



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 10:33 PM UTC

PDB ID : 3EJX / pdb_00003ejx
Title : Crystal structure of diaminopimelate epimerase from Arabidopsis thaliana in complex with LL-AziDAP
Authors : Pillai, B.; Moorthie, V.A.; Cherney, M.M.; Vederas, J.C.; James, M.N.G.
Deposited on : 2008-09-18
Resolution : 1.95 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

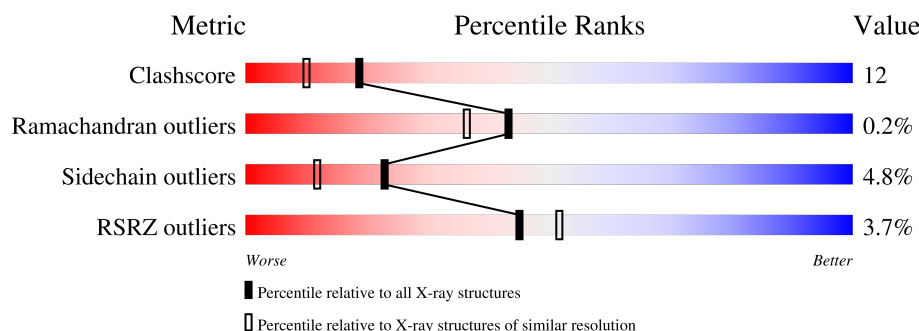
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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))
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

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	317	0% 73% 15% • 9%
1	B	317	2% 73% 15% • 9%
1	C	317	2% 73% 15% • 9%
1	D	317	4% 77% 17% • 5%
1	E	317	3% 72% 17% • 9%
1	F	317	9% 74% 17% • 5%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 15115 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 Diaminopimelate epimerase, chloroplastic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	287	Total	C	N	O	S	0	0	0
			2169	1363	377	413	16			
1	B	288	Total	C	N	O	S	0	0	0
			2179	1369	380	414	16			
1	C	287	Total	C	N	O	S	0	0	0
			2169	1363	377	413	16			
1	D	301	Total	C	N	O	S	6	0	0
			2273	1430	393	434	16			
1	E	287	Total	C	N	O	S	0	0	0
			2169	1363	377	413	16			
1	F	301	Total	C	N	O	S	6	0	0
			2273	1430	393	434	16			

There are 36 discrepancies between the modelled and reference sequences:

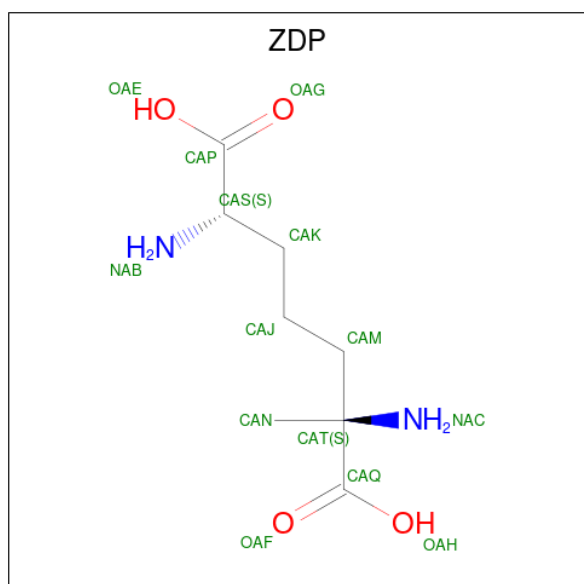
Chain	Residue	Modelled	Actual	Comment	Reference
A	312	HIS	-	expression tag	UNP Q9LFG2
A	313	HIS	-	expression tag	UNP Q9LFG2
A	314	HIS	-	expression tag	UNP Q9LFG2
A	315	HIS	-	expression tag	UNP Q9LFG2
A	316	HIS	-	expression tag	UNP Q9LFG2
A	317	HIS	-	expression tag	UNP Q9LFG2
B	312	HIS	-	expression tag	UNP Q9LFG2
B	313	HIS	-	expression tag	UNP Q9LFG2
B	314	HIS	-	expression tag	UNP Q9LFG2
B	315	HIS	-	expression tag	UNP Q9LFG2
B	316	HIS	-	expression tag	UNP Q9LFG2
B	317	HIS	-	expression tag	UNP Q9LFG2
C	312	HIS	-	expression tag	UNP Q9LFG2
C	313	HIS	-	expression tag	UNP Q9LFG2
C	314	HIS	-	expression tag	UNP Q9LFG2
C	315	HIS	-	expression tag	UNP Q9LFG2
C	316	HIS	-	expression tag	UNP Q9LFG2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	317	HIS	-	expression tag	UNP Q9LFG2
D	312	HIS	-	expression tag	UNP Q9LFG2
D	313	HIS	-	expression tag	UNP Q9LFG2
D	314	HIS	-	expression tag	UNP Q9LFG2
D	315	HIS	-	expression tag	UNP Q9LFG2
D	316	HIS	-	expression tag	UNP Q9LFG2
D	317	HIS	-	expression tag	UNP Q9LFG2
E	312	HIS	-	expression tag	UNP Q9LFG2
E	313	HIS	-	expression tag	UNP Q9LFG2
E	314	HIS	-	expression tag	UNP Q9LFG2
E	315	HIS	-	expression tag	UNP Q9LFG2
E	316	HIS	-	expression tag	UNP Q9LFG2
E	317	HIS	-	expression tag	UNP Q9LFG2
F	312	HIS	-	expression tag	UNP Q9LFG2
F	313	HIS	-	expression tag	UNP Q9LFG2
F	314	HIS	-	expression tag	UNP Q9LFG2
F	315	HIS	-	expression tag	UNP Q9LFG2
F	316	HIS	-	expression tag	UNP Q9LFG2
F	317	HIS	-	expression tag	UNP Q9LFG2

