



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 10:06 AM UTC

PDB ID : 2GIN / pdb_00002gin
Title : X-ray structure of the wt allene oxide cyclase 2 from arabidopsis thaliana
Authors : Hofmann, E.; Schaller, F.; Zerbe, P.
Deposited on : 2006-03-29
Resolution : 1.80 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

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
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

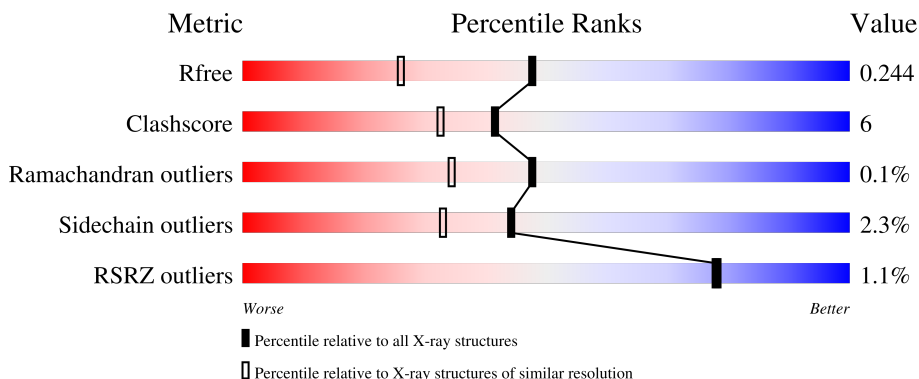
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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}	180053	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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 ≥ 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	188	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 79%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 12%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 8%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 8%; height: 10px; background-color: grey;"></div> </div>
1	B	188	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 77%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 14%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 8%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 8%; height: 10px; background-color: grey;"></div> </div>
1	C	188	<div style="display: flex; align-items: center;"> <div style="width: 83%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 9%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 8%; height: 10px; background-color: grey;"></div> </div>
1	D	188	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 78%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 12%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 8%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 8%; height: 10px; background-color: grey;"></div> </div>
1	E	188	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 80%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 12%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 8%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 8%; height: 10px; background-color: grey;"></div> </div>

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Mol	Chain	Length	Quality of chain
1	F	188	 85% 7% • 8%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 8876 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 Allene oxide cyclase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	173	1364	890	213	259	2	0	1	0
1	B	173	1364	890	213	259	2	0	1	0
1	C	173	1364	890	213	259	2	0	1	0
1	D	173	1364	890	213	259	2	0	1	0
1	E	173	1364	890	213	259	2	0	1	0
1	F	173	1364	890	213	259	2	0	1	0

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP Q9LS02
A	2	ARG	-	cloning artifact	UNP Q9LS02
A	3	GLY	-	cloning artifact	UNP Q9LS02
A	4	SER	-	cloning artifact	UNP Q9LS02
A	5	HIS	-	expression tag	UNP Q9LS02
A	6	HIS	-	expression tag	UNP Q9LS02
A	7	HIS	-	expression tag	UNP Q9LS02
A	8	HIS	-	expression tag	UNP Q9LS02
A	9	HIS	-	expression tag	UNP Q9LS02
A	10	HIS	-	expression tag	UNP Q9LS02
A	11	ARG	-	cloning artifact	UNP Q9LS02
A	12	SER	-	cloning artifact	UNP Q9LS02
B	1	MET	-	initiating methionine	UNP Q9LS02
B	2	ARG	-	cloning artifact	UNP Q9LS02
B	3	GLY	-	cloning artifact	UNP Q9LS02
B	4	SER	-	cloning artifact	UNP Q9LS02
B	5	HIS	-	expression tag	UNP Q9LS02

