Full wwPDB X-ray Structure Validation Report (i)

Sep 9, 2023 – 10:03 PM EDT

PDB ID	:	4H6C
Title	:	Crystal Structure of the Allene Oxide Cyclase 1 from Physcomitrella patens
Authors	:	Neumann, P.; Ficner, R.
Deposited on	:	2012-09-19
Resolution	:	1.35 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 (i) 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 (1)) were used in the production of this report:

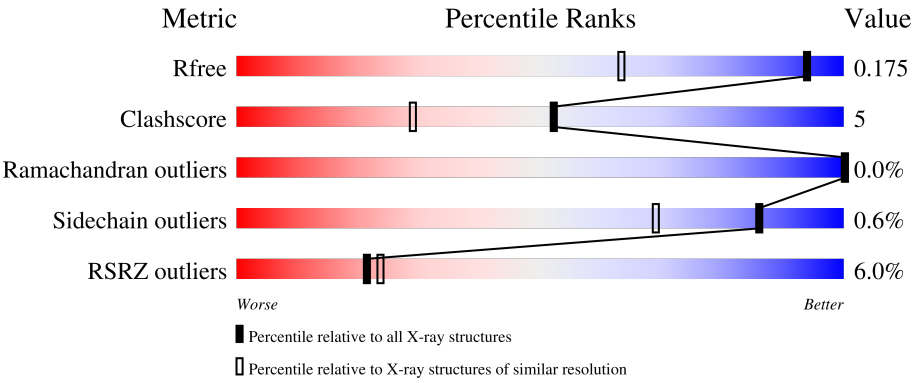
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 1.35 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}	130704	1509 (1.38-1.34)
Clashscore	141614	1551 (1.38-1.34)
Ramachandran outliers	138981	1530 (1.38-1.34)
Sidechain outliers	138945	1530 (1.38-1.34)
RSRZ outliers	127900	1487 (1.38-1.34)

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 <=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	195	4% 84% 9% 8%
1	B	195	5% 80% 11% 9%
1	C	195	8% 76% 14% 10%
1	D	195	2% 85% 7% • 8%
1	E	195	2% 83% 9% 8%

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Mol	Chain	Length	Quality of chain
1	F	195	4% 81% 8% 10%
1	G	195	7% 80% 10% 10%
1	H	195	8% 81% 9% 10%
1	I	195	3% 88% 8%
1	J	195	6% 82% 8% 10%
1	K	195	2% 86% 6% 8%
1	L	195	15% 78% 11% 10%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	HEZ	A	202	-	-	X	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 19586 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	180	Total	C	N	O	S	0	4	0
			1437	932	233	267	5			
1	D	180	Total	C	N	O	S	0	3	0
			1422	924	231	262	5			
1	C	175	Total	C	N	O	S	0	2	0
			1381	899	224	253	5			
1	B	177	Total	C	N	O	S	0	3	0
			1408	916	229	258	5			
1	E	180	Total	C	N	O	S	0	4	0
			1431	930	233	263	5			
1	F	175	Total	C	N	O	S	0	2	0
			1379	897	224	253	5			
1	G	175	Total	C	N	O	S	0	5	0
			1412	921	229	257	5			
1	H	175	Total	C	N	O	S	0	1	0
			1375	895	224	251	5			
1	I	180	Total	C	N	O	S	0	1	0
			1405	912	228	260	5			
1	J	175	Total	C	N	O	S	0	2	0
			1383	899	225	254	5			
1	K	180	Total	C	N	O	S	0	5	0
			1442	937	234	266	5			
1	L	175	Total	C	N	O	S	0	2	0
			1384	901	225	253	5			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	GLY	-	expression tag	UNP Q8GS38
A	-4	GLY	-	expression tag	UNP Q8GS38
A	-3	PRO	-	expression tag	UNP Q8GS38
A	-2	LEU	-	expression tag	UNP Q8GS38
A	-1	GLY	-	expression tag	UNP Q8GS38

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Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	expression tag	UNP Q8GS38
D	-5	GLY	-	expression tag	UNP Q8GS38
D	-4	GLY	-	expression tag	UNP Q8GS38
D	-3	PRO	-	expression tag	UNP Q8GS38
D	-2	LEU	-	expression tag	UNP Q8GS38
D	-1	GLY	-	expression tag	UNP Q8GS38
D	0	SER	-	expression tag	UNP Q8GS38
C	-5	GLY	-	expression tag	UNP Q8GS38
C	-4	GLY	-	expression tag	UNP Q8GS38
C	-3	PRO	-	expression tag	UNP Q8GS38
C	-2	LEU	-	expression tag	UNP Q8GS38
C	-1	GLY	-	expression tag	UNP Q8GS38
C	0	SER	-	expression tag	UNP Q8GS38
B	-5	GLY	-	expression tag	UNP Q8GS38
B	-4	GLY	-	expression tag	UNP Q8GS38
B	-3	PRO	-	expression tag	UNP Q8GS38
B	-2	LEU	-	expression tag	UNP Q8GS38
B	-1	GLY	-	expression tag	UNP Q8GS38
B	0	SER	-	expression tag	UNP Q8GS38
E	-5	GLY	-	expression tag	UNP Q8GS38
E	-4	GLY	-	expression tag	UNP Q8GS38
E	-3	PRO	-	expression tag	UNP Q8GS38
E	-2	LEU	-	expression tag	UNP Q8GS38
E	-1	GLY	-	expression tag	UNP Q8GS38
E	0	SER	-	expression tag	UNP Q8GS38
F	-5	GLY	-	expression tag	UNP Q8GS38
F	-4	GLY	-	expression tag	UNP Q8GS38
F	-3	PRO	-	expression tag	UNP Q8GS38
F	-2	LEU	-	expression tag	UNP Q8GS38
F	-1	GLY	-	expression tag	UNP Q8GS38
F	0	SER	-	expression tag	UNP Q8GS38
G	-5	GLY	-	expression tag	UNP Q8GS38
G	-4	GLY	-	expression tag	UNP Q8GS38
G	-3	PRO	-	expression tag	UNP Q8GS38
G	-2	LEU	-	expression tag	UNP Q8GS38
G	-1	GLY	-	expression tag	UNP Q8GS38
G	0	SER	-	expression tag	UNP Q8GS38
H	-5	GLY	-	expression tag	UNP Q8GS38
H	-4	GLY	-	expression tag	UNP Q8GS38
H	-3	PRO	-	expression tag	UNP Q8GS38
H	-2	LEU	-	expression tag	UNP Q8GS38
H	-1	GLY	-	expression tag	UNP Q8GS38

