



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 01:22 AM UTC

PDB ID : 4H6C / pdb_00004h6c
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 ⓘ 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:

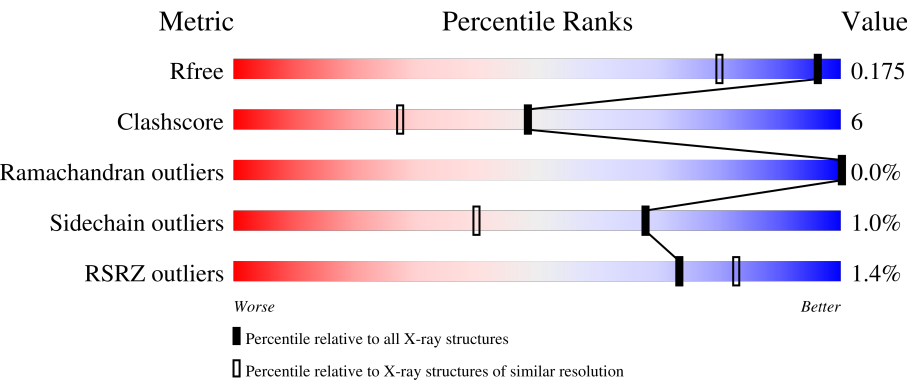
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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 1.35 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}	180053	1216 (1.36-1.36)
Clashscore	190562	1232 (1.36-1.36)
Ramachandran outliers	187476	1220 (1.36-1.36)
Sidechain outliers	187428	1220 (1.36-1.36)
RSRZ outliers	180081	1214 (1.36-1.36)

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	195	% 84%8%8%
1	B	195	% 81%10%9%
1	C	195	3% 76%13%10%
1	D	195	84%7%8%
1	E	195	84%9%8%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	195	2% 79% 9% 10%
1	G	195	% 79% 10% 10%
1	H	195	3% 81% 9% 10%
1	I	195	87% 5% 8%
1	J	195	4% 81% 8% 10%
1	K	195	% 86% 6% 8%
1	L	195	% 78% 10% 10%

2 Entry composition

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

Continued on next page...

Continued from previous page...

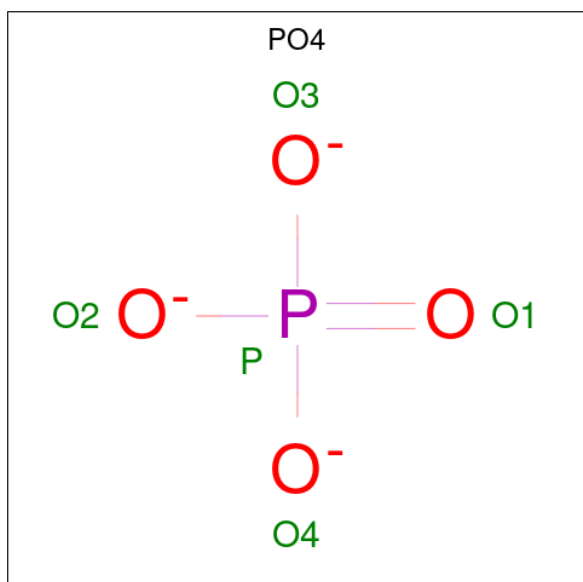
Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	expression tag	UNP Q8GS38
D	-5	GLY	-	expression tag	UNP Q8GS38
D	-4	GLY	-	expression tag	UNP Q8GS38
D	-3	PRO	-	expression tag	UNP Q8GS38
D	-2	LEU	-	expression tag	UNP Q8GS38
D	-1	GLY	-	expression tag	UNP Q8GS38
D	0	SER	-	expression tag	UNP Q8GS38
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

Continued on next page...

Continued from previous page...

