG22	1:C:352:ARG:O	1.98	0.63
1:B:741:GLN:HE22	1:B:769:GLY:H	1.45	0.62
1:A:282:SER:HG	2:A:801:PGR:H12	1.63	0.62
1:B:435:GLU:CD	2:B:801:PGR:O1	2.43	0.62
1:C:756:ASN:HB3	1:C:759:GLN:NE2	2.13	0.62
1:B:76:VAL:HG13	1:B:276:ILE:HG12	1.81	0.61
1:A:83:THR:HG21	1:A:324:THR:HG22	1.82	0.61
1:B:433:CYS:SG	2:B:801:PGR:H33	2.40	0.61
1:C:656:LYS:HA	1:C:668:LYS:HA	1.82	0.61
1:C:443:GLU:HB2	1:C:536:LEU:HD22	1.82	0.61
1:C:478:MET:HE1	1:C:578:LEU:HD22	1.81	0.61
1:D:45:LEU:HD13	1:D:49:MET:HB3	1.81	0.61
1:B:165:VAL:HA	1:B:437:GLN:HE22	1.64	0.61
1:D:447:ASP:OD2	2:D:801:PGR:H2	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:551:PHE:CZ	1:D:654:PHE:HD2	2.19	0.61
1:D:147:MET:HE3	1:D:153:THR:HA	1.82	0.61
1:B:401:GLY:CA	1:B:766:ARG:HG2	2.30	0.60
1:B:443:GLU:HB2	1:B:536:LEU:HD22	1.84	0.60
1:D:218:PHE:HD2	1:D:273:MET:HE2	1.66	0.60
1:B:177:PHE:CE2	1:B:253:PRO:HG2	2.36	0.60
1:A:431:ILE:HG12	1:A:437:GLN:HG2	1.84	0.60
1:B:104:ARG:HD2	1:B:327:GLU:HG2	1.84	0.60
1:B:435:GLU:CD	2:B:801:PGR:HO1	2.09	0.60
1:B:526:VAL:HG21	1:B:536:LEU:HD11	1.84	0.60
1:A:252:VAL:HB	1:A:266:THR:OG1	2.02	0.59
1:D:600:HIS:O	1:D:604:ASN:ND2	2.35	0.59
1:C:720:LYS:HD3	1:C:723:ARG:HH12	1.67	0.59
1:C:412:ILE:O	1:C:416:GLN:HG3	2.03	0.59
1:A:70:GLU:HB2	1:A:73:VAL:HG12	1.84	0.59
1:C:406:TYR:OH	1:C:433:CYS:O	2.21	0.58
1:B:438:ALA:HB1	1:B:441:ARG:HD2	1.84	0.58
1:B:132:SER:HB3	1:B:158:PHE:O	2.04	0.58
1:A:7:THR:OG1	1:A:364:GLU:OE1	2.21	0.58
1:D:282:SER:OG	2:D:801:PGR:H11	2.02	0.58
1:A:162:ILE:HD12	1:A:537:GLN:HE21	1.68	0.58
1:B:219:ALA:HB2	1:B:253:PRO:HD2	1.86	0.58
1:D:526:VAL:HG21	1:D:536:LEU:HD11	1.86	0.58
1:C:318:LEU:O	1:C:340:GLN:NE2	2.37	0.57
1:C:574:THR:HB	1:C:577:GLU:H	1.68	0.57
1:C:350:ASP:HB2	1:C:352:ARG:HG3	1.86	0.57
1:A:253:PRO:HD3	1:A:269:PHE:CD2	2.39	0.57
1:A:364:GLU:OE2	1:A:391:ARG:NH2	2.38	0.57
1:A:741:GLN:HE22	1:A:769:GLY:N	2.01	0.57
1:C:81:ARG:HG2	1:C:322:ASN:HD22	1.68	0.57
1:C:665:ARG:NH1	1:C:669:GLU:O	2.38	0.57
1:B:394:GLU:O	1:B:397:ARG:HG2	2.04	0.57
1:D:269:PHE:HB3	1:D:273:MET:HE3	1.86	0.57
1:C:253:PRO:HD3	1:C:269:PHE:CD2	2.39	0.57
1:C:237:THR:HG22	1:C:240:ARG:NH1	2.20	0.57
1:A:21:LEU:HD21	1:A:762:ASP:HB3	1.86	0.56
1:A:177:PHE:CE2	1:A:253:PRO:HG2	2.41	0.56
1:C:253:PRO:HB3	1:C:266:THR:HG23	1.87	0.56
1:D:439:PRO:O	1:D:441:ARG:HD3	2.04	0.56
1:D:468:ASN:C	1:D:469:LYS:HD2	2.29	0.56
1:C:433:CYS:SG	2:C:801:PGR:H33	2.45	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:76:VAL:HG13	1:C:276:ILE:HG12	1.87	0.56
1:B:114:LYS:HD2	1:B:114:LYS:H	1.70	0.56
1:C:212:TYR:HA	1:C:215:ALA:HB3	1.87	0.56
1:C:344:VAL:HB	1:C:359:THR:HG23	1.88	0.56
1:D:3:GLU:HG2	1:D:397:ARG:HH22	1.69	0.56
1:D:559:SER:HB3	1:D:662:PRO:HD2	1.87	0.56
1:D:20:ILE:HG21	1:D:319:ASN:HB3	1.88	0.56
1:A:406:TYR:OH	1:A:433:CYS:O	2.23	0.56
1:D:566:GLN:HG3	1:D:602:LEU:HD23	1.87	0.55
1:B:53:LYS:HE3	1:B:56:GLU:OE2	2.06	0.55
1:C:29:SER:O	1:C:33:VAL:HG23	2.05	0.55
1:D:435:GLU:HG2	1:D:446:HIS:HB3	1.87	0.55
1:B:451:PHE:HD1	1:B:452:ASN:N	2.05	0.55
1:C:135:ALA:O	1:C:139:MET:HG3	2.06	0.55
1:D:519:LEU:HD12	1:D:522:LEU:HD23	1.88	0.55
1:A:318:LEU:O	1:A:340:GLN:NE2	2.40	0.55
1:C:226:ALA:HB3	1:C:246:ALA:HB2	1.89	0.55
1:B:90:SER:HA	1:B:130:THR:HG21	1.88	0.55
1:A:126:TRP:O	1:A:127:PRO:C	2.50	0.55
1:A:268:TRP:CE2	1:A:317:LYS:HG3	2.42	0.55
1:C:13:VAL:HG13	1:C:316:ILE:HD11	1.88	0.55
1:A:433:CYS:SG	2:A:801:PGR:H33	2.47	0.54
1:B:741:GLN:HE22	1:B:769:GLY:N	2.05	0.54
1:C:218:PHE:CD2	1:C:273:MET:HE2	2.42	0.54
1:D:693:VAL:HG21	1:D:707:TYR:CE1	2.42	0.54
1:C:269:PHE:CD1	1:C:273:MET:HE3	2.42	0.54
1:A:344:VAL:HB	1:A:359:THR:HG23	1.89	0.54
1:B:410:VAL:HG22	1:B:699:PHE:CZ	2.43	0.54
1:D:547:GLY:HA2	1:D:642:GLN:O	2.07	0.54
1:A:268:TRP:CD2	1:A:317:LYS:HG3	2.43	0.54
1:C:370:ARG:HG2	1:C:400:LEU:HD11	1.89	0.54
1:C:37:GLU:O	1:C:41:GLU:HG2	2.07	0.54
1:A:766:ARG:HD2	1:A:770:TYR:O	2.08	0.53
1:A:62:LEU:HD12	1:A:63:PRO:HD2	1.90	0.53
1:B:260:PHE:CE1	1:B:296:LEU:HB2	2.43	0.53
1:C:35:ALA:HB2	1:C:58:ILE:HD11	1.90	0.53
1:D:406:TYR:OH	1:D:433:CYS:O	2.22	0.53
1:B:655:GLY:HA2	1:B:671:LEU:HG	1.90	0.53
1:B:650:ALA:HB1	1:B:654:PHE:CD2	2.44	0.53
1:C:282:SER:OG	2:C:801:PGR:H11	2.09	0.53
1:C:686:PRO:HB3	1:C:791:GLN:HB3	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:432:GLY:HA3	2:B:801:PGR:C1	2.39	0.53
1:B:92:ASP:OD1	1:B:93:TRP:N	2.42	0.53
1:C:731:ASN:OD1	1:C:735:LYS:HE3	2.09	0.53
1:C:432:GLY:HA3	2:C:801:PGR:O1	2.09	0.52
1:C:492:LYS:HE2	1:C:625:ILE:HD12	1.91	0.52
1:D:259:THR:OG1	1:D:262:GLU:HG3	2.10	0.52
1:D:634:THR:HG22	1:D:640:ARG:HH21	1.75	0.52
1:D:175:ILE:HD12	1:D:179:GLY:HA3	1.90	0.52
1:B:218:PHE:HB3	1:B:273:MET:HE2	1.92	0.52
1:B:578:LEU:O	1:B:582:LEU:HG	2.08	0.52
1:C:10:THR:HB	1:C:13:VAL:HG23	1.92	0.52
1:A:678:ARG:NH2	1:A:681:LYS:HE3	2.24	0.52
1:B:319:ASN:ND2	1:B:373:GLN:O	2.43	0.52
1:B:254:GLU:HG2	1:B:255:TYR:CD2	2.44	0.52