- Molecule 2 is (2S,6S)-2,6-DIAMINO-2-METHYLHEPTANEDIOIC ACID (CCD ID: ZDP) (formula: $C_8H_{16}N_2O_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	2	4		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	N	O	0	0
			14	8	2	4		
2	C	1	Total	C	N	O	0	0
			14	8	2	4		
2	D	1	Total	C	N	O	0	0
			14	8	2	4		
2	E	1	Total	C	N	O	0	0
			14	8	2	4		
2	F	1	Total	C	N	O	0	0
			14	8	2	4		

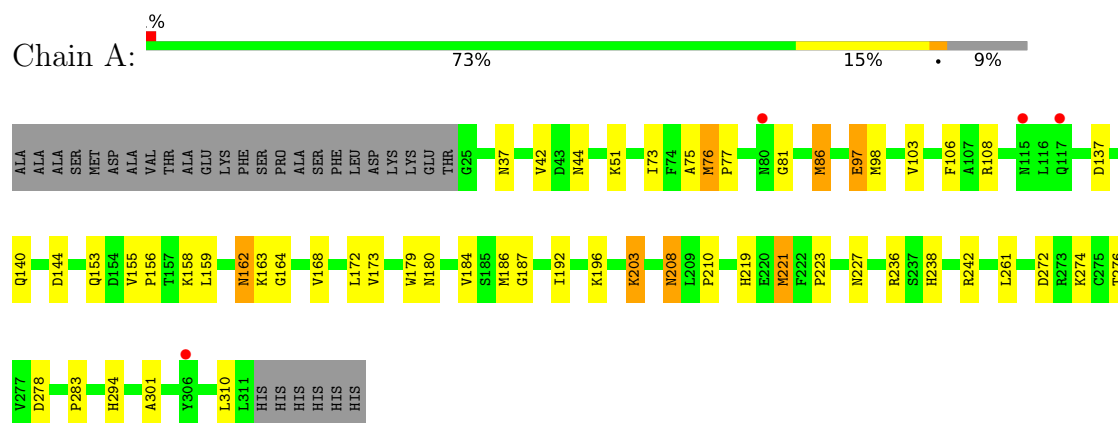
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	339	Total	O	0	0
			339	339		
3	B	338	Total	O	0	0
			338	338		
3	C	317	Total	O	0	0
			317	317		
3	D	280	Total	O	0	0
			280	280		
3	E	293	Total	O	0	0
			293	293		
3	F	232	Total	O	0	0
			232	232		