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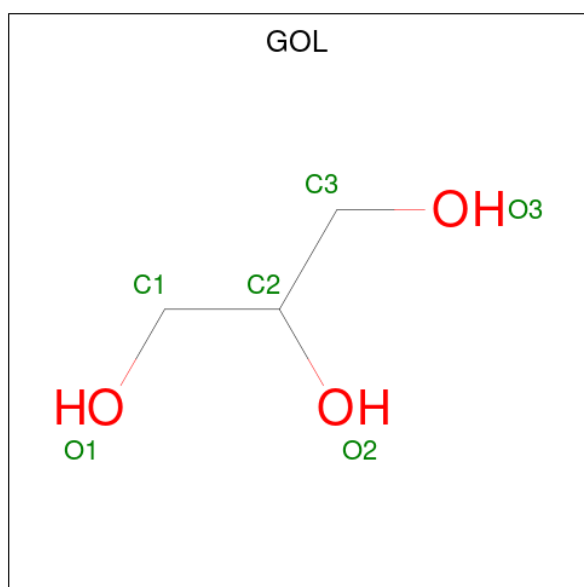
Chain	Residue	Modelled	Actual	Comment	Reference
B	6	HIS	-	expression tag	UNP Q9LS02
B	7	HIS	-	expression tag	UNP Q9LS02
B	8	HIS	-	expression tag	UNP Q9LS02
B	9	HIS	-	expression tag	UNP Q9LS02
B	10	HIS	-	expression tag	UNP Q9LS02
B	11	ARG	-	cloning artifact	UNP Q9LS02
B	12	SER	-	cloning artifact	UNP Q9LS02
C	1	MET	-	initiating methionine	UNP Q9LS02
C	2	ARG	-	cloning artifact	UNP Q9LS02
C	3	GLY	-	cloning artifact	UNP Q9LS02
C	4	SER	-	cloning artifact	UNP Q9LS02
C	5	HIS	-	expression tag	UNP Q9LS02
C	6	HIS	-	expression tag	UNP Q9LS02
C	7	HIS	-	expression tag	UNP Q9LS02
C	8	HIS	-	expression tag	UNP Q9LS02
C	9	HIS	-	expression tag	UNP Q9LS02
C	10	HIS	-	expression tag	UNP Q9LS02
C	11	ARG	-	cloning artifact	UNP Q9LS02
C	12	SER	-	cloning artifact	UNP Q9LS02
D	1	MET	-	initiating methionine	UNP Q9LS02
D	2	ARG	-	cloning artifact	UNP Q9LS02
D	3	GLY	-	cloning artifact	UNP Q9LS02
D	4	SER	-	cloning artifact	UNP Q9LS02
D	5	HIS	-	expression tag	UNP Q9LS02
D	6	HIS	-	expression tag	UNP Q9LS02
D	7	HIS	-	expression tag	UNP Q9LS02
D	8	HIS	-	expression tag	UNP Q9LS02
D	9	HIS	-	expression tag	UNP Q9LS02
D	10	HIS	-	expression tag	UNP Q9LS02
D	11	ARG	-	cloning artifact	UNP Q9LS02
D	12	SER	-	cloning artifact	UNP Q9LS02
E	1	MET	-	initiating methionine	UNP Q9LS02
E	2	ARG	-	cloning artifact	UNP Q9LS02
E	3	GLY	-	cloning artifact	UNP Q9LS02
E	4	SER	-	cloning artifact	UNP Q9LS02
E	5	HIS	-	expression tag	UNP Q9LS02
E	6	HIS	-	expression tag	UNP Q9LS02
E	7	HIS	-	expression tag	UNP Q9LS02
E	8	HIS	-	expression tag	UNP Q9LS02
E	9	HIS	-	expression tag	UNP Q9LS02
E	10	HIS	-	expression tag	UNP Q9LS02
E	11	ARG	-	cloning artifact	UNP Q9LS02

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Chain	Residue	Modelled	Actual	Comment	Reference
E	12	SER	-	cloning artifact	UNP Q9LS02
F	1	MET	-	initiating methionine	UNP Q9LS02
F	2	ARG	-	cloning artifact	UNP Q9LS02
F	3	GLY	-	cloning artifact	UNP Q9LS02
F	4	SER	-	cloning artifact	UNP Q9LS02
F	5	HIS	-	expression tag	UNP Q9LS02
F	6	HIS	-	expression tag	UNP Q9LS02
F	7	HIS	-	expression tag	UNP Q9LS02
F	8	HIS	-	expression tag	UNP Q9LS02
F	9	HIS	-	expression tag	UNP Q9LS02
F	10	HIS	-	expression tag	UNP Q9LS02
F	11	ARG	-	cloning artifact	UNP Q9LS02
F	12	SER	-	cloning artifact	UNP Q9LS02