1:B:216:ILE:HG23	1:B:254:GLU:HB2	1.93	0.51
1:B:339:PHE:O	1:B:432:GLY:HA2	2.10	0.51
1:C:444:GLY:HA3	1:C:446:HIS:NE2	2.24	0.51
1:C:746:ASP:OD1	1:C:746:ASP:N	2.42	0.51
1:C:442:THR:HG23	1:C:543:TYR:HB2	1.93	0.51
1:D:12:ARG:HD3	1:D:69:ASP:O	2.11	0.51
1:D:551:PHE:HZ	1:D:654:PHE:HD2	1.58	0.51
1:B:105:VAL:HG13	1:B:106:ALA:H	1.75	0.51
1:D:743:ASN:ND2	1:D:766:ARG:O	2.44	0.51
1:B:431:ILE:HG13	1:B:437:GLN:HE21	1.76	0.51
1:B:613:ASP:O	1:B:617:LEU:HG	2.11	0.51
1:D:318:LEU:HD13	1:D:374:PRO:HB3	1.93	0.51
1:B:550:ALA:HB2	1:B:626:TYR:CE2	2.46	0.51
1:B:507:ASN:O	1:B:511:ILE:HG13	2.11	0.50
1:A:9:PRO:HB3	1:A:368:HIS:HB3	1.92	0.50
1:A:438:ALA:HB1	1:A:441:ARG:HD2	1.93	0.50
1:C:147:MET:HE3	1:C:153:THR:HA	1.94	0.50
1:D:175:ILE:HB	1:D:179:GLY:HA3	1.92	0.50
1:D:212:TYR:HA	1:D:215:ALA:HB3	1.92	0.50
1:A:5:GLY:O	1:A:391:ARG:NH1	2.43	0.50
1:A:411:ILE:HG21	1:A:428:TYR:CE2	2.46	0.50
1:D:411:ILE:HD13	1:D:436:PRO:HB3	1.92	0.50
1:C:53:LYS:HA	1:C:56:GLU:HG2	1.93	0.50
1:C:193:ARG:HA	1:C:198:TYR:CD2	2.47	0.50
1:D:154:VAL:HG12	1:D:449:ALA:HB2	1.93	0.50
1:A:67:ARG:NH2	1:A:77:THR:O	2.44	0.50
1:A:145:GLU:HG2	1:A:469:LYS:NZ	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:704:GLY:HA2	1:C:738:MET:SD	2.52	0.50
1:B:151:VAL:HG11	1:B:498:PHE:CD1	2.47	0.50
1:B:248:ASN:O	1:B:252:VAL:HG22	2.11	0.50
1:D:784:ASP:O	1:D:787:SER:OG	2.21	0.50
1:A:67:ARG:O	1:A:70:GLU:HG3	2.12	0.49
1:D:32:ALA:HB2	1:D:85:ILE:HB	1.94	0.49
1:A:462:ASN:OD1	1:A:579:LYS:HE3	2.13	0.49
1:B:114:LYS:HD2	1:B:114:LYS:N	2.27	0.49
1:D:551:PHE:HZ	1:D:654:PHE:CD2	2.31	0.49
1:B:282:SER:OG	2:B:801:PGR:H12	2.11	0.49
1:C:27:VAL:HB	1:C:111:ILE:HG12	1.95	0.49
1:C:31:ARG:NH1	1:C:88:GLU:OE2	2.45	0.49
1:D:27:VAL:HG13	1:D:85:ILE:HD11	1.94	0.49
1:C:97:GLU:OE2	1:C:104:ARG:NH1	2.45	0.49
1:C:135:ALA:HB1	1:C:509:VAL:HG22	1.94	0.49
1:C:565:LYS:HA	1:C:569:GLU:HB3	1.95	0.49
1:D:147:MET:HE1	1:D:154:VAL:HG22	1.95	0.49
1:C:139:MET:HE3	1:C:144:LYS:HG2	1.94	0.49
1:C:193:ARG:HH12	1:C:202:GLU:CD	2.20	0.49
1:C:712:LEU:HD23	1:C:746:ASP:HB3	1.95	0.49
1:D:396:VAL:HG22	1:D:403:PRO:HD2	1.95	0.49
1:D:572:ARG:HB2	1:D:573:LEU:HD12	1.94	0.49
1:A:253:PRO:HB3	1:A:266:THR:HG23	1.95	0.49
1:D:188:LEU:HD11	1:D:202:GLU:HG3	1.94	0.49
1:D:435:GLU:CG	1:D:446:HIS:HB3	2.43	0.49
1:D:446:HIS:O	1:D:703:ASN:ND2	2.40	0.49
1:A:432:GLY:HA3	2:A:801:PGR:C1	2.42	0.48
1:C:10:THR:HG22	1:C:12:ARG:N	2.22	0.48
1:D:318:LEU:O	1:D:340:GLN:NE2	2.46	0.48
1:D:157:TYR:CE2	1:D:448:ALA:HA	2.48	0.48
1:A:754:GLN:HG2	1:A:782:GLN:OE1	2.13	0.48
1:B:188:LEU:HD11	1:B:202:GLU:HG3	1.96	0.48
1:C:478:MET:HE1	1:C:578:LEU:HD23	1.96	0.48
1:B:650:ALA:HB1	1:B:654:PHE:CE2	2.48	0.48
1:B:288:PHE:O	1:B:292:MET:HB2	2.13	0.48
1:C:549:GLN:NE2	1:C:646:TYR:CZ	2.82	0.48
1:C:750:LEU:HD22	1:C:774:PHE:CE1	2.49	0.48
1:B:212:TYR:HA	1:B:215:ALA:HB3	1.96	0.48
1:B:660:ALA:HA	1:B:665:ARG:O	2.13	0.48
1:C:574:THR:HG22	1:C:576:GLN:H	1.79	0.48
1:D:650:ALA:HB1	1:D:654:PHE:CD2	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:720:LYS:HD3	1:C:723:ARG:NH1	2.29	0.48
1:B:215:ALA:O	1:B:273:MET:HE1	2.15	0.47
1:B:253:PRO:HD3	1:B:269:PHE:CD2	2.49	0.47
1:D:106:ALA:HB2	1:D:331:GLN:HG2	1.96	0.47
1:C:372:PRO:HB3	1:C:771:SER:O	2.15	0.47
1:D:252:VAL:HB	1:D:266:THR:OG1	2.15	0.47
1:D:404:ALA:HB2	1:D:766:ARG:NH2	2.29	0.47
1:A:527:ASP:HA	1:A:528:ASP:HA	1.67	0.47
1:D:56:GLU:OE1	1:D:210:LEU:HD11	2.14	0.47
1:D:261:TRP:HA	1:D:310:LEU:HD13	1.97	0.47
1:D:288:PHE:CE1	1:D:292:MET:HG3	2.49	0.47
1:C:275:GLN:HG3	1:C:283:ILE:HG13	1.96	0.47
1:C:610:ASN:CB	1:C:684:LEU:HD23	2.45	0.47
1:D:376:PHE:HB3	1:D:402:VAL:HB	1.97	0.47
1:C:13:VAL:HG11	1:C:312:ASP:HB3	1.96	0.47
1:C:428:TYR:HA	1:C:439:PRO:HD3	1.97	0.47
1:A:252:VAL:HG11	1:A:262:GLU:HB3	1.96	0.46
1:B:253:PRO:HB3	1:B:266:THR:HG23	1.97	0.46
1:B:626:TYR:O	1:B:630:VAL:HG23	2.15	0.46
1:C:52:ALA:HB2	1:C:207:ALA:HB1	1.97	0.46
1:C:136:ALA:O	1:C:144:LYS:HE2	2.16	0.46
1:D:155:GLY:HA2	1:D:158:PHE:HB3	1.97	0.46
1:A:396:VAL:HG23	1:A:403:PRO:HD2	1.98	0.46
1:A:475:THR:HG21	1:A:493:LYS:HB2	1.97	0.46
1:C:396:VAL:HG11	1:C:725:PHE:CZ	2.51	0.46
1:C:473:PRO:HD2	1:C:494:GLN:OE1	2.15	0.46
1:D:651:ASN:OD1	1:D:651:ASN:N	2.47	0.46
1:A:404:ALA:HB2	1:A:766:ARG:NH2	2.28	0.46
1:B:56:GLU:HA	1:B:214:ALA:CB	2.46	0.46
1:C:97:GLU:HA	1:C:100:THR:OG1	2.15	0.46
1:A:713:PRO:HG2	1:A:746:ASP:OD1	2.15	0.46
1:B:431:ILE:CG1	1:B:437:GLN:HG2	2.45	0.46
1:C:138:TYR:CE1	1:D:203:GLN:HG3	2.51	0.46
1:D:64:VAL:HG13	1:D:222:TYR:CE1	2.51	0.46
1:D:93:TRP:O	1:D:97:GLU:HB2	2.16	0.46
1:A:514:GLY:HA2	1:A:537:GLN:HB3	1.96	0.46
1:C:758:GLN:NE2	1:C:759:GLN:HE21	2.14	0.46
1:D:51:ARG:NH1	1:D:88:GLU:OE1	2.41	0.46
1:D:424:ASP:O	1:D:441:ARG:NH2	2.48	0.46
1:A:451:PHE:CD1	1:A:502:LEU:HD22	2.51	0.46
1:C:555:ASP:HA	1:C:678:ARG:HD3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:730:ARG:HG3	1:D:730:ARG:HH11	1.81	0.46