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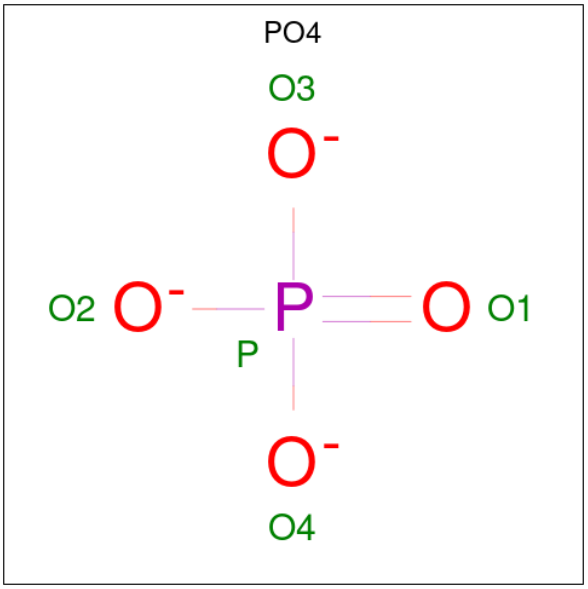
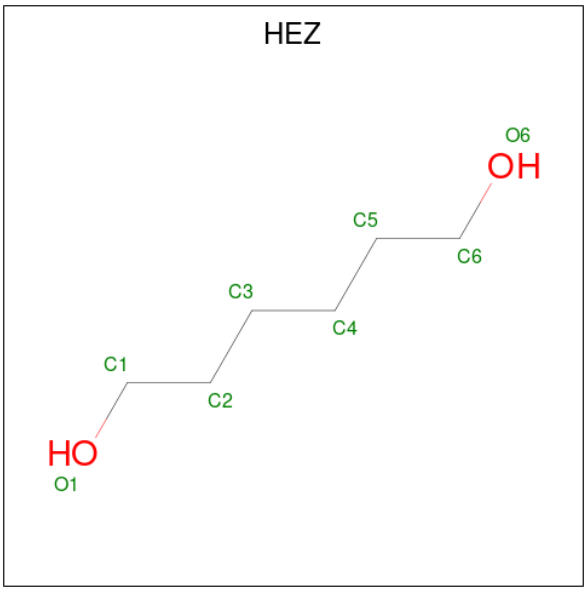
Chain	Residue	Modelled	Actual	Comment	Reference
H	0	SER	-	expression tag	UNP Q8GS38
I	-5	GLY	-	expression tag	UNP Q8GS38
I	-4	GLY	-	expression tag	UNP Q8GS38
I	-3	PRO	-	expression tag	UNP Q8GS38
I	-2	LEU	-	expression tag	UNP Q8GS38
I	-1	GLY	-	expression tag	UNP Q8GS38
I	0	SER	-	expression tag	UNP Q8GS38
J	-5	GLY	-	expression tag	UNP Q8GS38
J	-4	GLY	-	expression tag	UNP Q8GS38
J	-3	PRO	-	expression tag	UNP Q8GS38
J	-2	LEU	-	expression tag	UNP Q8GS38
J	-1	GLY	-	expression tag	UNP Q8GS38
J	0	SER	-	expression tag	UNP Q8GS38
K	-5	GLY	-	expression tag	UNP Q8GS38
K	-4	GLY	-	expression tag	UNP Q8GS38
K	-3	PRO	-	expression tag	UNP Q8GS38
K	-2	LEU	-	expression tag	UNP Q8GS38
K	-1	GLY	-	expression tag	UNP Q8GS38
K	0	SER	-	expression tag	UNP Q8GS38
L	-5	GLY	-	expression tag	UNP Q8GS38
L	-4	GLY	-	expression tag	UNP Q8GS38
L	-3	PRO	-	expression tag	UNP Q8GS38
L	-2	LEU	-	expression tag	UNP Q8GS38
L	-1	GLY	-	expression tag	UNP Q8GS38
L	0	SER	-	expression tag	UNP Q8GS38

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O P 5 4 1	0	0
2	D	1	Total O P 5 4 1	0	0
2	C	1	Total O P 5 4 1	0	0
2	B	1	Total O P 5 4 1	0	0
2	B	1	Total O P 5 4 1	0	0
2	E	1	Total O P 5 4 1	0	0
2	F	1	Total O P 5 4 1	0	0
2	G	1	Total O P 5 4 1	0	0
2	G	1	Total O P 5 4 1	0	0
2	H	1	Total O P 5 4 1	0	0
2	H	1	Total O P 5 4 1	0	0
2	I	1	Total O P 5 4 1	0	0
2	I	1	Total O P 5 4 1	0	0
2	J	1	Total O P 5 4 1	0	0
2	J	1	Total O P 5 4 1	0	0
2	K	1	Total O P 5 4 1	0	0
2	L	1	Total O P 5 4 1	0	0

- Molecule 3 is HEXANE-1,6-DIOL (three-letter code: HEZ) (formula: $C_6H_{14}O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 8 6 2	0	0
3	D	1	Total C O 8 6 2	0	0
3	B	1	Total C O 8 6 2	0	0
3	E	1	Total C O 8 6 2	0	0
3	F	1	Total C O 8 6 2	0	0
3	G	1	Total C O 8 6 2	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	238	Total O 238 238	0	0
4	D	302	Total O 302 302	0	0
4	C	197	Total O 197 197	0	0
4	B	245	Total O 245 245	0	0
4	E	280	Total O 280 280	0	0
4	F	209	Total O 209 209	0	0

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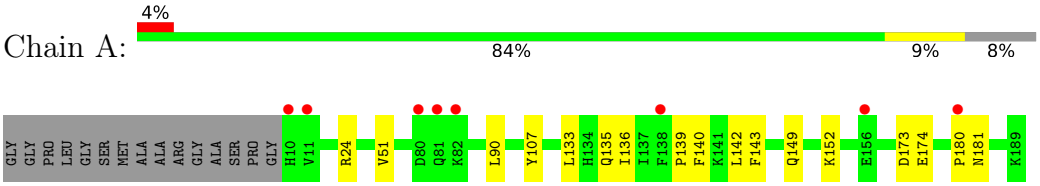
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	G	192	Total O 192 192	0	0
4	H	196	Total O 196 196	0	0
4	I	211	Total O 211 211	0	0
4	J	162	Total O 163 163	0	1
4	K	238	Total O 239 239	0	1
4	L	121	Total O 122 122	0	1

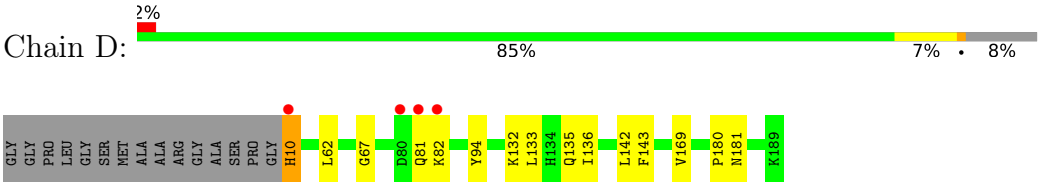
3 Residue-property plots (i)

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.