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		
2	D	1	Total	C	O	0	0
			6	3	3		
2	D	1	Total	C	O	0	0
			6	3	3		
2	F	1	Total	C	O	0	0
			6	3	3		

- Molecule 3 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total 1	Na 1	0	0
3	D	1	Total 1	Na 1	0	0

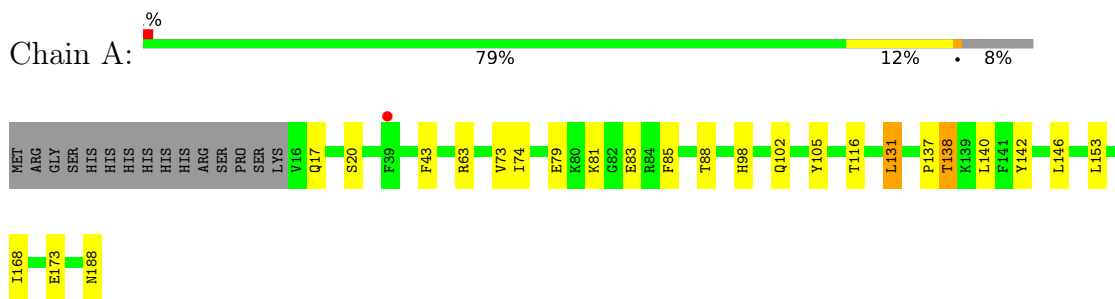
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	108	Total 108	O 108	0	0
4	B	118	Total 118	O 118	0	0
4	C	108	Total 108	O 108	0	0
4	D	104	Total 104	O 104	0	0
4	E	117	Total 117	O 117	0	0
4	F	105	Total 105	O 105	0	0

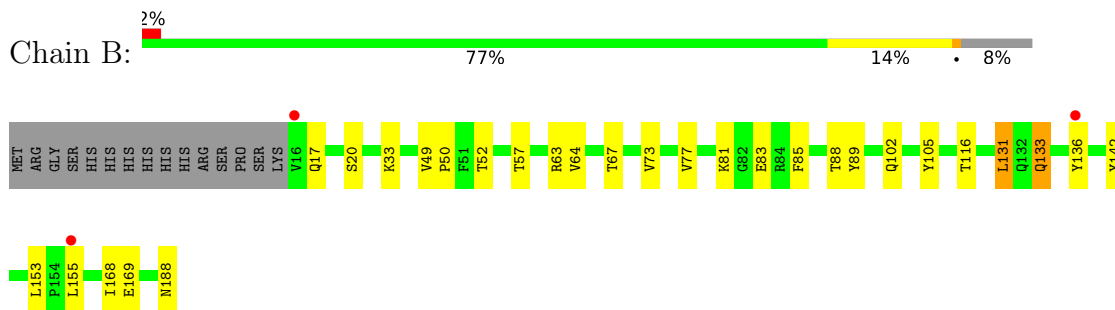
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