1:A:400:LEU:HB2	1:A:402:VAL:HG22	1.96	0.46
1:C:587:GLY:CA	1:C:590:SER:HB3	2.46	0.46
1:D:73:VAL:O	1:D:265:GLN:NE2	2.42	0.46
1:D:443:GLU:HB2	1:D:536:LEU:HD22	1.98	0.46
1:B:704:GLY:HA2	1:B:738:MET:SD	2.56	0.46
1:C:36:THR:HG23	1:C:126:TRP:NE1	2.31	0.46
1:D:230:ALA:O	1:D:239:GLN:NE2	2.44	0.46
1:D:549:GLN:HA	1:D:644:GLY:O	2.16	0.46
1:A:25:PRO:HG2	1:A:336:TYR:CZ	2.51	0.45
1:A:86:CYS:SG	1:A:279:SER:HB3	2.56	0.45
1:B:173:LEU:HB3	1:B:295:TYR:CZ	2.51	0.45
1:B:408:ASP:HB3	1:B:412:ILE:HD12	1.97	0.45
1:C:613:ASP:O	1:C:617:LEU:HG	2.16	0.45
1:D:698:HIS:CD2	1:D:737:GLY:HA2	2.51	0.45
1:B:67:ARG:O	1:B:70:GLU:HG3	2.16	0.45
1:C:504:GLU:HG3	1:D:198:TYR:OH	2.15	0.45
1:C:590:SER:OG	1:C:591:GLY:N	2.49	0.45
1:C:185:THR:HG23	1:C:209:ILE:HD11	1.97	0.45
1:C:594:ARG:O	1:C:598:ILE:HG13	2.17	0.45
1:D:465:ARG:NH1	1:D:477:GLU:OE2	2.45	0.45
1:A:204:PHE:O	1:A:208:VAL:HG23	2.16	0.45
1:B:289:ASP:HB3	1:B:344:VAL:HG12	1.98	0.45
1:C:621:GLN:O	1:C:625:ILE:HG12	2.16	0.45
1:A:248:ASN:O	1:A:252:VAL:HG22	2.16	0.45
1:A:620:ARG:NH1	1:A:624:LEU:HD11	2.32	0.45
1:B:165:VAL:HA	1:B:437:GLN:NE2	2.28	0.45
1:B:716:LEU:HD22	1:B:725:PHE:HB2	1.98	0.45
1:C:251:ARG:HG2	1:C:262:GLU:OE2	2.15	0.45
1:A:155:GLY:HA2	1:A:158:PHE:HB3	1.97	0.45
1:A:475:THR:HG22	1:A:493:LYS:HD2	1.99	0.45
1:A:496:ALA:HA	1:A:629:GLU:OE1	2.16	0.45
1:C:51:ARG:O	1:C:55:VAL:HG23	2.16	0.45
1:C:348:THR:HG23	1:C:350:ASP:H	1.82	0.45
1:C:648:VAL:O	1:C:768:ALA:HB3	2.17	0.45
1:D:223:ALA:HA	1:D:246:ALA:HA	1.99	0.45
1:D:433:CYS:HB3	1:D:769:GLY:HA3	1.99	0.45
1:A:97:GLU:HG2	3:A:904:HOH:O	2.17	0.45
1:B:147:MET:HE3	1:B:154:VAL:H	1.82	0.45
1:C:147:MET:HE1	1:C:154:VAL:HG22	1.99	0.45
1:C:631:GLU:CD	1:C:700:ILE:HD11	2.42	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:659:SER:O	1:C:665:ARG:NH2	2.49	0.45
1:B:12:ARG:HG3	1:B:69:ASP:HB3	1.99	0.45
1:B:452:ASN:ND2	1:B:654:PHE:HB3	2.31	0.45
1:B:484:MET:HE2	1:B:564:GLN:HB2	1.98	0.45
1:C:376:PHE:HB3	1:C:402:VAL:HB	1.99	0.45
1:C:773:GLN:O	1:C:776:VAL:HG22	2.17	0.45
1:C:741:GLN:HE21	1:C:741:GLN:HB3	1.63	0.45
1:D:520:PRO:HD2	3:D:906:HOH:O	2.17	0.45
1:C:459:ILE:HG22	1:C:464:GLY:HA2	1.98	0.44
1:B:514:GLY:HA2	1:B:537:GLN:HB3	1.98	0.44
1:C:578:LEU:O	1:C:582:LEU:HG	2.17	0.44
1:D:723:ARG:HG2	1:D:723:ARG:NH1	2.26	0.44
1:C:455:LYS:O	1:C:459:ILE:HG13	2.17	0.44
1:D:16:LEU:HB3	1:D:316:ILE:HG21	2.00	0.44
1:D:445:TRP:CH2	1:D:509:VAL:HG12	2.53	0.44
1:A:624:LEU:HD22	1:A:628:GLN:NE2	2.33	0.44
1:B:188:LEU:HD13	1:B:205:TYR:CB	2.47	0.44
1:C:373:GLN:HA	1:C:374:PRO:C	2.43	0.44
1:D:285:PRO:HG2	1:D:342:LEU:HD12	1.99	0.44
1:A:145:GLU:HG2	1:A:469:LYS:HZ1	1.83	0.44
1:D:445:TRP:CH2	1:D:510:ASP:HA	2.53	0.44
1:C:45:LEU:O	1:C:50:ARG:NH2	2.51	0.44
1:C:587:GLY:HA2	1:C:590:SER:HB3	1.98	0.44
1:D:288:PHE:CD1	1:D:292:MET:HG3	2.52	0.44
1:A:50:ARG:HH11	1:A:50:ARG:HB2	1.82	0.44
1:A:184:VAL:O	1:A:188:LEU:HB2	2.18	0.44
1:C:172:VAL:HG11	1:C:270:ILE:HD11	1.99	0.44
1:D:13:VAL:HG13	1:D:316:ILE:HD11	2.00	0.44
1:B:435:GLU:OE1	2:B:801:PGR:O1	2.35	0.43
1:C:573:LEU:HD21	1:C:598:ILE:HG23	1.99	0.43
1:C:616:ASP:OD2	1:C:695:LYS:NZ	2.49	0.43
1:A:655:GLY:HA2	1:A:671:LEU:HG	1.99	0.43
1:A:381:TRP:CZ3	1:C:736:LYS:HE2	2.54	0.43
1:B:347:GLN:HG3	1:B:408:ASP:OD2	2.19	0.43
1:C:706:LEU:HD11	1:C:768:ALA:C	2.43	0.43
1:A:172:VAL:HG11	1:A:270:ILE:HD11	2.00	0.43
1:A:673:ASP:OD1	1:A:673:ASP:N	2.46	0.43
1:C:204:PHE:O	1:C:208:VAL:HG23	2.18	0.43
1:C:396:VAL:HG11	1:C:725:PHE:HZ	1.83	0.43
1:C:343:CYS:HA	1:C:377:SER:O	2.18	0.43
1:A:85:ILE:HG22	1:A:87:PRO:HD3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:93:TRP:CE3	1:C:326:ASP:HA	2.53	0.43
1:D:686:PRO:HB3	1:D:791:GLN:HB3	2.01	0.43
1:A:57:LYS:O	1:A:61:GLU:HB2	2.19	0.43
1:A:648:VAL:HG21	2:A:801:PGR:H31	2.00	0.43
1:B:62:LEU:HD12	1:B:63:PRO:HD2	2.01	0.43
1:B:126:TRP:O	1:B:127:PRO:C	2.61	0.43
1:D:527:ASP:HA	1:D:528:ASP:HA	1.77	0.43
1:C:275:GLN:OE1	1:C:321:ILE:HD13	2.19	0.43
1:D:175:ILE:HD12	1:D:179:GLY:C	2.44	0.43
1:A:83:THR:HG21	1:A:324:THR:CG2	2.47	0.43
1:A:712:LEU:HD23	1:A:712:LEU:HA	1.89	0.43
1:B:35:ALA:HB2	1:B:58:ILE:HD11	2.00	0.43
1:B:177:PHE:O	1:B:181:ILE:HG13	2.19	0.43
1:B:499:VAL:O	1:B:503:VAL:HG23	2.19	0.43
1:C:412:ILE:HB	1:C:413:PRO:HD3	1.99	0.43
1:A:17:LYS:HD2	1:A:369:VAL:O	2.18	0.43
1:A:381:TRP:HZ3	1:C:736:LYS:HE2	1.84	0.43
1:C:668:LYS:HE2	1:C:668:LYS:HB2	1.60	0.42
1:D:30:GLU:HG2	1:D:63:PRO:HG2	2.00	0.42
1:D:64:VAL:CG1	1:D:225:GLU:HG3	2.49	0.42
1:D:253:PRO:HD3	1:D:269:PHE:CD2	2.54	0.42
1:D:550:ALA:HB2	1:D:626:TYR:CE2	2.54	0.42
1:D:551:PHE:CZ	1:D:654:PHE:CD2	3.04	0.42
1:A:564:GLN:O	1:A:569:GLU:HG3	2.18	0.42
1:B:12:ARG:HH12	1:B:241:GLU:CD	2.27	0.42
1:B:318:LEU:HD13	1:B:374:PRO:HB3	2.00	0.42
1:B:706:LEU:HA	1:B:739:HIS:ND1	2.33	0.42
1:C:526:VAL:HG11	1:C:536:LEU:HD21	2.02	0.42
1:D:188:LEU:HD13	1:D:205:TYR:CD2	2.54	0.42