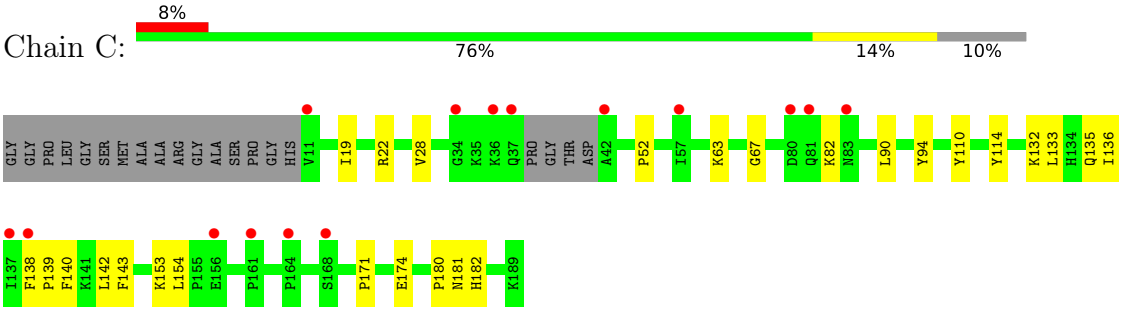
• Molecule 1: Allene oxide cyclase



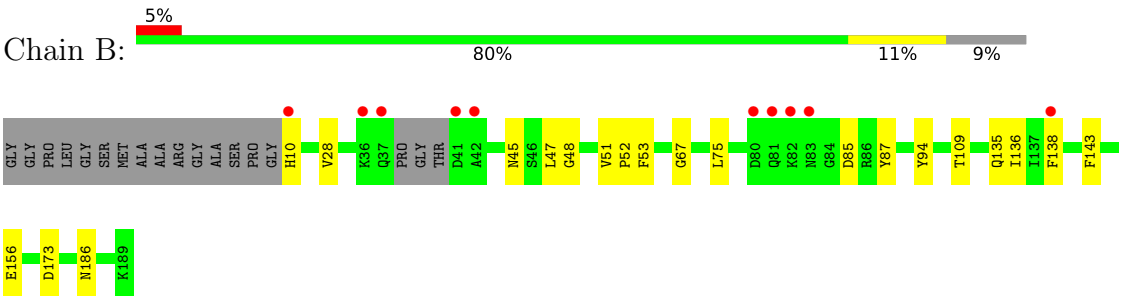
• Molecule 1: Allene oxide cyclase



• Molecule 1: Allene oxide cyclase

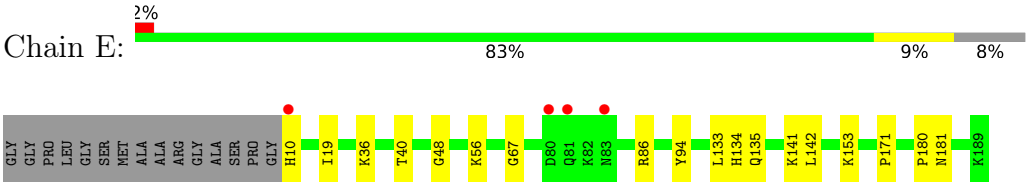


• Molecule 1: Allene oxide cyclase



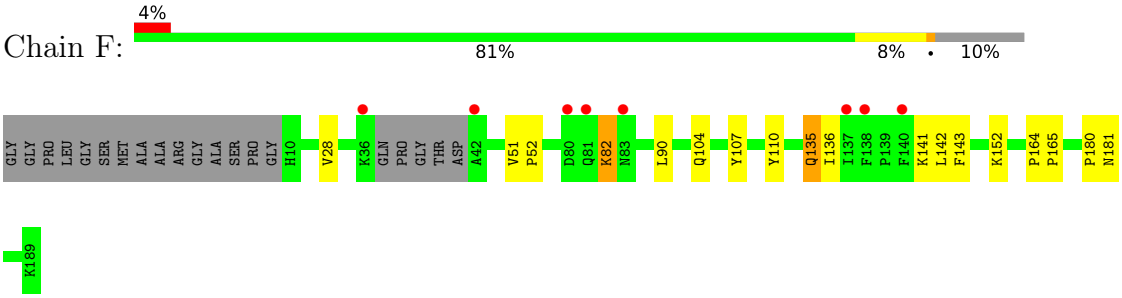
• Molecule 1: Allene oxide cyclase

Chain E:



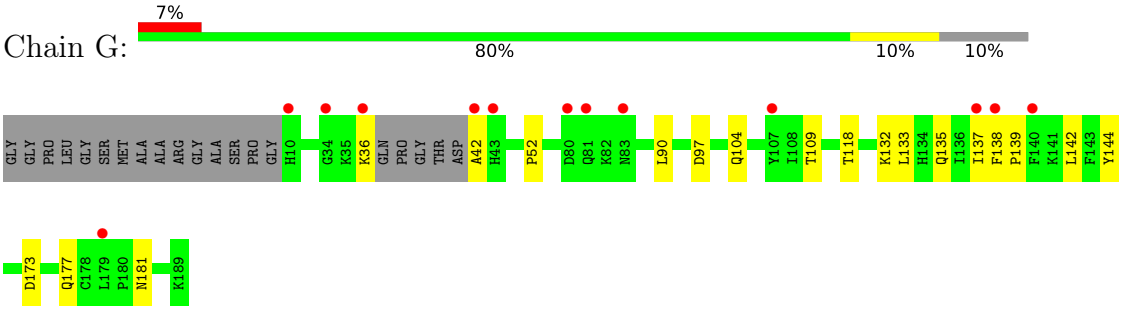
• Molecule 1: Allene oxide cyclase

Chain F:



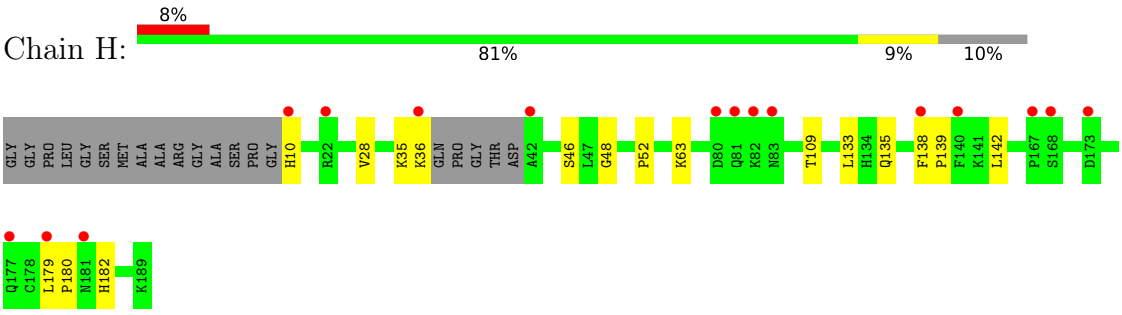
• Molecule 1: Allene oxide cyclase

Chain G:



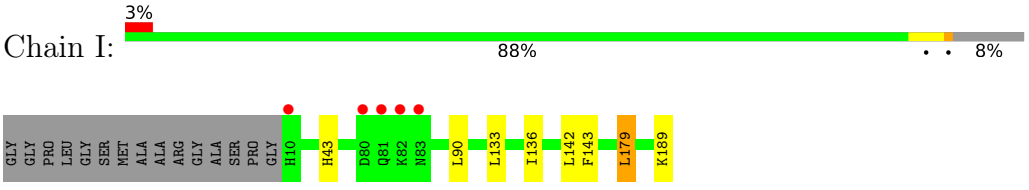
• Molecule 1: Allene oxide cyclase

Chain H:



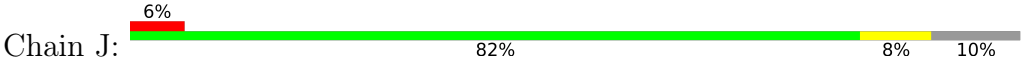
• Molecule 1: Allene oxide cyclase

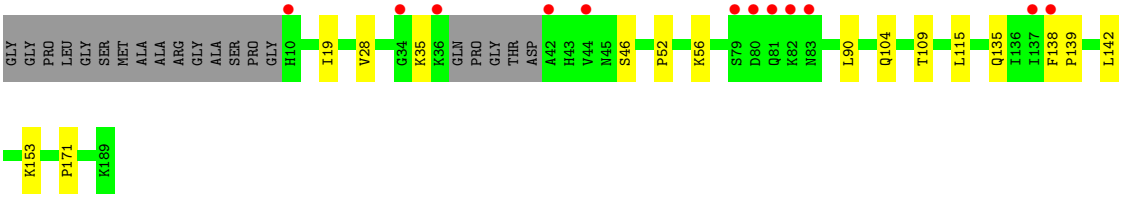
Chain I:



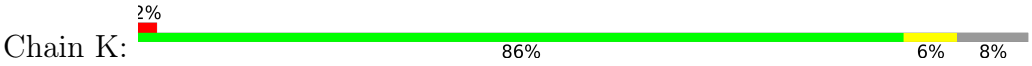
• Molecule 1: Allene oxide cyclase

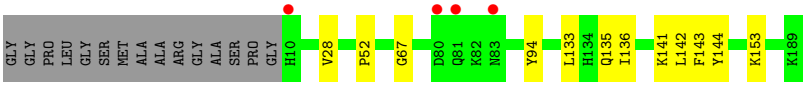
Chain J:



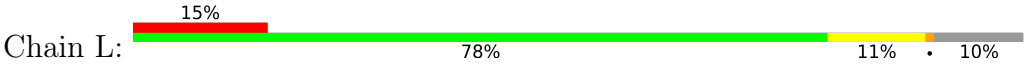


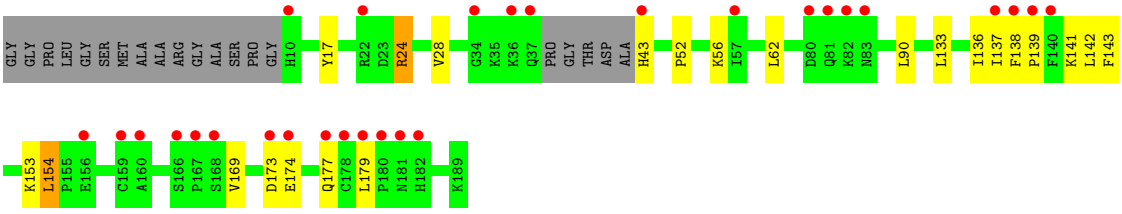
• Molecule 1: Allene oxide cyclase





• Molecule 1: Allene oxide cyclase





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	67.32Å 67.43Å 161.78Å 84.61° 79.32° 61.99°	Depositor
Resolution (Å)	19.80 – 1.35 19.80 – 1.35	Depositor EDS
% Data completeness (in resolution range)	82.4 (19.80-1.35) 82.4 (19.80-1.35)	Depositor EDS
R_{merge}	0.02	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.87 (at 1.35Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.138 , 0.174 0.139 , 0.175	Depositor DCC
R_{free} test set	22342 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	14.4	Xtriage
Anisotropy	0.238	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.41 , 62.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.042 for h,h-k,h-l 0.024 for -h,-h+k,-l 0.022 for -h,-k,-h+l	Xtriage
F_o,F_c correlation	0.98	EDS
Total number of atoms	19586	wwPDB-VP
Average B, all atoms (Å^2)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.70% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: PO4, HEZ

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	0.82	0/1481	0.82	3/2011 (0.1%)
1	B	0.74	0/1449	0.73	1/1965 (0.1%)
1	C	0.75	0/1421	0.71	0/1927
1	D	0.80	0/1465	0.81	0/1991
1	E	0.75	0/1474	0.77	1/2002 (0.0%)
1	F	0.79	0/1419	0.72	0/1924
1	G	0.73	0/1454	0.71	0/1972
1	H	0.72	0/1416	0.71	0/1920
1	I	0.73	0/1447	0.69	0/1965
1	J	0.69	0/1424	0.68	0/1931
1	K	0.72	0/1485	0.70	0/2017
1	L	0.67	0/1424	0.66	0/1929
All	All	0.74	0/17359	0.73	5/23554 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	86	ARG	NE-CZ-NH1	8.16	124.38	120.30
1	A	173	ASP	CB-CG-OD2	-5.63	113.24	118.30
1	A	24	ARG	NE-CZ-NH2	-5.18	117.71	120.30
1	A	173	ASP	CB-CG-OD1	5.09	122.88	118.30
1	B	173	ASP	CB-CG-OD1	5.08	122.87	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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	1437	0	1388	17	0
1	B	1408	0	1373	21	0
1	C	1381	0	1350	23	0
1	D	1422	0	1380	14	0
1	E	1431	0	1392	17	0
1	F	1379	0	1343	16	0
1	G	1412	0	1376	17	0
1	H	1375	0	1341	13	0
1	I	1405	0	1366	6	0
1	J	1383	0	1344	13	0
1	K	1442	0	1404	8	0
1	L	1384	0	1353	18	0
2	A	5	0	0	0	0
2	B	10	0	0	1	0
2	C	5	0	0	0	0
2	D	5	0	0	0	0
2	E	5	0	0	0	0
2	F	5	0	0	0	0
2	G	10	0	0	0	0
2	H	10	0	0	0	0
2	I	10	0	0	0	0
2	J	10	0	0	0	0
2	K	5	0	0	0	0
2	L	5	0	0	0	0
3	A	8	0	14	10	0
3	B	8	0	14	4	0
3	D	8	0	13	1	0
3	E	8	0	14	0	0
3	F	8	0	14	3	0
3	G	8	0	14	1	0
4	A	238	0	0	4	0
4	B	245	0	0	9	2
4	C	197	0	0	2	0
4	D	302	0	0	4	0
4	E	280	0	0	6	2
4	F	209	0	0	2	0
4	G	192	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	H	196	0	0	2	2
4	I	211	0	0	4	3
4	J	163	0	0	2	0
4	K	239	0	0	1	1
4	L	122	0	0	4	0
All	All	19586	0	16493	183	5

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 5.

