



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 12:10 PM UTC

PDB ID : 1EHY / pdb_00001ehy
Title : X-ray structure of the epoxide hydrolase from agrobacterium radiobacter ad1
Authors : Nardini, M.; Ridder, I.S.; Rozeboom, H.J.; Kalk, K.H.; Rink, R.; Janssen, D.B.; Dijkstra, B.W.
Deposited on : 1998-10-17
Resolution : 2.10 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
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

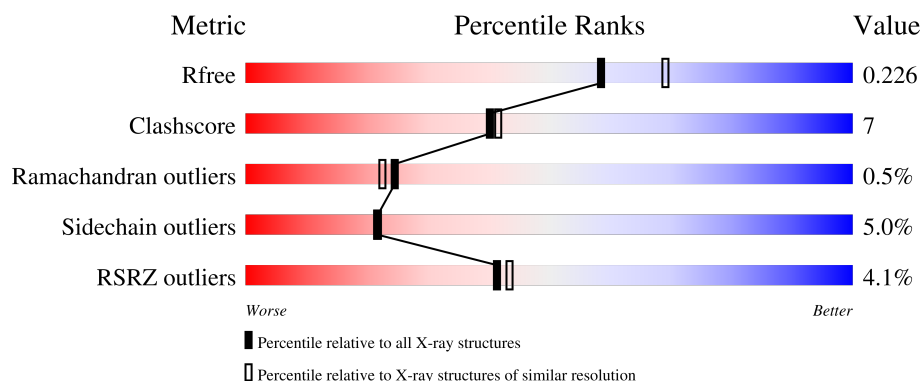
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

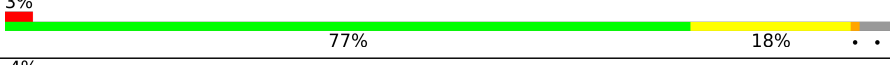
The reported resolution of this entry is 2.10 Å.

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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	294	
1	B	294	
1	C	294	
1	D	294	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9876 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 PROTEIN (SOLUBLE EPOXIDE HYDROLASE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	282	Total	C	N	O	S	0	0	0
			2317	1503	380	424	10			
1	B	282	Total	C	N	O	S	0	0	0
			2317	1503	380	424	10			
1	C	282	Total	C	N	O	S	0	0	0
			2311	1500	377	424	10			
1	D	282	Total	C	N	O	S	0	0	0
			2317	1503	380	424	10			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	ALA	THR	cloning artifact	UNP O31243
B	2	ALA	THR	cloning artifact	UNP O31243
C	2	ALA	THR	cloning artifact	UNP O31243
D	2	ALA	THR	cloning artifact	UNP O31243

- Molecule 2 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	K	0	0
			1	1		
2	B	1	Total	K	0	0
			1	1		
2	C	1	Total	K	0	0
			1	1		
2	D	1	Total	K	0	0
			1	1		

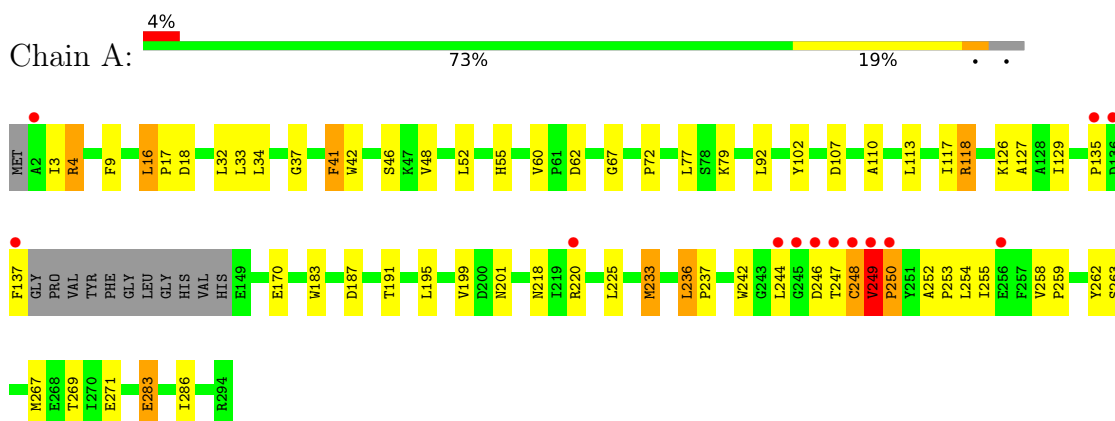
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	134	Total 138	O 138	0	4
3	B	154	Total 167	O 167	0	13
3	C	139	Total 147	O 147	0	8
3	D	150	Total 158	O 158	0	8