1:B:21:LEU:HD12	1:B:21:LEU:HA	1.91	0.42
1:B:73:VAL:O	1:B:265:GLN:NE2	2.39	0.42
1:B:597:GLU:O	1:B:601:ILE:HG13	2.19	0.42
1:B:663:ASP:HB2	1:B:678:ARG:HH12	1.83	0.42
1:D:55:VAL:CG1	1:D:277:GLU:HB2	2.49	0.42
1:D:435:GLU:CB	1:D:446:HIS:HB3	2.48	0.42
1:B:39:TYR:CE1	1:B:54:VAL:HG21	2.53	0.42
1:B:586:PHE:CE2	1:B:660:ALA:HB1	2.55	0.42
1:D:510:ASP:OD2	1:D:637:ARG:NH2	2.44	0.42
1:B:658:VAL:HG12	1:B:659:SER:O	2.20	0.42
1:C:484:MET:HB3	1:C:484:MET:HE3	1.72	0.42
1:A:470:GLN:NE2	1:A:474:MET:HG2	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:381:TRP:HZ3	1:D:736:LYS:HD3	1.85	0.42
1:C:15:ARG:HH21	1:C:69:ASP:CG	2.27	0.42
1:C:32:ALA:HB2	1:C:85:ILE:HB	2.02	0.42
1:C:173:LEU:HD23	1:C:173:LEU:HA	1.92	0.42
1:D:97:GLU:OE2	1:D:327:GLU:HG3	2.19	0.42
1:D:173:LEU:HB3	1:D:295:TYR:CZ	2.54	0.42
1:D:274:LEU:HD23	1:D:274:LEU:HA	1.92	0.42
1:A:711:PHE:CD1	1:A:716:LEU:HD11	2.54	0.42
1:C:173:LEU:HB3	1:C:295:TYR:CZ	2.55	0.42
1:B:535:SER:OG	1:B:538:GLU:HG3	2.19	0.42
1:C:366:THR:HG21	1:C:402:VAL:HG21	2.01	0.42
1:C:722:LEU:O	1:C:725:PHE:HB3	2.20	0.42
1:D:478:MET:HE1	1:D:578:LEU:HG	2.01	0.42
1:D:712:LEU:HB2	1:D:790:GLU:OE2	2.20	0.42
1:A:268:TRP:CE2	1:A:272:SER:HB3	2.55	0.42
1:C:431:ILE:HG13	1:C:437:GLN:HG2	2.02	0.42
1:D:64:VAL:HG13	1:D:222:TYR:CD1	2.55	0.42
1:C:428:TYR:CD1	1:C:428:TYR:C	2.98	0.42
1:C:438:ALA:HB1	1:C:441:ARG:HD2	2.01	0.42
1:D:305:GLU:CD	1:D:305:GLU:H	2.28	0.42
1:D:438:ALA:HB1	1:D:441:ARG:HE	1.85	0.42
1:C:269:PHE:HD1	1:C:273:MET:HE3	1.83	0.41
1:D:242:LEU:HD23	1:D:242:LEU:HA	1.95	0.41
1:D:706:LEU:HD11	1:D:768:ALA:C	2.45	0.41
1:A:45:LEU:HD13	1:A:49:MET:HG3	2.02	0.41
1:A:547:GLY:HA3	1:A:703:ASN:ND2	2.35	0.41
1:B:526:VAL:HG11	1:B:536:LEU:HD21	2.01	0.41
1:B:288:PHE:CE2	1:B:292:MET:HG3	2.55	0.41
1:C:67:ARG:NH1	1:C:320:ASP:OD2	2.52	0.41
1:C:522:LEU:HD12	1:C:522:LEU:O	2.20	0.41
1:D:567:VAL:HG22	1:D:573:LEU:HB2	2.01	0.41
1:B:283:ILE:O	1:B:340:GLN:HB3	2.21	0.41
1:B:444:GLY:HA3	1:B:446:HIS:CD2	2.56	0.41
1:B:527:ASP:HA	1:B:528:ASP:HA	1.83	0.41
1:C:66:ILE:HD12	1:C:225:GLU:HG3	2.01	0.41
1:D:208:VAL:HG22	1:D:520:PRO:O	2.20	0.41
1:D:223:ALA:HB2	1:D:249:CYS:HB2	2.03	0.41
1:D:268:TRP:CH2	1:D:317:LYS:O	2.73	0.41
1:C:85:ILE:HD12	1:C:94:VAL:HG11	2.03	0.41
1:D:563:ILE:O	1:D:567:VAL:HB	2.21	0.41
1:A:381:TRP:HB3	1:A:408:ASP:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:153:THR:HG21	1:B:654:PHE:CZ	2.56	0.41
1:B:451:PHE:HE1	1:B:456:VAL:HG21	1.86	0.41
1:B:550:ALA:HB2	1:B:626:TYR:CD2	2.55	0.41
1:D:377:SER:HB3	1:D:406:TYR:CE2	2.56	0.41
1:C:451:PHE:CD2	1:C:502:LEU:HD22	2.56	0.41
1:D:372:PRO:HB3	1:D:771:SER:O	2.20	0.41
1:D:499:VAL:O	1:D:503:VAL:HG23	2.21	0.41
1:B:126:TRP:N	1:B:127:PRO:CD	2.84	0.41
1:C:282:SER:HA	1:C:339:PHE:O	2.21	0.41
1:D:376:PHE:CD2	1:D:403:PRO:HB3	2.56	0.41
1:A:27:VAL:HB	1:A:111:ILE:HG12	2.02	0.41
1:A:95:GLU:HA	1:A:98:PHE:CE1	2.56	0.41
1:A:173:LEU:HB3	1:A:295:TYR:CZ	2.56	0.41
1:A:647:PRO:HG3	1:A:673:ASP:HB2	2.02	0.41
1:B:29:SER:HB3	1:B:115:THR:HG23	2.02	0.41
1:B:74:GLY:HA2	1:B:222:TYR:CE2	2.56	0.41
1:B:555:ASP:OD1	1:B:678:ARG:HD2	2.21	0.41
1:D:90:SER:HA	1:D:130:THR:HG21	2.03	0.41
1:A:443:GLU:HB2	1:A:536:LEU:HD22	2.03	0.41
1:B:49:MET:O	1:B:53:LYS:HG2	2.21	0.41
1:C:114:LYS:O	1:C:117:ASP:HB2	2.21	0.41
1:C:652:VAL:HG11	1:C:780:GLU:HB2	2.03	0.41
1:A:55:VAL:HG22	1:A:59:PHE:CE2	2.56	0.40
1:A:526:VAL:HG11	1:A:536:LEU:HD21	2.02	0.40
1:A:559:SER:HB3	1:A:662:PRO:HD2	2.01	0.40
1:B:55:VAL:CG1	1:B:277:GLU:HG3	2.51	0.40
1:B:154:VAL:HG12	1:B:449:ALA:HB2	2.02	0.40
1:B:277:GLU:CD	1:B:521:PHE:HB3	2.45	0.40
1:B:445:TRP:CH2	1:B:510:ASP:HA	2.55	0.40
1:C:433:CYS:HB3	1:C:769:GLY:HA3	2.02	0.40
1:C:766:ARG:HG3	1:C:770:TYR:O	2.20	0.40
1:B:431:ILE:HG12	1:B:437:GLN:HG2	2.03	0.40
1:C:268:TRP:CH2	1:C:317:LYS:O	2.74	0.40
1:D:226:ALA:HB3	1:D:246:ALA:HB2	2.04	0.40
1:D:704:GLY:HA2	1:D:738:MET:SD	2.62	0.40
1:B:68:PRO:O	1:B:69:ASP:HB2	2.21	0.40
1:B:432:GLY:HA3	2:B:801:PGR:H11	2.04	0.40
1:D:147:MET:CE	1:D:154:VAL:HG22	2.52	0.40
1:D:264:CYS:HB3	1:D:314:CYS:SG	2.61	0.40
1:A:369:VAL:HG12	1:A:371:LEU:HG	2.03	0.40
1:B:177:PHE:HB2	1:B:254:GLU:HA	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:679:GLN:NE2	1:B:784:ASP:OD1	2.51	0.40
1:D:162:ILE:HD11	1:D:513:HIS:CG	2.57	0.40
1:D:356:ASN:O	1:D:359:THR:HB	2.21	0.40
1:D:445:TRP:HH2	1:D:509:VAL:HG12	1.85	0.40
1:A:215:ALA:HB1	1:A:273:MET:HE1	2.02	0.40
1:B:340:GLN:H	1:B:340:GLN:HG2	1.68	0.40
1:B:451:PHE:CD1	1:B:451:PHE:C	3.00	0.40
1:C:447:ASP:HA	1:C:549:GLN:HE22	1.87	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	790/816 (97%)	745 (94%)	44 (6%)	1 (0%)	48	77
1	B	791/816 (97%)	750 (95%)	39 (5%)	2 (0%)	37	67
1	C	790/816 (97%)	736 (93%)	53 (7%)	1 (0%)	48	77
1	D	792/816 (97%)	746 (94%)	45 (6%)	1 (0%)	48	77
All	All	3163/3264 (97%)	2977 (94%)	181 (6%)	5 (0%)	44	73