All (183) 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:G:90:LEU:HD13	1:G:104[B]:GLN:HG2	1.34	1.08
1:A:107[B]:TYR:CE2	3:A:202:HEZ:C5	2.48	0.97
1:A:107[B]:TYR:CE2	3:A:202:HEZ:H51	2.06	0.91
1:G:90:LEU:CD1	1:G:104[B]:GLN:HG2	2.02	0.87
3:B:201:HEZ:H42	4:B:475:HOH:O	1.78	0.83
1:F:107:TYR:HE1	1:F:135:GLN:HE22	1.25	0.82
1:D:81:GLN:HE21	1:D:82:LYS:HE3	1.43	0.81
1:G:133[B]:LEU:HD11	1:G:142:LEU:HD23	1.62	0.80
1:J:56:LYS:NZ	4:J:372:HOH:O	2.15	0.78
1:A:107[B]:TYR:CZ	3:A:202:HEZ:H52	2.19	0.78
1:L:43:HIS:N	4:L:372:HOH:O	2.18	0.77
1:A:107[B]:TYR:CE2	3:A:202:HEZ:H52	2.19	0.77
1:B:51:VAL:HG11	3:B:201:HEZ:H22	1.66	0.76
1:D:133[A]:LEU:HD11	1:D:142:LEU:HD23	1.68	0.75
1:B:186:ASN:OD1	4:B:511:HOH:O	2.04	0.73
1:E:10:HIS:N	4:E:535:HOH:O	2.20	0.73
1:I:43:HIS:ND1	4:I:510:HOH:O	2.20	0.73
1:D:62:LEU:CD1	1:D:169:VAL:HG13	2.20	0.72
1:C:135:GLN:NE2	1:C:138:PHE:HB2	2.02	0.72
1:G:36:LYS:HZ1	1:G:42:ALA:N	1.87	0.72
1:K:153:LYS:HD2	4:K:522:HOH:O	1.90	0.71
1:B:109:THR:O	1:B:135:GLN:NE2	2.24	0.69
1:A:107[B]:TYR:CZ	3:A:202:HEZ:C5	2.76	0.69
1:C:82:LYS:HD3	1:C:110:TYR:CE2	2.28	0.69
1:I:179:LEU:HD23	4:I:507:HOH:O	1.93	0.69
1:G:181:ASN:ND2	4:G:439:HOH:O	2.25	0.69
1:E:36:LYS:HE2	4:E:515:HOH:O	1.93	0.68
1:D:135:GLN:HG2	4:D:528:HOH:O	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:97:ASP:OD1	4:G:467:HOH:O	2.13	0.65
1:D:62:LEU:HD11	1:D:169:VAL:HG13	1.80	0.64
1:E:135:GLN:HG2	4:E:411:HOH:O	1.98	0.64
1:G:135:GLN:NE2	1:G:138:PHE:HB2	2.14	0.63
1:D:62:LEU:HD11	1:D:169:VAL:CG1	2.29	0.63
1:E:48:GLY:N	4:E:471:HOH:O	2.21	0.62
1:D:135:GLN:CG	4:D:528:HOH:O	2.48	0.62
1:B:75[A]:LEU:HD11	1:B:85:ASP:HB3	1.82	0.62
1:F:82:LYS:HD3	1:F:110:TYR:CE2	2.35	0.61
1:B:45:ASN:HB3	1:B:75[A]:LEU:HD21	1.81	0.61
1:B:75[A]:LEU:HD13	1:B:87:TYR:CE1	2.36	0.61
1:A:107[B]:TYR:CD2	3:A:202:HEZ:H51	2.36	0.60
1:J:135:GLN:NE2	1:J:138:PHE:HB2	2.16	0.60
1:A:90:LEU:HD13	1:C:90:LEU:HD13	1.83	0.60
3:A:202:HEZ:H12	4:A:534:HOH:O	2.00	0.60
1:C:135:GLN:HE21	1:C:138:PHE:HB2	1.66	0.60
1:C:135:GLN:HA	1:C:142:LEU:HD23	1.83	0.60
1:L:62:LEU:HD11	1:L:169:VAL:HG13	1.84	0.60
1:J:35:LYS:HE2	1:J:46:SER:HB2	1.84	0.59
1:B:48:GLY:N	4:B:480:HOH:O	2.21	0.59
1:C:114:TYR:OH	1:C:132:LYS:HE2	2.03	0.59
1:J:90:LEU:HD13	1:L:90:LEU:HD13	1.85	0.59
1:L:174:GLU:HG2	1:L:179:LEU:HD12	1.83	0.58
1:C:22:ARG:HD3	1:C:140:PHE:CE1	2.38	0.58
1:E:48:GLY:CA	4:E:471:HOH:O	2.52	0.57
2:B:203:PO4:O4	4:B:528:HOH:O	2.17	0.56
1:D:62:LEU:HD13	1:D:169:VAL:HG13	1.86	0.56
1:G:132:LYS:NZ	4:G:448:HOH:O	2.38	0.56
1:E:133[B]:LEU:HD11	1:E:142:LEU:HD23	1.87	0.56
1:I:189:LYS:NZ	4:I:314:HOH:O	2.36	0.56
1:L:62:LEU:CD1	1:L:169:VAL:HG13	2.36	0.56
1:C:136:ILE:HD11	1:C:143:PHE:HB2	1.88	0.55
1:C:19:ILE:CD1	1:C:171:PRO:HD3	2.36	0.55
1:F:51:VAL:HG11	3:F:201:HEZ:H22	1.88	0.55
1:B:48:GLY:CA	4:B:480:HOH:O	2.53	0.55
1:L:137:ILE:HD12	1:L:141[B]:LYS:HE3	1.87	0.55
1:F:164:PRO:HD3	4:F:372:HOH:O	2.05	0.55
4:B:536:HOH:O	3:G:202:HEZ:H11	2.05	0.54
1:F:152:LYS:HG2	4:F:448:HOH:O	2.08	0.54
1:C:135:GLN:HA	1:C:142:LEU:CD2	2.37	0.54
1:H:36:LYS:O	4:H:362:HOH:O	2.19	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:19[B]:ILE:CD1	1:E:171:PRO:HD3	2.39	0.53
3:A:202:HEZ:C1	4:A:534:HOH:O	2.54	0.53
1:G:104[B]:GLN:HG3	1:G:118:THR:HG21	1.91	0.53
1:D:132:LYS:NZ	4:D:675:HOH:O	2.42	0.53
1:B:52:PRO:HG2	1:E:48:GLY:HA2	1.91	0.52
1:I:136:ILE:HD11	1:I:143:PHE:HB2	1.90	0.52
1:B:48:GLY:HA2	1:F:52:PRO:HG2	1.92	0.52
1:G:104[B]:GLN:CG	1:G:118:THR:HG21	2.41	0.50
1:H:63:LYS:O	1:H:182:HIS:HD2	1.94	0.50
1:H:135:GLN:HA	1:H:142:LEU:CD2	2.41	0.50
1:L:24:ARG:NH2	4:L:421[A]:HOH:O	2.34	0.50
1:A:107[B]:TYR:CZ	3:A:202:HEZ:H51	2.45	0.50
1:A:149:GLN:OE1	4:A:474:HOH:O	2.20	0.49
1:L:56:LYS:NZ	4:L:413:HOH:O	2.44	0.49
1:H:10:HIS:N	4:H:371:HOH:O	2.44	0.49
1:E:19[B]:ILE:HD13	1:E:171:PRO:HD3	1.95	0.49
1:C:180:PRO:O	1:C:181:ASN:HB2	2.13	0.49
1:F:180:PRO:O	1:F:181:ASN:HB2	2.13	0.49
1:D:10:HIS:HA	4:D:677:HOH:O	2.11	0.48
1:C:63:LYS:HE3	4:C:493:HOH:O	2.12	0.48
1:K:28:VAL:O	1:K:52:PRO:HD2	2.13	0.48
1:H:135:GLN:OE1	1:H:138:PHE:HB2	2.13	0.48