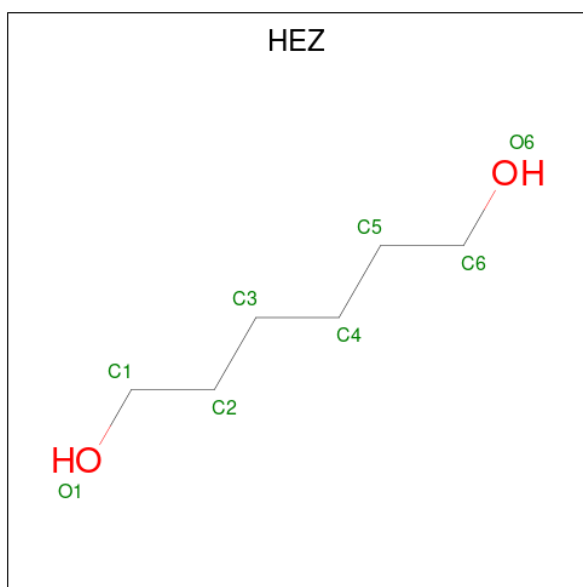
Chain	Residue	Modelled	Actual	Comment	Reference
H	0	SER	-	expression tag	UNP Q8GS38
I	-5	GLY	-	expression tag	UNP Q8GS38
I	-4	GLY	-	expression tag	UNP Q8GS38
I	-3	PRO	-	expression tag	UNP Q8GS38
I	-2	LEU	-	expression tag	UNP Q8GS38
I	-1	GLY	-	expression tag	UNP Q8GS38
I	0	SER	-	expression tag	UNP Q8GS38
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 (CCD ID: PO4) (formula: O₄P).



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 (CCD ID: HEZ) (formula: C₆H₁₄O₂).



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

- Molecule 4 is water.

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

Continued on next page...

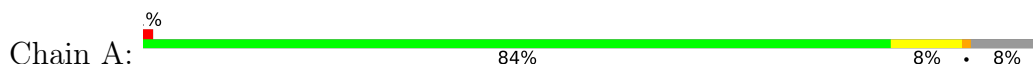
Continued from previous page...

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

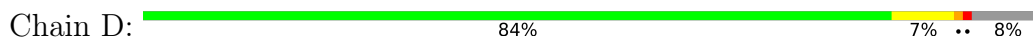
3 Residue-property plots [i](#)

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.

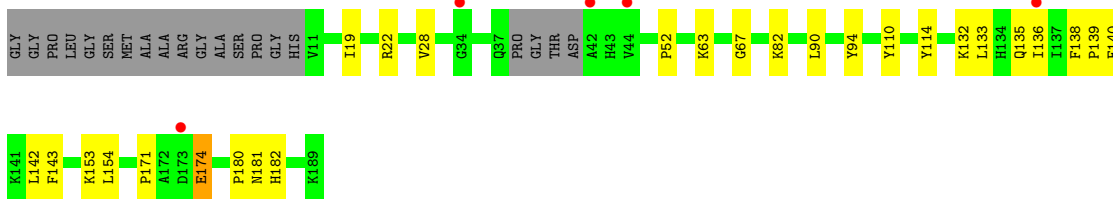
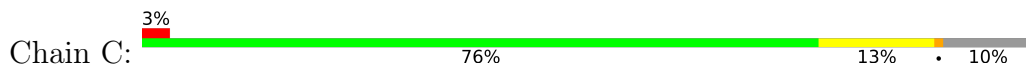
- Molecule 1: Allene oxide cyclase



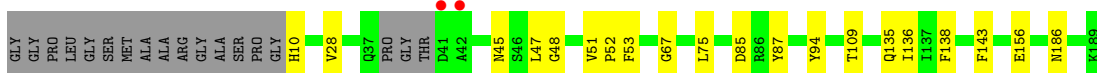
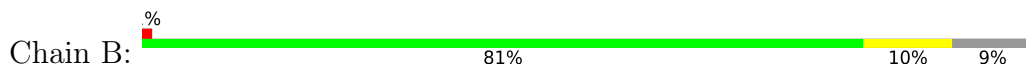
- Molecule 1: Allene oxide cyclase