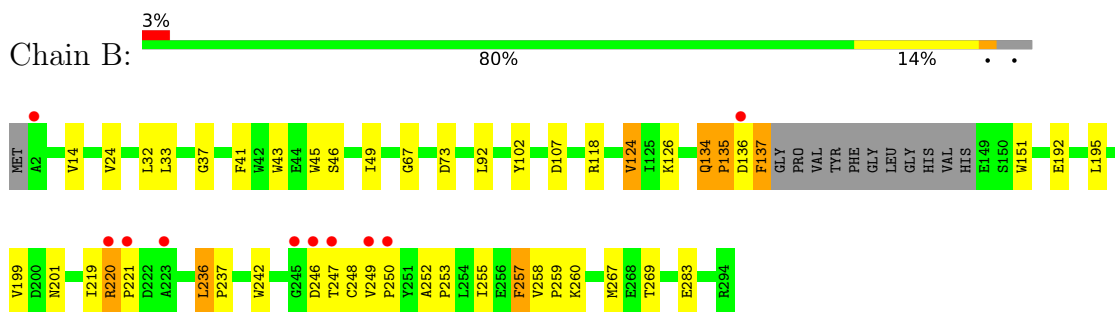
3 Residue-property plots [i](#)

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.

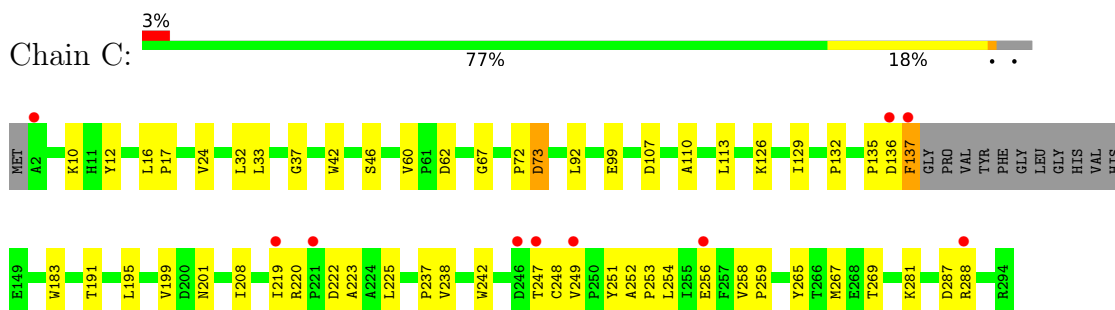
- Molecule 1: PROTEIN (SOLUBLE EPOXIDE HYDROLASE)



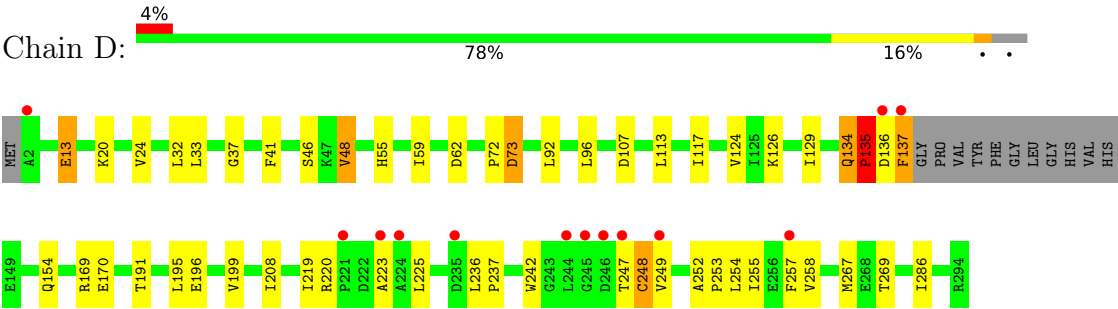
- Molecule 1: PROTEIN (SOLUBLE EPOXIDE HYDROLASE)