1:E:56:LYS:NZ	4:E:464:HOH:O	2.42	0.48
1:A:136:ILE:HD11	1:A:143:PHE:HB2	1.95	0.47
1:L:136:ILE:HD12	1:L:141[A]:LYS:HG2	1.96	0.47
1:F:136:ILE:HD11	1:F:143:PHE:HB2	1.96	0.47
1:H:35:LYS:HE3	1:H:46:SER:HB3	1.96	0.47
1:G:109:THR:O	1:G:135:GLN:NE2	2.47	0.47
1:C:153:LYS:HD3	1:C:154:LEU:N	2.29	0.47
1:B:75[A]:LEU:HD13	1:B:87:TYR:CZ	2.50	0.47
1:F:141:LYS:O	1:F:142:LEU:HD23	2.15	0.47
1:L:136:ILE:HD11	1:L:143:PHE:HB2	1.97	0.47
1:E:141:LYS:C	1:E:142:LEU:HD12	2.35	0.47
1:L:17:TYR:CE1	1:L:169:VAL:HG11	2.50	0.47
1:H:135:GLN:HA	1:H:142:LEU:HD22	1.96	0.47
1:A:174:GLU:HG3	4:A:441:HOH:O	2.15	0.46
1:E:67:GLY:HA3	1:E:94:TYR:O	2.15	0.46
1:B:53:PHE:CD2	3:B:201:HEZ:H51	2.50	0.46
1:A:180:PRO:O	1:A:181:ASN:HB2	2.15	0.46
1:A:152:LYS:HB2	1:A:152:LYS:HE3	1.51	0.45
1:D:180:PRO:O	1:D:181:ASN:HB2	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:67:GLY:HA3	1:D:94:TYR:O	2.16	0.45
1:K:135:GLN:OE1	1:K:142:LEU:CD2	2.64	0.45
3:D:301:HEZ:H12	1:E:40:THR:HA	1.99	0.45
1:B:156:GLU:HG2	4:B:446:HOH:O	2.17	0.45
1:H:109:THR:O	1:H:135:GLN:OE1	2.35	0.45
1:A:51:VAL:HG11	3:A:202:HEZ:H12	1.99	0.45
1:H:138:PHE:HA	1:H:139:PRO:HA	1.79	0.45
1:K:67:GLY:HA3	1:K:94:TYR:O	2.17	0.45
1:L:153:LYS:HD3	1:L:154:LEU:N	2.31	0.45
1:C:133:LEU:C	1:C:133:LEU:HD23	2.37	0.45
1:A:142:LEU:HD12	1:A:142:LEU:N	2.32	0.45
1:E:133[A]:LEU:C	1:E:133[A]:LEU:HD23	2.37	0.45
1:E:153[B]:LYS:C	1:E:153[B]:LYS:HD3	2.37	0.44
1:G:36:LYS:HA	1:G:42:ALA:O	2.17	0.44
1:H:135:GLN:HE22	1:H:138:PHE:HD1	1.66	0.44
1:J:115[A]:LEU:HD12	1:J:115[A]:LEU:N	2.33	0.44
1:C:153:LYS:HD3	1:C:154:LEU:O	2.17	0.44
1:E:180:PRO:O	1:E:181:ASN:HB2	2.17	0.44
1:B:135:GLN:NE2	1:B:138:PHE:HB2	2.33	0.44
1:L:138:PHE:HA	1:L:139:PRO:HA	1.74	0.44
1:C:19:ILE:HD12	1:C:171:PRO:HD3	2.00	0.44
1:I:133[B]:LEU:HD11	1:I:142:LEU:HD23	1.99	0.44
1:G:173:ASP:OD2	1:G:177:GLN:NE2	2.51	0.43
1:J:109:THR:O	1:J:135:GLN:NE2	2.50	0.43
1:C:135:GLN:HB2	4:C:337:HOH:O	2.19	0.43
1:B:186:ASN:ND2	4:B:493:HOH:O	2.50	0.43
1:F:143:PHE:CD2	1:F:165:PRO:HG3	2.52	0.43
1:A:107[B]:TYR:CD2	1:A:133:LEU:HD11	2.52	0.43
1:D:81:GLN:HG2	1:D:82:LYS:HG2	2.00	0.43
1:C:174:GLU:CD	1:C:174:GLU:H	2.22	0.43
1:H:133:LEU:C	1:H:133:LEU:HD23	2.38	0.43
1:K:133[B]:LEU:HD13	1:K:144:TYR:CZ	2.53	0.43
1:L:28:VAL:O	1:L:52:PRO:HD2	2.19	0.43
1:B:10:HIS:N	4:B:479:HOH:O	2.51	0.43
1:C:28:VAL:O	1:C:52:PRO:HD2	2.19	0.43
1:F:107:TYR:HE2	3:F:201:HEZ:H31	1.83	0.43
1:H:28:VAL:O	1:H:52:PRO:HD2	2.19	0.43
1:J:19:ILE:CD1	1:J:171:PRO:HD3	2.49	0.43
1:B:47:LEU:HA	1:B:75[A]:LEU:O	2.18	0.42
1:F:51:VAL:HG11	3:F:201:HEZ:H52	2.00	0.42
1:G:104[B]:GLN:CD	1:G:118:THR:HG21	2.39	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:90:LEU:HD23	1:J:104:GLN:HG3	2.01	0.42
1:C:138:PHE:HA	1:C:139:PRO:HA	1.80	0.42
1:K:141:LYS:O	1:K:142:LEU:HD23	2.19	0.42
1:G:138:PHE:HA	1:G:139:PRO:HA	1.82	0.42
1:I:133[A]:LEU:C	1:I:133[A]:LEU:HD23	2.40	0.42
1:J:138:PHE:CE1	1:J:139:PRO:HB3	2.55	0.42
1:F:90:LEU:HD23	1:F:104[B]:GLN:HG3	2.01	0.42
1:L:133:LEU:C	1:L:133:LEU:HD23	2.41	0.42
1:F:180:PRO:HA	4:I:480:HOH:O	2.19	0.42
1:C:135:GLN:OE1	1:C:142:LEU:HD21	2.19	0.41
1:B:136:ILE:HD11	1:B:143:PHE:HB2	2.02	0.41
1:E:133[A]:LEU:HD23	1:E:134:HIS:N	2.35	0.41
1:D:136:ILE:HD11	1:D:143:PHE:HB2	2.02	0.41
1:B:67:GLY:HA3	1:B:94:TYR:O	2.21	0.41
1:K:136:ILE:HD11	1:K:143:PHE:HB2	2.02	0.41
1:C:174:GLU:HG3	1:C:182:HIS:CE1	2.56	0.41
1:L:24:ARG:HG3	4:L:316:HOH:O	2.20	0.41
1:G:52:PRO:HG2	1:H:48:GLY:HA2	2.02	0.41
1:K:133[A]:LEU:HD23	1:K:133[A]:LEU:C	2.40	0.41
1:F:28:VAL:O	1:F:52:PRO:HD2	2.21	0.41
1:L:141[B]:LYS:C	1:L:142:LEU:HD12	2.40	0.41
1:L:173:ASP:OD2	1:L:177:GLN:NE2	2.53	0.41
1:A:139:PRO:HD2	1:A:140:PHE:CD2	2.55	0.40
1:C:67:GLY:HA3	1:C:94:TYR:O	2.21	0.40
1:B:53:PHE:CE2	3:B:201:HEZ:H51	2.55	0.40
1:J:138:PHE:HA	1:J:139:PRO:HA	1.76	0.40
1:F:164:PRO:HA	1:F:165:PRO:HD3	1.99	0.40
1:J:28:VAL:O	1:J:52:PRO:HD2	2.22	0.40
1:G:133[B]:LEU:HD13	1:G:144:TYR:CE1	2.57	0.40
1:B:28:VAL:O	1:B:52:PRO:HD2	2.20	0.40
1:J:46:SER:HB3	4:J:368:HOH:O	2.22	0.40
1:J:142:LEU:HD12	1:J:142:LEU:N	2.37	0.40