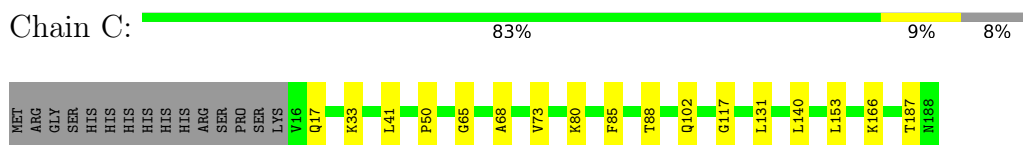
- Molecule 1: Allene oxide cyclase 2



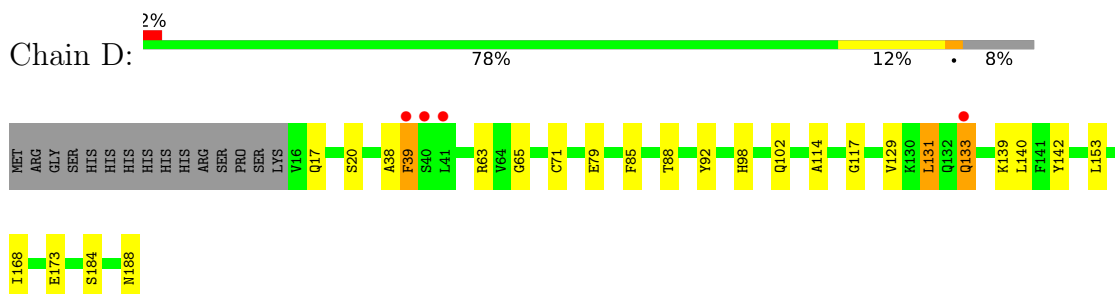
- Molecule 1: Allene oxide cyclase 2



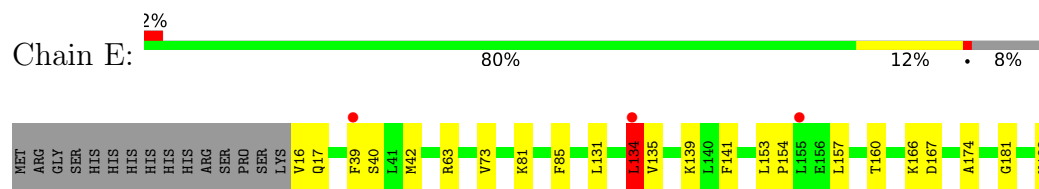
- Molecule 1: Allene oxide cyclase 2



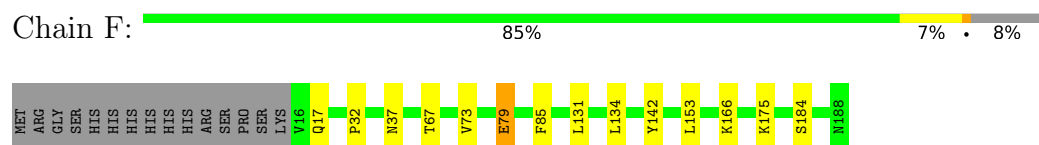
- Molecule 1: Allene oxide cyclase 2



- Molecule 1: Allene oxide cyclase 2



- Molecule 1: Allene oxide cyclase 2



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	66.90Å 104.20Å 86.70Å 90.00° 95.10° 90.00°	Depositor
Resolution (Å)	50.00 – 1.80 50.00 – 1.80	Depositor EDS
% Data completeness (in resolution range)	97.7 (50.00-1.80) 98.5 (50.00-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.38 (at 1.79Å)	Xtrriage
Refinement program	REFMAC refmac_5.2.0019	Depositor
R, R_{free}	0.207 , 0.248 0.204 , 0.244	Depositor DCC
R_{free} test set	5393 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	24.2	Xtrriage
Anisotropy	0.146	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 31.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8876	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.74% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	1.24	0/1400	1.03	2/1901 (0.1%)
1	B	1.26	4/1400 (0.3%)	1.03	4/1901 (0.2%)
1	C	1.24	1/1400 (0.1%)	1.04	0/1901
1	D	1.30	3/1400 (0.2%)	1.03	0/1901
1	E	1.26	0/1400	1.07	4/1901 (0.2%)
1	F	1.26	1/1400 (0.1%)	0.98	0/1901
All	All	1.26	9/8400 (0.1%)	1.03	10/11406 (0.1%)

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	129	VAL	CA-CB	6.41	1.63	1.54
1	C	117	GLY	N-CA	5.94	1.50	1.45
1	B	57	THR	CA-CB	5.89	1.62	1.53
1	B	168	ILE	CA-CB	5.79	1.59	1.54
1	D	117	GLY	N-CA	5.28	1.50	1.45
1	F	67	THR	N-CA	5.17	1.51	1.45
1	D	114	ALA	CA-CB	5.13	1.61	1.53
1	B	67	THR	N-CA	5.01	1.51	1.45
1	B	52	THR	CA-CB	5.00	1.64	1.53