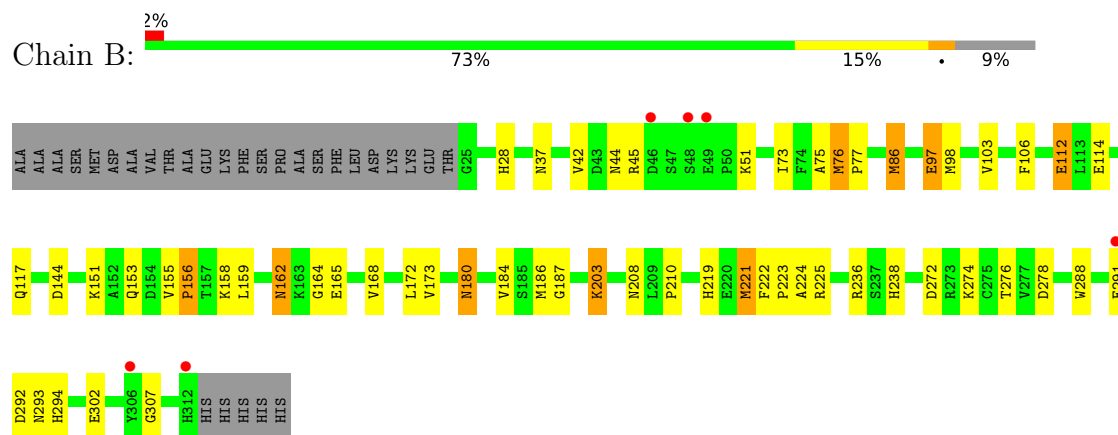
3 Residue-property plots [i](#)

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.

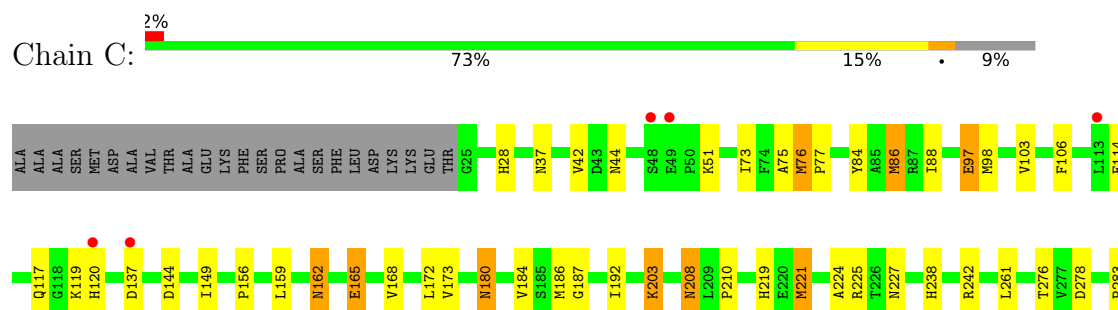
- Molecule 1: Diaminopimelate epimerase, chloroplastic



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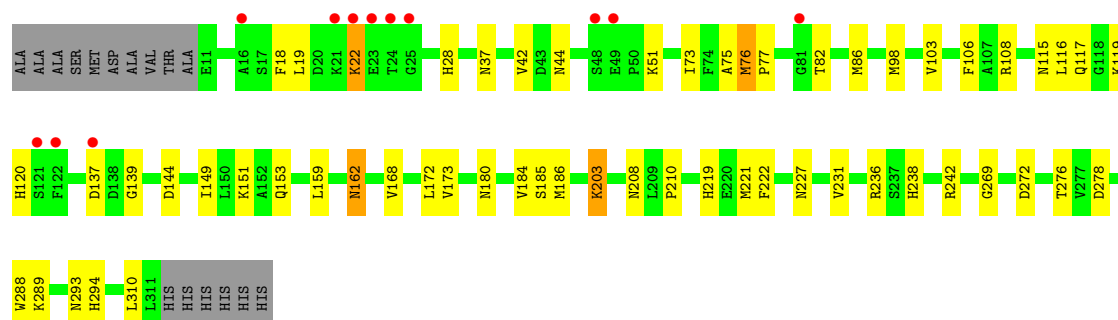
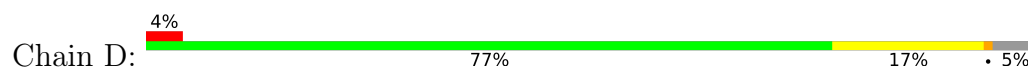