All (5) 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)
4:B:537:HOH:O	4:E:579:HOH:O[1_565]	1.81	0.39
4:H:493:HOH:O	4:I:508:HOH:O[1_565]	2.00	0.20
4:B:432:HOH:O	4:E:468:HOH:O[1_565]	2.03	0.17

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:493:HOH:O	4:I:509:HOH:O[1_565]	2.05	0.15
4:I:500:HOH:O	4:K:524:HOH:O[1_656]	2.19	0.01

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	182/195 (93%)	180 (99%)	2 (1%)	0	100	100
1	B	176/195 (90%)	176 (100%)	0	0	100	100
1	C	173/195 (89%)	172 (99%)	1 (1%)	0	100	100
1	D	181/195 (93%)	179 (99%)	2 (1%)	0	100	100
1	E	182/195 (93%)	181 (100%)	1 (0%)	0	100	100
1	F	173/195 (89%)	172 (99%)	1 (1%)	0	100	100
1	G	176/195 (90%)	175 (99%)	1 (1%)	0	100	100
1	H	172/195 (88%)	170 (99%)	1 (1%)	1 (1%)	25	6
1	I	179/195 (92%)	178 (99%)	1 (1%)	0	100	100
1	J	173/195 (89%)	172 (99%)	1 (1%)	0	100	100
1	K	183/195 (94%)	181 (99%)	2 (1%)	0	100	100
1	L	173/195 (89%)	170 (98%)	3 (2%)	0	100	100
All	All	2123/2340 (91%)	2106 (99%)	16 (1%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	180	PRO

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	154/157 (98%)	153 (99%)	1 (1%)	86 69
1	B	151/157 (96%)	151 (100%)	0	100 100
1	C	148/157 (94%)	148 (100%)	0	100 100
1	D	152/157 (97%)	151 (99%)	1 (1%)	84 64
1	E	153/157 (98%)	153 (100%)	0	100 100
1	F	147/157 (94%)	145 (99%)	2 (1%)	67 36
1	G	151/157 (96%)	150 (99%)	1 (1%)	84 64
1	H	147/157 (94%)	146 (99%)	1 (1%)	84 64
1	I	150/157 (96%)	148 (99%)	2 (1%)	69 37
1	J	148/157 (94%)	147 (99%)	1 (1%)	84 64
1	K	155/157 (99%)	155 (100%)	0	100 100
1	L	148/157 (94%)	146 (99%)	2 (1%)	67 36
All	All	1804/1884 (96%)	1793 (99%)	11 (1%)	86 69

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	135	GLN
1	D	10	HIS
1	F	82	LYS
1	F	135	GLN
1	G	137	ILE
1	H	179	LEU
1	I	90	LEU
1	I	179	LEU
1	J	153	LYS
1	L	24	ARG
1	L	154	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	81	GLN
1	F	135	GLN
1	G	43	HIS
1	G	177	GLN
1	H	135	GLN
1	H	182	HIS
1	I	43	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 monosaccharides in this entry.

5.6 Ligand geometry

23 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	PO4	J	201	-	4,4,4	0.69	0	6,6,6	1.76	2 (33%)
3	HEZ	E	201	-	7,7,7	0.65	0	6,6,6	0.53	0
2	PO4	L	201	-	4,4,4	1.01	0	6,6,6	0.80	0
3	HEZ	D	301	-	7,7,7	1.39	2 (28%)	6,6,6	0.84	0
2	PO4	A	201	-	4,4,4	1.47	1 (25%)	6,6,6	1.33	1 (16%)
2	PO4	J	202	-	4,4,4	0.87	0	6,6,6	0.64	0
2	PO4	B	202	-	4,4,4	2.41	1 (25%)	6,6,6	1.46	1 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	HEZ	A	202	-	7,7,7	0.44	0	6,6,6	1.09	0
3	HEZ	B	201	-	7,7,7	0.46	0	6,6,6	0.86	0
2	PO4	B	203	-	4,4,4	0.91	0	6,6,6	1.07	1 (16%)
2	PO4	G	201	-	4,4,4	0.95	0	6,6,6	1.28	1 (16%)
2	PO4	D	302	-	4,4,4	0.95	0	6,6,6	0.89	0
2	PO4	I	202	-	4,4,4	0.68	0	6,6,6	0.67	0
2	PO4	H	202	-	4,4,4	1.09	0	6,6,6	0.78	0
3	HEZ	F	201	-	7,7,7	0.34	0	6,6,6	0.48	0
2	PO4	G	203	-	4,4,4	0.51	0	6,6,6	1.17	1 (16%)
2	PO4	I	201	-	4,4,4	1.40	1 (25%)	6,6,6	0.95	0
2	PO4	C	201	-	4,4,4	0.41	0	6,6,6	1.18	0
2	PO4	H	201	-	4,4,4	0.65	0	6,6,6	1.27	0
2	PO4	F	202	-	4,4,4	1.27	1 (25%)	6,6,6	0.88	0
2	PO4	K	201	-	4,4,4	1.22	0	6,6,6	0.78	0
3	HEZ	G	202	-	7,7,7	0.56	0	6,6,6	0.51	0
2	PO4	E	202	-	4,4,4	1.30	1 (25%)	6,6,6	1.82	2 (33%)

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	HEZ	E	201	-	-	0/5/5/5	-
3	HEZ	F	201	-	-	0/5/5/5	-
3	HEZ	B	201	-	-	0/5/5/5	-
3	HEZ	A	202	-	-	0/5/5/5	-
3	HEZ	G	202	-	-	0/5/5/5	-
3	HEZ	D	301	-	-	1/5/5/5	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	202	PO4	P-O1	4.58	1.61	1.50
2	I	201	PO4	P-O1	2.46	1.56	1.50
3	D	301	HEZ	O6-C6	2.40	1.54	1.42
2	A	201	PO4	P-O1	2.37	1.56	1.50
2	F	202	PO4	P-O1	2.37	1.56	1.50
2	E	202	PO4	P-O1	2.34	1.56	1.50
3	D	301	HEZ	C5-C6	2.30	1.63	1.50

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	202	PO4	O2-P-O1	-3.53	97.98	110.89
2	B	202	PO4	O2-P-O1	-3.08	99.64	110.89
2	J	201	PO4	O2-P-O1	-2.60	101.39	110.89
2	G	203	PO4	O4-P-O2	2.47	115.91	107.97
2	G	201	PO4	O3-P-O1	-2.42	102.02	110.89
2	E	202	PO4	O3-P-O2	2.31	115.38	107.97
2	A	201	PO4	O4-P-O3	-2.20	100.89	107.97
2	J	201	PO4	O4-P-O2	2.20	115.03	107.97
2	B	203	PO4	O3-P-O1	2.08	118.51	110.89

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	301	HEZ	C2-C3-C4-C5

There are no ring outliers.