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	77	VAL	CA-C-N	6.15	126.33	119.32
1	B	77	VAL	C-N-CA	6.15	126.33	119.32
1	B	89	TYR	N-CA-C	6.12	117.54	108.60
1	E	134	LEU	CA-CB-CG	5.49	135.51	116.30
1	A	146	LEU	N-CA-C	5.22	117.24	109.25
1	E	167	ASP	N-CA-C	5.22	119.35	112.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	160	THR	CA-C-N	-5.17	114.45	119.78
1	E	160	THR	C-N-CA	-5.17	114.45	119.78
1	B	64	VAL	N-CA-C	5.08	116.18	111.81
1	A	138	THR	N-CA-C	5.02	120.79	114.31

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1364	0	1350	20	0
1	B	1364	0	1350	24	0
1	C	1364	0	1350	12	0
1	D	1364	0	1350	22	0
1	E	1364	0	1350	17	0
1	F	1364	0	1350	10	0
2	A	6	0	8	2	0
2	B	6	0	8	1	0
2	D	12	0	16	2	0
2	F	6	0	8	1	0
3	B	1	0	0	0	0
3	D	1	0	0	0	0
4	A	108	0	0	3	0
4	B	118	0	0	8	0
4	C	108	0	0	3	0
4	D	104	0	0	6	0
4	E	117	0	0	5	0
4	F	105	0	0	1	0
All	All	8876	0	8140	105	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 6.