- Molecule 1: Diaminopimelate epimerase, chloroplastic

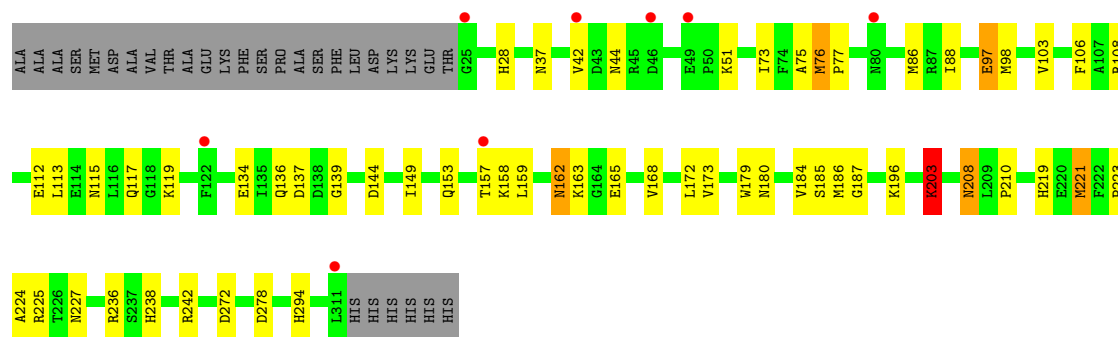




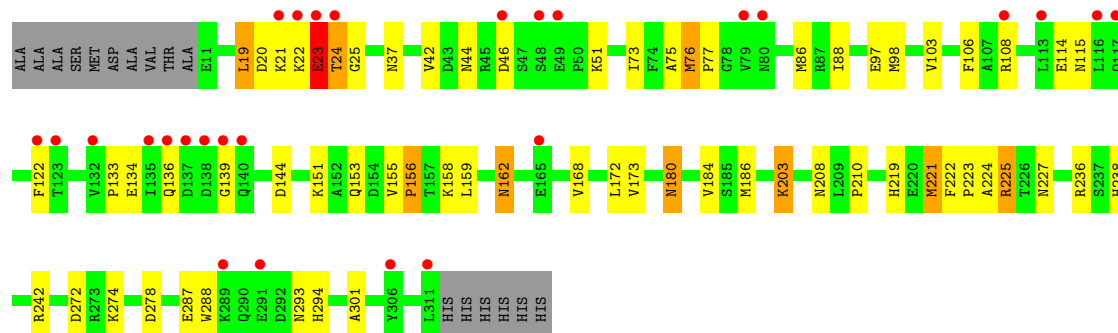
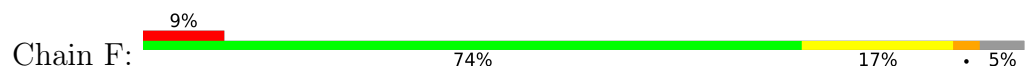
- Molecule 1: Diaminopimelate epimerase, chloroplastic



- Molecule 1: Diaminopimelate epimerase, chloroplastic



- Molecule 1: Diaminopimelate epimerase, chloroplastic



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	102.54Å 136.44Å 102.57Å 90.00° 119.54° 90.00°	Depositor
Resolution (Å)	50.00 – 1.95 50.00 – 1.95	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-1.95) 98.0 (50.00-1.95)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.46 (at 1.95Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.179 , 0.208 0.189 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	23.8	Xtriage
Anisotropy	0.250	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 50.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.001 for -h-l,k,h 0.001 for l,k,-h-l 0.014 for h,-k,-h-l 0.013 for -h-l,-k,l 0.014 for l,-k,h	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	15115	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.18% 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: ZDP

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	0.69	2/2214 (0.1%)	1.00	7/2998 (0.2%)
1	B	0.68	2/2225 (0.1%)	0.99	8/3013 (0.3%)
1	C	0.67	2/2214 (0.1%)	1.00	5/2998 (0.2%)
1	D	0.63	0/2321	0.98	8/3141 (0.3%)
1	E	0.64	1/2214 (0.0%)	0.98	4/2998 (0.1%)
1	F	0.58	1/2321 (0.0%)	1.00	10/3141 (0.3%)
All	All	0.65	8/13509 (0.1%)	0.99	42/18289 (0.2%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	221	MET	SD-CE	-8.39	1.58	1.79
1	A	221	MET	SD-CE	-7.89	1.59	1.79
1	C	221	MET	SD-CE	-7.28	1.61	1.79
1	E	221	MET	SD-CE	-6.58	1.63	1.79
1	C	86	MET	SD-CE	-6.51	1.63	1.79
1	B	86	MET	SD-CE	-5.61	1.65	1.79
1	A	86	MET	SD-CE	-5.18	1.66	1.79
1	F	221	MET	SD-CE	-5.03	1.67	1.79