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4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	146.62Å 100.20Å 96.88Å 90.00° 100.68° 90.00°	Depositor
Resolution (Å)	25.00 – 2.10 25.00 – 2.10	Depositor EDS
% Data completeness (in resolution range)	91.5 (25.00-2.10) 85.5 (25.00-2.10)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.17 (at 2.10Å)	Xtriage
Refinement program	X-PLOR 3.843	Depositor
R, R_{free}	0.190 , 0.227 0.195 , 0.226	Depositor DCC
R_{free} test set	3757 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å ²)	23.4	Xtriage
Anisotropy	0.225	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 54.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	9876	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.46% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.57	2/2390 (0.1%)	0.96	9/3248 (0.3%)
1	B	0.53	0/2390	0.94	8/3248 (0.2%)
1	C	0.52	0/2384	0.96	8/3241 (0.2%)
1	D	0.53	0/2390	0.96	9/3248 (0.3%)
All	All	0.54	2/9554 (0.0%)	0.96	34/12985 (0.3%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	249	VAL	CA-C	7.86	1.61	1.52
1	A	248	CYS	C-N	6.46	1.40	1.33

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	249	VAL	O-C-N	-9.01	110.83	121.10
1	D	134	GLN	CA-C-N	7.75	129.52	119.84
1	D	134	GLN	C-N-CA	7.75	129.52	119.84
1	B	134	GLN	CA-C-N	6.67	128.18	119.84
1	B	134	GLN	C-N-CA	6.67	128.18	119.84
1	D	46	SER	N-CA-C	6.31	119.83	111.75
1	C	46	SER	N-CA-C	6.19	119.68	111.75
1	A	110	ALA	N-CA-C	-6.03	104.79	111.36
1	B	257	PHE	N-CA-C	6.01	120.34	112.89
1	D	191	THR	N-CA-C	-5.86	102.98	110.53
1	C	110	ALA	N-CA-C	-5.83	105.01	111.36
1	D	62	ASP	N-CA-C	-5.69	100.40	109.96
1	A	191	THR	N-CA-C	-5.67	103.22	110.53
1	B	220	ARG	CA-C-N	5.66	126.92	119.84
1	B	220	ARG	C-N-CA	5.66	126.92	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	250	PRO	O-C-N	-5.64	115.02	122.64
1	A	187	ASP	N-CA-C	5.61	117.40	111.28
1	D	249	VAL	CB-CA-C	-5.59	108.42	114.35
1	C	191	THR	N-CA-C	-5.54	103.38	110.53
1	A	16	LEU	N-CA-C	-5.50	102.99	110.36
1	C	249	VAL	N-CA-C	5.38	120.41	112.61
1	C	62	ASP	N-CA-C	-5.36	100.56	109.46
1	A	102	TYR	N-CA-C	-5.36	101.74	110.20
1	A	3	ILE	N-CA-C	5.27	116.38	109.21
1	C	251	TYR	N-CA-C	5.21	119.74	113.17
1	C	281	LYS	CA-C-N	5.21	124.66	119.24
1	C	281	LYS	C-N-CA	5.21	124.66	119.24
1	D	257	PHE	N-CA-C	5.20	118.78	112.23
1	A	46	SER	N-CA-C	5.20	118.41	111.75
1	B	102	TYR	N-CA-C	-5.18	102.01	110.20
1	B	43	TRP	N-CA-C	5.17	118.68	112.38
1	D	248	CYS	CA-C-N	5.14	123.48	120.24
1	D	248	CYS	C-N-CA	5.14	123.48	120.24
1	B	46	SER	N-CA-C	5.06	118.23	111.75

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	2317	0	2216	43	0
1	B	2317	0	2216	24	0
1	C	2311	0	2204	30	0
1	D	2317	0	2215	26	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	138	0	0	3	0
3	B	167	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	147	0	0	4	0
3	D	158	0	0	2	0
All	All	9876	0	8851	120	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 7.