All (105) 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:102[B]:GLN:HE21	1:B:116:THR:HG21	1.26	0.99
1:B:155:LEU:HB3	4:B:996:HOH:O	1.64	0.96
1:A:63:ARG:HH22	1:A:188:ASN:HD22	1.14	0.92
1:E:63:ARG:HH22	1:E:188:ASN:HD22	1.18	0.91
1:D:63:ARG:HH22	1:D:188:ASN:HD22	1.20	0.89
2:A:901:GOL:H32	4:A:1000:HOH:O	1.73	0.86
1:B:102[B]:GLN:HE21	1:B:116:THR:CG2	1.92	0.82
1:B:102[B]:GLN:NE2	1:B:116:THR:HG21	1.94	0.81
1:D:38:ALA:O	4:D:998:HOH:O	1.99	0.80
2:D:902:GOL:H32	4:E:294:HOH:O	1.82	0.80
1:B:133:GLN:NE2	4:B:1022:HOH:O	2.15	0.80
1:F:17:GLN:HE22	1:F:153:LEU:H	1.31	0.78
1:B:105:TYR:CD2	4:B:1022:HOH:O	2.38	0.77
1:D:17:GLN:HE22	1:D:153:LEU:H	1.29	0.76
1:C:102[B]:GLN:NE2	4:C:278:HOH:O	2.19	0.76
1:E:17:GLN:HE22	1:E:153:LEU:H	1.34	0.74
1:A:17:GLN:HE22	1:A:153:LEU:H	1.36	0.72
1:D:39:PHE:HD1	4:D:907:HOH:O	1.71	0.71
1:C:131:LEU:HD11	1:C:140:LEU:HD23	1.72	0.71
1:B:17:GLN:HE22	1:B:153:LEU:H	1.39	0.71
1:C:73:VAL:HG22	1:C:85:PHE:CE1	2.31	0.66
1:E:16:VAL:N	4:E:304:HOH:O	2.30	0.65
1:B:63:ARG:HH22	1:B:188:ASN:HD22	1.42	0.63
1:E:73:VAL:HG22	1:E:85:PHE:CE1	2.34	0.63
1:B:105:TYR:CE2	4:B:1022:HOH:O	2.52	0.63
1:D:98:HIS:HD2	4:E:196:HOH:O	1.82	0.63
1:E:166:LYS:HG3	4:E:300:HOH:O	1.99	0.63
1:E:134:LEU:HD21	1:E:141:PHE:HB3	1.81	0.62
1:F:166:LYS:HG3	4:F:938:HOH:O	2.00	0.62
1:A:98:HIS:HD2	4:B:919:HOH:O	1.82	0.62
1:E:134:LEU:HD21	1:E:141:PHE:CB	2.30	0.62
1:E:63:ARG:NH2	1:E:188:ASN:HD22	1.96	0.61
1:A:63:ARG:HH22	1:A:188:ASN:ND2	1.94	0.60
1:A:63:ARG:NH2	1:A:188:ASN:HD22	1.94	0.60
1:A:88:THR:OG1	1:A:102[B]:GLN:NE2	2.33	0.60
1:D:63:ARG:NH2	1:D:188:ASN:HD22	1.97	0.60
1:E:135:VAL:HG22	1:E:166:LYS:HD3	1.84	0.59
1:A:116:THR:OG1	1:B:102[B]:GLN:NE2	2.35	0.59
1:F:79:GLU:CD	1:F:79:GLU:H	2.11	0.59
1:C:17:GLN:HE22	1:C:153:LEU:H	1.51	0.58
1:E:63:ARG:HH22	1:E:188:ASN:ND2	1.95	0.57
1:B:88:THR:OG1	1:B:102[A]:GLN:NE2	2.33	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:131:LEU:HD23	1:B:131:LEU:C	2.31	0.56
1:B:73:VAL:HG22	1:B:85:PHE:CE1	2.42	0.55
1:D:39:PHE:CD1	4:D:907:HOH:O	2.53	0.55
1:D:63:ARG:HH22	1:D:188:ASN:ND2	1.96	0.55
1:F:131:LEU:HD13	1:F:142:TYR:CE2	2.42	0.55
1:A:43:PHE:CD2	1:A:83:GLU:HG3	2.43	0.54
1:D:184:SER:O	4:D:996:HOH:O	2.18	0.54
1:E:135:VAL:HB	1:E:139:LYS:HB2	1.89	0.54
1:C:131:LEU:CD1	1:C:140:LEU:HD23	2.38	0.53
1:F:17:GLN:NE2	1:F:153:LEU:H	2.04	0.52
1:F:32:PRO:HB3	2:F:903:GOL:H11	1.91	0.51
1:A:73:VAL:HG22	1:A:85:PHE:CE1	2.45	0.51
1:A:173:GLU:HG2	4:A:992:HOH:O	2.10	0.51
1:A:74:ILE:HG13	1:C:68:ALA:HB1	1.92	0.50