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	225	ARG	NE-CZ-NH2	7.39	125.85	119.20
1	F	25	GLY	N-CA-C	7.33	122.92	112.81
1	F	225	ARG	NE-CZ-NH1	-7.03	114.47	121.50
1	F	186	MET	N-CA-C	-6.87	102.19	111.87
1	D	186	MET	N-CA-C	-6.76	102.34	111.87
1	C	186	MET	N-CA-C	-6.61	102.55	111.87
1	B	186	MET	N-CA-C	-6.54	101.95	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	23	GLU	N-CA-C	6.51	124.67	110.80
1	E	186	MET	N-CA-C	-6.40	102.15	111.30
1	A	186	MET	N-CA-C	-6.38	102.18	111.30
1	C	37	ASN	N-CA-C	-6.35	97.31	108.23
1	A	37	ASN	N-CA-C	-6.20	97.56	108.23
1	B	276	THR	N-CA-C	-6.01	99.44	109.24
1	E	37	ASN	N-CA-C	-5.91	98.07	108.23
1	A	276	THR	N-CA-C	-5.85	99.70	109.24
1	A	164	GLY	N-CA-C	-5.78	100.23	110.86
1	D	227	ASN	N-CA-C	-5.74	101.19	110.32
1	B	164	GLY	N-CA-C	-5.74	101.60	111.47
1	D	276	THR	N-CA-C	-5.68	99.98	109.24
1	B	37	ASN	N-CA-C	-5.65	98.51	108.23
1	B	222	PHE	CA-C-N	5.62	125.73	119.32
1	B	222	PHE	C-N-CA	5.62	125.73	119.32
1	D	37	ASN	N-CA-C	-5.56	98.21	107.99
1	B	203	LYS	N-CA-C	-5.54	96.22	107.41
1	E	227	ASN	N-CA-C	-5.51	101.55	110.32
1	F	37	ASN	N-CA-C	-5.48	98.81	108.23
1	E	203	LYS	N-CA-C	-5.45	96.40	107.41
1	F	203	LYS	N-CA-C	-5.45	96.40	107.41
1	D	203	LYS	N-CA-C	-5.43	96.44	107.41
1	F	227	ASN	N-CA-C	-5.39	101.75	110.32
1	C	203	LYS	N-CA-C	-5.29	96.73	107.41
1	C	227	ASN	N-CA-C	-5.28	101.93	110.32
1	A	203	LYS	N-CA-C	-5.24	96.83	107.41
1	B	307	GLY	N-CA-C	5.20	120.53	110.66
1	F	222	PHE	CA-C-N	5.19	125.49	119.47
1	F	222	PHE	C-N-CA	5.19	125.49	119.47
1	A	227	ASN	N-CA-C	-5.18	102.08	110.32
1	A	81	GLY	N-CA-C	5.18	121.65	114.92
1	D	231	VAL	N-CA-C	5.12	115.86	108.48
1	C	276	THR	N-CA-C	-5.05	101.02	109.24
1	D	222	PHE	CA-C-N	5.01	125.28	119.47
1	D	222	PHE	C-N-CA	5.01	125.28	119.47

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	2169	0	2121	50	0
1	B	2179	0	2128	54	0
1	C	2169	0	2121	52	0
1	D	2273	0	2217	59	0
1	E	2169	0	2121	51	0
1	F	2273	0	2217	53	0
2	A	14	0	13	0	0
2	B	14	0	13	0	0
2	C	14	0	13	0	0
2	D	14	0	13	0	0
2	E	14	0	13	0	0
2	F	14	0	13	0	0
3	A	339	0	0	8	0
3	B	338	0	0	6	0
3	C	317	0	0	7	0
3	D	280	0	0	7	0
3	E	293	0	0	3	0
3	F	232	0	0	4	0
All	All	15115	0	13003	312	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 12.