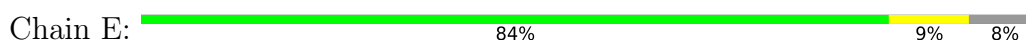
- Molecule 1: Allene oxide cyclase



- Molecule 1: Allene oxide cyclase

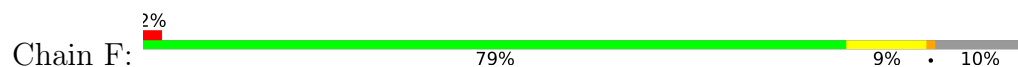


- Molecule 1: Allene oxide cyclase

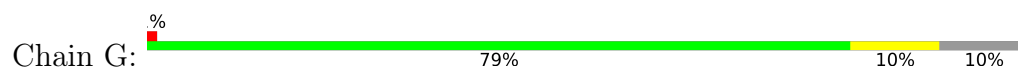




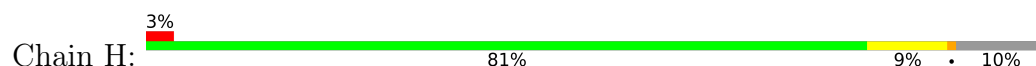
- Molecule 1: Allene oxide cyclase



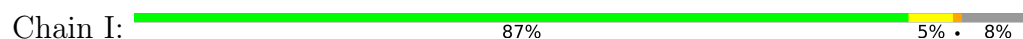
- Molecule 1: Allene oxide cyclase



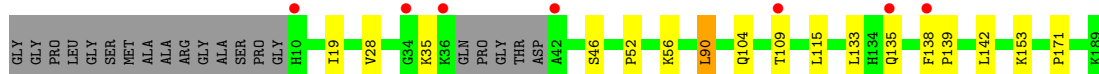
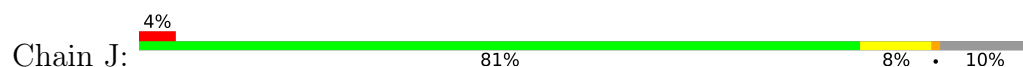
- Molecule 1: Allene oxide cyclase



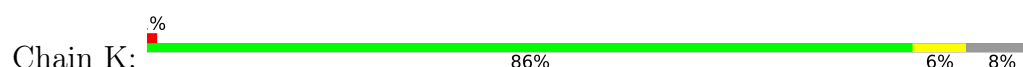
- Molecule 1: Allene oxide cyclase



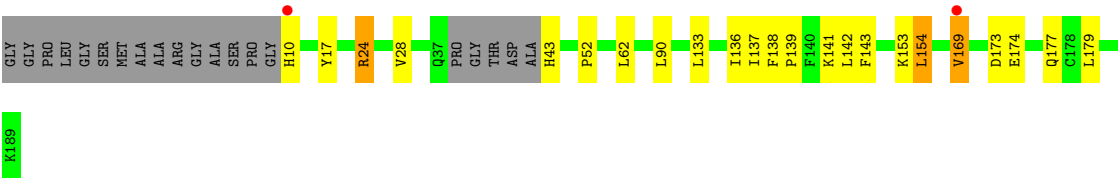
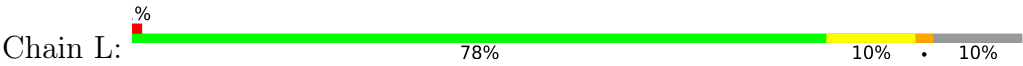
- Molecule 1: Allene oxide cyclase



- Molecule 1: Allene oxide cyclase



● Molecule 1: Allene oxide cyclase



4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ 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)	0.40 , 58.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	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.*

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: HEZ, PO4

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	0.96	2/1481 (0.1%)	0.90	0/2011
1	B	0.86	0/1449	0.83	0/1965
1	C	0.85	0/1421	0.81	0/1927
1	D	0.96	1/1465 (0.1%)	0.89	0/1991
1	E	0.86	0/1474	0.85	2/2002 (0.1%)
1	F	0.85	0/1419	0.81	0/1924
1	G	0.82	1/1454 (0.1%)	0.78	0/1972
1	H	0.83	0/1416	0.81	0/1920
1	I	0.83	0/1447	0.79	0/1965
1	J	0.76	0/1424	0.80	0/1931
1	K	0.82	0/1485	0.80	0/2017
1	L	0.75	0/1424	0.79	0/1929
All	All	0.85	4/17359 (0.0%)	0.82	2/23554 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	169	VAL	CA-CB	8.22	1.62	1.54
1	A	66	LEU	N-CA	5.76	1.53	1.46
1	A	99	GLY	C-O	5.50	1.28	1.24
1	G	169	VAL	CA-CB	5.46	1.59	1.54

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	47	LEU	CA-C-N	-6.24	116.02	123.44
1	E	47	LEU	C-N-CA	-6.24	116.02	123.44

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	1437	0	1388	11	0
1	B	1408	0	1373	21	0
1	C	1381	0	1350	24	0
1	D	1422	0	1380	15	0
1	E	1431	0	1392	16	0
1	F	1379	0	1343	18	0
1	G	1412	0	1376	17	0
1	H	1375	0	1341	14	0
1	I	1405	0	1366	8	0
1	J	1383	0	1344	15	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	3	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	5	2
4	F	209	0	0	3	0
4	G	192	0	0	3	0

Continued on next page...

Continued from previous page...

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	3	0
All	All	19586	0	16493	185	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 6.