1:C:102[B]:GLN:CD	4:C:296:HOH:O	2.53	0.50
1:B:102[B]:GLN:NE2	1:B:116:THR:CG2	2.63	0.50
1:B:136:TYR:HE1	4:B:980:HOH:O	1.94	0.49
1:D:71:CYS:HB3	1:D:85:PHE:CD1	2.47	0.49
1:B:169:GLU:HA	1:B:169:GLU:OE1	2.11	0.49
1:D:17:GLN:NE2	1:D:153:LEU:H	2.07	0.48
1:A:20:SER:HA	1:A:142:TYR:O	2.13	0.48
1:C:33:LYS:O	1:C:50:PRO:HD2	2.13	0.48
1:D:88:THR:OG1	1:D:102[B]:GLN:NE2	2.38	0.47
1:E:154:PRO:HG2	1:E:157:LEU:HD12	1.97	0.47
1:D:168:ILE:C	1:D:168:ILE:HD12	2.41	0.46
1:A:116:THR:CB	1:B:102[B]:GLN:HE22	2.28	0.46
1:A:137:PRO:HD2	1:A:138:THR:HG23	1.97	0.46
1:E:134:LEU:HD21	1:E:141:PHE:HB2	1.97	0.46
1:D:131:LEU:C	1:D:131:LEU:HD23	2.41	0.46
1:B:63:ARG:HH22	1:B:188:ASN:ND2	2.13	0.45
1:A:173:GLU:H	1:A:173:GLU:CD	2.25	0.45
1:C:88:THR:OG1	1:C:102[A]:GLN:OE1	2.14	0.45
1:F:131:LEU:HD13	1:F:142:TYR:CZ	2.52	0.45
1:B:49:VAL:HG11	2:B:904:GOL:H32	1.99	0.44
1:D:139:LYS:O	1:D:140:LEU:HD12	2.17	0.44
1:B:33:LYS:O	1:B:50:PRO:HD2	2.17	0.44
1:D:133:GLN:O	1:D:133:GLN:HG3	2.17	0.44
1:D:139:LYS:C	1:D:140:LEU:HD12	2.43	0.44
1:F:73:VAL:HG22	1:F:85:PHE:CE1	2.53	0.44
1:D:17:GLN:HE22	1:D:153:LEU:N	2.06	0.44
1:A:131:LEU:C	1:A:131:LEU:HD23	2.43	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:901:GOL:C3	4:A:1000:HOH:O	2.45	0.43
1:B:17:GLN:NE2	1:B:153:LEU:H	2.13	0.43
1:B:20:SER:HA	1:B:142:TYR:O	2.18	0.43
1:B:136:TYR:CE1	4:B:1008:HOH:O	2.68	0.43
1:E:42:MET:HA	1:E:42:MET:HE2	2.00	0.43
1:D:133:GLN:CB	4:D:1007:HOH:O	2.66	0.43
1:C:17:GLN:HE22	1:C:153:LEU:N	2.15	0.43
1:F:17:GLN:HE22	1:F:153:LEU:N	2.08	0.42
1:D:133:GLN:NE2	4:D:932:HOH:O	2.52	0.42
1:B:136:TYR:CE1	4:B:980:HOH:O	2.57	0.42
1:E:81:LYS:HE2	1:E:81:LYS:HB3	1.77	0.42
2:D:902:GOL:H11	1:F:37:ASN:HD21	1.84	0.42
1:A:168:ILE:C	1:A:168:ILE:HD12	2.45	0.42
1:A:17:GLN:NE2	1:A:153:LEU:H	2.11	0.41
1:A:105:TYR:OH	1:A:140:LEU:HD21	2.20	0.41
1:D:20:SER:HA	1:D:142:TYR:O	2.20	0.41
1:C:166:LYS:HD3	4:C:261:HOH:O	2.19	0.41
1:A:43:PHE:HD2	1:A:83:GLU:HG3	1.85	0.41
1:D:65:GLY:HA3	1:D:92:TYR:O	2.21	0.40
1:E:174:ALA:HA	1:E:181:GLY:O	2.21	0.40
1:E:39:PHE:C	4:E:282:HOH:O	2.64	0.40
1:C:65:GLY:HA2	1:C:187:THR:O	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	172/188 (92%)	169 (98%)	3 (2%)	0	100	100
1	B	172/188 (92%)	171 (99%)	1 (1%)	0	100	100
1	C	172/188 (92%)	168 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	172/188 (92%)	168 (98%)	3 (2%)	1 (1%)	21	11
1	E	172/188 (92%)	168 (98%)	4 (2%)	0	100	100
1	F	172/188 (92%)	167 (97%)	5 (3%)	0	100	100
All	All	1032/1128 (92%)	1011 (98%)	20 (2%)	1 (0%)	48	34