All (120) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:135:PRO:HG2	1:C:183:TRP:CD1	2.05	0.91
1:D:220:ARG:HE	1:D:223:ALA:HB2	1.36	0.89
1:A:135:PRO:HG2	1:A:183:TRP:CD1	2.08	0.89
1:A:233:MET:HE1	1:A:263:SER:HB3	1.65	0.78
1:C:126:LYS:HG2	1:C:237:PRO:HG2	1.68	0.73
1:B:126:LYS:HG2	1:B:237:PRO:HG2	1.71	0.71
1:D:126:LYS:HG2	1:D:237:PRO:HG2	1.71	0.70
1:A:48:VAL:HG13	1:A:286:ILE:HG12	1.75	0.68
1:D:13:GLU:HG2	1:D:20:LYS:HE2	1.76	0.67
1:C:16:LEU:HB3	1:C:17:PRO:HD2	1.78	0.66
1:A:249:VAL:HG13	1:B:248:CYS:SG	2.36	0.65
1:A:126:LYS:HG2	1:A:237:PRO:HG2	1.79	0.65
1:C:135:PRO:HG2	1:C:183:TRP:CG	2.31	0.65
1:D:113:LEU:HD23	1:D:129:ILE:HD13	1.81	0.62
1:D:37:GLY:HA3	1:D:107:ASP:HB3	1.82	0.61
1:A:42:TRP:HB2	1:A:60:VAL:HG12	1.82	0.61
1:D:48:VAL:HG22	1:D:286:ILE:HG13	1.82	0.61
1:B:124:VAL:HG13	1:B:236:LEU:HD11	1.83	0.60
1:C:137:PHE:HZ	1:C:219:ILE:HG21	1.66	0.59
1:A:244:LEU:HD11	1:A:271:GLU:HG2	1.85	0.59
1:B:220:ARG:HG3	1:B:221:PRO:HD2	1.83	0.59
1:B:255:ILE:HA	1:B:267:MET:HE1	1.85	0.58
1:A:255:ILE:HA	1:A:267:MET:HE1	1.85	0.57
1:B:67:GLY:HA2	1:B:201:ASN:OD1	2.04	0.57
1:B:37:GLY:HA3	1:B:107:ASP:HB3	1.86	0.56
1:A:48:VAL:HG12	1:A:52:LEU:HD12	1.86	0.56
1:C:252:ALA:N	1:C:253:PRO:HD2	2.21	0.56
1:A:4:ARG:HD2	1:A:9:PHE:CE1	2.40	0.56
1:A:48:VAL:HG12	1:A:52:LEU:CD1	2.37	0.55
1:A:135:PRO:HG2	1:A:183:TRP:CG	2.40	0.55
1:A:244:LEU:CD1	1:A:271:GLU:OE2	2.53	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:242:TRP:HH2	1:C:267:MET:HE2	1.71	0.55
1:A:254:LEU:O	1:A:258:VAL:HG23	2.07	0.54
1:D:252:ALA:N	1:D:253:PRO:HD2	2.22	0.54
1:A:252:ALA:N	1:A:253:PRO:HD2	2.23	0.54
1:C:242:TRP:CH2	1:C:267:MET:HE2	2.43	0.54
1:C:67:GLY:HA2	1:C:201:ASN:OD1	2.08	0.53
1:A:248:CYS:O	1:A:249:VAL:HB	2.08	0.53
1:C:113:LEU:HD23	1:C:129:ILE:HD13	1.91	0.52
1:A:242:TRP:O	1:A:269:THR:HA	2.10	0.52
1:A:244:LEU:CD1	1:A:271:GLU:HG2	2.39	0.52