All (185) 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: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:L:43:HIS:N	4:L:372:HOH:O	2.18	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	1.88	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: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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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
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: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:E:141:LYS:C	1:E:142:LEU:HD12	2.35	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:133[A]:LEU:C	1:E:133[A]:LEU:HD23	2.37	0.50
1:A:149:GLN:OE1	4:A:474:HOH:O	2.20	0.49
1:C:133:LEU:C	1:C:133:LEU:HD23	2.37	0.49
1:E:153[B]:LYS:C	1:E:153[B]:LYS:HD3	2.37	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:H:133:LEU:C	1:H:133:LEU:HD23	2.38	0.48
1:A:136:ILE:HD11	1:A:143:PHE:HB2	1.95	0.47
1:C:174:GLU:H	1:C:174:GLU:CD	2.22	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:G:104[B]:GLN:CD	1:G:118:THR:HG21	2.39	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: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:I:133[A]:LEU:C	1:I:133[A]:LEU:HD23	2.40	0.47
1:L:133:LEU:C	1:L:133:LEU:HD23	2.41	0.46
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:L:141[B]:LYS:C	1:L:142:LEU:HD12	2.40	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:G:132:LYS:NZ	4:G:448:HOH:O	2.38	0.46
1:D:132:LYS:NZ	4:D:675:HOH:O	2.42	0.46
1:K:133[A]:LEU:HD23	1:K:133[A]:LEU:C	2.40	0.46
1:A:152:LYS:HB2	1:A:152:LYS:HE3	1.51	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:180:PRO:O	1:D:181:ASN:HB2	2.15	0.45
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:F:56:LYS:NZ	4:F:430:HOH:O	2.30	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:A:142:LEU:HD12	1:A:142:LEU:N	2.32	0.45
1:J:133:LEU:C	1:J:133:LEU:HD23	2.42	0.44
1:J:153:LYS:HD3	1:J:153:LYS:C	2.41	0.44
1:C:153:LYS:HD3	1:C:153:LYS:C	2.42	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:A:133:LEU:HD23	1:A:133:LEU:C	2.42	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:L:141[A]:LYS:C	1:L:142:LEU:HD12	2.42	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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:133[B]:LEU:C	1:D:133[B]:LEU:HD23	2.44	0.42
1:F:51:VAL:HG11	3:F:201:HEZ:H52	2.00	0.42
1:J:90:LEU:HD23	1:J:104:GLN:HG3	2.01	0.42
1:H:174:GLU:CD	1:H:174:GLU:H	2.26	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: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: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:I:141:LYS:C	1:I:142:LEU:HD12	2.45	0.41
1:F:133:LEU:C	1:F:133:LEU:HD23	2.45	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:F:28:VAL:O	1:F:52:PRO:HD2	2.21	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:I:186:ASN:O	1:I:187:PHE:C	2.63	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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%)	21	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 ⓘ

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%)	152 (99%)	2 (1%)	61	30
1	B	151/157 (96%)	151 (100%)	0	100	100
1	C	148/157 (94%)	147 (99%)	1 (1%)	76	54
1	D	152/157 (97%)	149 (98%)	3 (2%)	48	16
1	E	153/157 (98%)	153 (100%)	0	100	100
1	F	147/157 (94%)	145 (99%)	2 (1%)	59	28
1	G	151/157 (96%)	150 (99%)	1 (1%)	76	54
1	H	147/157 (94%)	145 (99%)	2 (1%)	59	28
1	I	150/157 (96%)	148 (99%)	2 (1%)	61	30
1	J	148/157 (94%)	147 (99%)	1 (1%)	76	54
1	K	155/157 (99%)	155 (100%)	0	100	100
1	L	148/157 (94%)	144 (97%)	4 (3%)	39	9
All	All	1804/1884 (96%)	1786 (99%)	18 (1%)	68	40

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	135	GLN
1	A	152	LYS
1	D	10	HIS
1	D	75	LEU
1	D	169	VAL
1	C	174	GLU
1	F	82	LYS
1	F	135	GLN
1	G	137	ILE
1	H	174	GLU
1	H	179	LEU
1	I	90	LEU
1	I	179	LEU
1	J	90	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	L	10	HIS
1	L	24	ARG
1	L	154	LEU
1	L	169	VAL