6 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	301	HEZ	1	0
3	A	202	HEZ	10	0
3	B	201	HEZ	4	0
2	B	203	PO4	1	0
3	F	201	HEZ	3	0
3	G	202	HEZ	1	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

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, 95^{th} 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	180/195 (92%)	0.18	8 (4%) 34 39	12, 23, 39, 51	2 (1%)
1	B	177/195 (90%)	0.09	10 (5%) 24 27	12, 19, 39, 59	3 (1%)
1	C	175/195 (89%)	0.35	15 (8%) 10 12	12, 24, 39, 55	2 (1%)
1	D	180/195 (92%)	-0.11	4 (2%) 62 68	10, 16, 26, 45	2 (1%)
1	E	180/195 (92%)	-0.06	4 (2%) 62 68	12, 18, 29, 45	1 (0%)
1	F	175/195 (89%)	0.17	8 (4%) 32 37	13, 23, 41, 49	2 (1%)
1	G	175/195 (89%)	0.16	13 (7%) 14 16	16, 23, 40, 51	3 (1%)
1	H	175/195 (89%)	0.22	16 (9%) 9 11	16, 25, 43, 52	4 (2%)
1	I	180/195 (92%)	-0.02	5 (2%) 53 59	17, 25, 38, 48	3 (1%)
1	J	175/195 (89%)	0.33	12 (6%) 16 18	17, 27, 48, 58	3 (1%)
1	K	180/195 (92%)	-0.06	4 (2%) 62 68	16, 22, 34, 47	2 (1%)
1	L	175/195 (89%)	0.58	29 (16%) 1 1	19, 32, 49, 57	1 (0%)
All	All	2127/2340 (90%)	0.15	128 (6%) 21 24	10, 23, 42, 59	28 (1%)

All (128) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	42	ALA	7.6
1	C	42	ALA	6.9
1	F	42	ALA	6.1
1	J	36	LYS	5.4
1	J	42	ALA	5.3
1	L	81	GLN	5.3
1	A	10	HIS	5.1
1	H	81	GLN	5.1
1	L	179	LEU	4.8
1	L	177	GLN	4.7
1	A	81	GLN	4.7

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Mol	Chain	Res	Type	RSRZ
1	J	34	GLY	4.6
1	C	81	GLN	4.5
1	B	37	GLN	4.5
1	B	41	ASP	4.5
1	J	10	HIS	4.5
1	B	81	GLN	4.4
1	I	81	GLN	4.4
1	F	36	LYS	4.3
1	B	42	ALA	4.3
1	L	167	PRO	4.2
1	L	156	GLU	4.1
1	J	81	GLN	4.1
1	E	81	GLN	4.0
1	H	82	LYS	4.0
1	G	81	GLN	3.9
1	K	10	HIS	3.9
1	L	180	PRO	3.9
1	C	168	SER	3.9
1	C	37	GLN	3.9
1	H	42	ALA	3.9
1	L	83	ASN	3.9
1	H	80	ASP	3.8
1	G	137	ILE	3.7
1	L	138	PHE	3.7
1	H	10	HIS	3.7
1	B	36	LYS	3.7
1	J	83	ASN	3.6
1	F	81	GLN	3.6
1	L	37	GLN	3.6
1	J	80	ASP	3.5
1	K	81	GLN	3.5
1	C	36	LYS	3.5
1	G	10	HIS	3.4
1	F	83	ASN	3.4
1	G	36	LYS	3.4
1	L	181	ASN	3.3
1	H	36	LYS	3.3
1	L	36	LYS	3.3
1	L	80	ASP	3.3
1	J	138	PHE	3.2
1	E	10	HIS	3.2
1	L	22	ARG	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	11	VAL	3.2
1	F	137	ILE	3.1
1	L	140	PHE	3.1
1	D	81	GLN	3.0
1	H	181	ASN	3.0
1	L	139	PRO	3.0
1	D	80	ASP	3.0
1	B	80	ASP	3.0
1	J	137	ILE	2.9
1	C	161	PRO	2.9
1	L	43	HIS	2.9
1	H	168	SER	2.9
1	K	80	ASP	2.8
1	L	174	GLU	2.8
1	I	82	LYS	2.8
1	L	82	LYS	2.8
1	L	10	HIS	2.8
1	G	179	LEU	2.7
1	C	34	GLY	2.7
1	A	82	LYS	2.6
1	H	138	PHE	2.6
1	I	80	ASP	2.6
1	J	79	SER	2.6
1	G	107[A]	TYR	2.6
1	A	138	PHE	2.6
1	F	140	PHE	2.6
1	H	22	ARG	2.6
1	L	34	GLY	2.6
1	C	156	GLU	2.6
1	C	11	VAL	2.6
1	D	10	HIS	2.5
1	F	80	ASP	2.5
1	G	80	ASP	2.5
1	B	138	PHE	2.5
1	L	178	CYS	2.5
1	L	168	SER	2.5
1	E	80	ASP	2.5
1	E	83	ASN	2.5
1	L	173	ASP	2.5
1	F	138	PHE	2.5
1	B	82	LYS	2.4
1	J	44	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	I	83	ASN	2.4
1	L	57	ILE	2.3
1	A	156[A]	GLU	2.3
1	G	83	ASN	2.3
1	D	82	LYS	2.3
1	L	160	ALA	2.3
1	L	137	ILE	2.2
1	L	159	CYS	2.2
1	L	166	SER	2.2
1	B	83	ASN	2.2
1	H	83	ASN	2.2
1	H	167	PRO	2.2
1	H	173	ASP	2.2
1	L	182	HIS	2.2
1	G	34	GLY	2.2
1	B	10	HIS	2.1
1	C	138	PHE	2.1
1	C	164	PRO	2.1
1	K	83	ASN	2.1
1	C	137	ILE	2.1
1	C	83	ASN	2.1
1	C	80	ASP	2.1
1	G	140	PHE	2.1
1	H	140	PHE	2.1
1	H	179	LEU	2.1
1	I	10	HIS	2.1
1	H	177	GLN	2.1
1	J	82	LYS	2.1
1	A	180	PRO	2.1
1	G	43	HIS	2.0
1	A	80	ASP	2.0
1	C	57	ILE	2.0
1	G	138	PHE	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 (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, 95^{th} 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	PO4	G	203	5/5	0.80	0.18	26,34,43,43	5
2	PO4	B	203	5/5	0.82	0.18	21,31,38,43	5
2	PO4	H	202	5/5	0.85	0.20	29,41,43,44	5
3	HEZ	G	202	8/8	0.86	0.14	34,36,38,38	2
3	HEZ	B	201	8/8	0.87	0.22	40,42,47,50	2
3	HEZ	D	301	8/8	0.90	0.23	21,31,33,35	6
3	HEZ	F	201	8/8	0.91	0.17	39,41,42,43	5
3	HEZ	E	201	8/8	0.92	0.23	20,34,37,38	6
2	PO4	I	202	5/5	0.92	0.12	29,32,39,41	5
2	PO4	J	202	5/5	0.92	0.10	35,43,47,50	5
3	HEZ	A	202	8/8	0.93	0.17	31,33,39,42	5
2	PO4	B	202	5/5	0.97	0.07	19,20,23,23	5
2	PO4	C	201	5/5	0.97	0.08	26,26,28,29	5
2	PO4	J	201	5/5	0.98	0.07	22,24,25,26	5
2	PO4	A	201	5/5	0.98	0.07	23,24,26,27	5
2	PO4	K	201	5/5	0.99	0.05	26,26,27,27	5
2	PO4	L	201	5/5	0.99	0.05	28,29,29,30	5
2	PO4	H	201	5/5	0.99	0.05	28,28,29,29	5
2	PO4	E	202	5/5	0.99	0.05	19,20,22,23	5
2	PO4	I	201	5/5	0.99	0.05	23,24,27,27	5
2	PO4	F	202	5/5	0.99	0.05	21,23,25,27	5
2	PO4	G	201	5/5	0.99	0.04	22,23,25,26	5
2	PO4	D	302	5/5	0.99	0.06	17,17,19,20	5

6.5 Other polymers (i)

There are no such residues in this entry.