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	648	VAL
1	B	648	VAL
1	C	648	VAL
1	D	648	VAL
1	B	647	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	662/683 (97%)	655 (99%)	7 (1%)	70	90
1	B	663/683 (97%)	657 (99%)	6 (1%)	75	92
1	C	662/683 (97%)	654 (99%)	8 (1%)	67	89
1	D	663/683 (97%)	661 (100%)	2 (0%)	91	97
All	All	2650/2732 (97%)	2627 (99%)	23 (1%)	75	92

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	LYS
1	A	61	GLU
1	A	233	GLU
1	A	603	GLU
1	A	676	SER
1	A	743	ASN
1	A	789	THR
1	B	56	GLU
1	B	435	GLU
1	B	546	THR
1	B	714	SER
1	B	720	LYS
1	B	789	THR
1	C	56	GLU
1	C	130	THR
1	C	458	GLU
1	C	578	LEU
1	C	684	LEU
1	C	746	ASP
1	C	755	LYS
1	C	789	THR
1	D	88	GLU
1	D	746	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	190	ASN
1	A	382	GLN
1	A	497	HIS
1	A	537	GLN
1	A	566	GLN
1	A	743	ASN
1	A	759	GLN
1	A	760	HIS
1	B	149	ASN
1	B	382	GLN
1	B	437	GLN
1	B	452	ASN
1	B	497	HIS
1	B	566	GLN
1	B	576	GLN
1	B	756	ASN
1	C	220	HIS
1	C	290	GLN
1	C	549	GLN
1	C	703	ASN
1	C	759	GLN
1	C	761	GLN
1	D	462	ASN
1	D	468	ASN
1	D	698	HIS
1	D	731	ASN
1	D	739	HIS