1:C:10:LYS:HE2	3:C:563:HOH:O	2.08	0.52
1:A:37:GLY:HA3	1:A:107:ASP:HB3	1.92	0.52
1:C:242:TRP:NE1	1:C:269:THR:HG22	2.25	0.51
1:D:137:PHE:HZ	1:D:219:ILE:HG21	1.76	0.50
1:D:59:ILE:HD13	1:D:96:LEU:HD12	1.93	0.50
1:A:283:GLU:H	1:A:283:GLU:CD	2.18	0.50
1:C:238:VAL:O	1:C:265:TYR:HA	2.13	0.49
1:B:252:ALA:N	1:B:253:PRO:HD2	2.27	0.48
1:B:126:LYS:HG2	1:B:237:PRO:CG	2.42	0.48
1:C:99:GLU:HG2	3:C:665[B]:HOH:O	2.13	0.48
1:A:170:GLU:HG3	3:A:388:HOH:O	2.11	0.48
1:A:247:THR:O	1:A:248:CYS:HB2	2.12	0.48
1:A:55:HIS:HB3	3:A:329:HOH:O	2.13	0.48
1:B:249:VAL:HB	1:B:250:PRO:HD3	1.95	0.48
1:A:233:MET:CE	1:A:263:SER:HB3	2.41	0.47
1:A:244:LEU:HD12	1:A:271:GLU:HA	1.95	0.47
1:C:208:ILE:HG12	3:C:546:HOH:O	2.14	0.47
1:B:283:GLU:H	1:B:283:GLU:CD	2.23	0.47
1:C:287:ASP:OD2	1:C:288:ARG:NH1	2.47	0.47
1:A:48:VAL:HG13	1:A:286:ILE:CG1	2.44	0.46
1:A:233:MET:HE1	1:A:263:SER:CB	2.41	0.46
1:D:247:THR:HG22	1:D:248:CYS:H	1.80	0.46
1:B:220:ARG:HG3	1:B:221:PRO:CD	2.45	0.46
1:D:255:ILE:HA	1:D:267:MET:HE1	1.96	0.46
1:C:37:GLY:HA3	1:C:107:ASP:HB3	1.97	0.46
1:B:137:PHE:HZ	1:B:219:ILE:HG21	1.81	0.46
1:A:67:GLY:HA2	1:A:201:ASN:OD1	2.15	0.46
1:C:254:LEU:O	1:C:258:VAL:HG23	2.16	0.46
1:B:151:TRP:HB3	1:D:154:GLN:OE1	2.16	0.45
1:D:258:VAL:HG21	1:D:267:MET:HE3	1.97	0.45
1:D:134:GLN:O	1:D:137:PHE:HB2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:42:TRP:HB2	1:C:60:VAL:HG12	1.98	0.45
1:D:254:LEU:O	1:D:258:VAL:HG23	2.16	0.45
1:B:45:TRP:O	1:B:49:ILE:HG13	2.17	0.44
1:C:12:TYR:HB3	3:C:613:HOH:O	2.16	0.44
1:A:258:VAL:N	1:A:259:PRO:HD2	2.31	0.44
1:D:208:ILE:HG12	3:D:338:HOH:O	2.17	0.44
1:D:48:VAL:HG22	1:D:286:ILE:CG1	2.48	0.44
1:A:218:ASN:HB3	1:A:225:LEU:HD13	2.00	0.43
1:C:137:PHE:CZ	1:C:219:ILE:HG21	2.51	0.43
1:A:233:MET:HB3	1:A:233:MET:HE3	1.70	0.43
1:D:195:LEU:O	1:D:199:VAL:HG23	2.18	0.43
1:B:257:PHE:HD1	1:B:260:LYS:HD2	1.83	0.43