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	55	ASN
1	A	149	GLN
1	D	37	GLN
1	D	45	ASN
1	D	81	GLN
1	D	177	GLN
1	C	55	ASN
1	B	10	HIS
1	B	37	GLN
1	E	37	GLN
1	E	45	ASN
1	E	149	GLN
1	F	55	ASN
1	F	135	GLN
1	G	55	ASN
1	G	177	GLN
1	H	55	ASN
1	H	135	GLN
1	H	182	HIS
1	I	43	HIS
1	J	55	ASN
1	J	149	GLN
1	K	37	GLN
1	K	55	ASN
1	K	181	ASN
1	L	55	ASN
1	L	177	GLN

5.3.3 RNA ⓘ

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](#)

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	L	201	-	4,4,4	1.07	0	6,6,6	0.84	0
2	PO4	G	201	-	4,4,4	1.01	0	6,6,6	1.33	1 (16%)
2	PO4	H	201	-	4,4,4	0.70	0	6,6,6	1.33	0
2	PO4	J	201	-	4,4,4	0.72	0	6,6,6	1.83	2 (33%)
2	PO4	A	201	-	4,4,4	1.53	1 (25%)	6,6,6	1.37	1 (16%)
3	HEZ	E	201	-	7,7,7	0.66	0	6,6,6	0.53	0
2	PO4	B	202	-	4,4,4	2.50	1 (25%)	6,6,6	1.52	1 (16%)
2	PO4	H	202	-	4,4,4	1.14	0	6,6,6	0.82	0
2	PO4	K	201	-	4,4,4	1.27	0	6,6,6	0.82	0
2	PO4	I	202	-	4,4,4	0.73	0	6,6,6	0.70	0
2	PO4	D	302	-	4,4,4	1.00	0	6,6,6	0.92	0
2	PO4	G	203	-	4,4,4	0.55	0	6,6,6	1.22	1 (16%)
2	PO4	C	201	-	4,4,4	0.45	0	6,6,6	1.23	0
3	HEZ	D	301	-	7,7,7	1.42	2 (28%)	6,6,6	0.88	0
2	PO4	B	203	-	4,4,4	0.97	0	6,6,6	1.11	1 (16%)
2	PO4	J	202	-	4,4,4	0.91	0	6,6,6	0.67	0
3	HEZ	G	202	-	7,7,7	0.57	0	6,6,6	0.51	0
2	PO4	E	202	-	4,4,4	1.37	1 (25%)	6,6,6	1.89	2 (33%)
3	HEZ	B	201	-	7,7,7	0.46	0	6,6,6	0.87	0
2	PO4	I	201	-	4,4,4	1.47	1 (25%)	6,6,6	0.98	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	HEZ	A	202	-	7,7,7	0.45	0	6,6,6	1.13	0
3	HEZ	F	201	-	7,7,7	0.33	0	6,6,6	0.49	0
2	PO4	F	202	-	4,4,4	1.34	1 (25%)	6,6,6	0.91	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
3	HEZ	E	201	-	-	0/5/5/5	-
3	HEZ	B	201	-	-	0/5/5/5	-
3	HEZ	D	301	-	-	1/5/5/5	-
3	HEZ	A	202	-	-	0/5/5/5	-
3	HEZ	F	201	-	-	0/5/5/5	-
3	HEZ	G	202	-	-	0/5/5/5	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	202	PO4	P-O1	4.74	1.61	1.50
2	I	201	PO4	P-O1	2.58	1.56	1.50
2	A	201	PO4	P-O1	2.49	1.56	1.50
2	F	202	PO4	P-O1	2.49	1.56	1.50
2	E	202	PO4	P-O1	2.46	1.56	1.50
3	D	301	HEZ	O6-C6	2.43	1.54	1.42
3	D	301	HEZ	C5-C6	2.33	1.63	1.51

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	202	PO4	O2-P-O1	-3.67	97.98	110.95
2	B	202	PO4	O2-P-O1	-3.20	99.64	110.95
2	J	201	PO4	O2-P-O1	-2.70	101.39	110.95
2	G	203	PO4	O4-P-O2	2.57	115.91	107.91
2	G	201	PO4	O3-P-O1	-2.52	102.02	110.95
2	E	202	PO4	O3-P-O2	2.40	115.38	107.91
2	J	201	PO4	O4-P-O2	2.29	115.03	107.91
2	A	201	PO4	O4-P-O3	-2.26	100.89	107.91
2	B	203	PO4	O3-P-O1	2.14	118.51	110.95