### 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

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	PGR	A	801	-	3,4,4	0.27	0	1,4,4	0.17	0
2	PGR	D	801	-	3,4,4	0.19	0	1,4,4	0.15	0
2	PGR	B	801	-	3,4,4	0.22	0	1,4,4	1.19	0
2	PGR	C	801	-	3,4,4	0.23	0	1,4,4	0.31	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
2	PGR	A	801	-	-	2/2/2/2	-
2	PGR	D	801	-	-	2/2/2/2	-
2	PGR	B	801	-	-	2/2/2/2	-
2	PGR	C	801	-	-	1/2/2/2	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (7) torsion outliers are listed below:

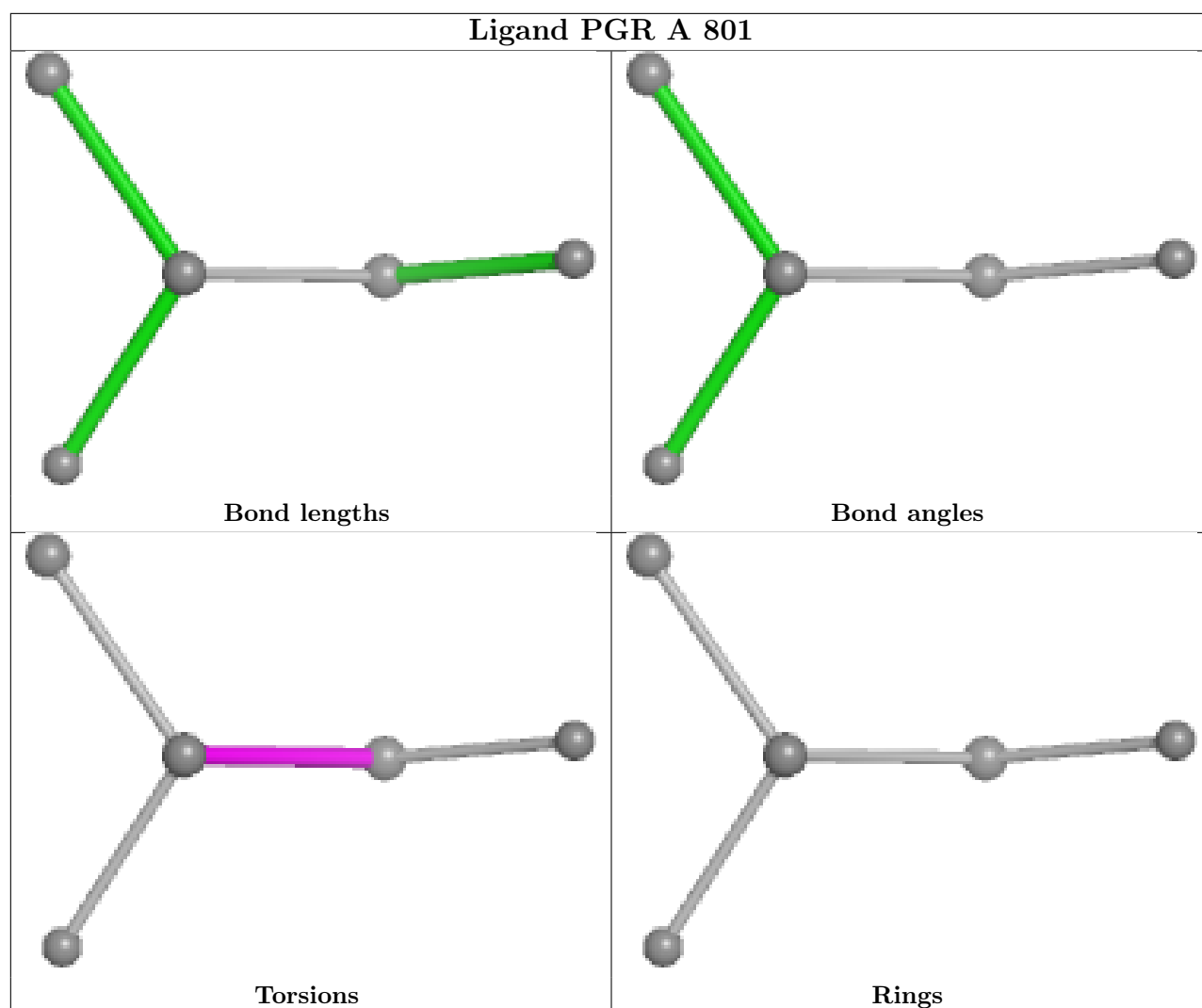
Mol	Chain	Res	Type	Atoms
2	A	801	PGR	O1-C1-C2-C3
2	A	801	PGR	O1-C1-C2-O2
2	B	801	PGR	O1-C1-C2-O2
2	D	801	PGR	O1-C1-C2-C3
2	D	801	PGR	O1-C1-C2-O2
2	B	801	PGR	O1-C1-C2-C3
2	C	801	PGR	O1-C1-C2-O2

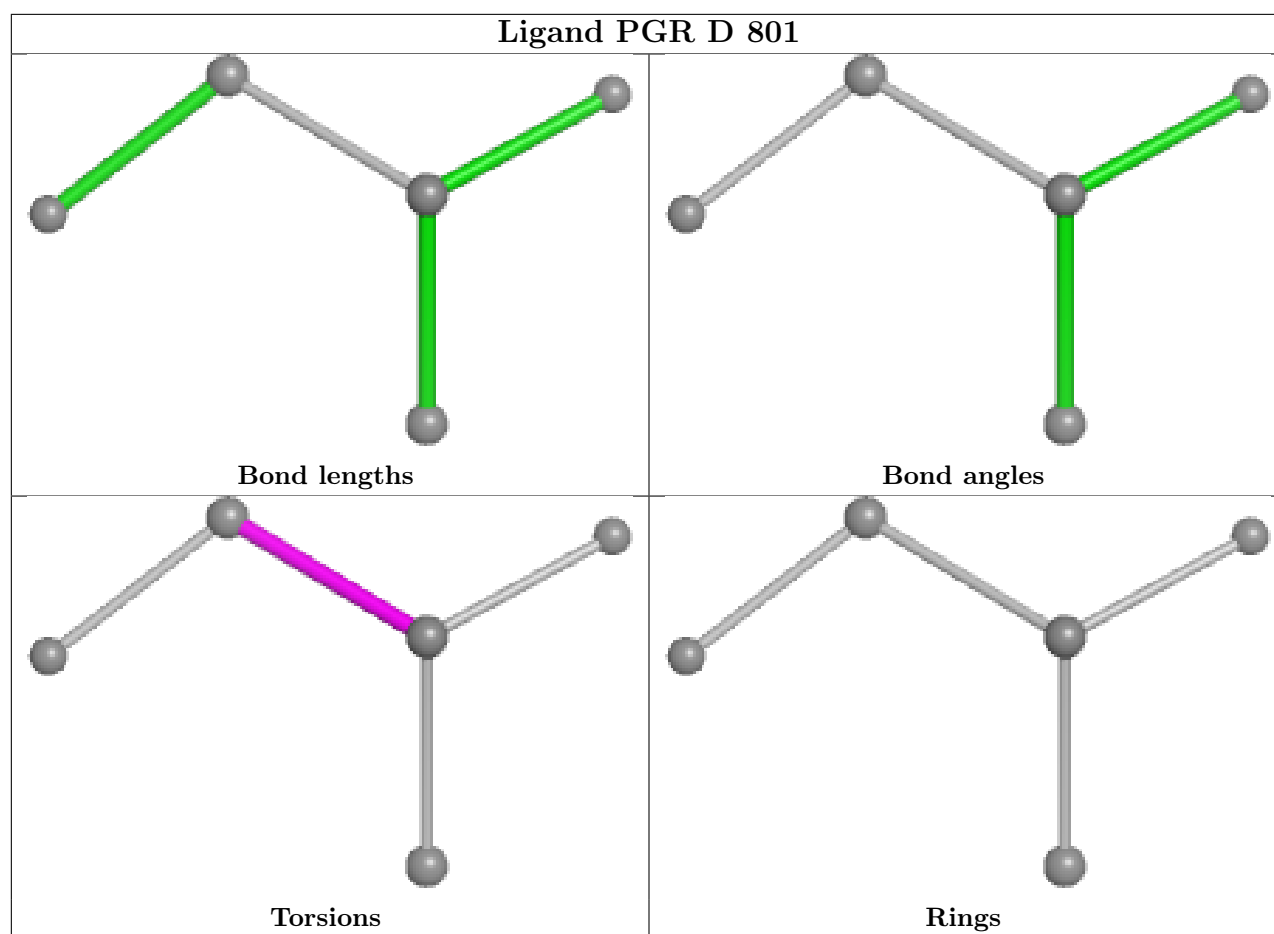
There are no ring outliers.

4 monomers are involved in 19 short contacts:

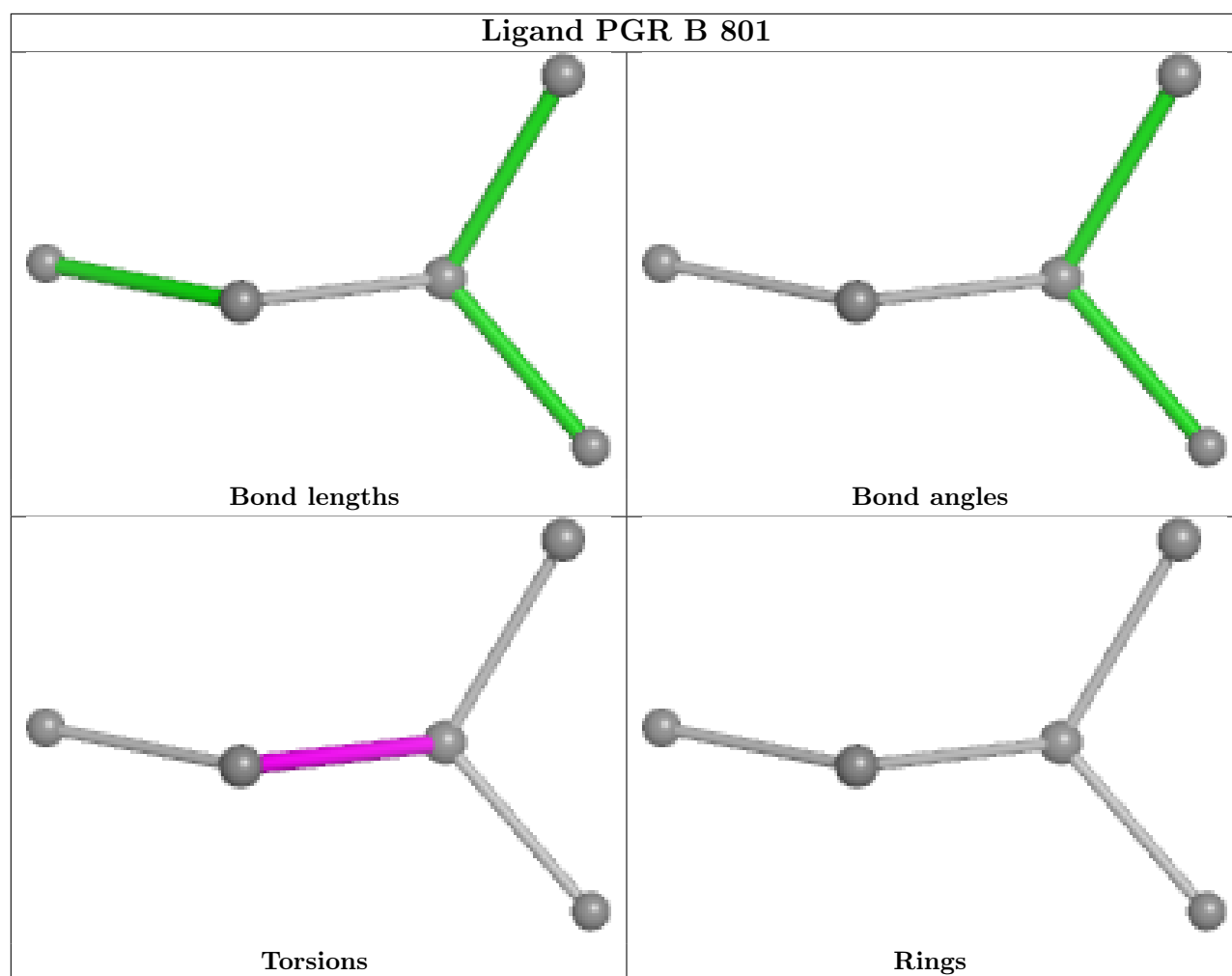
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	801	PGR	6	0
2	D	801	PGR	2	0
2	B	801	PGR	8	0
2	C	801	PGR	3	0

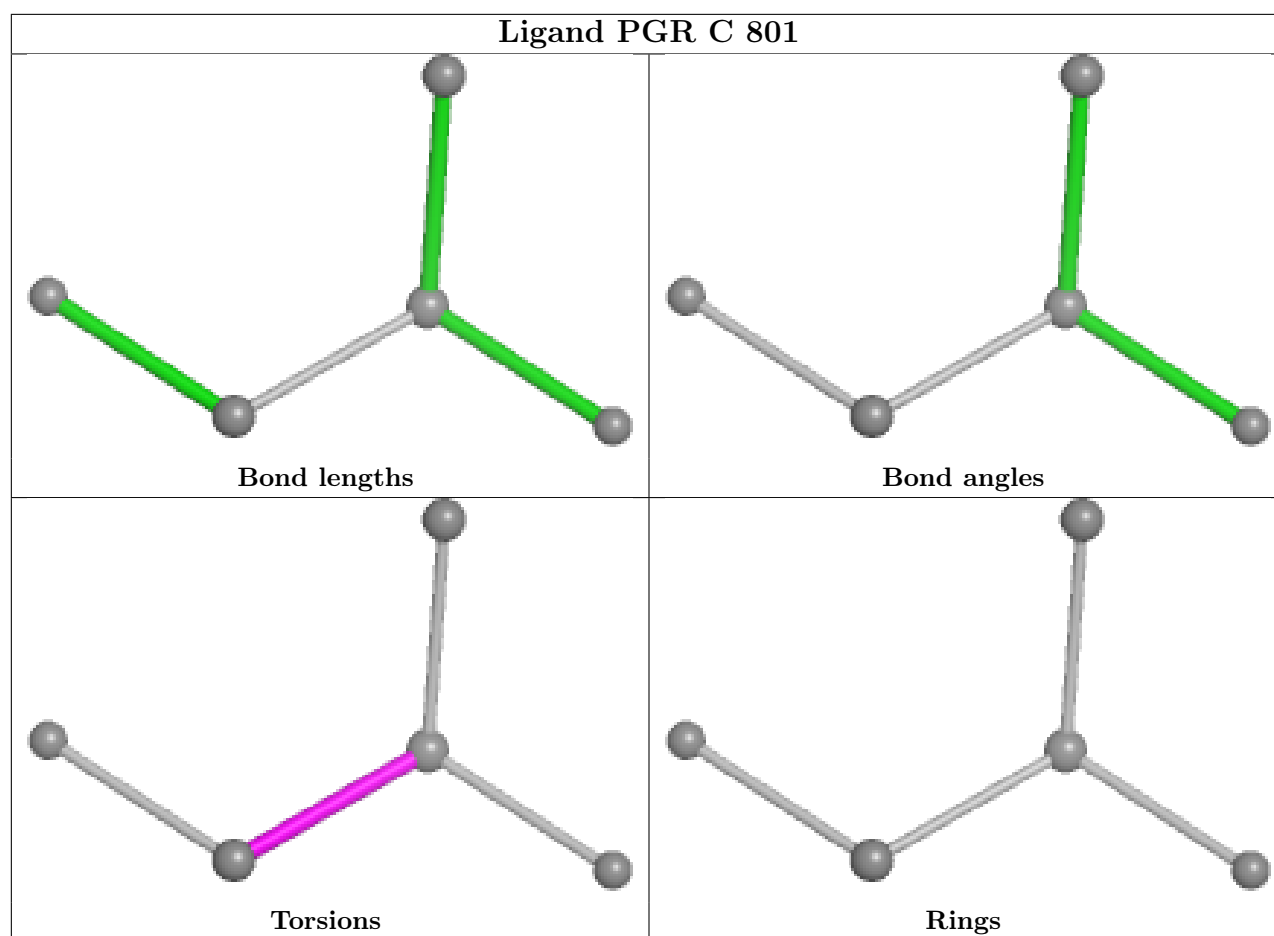
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 [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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	792/816 (97%)	-0.23	0 <a href="#">100</a> <a href="#">100</a>	14, 22, 36, 58	0
1	B	792/816 (97%)	-0.10	4 (0%) <a href="#">87</a> <a href="#">83</a>	14, 27, 43, 61	1 (0%)
1	C	792/816 (97%)	-0.03	2 (0%) <a href="#">90</a> <a href="#">87</a>	15, 29, 46, 87	0
1	D	794/816 (97%)	0.01	4 (0%) <a href="#">87</a> <a href="#">83</a>	19, 30, 45, 72	0
All	All	3170/3264 (97%)	-0.09	10 (0%) <a href="#">90</a> <a href="#">87</a>	14, 27, 43, 87	1 (0%)

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	0	MET	3.9
1	B	2	LEU	3.8
1	B	84[A]	GLU	3.5
1	B	551	PHE	3.3
1	C	551	PHE	2.6
1	D	551	PHE	2.5
1	D	441	ARG	2.2
1	C	591	GLY	2.1
1	B	297	ALA	2.0
1	D	8	HIS	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 monosaccharides in this entry.