1:C:247:THR:OG1	1:C:248:CYS:N	2.51	0.43
1:A:236:LEU:HD22	1:A:237:PRO:HD2	2.01	0.43
1:A:72:PRO:HB3	1:A:79:LYS:HD3	2.00	0.43
1:A:195:LEU:O	1:A:199:VAL:HG23	2.18	0.43
1:B:195:LEU:O	1:B:199:VAL:HG23	2.18	0.43
1:C:72:PRO:O	1:C:73:ASP:C	2.62	0.43
1:B:246:ASP:O	1:B:247:THR:HG23	2.19	0.42
1:C:220:ARG:HB2	1:C:223:ALA:HB2	2.00	0.42
1:C:258:VAL:N	1:C:259:PRO:HD2	2.34	0.42
1:D:55:HIS:HB3	3:D:330:HOH:O	2.18	0.42
1:A:250:PRO:HA	3:A:376:HOH:O	2.18	0.42
1:A:113:LEU:HD12	1:A:117:ILE:HG23	2.02	0.42
1:A:113:LEU:HD21	1:A:127:ALA:HB1	2.01	0.42
1:A:117:ILE:HD11	1:A:118:ARG:NH2	2.35	0.42
1:A:242:TRP:CH2	1:A:267:MET:HE2	2.55	0.42
1:C:195:LEU:O	1:C:199:VAL:HG23	2.19	0.41
1:D:13:GLU:CG	1:D:20:LYS:HE2	2.48	0.41
1:B:242:TRP:NE1	1:B:269:THR:HG22	2.34	0.41
1:C:129:ILE:HG22	1:C:132:PRO:HD3	2.02	0.41
1:D:242:TRP:NE1	1:D:269:THR:HG22	2.36	0.41
1:A:34:LEU:HB2	1:A:60:VAL:HG22	2.02	0.41
1:B:134:GLN:HA	1:B:135:PRO:HD3	1.89	0.41
1:C:220:ARG:H	1:C:223:ALA:HB2	1.85	0.41
1:A:41:PHE:HB2	1:A:62:ASP:OD1	2.20	0.41
1:B:258:VAL:N	1:B:259:PRO:HD2	2.36	0.41
1:D:134:GLN:HA	1:D:135:PRO:HD3	1.89	0.41
1:B:258:VAL:HG21	1:B:267:MET:HE3	2.01	0.41
1:D:72:PRO:O	1:D:73:ASP:C	2.64	0.41
1:A:118:ARG:NH2	1:A:262:TYR:OH	2.53	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:13:GLU:HG2	1:D:20:LYS:CE	2.49	0.40
1:A:16:LEU:HB3	1:A:17:PRO:HD2	2.03	0.40
1:B:257:PHE:CE1	1:C:222:ASP:HB3	2.56	0.40
1:D:113:LEU:HD12	1:D:117:ILE:HG23	2.03	0.40
1:B:124:VAL:HG22	1:B:236:LEU:HD21	2.04	0.40
1:C:288:ARG:HA	1:C:288:ARG:HD3	1.86	0.40
1:D:169:ARG:NH2	1:D:196:GLU:OE1	2.48	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	278/294 (95%)	264 (95%)	13 (5%)	1 (0%)	30	28
1	B	278/294 (95%)	265 (95%)	11 (4%)	2 (1%)	18	15
1	C	278/294 (95%)	265 (95%)	12 (4%)	1 (0%)	30	28
1	D	278/294 (95%)	266 (96%)	10 (4%)	2 (1%)	18	15
All	All	1112/1176 (95%)	1060 (95%)	46 (4%)	6 (0%)	24	22