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	39	PHE

5.3.2 Protein sidechains [i](#)

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	147/160 (92%)	144 (98%)	3 (2%)	48	38
1	B	147/160 (92%)	143 (97%)	4 (3%)	39	27
1	C	147/160 (92%)	145 (99%)	2 (1%)	59	52
1	D	147/160 (92%)	143 (97%)	4 (3%)	39	27
1	E	147/160 (92%)	144 (98%)	3 (2%)	48	38
1	F	147/160 (92%)	143 (97%)	4 (3%)	39	27
All	All	882/960 (92%)	862 (98%)	20 (2%)	44	33

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

Mol	Chain	Res	Type
1	A	79	GLU
1	A	81	LYS
1	A	131	LEU
1	B	81	LYS
1	B	83	GLU
1	B	131	LEU
1	B	133	GLN

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Mol	Chain	Res	Type
1	C	41	LEU
1	C	80	LYS
1	D	79	GLU
1	D	131	LEU
1	D	133	GLN
1	D	173	GLU
1	E	40	SER
1	E	131	LEU
1	E	134	LEU
1	F	79	GLU
1	F	134	LEU
1	F	175	LYS
1	F	184	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	GLN
1	A	98	HIS
1	A	132	GLN
1	A	188	ASN
1	B	17	GLN
1	B	188	ASN
1	C	17	GLN
1	D	17	GLN
1	D	53	ASN
1	D	98	HIS
1	D	188	ASN
1	E	17	GLN
1	E	37	ASN
1	E	53	ASN
1	E	132	GLN
1	E	188	ASN
1	F	17	GLN
1	F	37	ASN
1	F	53	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 2 are monoatomic - leaving 5 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	GOL	B	904	-	5,5,5	0.40	0	5,5,5	0.27	0
2	GOL	D	902	-	5,5,5	0.54	0	5,5,5	0.76	0
2	GOL	F	903	-	5,5,5	0.46	0	5,5,5	0.43	0
2	GOL	A	901	-	5,5,5	0.32	0	5,5,5	0.64	0
2	GOL	D	905	-	5,5,5	0.28	0	5,5,5	0.56	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	GOL	B	904	-	-	0/4/4/4	-
2	GOL	D	902	-	-	2/4/4/4	-
2	GOL	F	903	-	-	4/4/4/4	-
2	GOL	A	901	-	-	4/4/4/4	-
2	GOL	D	905	-	-	1/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	901	GOL	O2-C2-C3-O3
2	A	901	GOL	O1-C1-C2-C3
2	A	901	GOL	C1-C2-C3-O3
2	D	902	GOL	C1-C2-C3-O3
2	F	903	GOL	O1-C1-C2-C3
2	F	903	GOL	C1-C2-C3-O3
2	A	901	GOL	O1-C1-C2-O2
2	D	902	GOL	O2-C2-C3-O3
2	F	903	GOL	O1-C1-C2-O2
2	D	905	GOL	O1-C1-C2-O2
2	F	903	GOL	O2-C2-C3-O3

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	904	GOL	1	0
2	D	902	GOL	2	0
2	F	903	GOL	1	0
2	A	901	GOL	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	173/188 (92%)	-0.02	1 (0%) 85 86	7, 23, 34, 38	1 (0%)
1	B	173/188 (92%)	-0.12	3 (1%) 69 69	7, 22, 32, 38	1 (0%)
1	C	173/188 (92%)	0.02	0 100 100	7, 23, 35, 38	1 (0%)
1	D	173/188 (92%)	-0.14	4 (2%) 61 61	7, 21, 33, 36	1 (0%)
1	E	173/188 (92%)	-0.03	3 (1%) 69 69	7, 22, 34, 39	1 (0%)
1	F	173/188 (92%)	-0.17	0 100 100	7, 22, 32, 38	1 (0%)
All	All	1038/1128 (92%)	-0.08	11 (1%) 78 78	7, 22, 33, 39	6 (0%)

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	39	PHE	4.5
1	B	136	TYR	4.5
1	E	39	PHE	3.6
1	A	39	PHE	3.5
1	E	134	LEU	3.1
1	D	133	GLN	3.0
1	D	40	SER	2.4
1	D	41	LEU	2.3
1	E	155	LEU	2.3
1	B	155	LEU	2.2
1	B	16	VAL	2.1

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	GOL	B	904	6/6	0.80	0.17	54,55,55,56	0
2	GOL	F	903	6/6	0.85	0.15	46,49,50,51	0
2	GOL	D	905	6/6	0.92	0.10	24,29,34,39	0
2	GOL	D	902	6/6	0.92	0.09	23,28,29,33	0
2	GOL	A	901	6/6	0.94	0.08	27,27,30,31	0
3	NA	B	801	1/1	0.96	0.21	23,23,23,23	0
3	NA	D	802	1/1	0.99	0.15	14,14,14,14	0

6.5 Other polymers [i](#)

There are no such residues in this entry.