## 6.4 Ligands

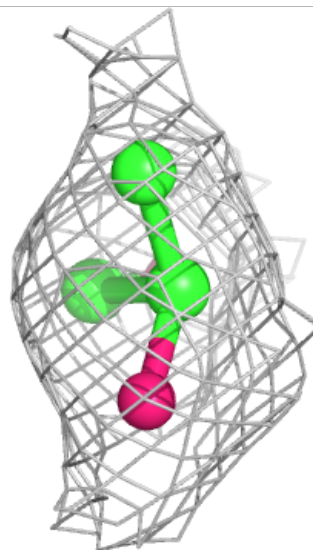
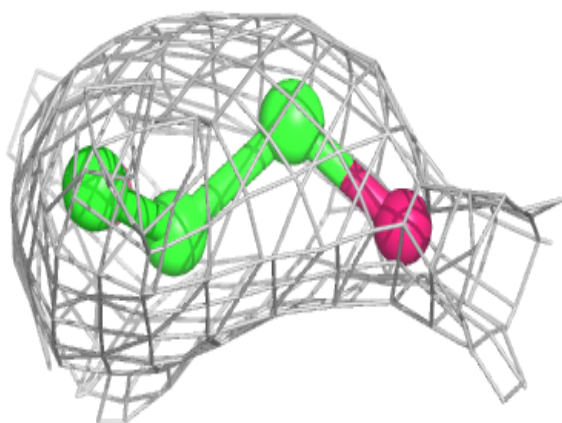
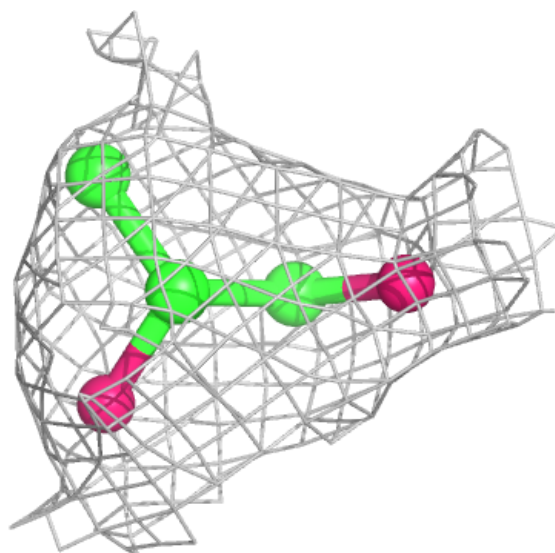
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	PGR	A	801	5/5	0.88	0.13	22,22,23,23	0
2	PGR	B	801	5/5	0.88	0.13	22,23,25,28	0
2	PGR	D	801	5/5	0.92	0.12	26,26,27,27	0
2	PGR	C	801	5/5	0.94	0.10	22,23,24,25	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.

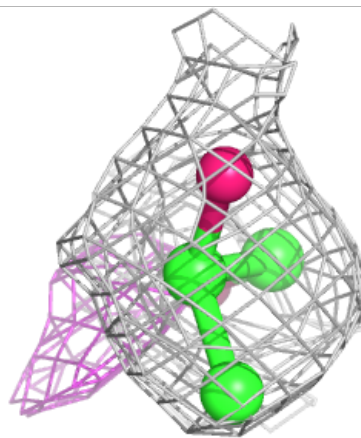
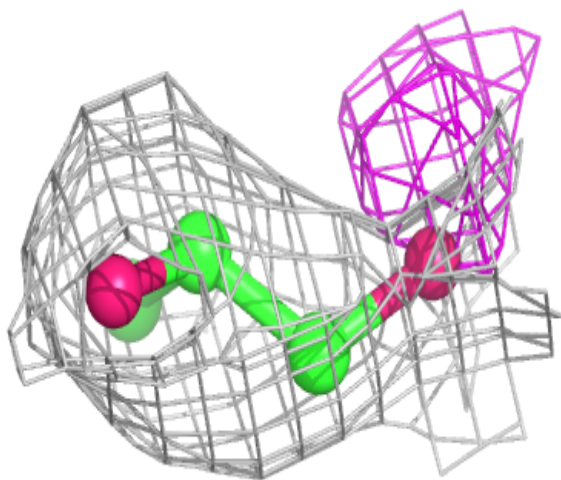
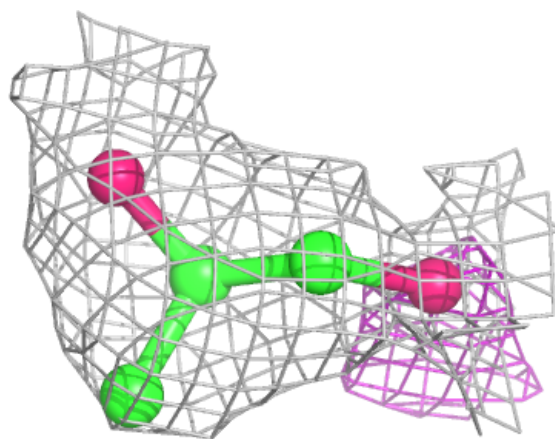
**Electron density around PGR A 801:**

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



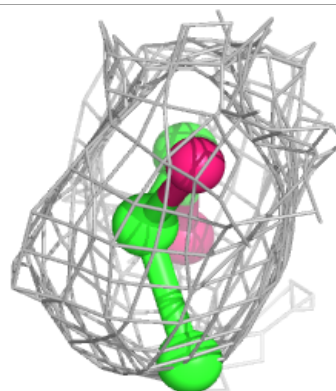
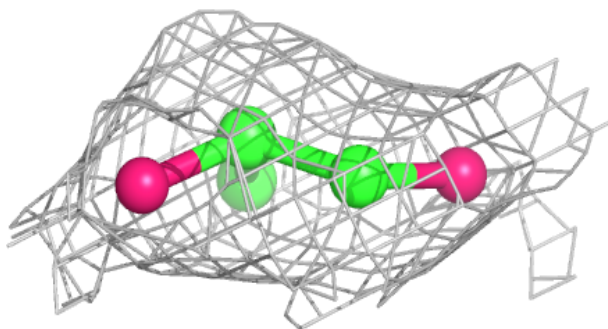
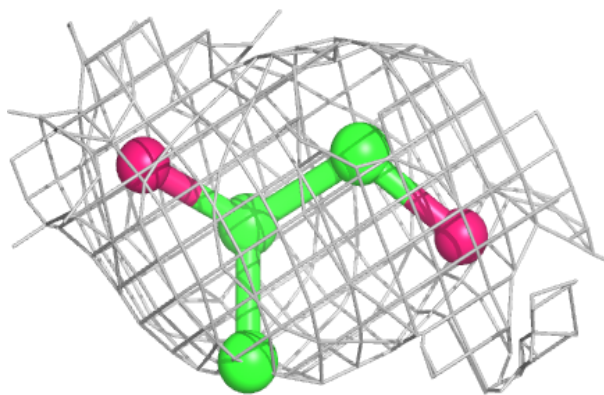
**Electron density around PGR B 801:**

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



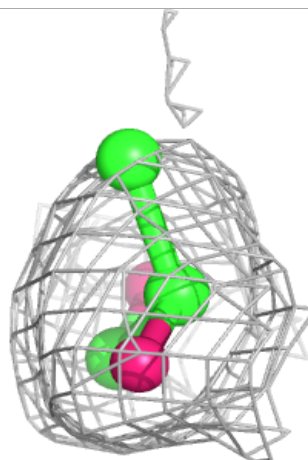
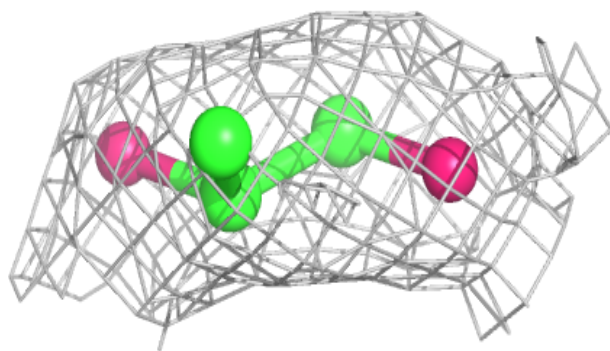
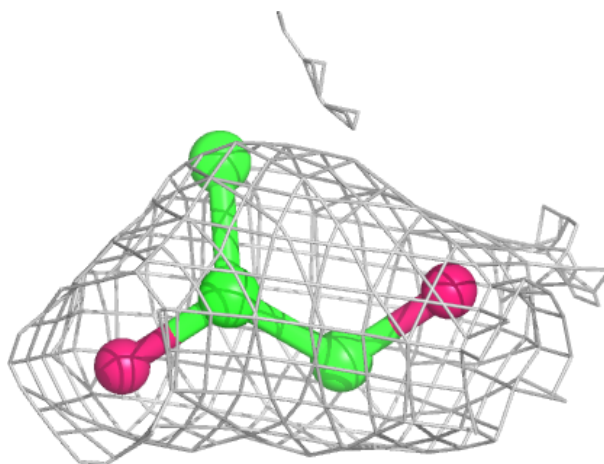
**Electron density around PGR D 801:**

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



**Electron density around PGR C 801:**

$2mF_o-DF_c$  (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.