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	249	VAL
1	D	135	PRO
1	B	73	ASP
1	C	73	ASP
1	D	73	ASP
1	B	135	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	247/256 (96%)	232 (94%)	15 (6%)	17	15
1	B	247/256 (96%)	235 (95%)	12 (5%)	22	22
1	C	246/256 (96%)	238 (97%)	8 (3%)	33	37
1	D	247/256 (96%)	233 (94%)	14 (6%)	18	17
All	All	987/1024 (96%)	938 (95%)	49 (5%)	22	22

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ARG
1	A	18	ASP
1	A	32	LEU
1	A	33	LEU
1	A	41	PHE
1	A	77	LEU
1	A	92	LEU
1	A	118	ARG
1	A	129	ILE
1	A	137	PHE
1	A	220	ARG
1	A	233	MET
1	A	236	LEU
1	A	246	ASP
1	A	283	GLU
1	B	14	VAL
1	B	24	VAL
1	B	32	LEU
1	B	33	LEU
1	B	41	PHE
1	B	92	LEU
1	B	118	ARG
1	B	124	VAL
1	B	136	ASP

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Mol	Chain	Res	Type
1	B	137	PHE
1	B	192	GLU
1	B	236	LEU
1	C	24	VAL
1	C	32	LEU
1	C	33	LEU
1	C	92	LEU
1	C	136	ASP
1	C	137	PHE
1	C	225	LEU
1	C	256	GLU
1	D	13	GLU
1	D	24	VAL
1	D	32	LEU
1	D	33	LEU
1	D	41	PHE
1	D	48	VAL
1	D	92	LEU
1	D	124	VAL
1	D	135	PRO
1	D	136	ASP
1	D	137	PHE
1	D	170	GLU
1	D	225	LEU
1	D	236	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	89	GLN
1	A	154	GLN
1	B	89	GLN
1	C	55	HIS
1	C	89	GLN
1	D	89	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](#)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	282/294 (95%)	0.02	13 (4%) 37 39	16, 28, 54, 74	0
1	B	282/294 (95%)	-0.29	10 (3%) 47 49	12, 22, 48, 66	0
1	C	282/294 (95%)	-0.13	10 (3%) 47 49	14, 25, 55, 71	0
1	D	282/294 (95%)	-0.17	13 (4%) 37 39	12, 23, 53, 68	0
All	All	1128/1176 (95%)	-0.14	46 (4%) 41 43	12, 25, 54, 74	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	246	ASP	5.2
1	A	249	VAL	4.9
1	A	247	THR	4.5
1	C	2	ALA	3.7
1	D	2	ALA	3.5
1	A	2	ALA	3.4
1	B	136	ASP	3.2
1	D	136	ASP	3.2
1	A	250	PRO	3.2
1	C	288	ARG	3.1
1	B	247	THR	3.1
1	A	248	CYS	3.0
1	A	245	GLY	3.0
1	A	137	PHE	3.0
1	C	137	PHE	2.8
1	D	247	THR	2.8
1	B	2	ALA	2.7
1	A	256	GLU	2.6
1	B	250	PRO	2.6
1	C	136	ASP	2.6
1	C	249	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	137	PHE	2.5
1	C	219	ILE	2.5
1	B	221	PRO	2.4
1	D	221	PRO	2.4
1	C	247	THR	2.4
1	C	221	PRO	2.4
1	C	246	ASP	2.3
1	B	223	ALA	2.3
1	D	244	LEU	2.3
1	D	224	ALA	2.3
1	B	245	GLY	2.3
1	A	135	PRO	2.2
1	D	235	ASP	2.2
1	D	245	GLY	2.2
1	D	257	PHE	2.2
1	C	256	GLU	2.2
1	D	223	ALA	2.2
1	A	220	ARG	2.2
1	B	246	ASP	2.2
1	B	249	VAL	2.1
1	B	220	ARG	2.1
1	D	246	ASP	2.1
1	A	136	ASP	2.1
1	D	249	VAL	2.1
1	A	244	LEU	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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($\text{\AA}^2$)	Q<0.9
2	K	B	296	1/1	0.95	0.05	29,29,29,29	0
2	K	C	297	1/1	0.95	0.06	33,33,33,33	0
2	K	A	295	1/1	0.96	0.09	36,36,36,36	0
2	K	D	298	1/1	0.96	0.05	33,33,33,33	0

6.5 Other polymers [i](#)

There are no such residues in this entry.