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 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	301	HEZ	1	0
2	B	203	PO4	1	0
3	G	202	HEZ	1	0
3	B	201	HEZ	4	0
3	A	202	HEZ	3	0
3	F	201	HEZ	3	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, 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	180/195 (92%)	-0.13	2 (1%) 78 86	9, 23, 39, 44	6 (3%)
1	B	177/195 (90%)	-0.32	2 (1%) 78 86	8, 19, 37, 59	6 (3%)
1	C	175/195 (89%)	-0.03	5 (2%) 53 63	8, 23, 39, 55	4 (2%)
1	D	180/195 (92%)	-0.49	0 100 100	6, 16, 26, 45	5 (2%)
1	E	180/195 (92%)	-0.39	0 100 100	7, 18, 29, 45	5 (2%)
1	F	175/195 (89%)	-0.07	3 (1%) 69 79	6, 23, 41, 49	4 (2%)
1	G	175/195 (89%)	-0.15	2 (1%) 78 86	8, 23, 39, 51	8 (4%)
1	H	175/195 (89%)	-0.03	5 (2%) 53 63	11, 25, 42, 51	5 (2%)
1	I	180/195 (92%)	-0.10	0 100 100	11, 25, 37, 48	4 (2%)
1	J	175/195 (89%)	0.10	7 (4%) 42 53	11, 27, 45, 58	5 (2%)
1	K	180/195 (92%)	-0.19	1 (0%) 85 91	9, 22, 33, 47	7 (3%)
1	L	175/195 (89%)	0.37	2 (1%) 78 86	11, 32, 49, 57	3 (1%)
All	All	2127/2340 (90%)	-0.12	29 (1%) 73 83	6, 23, 41, 59	62 (2%)

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	42	ALA	5.0
1	H	10	HIS	4.5
1	C	42	ALA	3.8
1	J	42	ALA	3.7
1	C	44[A]	VAL	3.6
1	L	169	VAL	3.6
1	J	138	PHE	2.9
1	K	10	HIS	2.6
1	J	10	HIS	2.5
1	H	42	ALA	2.4
1	B	41	ASP	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	L	10	HIS	2.3
1	B	42	ALA	2.3
1	J	109	THR	2.3
1	C	173	ASP	2.3
1	J	34	GLY	2.2
1	F	138	PHE	2.2
1	H	138	PHE	2.2
1	J	135	GLN	2.2
1	F	163	VAL	2.1
1	H	177	GLN	2.1
1	C	34	GLY	2.1
1	H	140	PHE	2.1
1	C	136	ILE	2.1
1	F	42	ALA	2.1
1	A	10	HIS	2.1
1	J	36	LYS	2.0
1	A	138	PHE	2.0
1	G	137	ILE	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	PO4	G	203	5/5	0.83	0.15	26,34,43,43	5
2	PO4	B	203	5/5	0.85	0.15	21,31,38,43	5
2	PO4	H	202	5/5	0.89	0.11	29,41,43,44	5
2	PO4	J	202	5/5	0.90	0.10	35,43,47,50	5
3	HEZ	D	301	8/8	0.90	0.12	21,31,33,35	6

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	HEZ	E	201	8/8	0.91	0.14	20,34,37,38	6
3	HEZ	F	201	8/8	0.91	0.10	39,41,42,43	5
3	HEZ	G	202	8/8	0.91	0.11	34,36,38,38	2
3	HEZ	B	201	8/8	0.92	0.10	40,42,47,50	2
2	PO4	I	202	5/5	0.92	0.10	29,32,39,41	5
3	HEZ	A	202	8/8	0.94	0.09	31,33,39,42	5
2	PO4	C	201	5/5	0.95	0.10	26,26,28,29	5
2	PO4	B	202	5/5	0.96	0.07	19,20,23,23	5
2	PO4	J	201	5/5	0.97	0.07	22,24,25,26	5
2	PO4	E	202	5/5	0.98	0.05	19,20,22,23	5
2	PO4	A	201	5/5	0.98	0.08	23,24,26,27	5
2	PO4	L	201	5/5	0.98	0.07	28,29,29,30	5
2	PO4	I	201	5/5	0.99	0.05	23,24,27,27	5
2	PO4	G	201	5/5	0.99	0.04	22,23,25,26	5
2	PO4	D	302	5/5	0.99	0.04	17,17,19,20	5
2	PO4	H	201	5/5	0.99	0.04	28,28,29,29	5
2	PO4	K	201	5/5	0.99	0.05	26,26,27,27	5
2	PO4	F	202	5/5	0.99	0.05	21,23,25,27	5

6.5 Other polymers [i](#)

There are no such residues in this entry.