All (312) 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:E:162:ASN:HD21	1:E:168:VAL:H	1.09	0.99
1:E:157:THR:HG22	1:E:159:LEU:H	1.31	0.96
1:A:162:ASN:HD21	1:A:168:VAL:H	1.12	0.95
1:F:162:ASN:HD21	1:F:168:VAL:H	1.07	0.94
1:C:73:ILE:HG21	1:C:86:MET:HE2	1.50	0.94
1:C:162:ASN:HD21	1:C:168:VAL:H	1.08	0.92
1:E:219:HIS:HD2	1:E:221:MET:H	1.16	0.91
1:C:219:HIS:HD2	1:C:221:MET:H	1.19	0.90
1:D:219:HIS:HD2	1:D:221:MET:H	1.19	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:219:HIS:HD2	1:F:221:MET:H	1.21	0.87
1:A:73:ILE:HG21	1:A:86:MET:HE2	1.54	0.87
1:B:162:ASN:HD21	1:B:168:VAL:H	1.18	0.87
1:A:219:HIS:HD2	1:A:221:MET:H	1.20	0.87
1:B:219:HIS:HD2	1:B:221:MET:H	1.18	0.86
1:D:162:ASN:HD21	1:D:168:VAL:H	1.19	0.85
1:B:73:ILE:HG21	1:B:86:MET:HE2	1.59	0.84
1:F:73:ILE:HG21	1:F:86:MET:HE2	1.60	0.84
1:D:73:ILE:HG21	1:D:86:MET:HE2	1.61	0.83
1:E:73:ILE:HG21	1:E:86:MET:HE2	1.61	0.82
1:A:86:MET:HE3	1:A:106:PHE:CD2	2.15	0.81
1:B:291:GLU:CD	1:B:291:GLU:H	1.87	0.81
1:F:162:ASN:HD22	1:F:162:ASN:H	1.26	0.80
1:E:162:ASN:HD22	1:E:162:ASN:H	1.27	0.80
1:C:162:ASN:HD22	1:C:162:ASN:H	1.30	0.78
1:C:159:LEU:HD23	1:C:221:MET:HE2	1.65	0.78
1:D:86:MET:HE3	1:D:106:PHE:CD2	2.18	0.78
1:E:86:MET:HE3	1:E:106:PHE:CD2	2.18	0.78
1:A:162:ASN:HD22	1:A:162:ASN:H	1.33	0.77
1:F:44:ASN:HD21	1:F:51:LYS:H	1.29	0.77
1:C:86:MET:HE3	1:C:106:PHE:CD2	2.20	0.76
1:C:44:ASN:HD21	1:C:51:LYS:H	1.34	0.76
1:B:158:LYS:HE3	1:B:223:PRO:HG3	1.66	0.75
1:C:73:ILE:CG2	1:C:86:MET:HE2	2.16	0.75
1:D:159:LEU:HD23	1:D:221:MET:HE2	1.68	0.75
1:A:73:ILE:CG2	1:A:86:MET:HE2	2.18	0.74
1:F:86:MET:HE3	1:F:106:PHE:CD2	2.22	0.74
1:B:44:ASN:HD21	1:B:51:LYS:H	1.37	0.72
1:D:44:ASN:HD21	1:D:51:LYS:H	1.37	0.72
1:B:159:LEU:HD23	1:B:221:MET:HE2	1.72	0.72
1:A:44:ASN:HD21	1:A:51:LYS:H	1.37	0.72
1:A:137:ASP:HB3	1:C:28:HIS:CD2	2.25	0.72
1:B:162:ASN:H	1:B:162:ASN:HD22	1.36	0.71
1:A:153:GLN:HG2	3:A:803:HOH:O	1.92	0.70
1:E:44:ASN:HD21	1:E:51:LYS:H	1.37	0.69
1:F:158:LYS:HE3	1:F:223:PRO:HG3	1.74	0.69
1:A:159:LEU:HD23	1:A:221:MET:HE2	1.73	0.69
1:B:73:ILE:CG2	1:B:86:MET:HE2	2.21	0.69
1:B:86:MET:HE3	1:B:106:PHE:CD2	2.28	0.69
1:C:144:ASP:OD1	1:C:294:HIS:HD2	1.76	0.69
1:F:44:ASN:HD21	1:F:51:LYS:N	1.90	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:242:ARG:HD3	3:C:984:HOH:O	1.92	0.68
1:C:162:ASN:ND2	1:C:168:VAL:H	1.89	0.68
1:A:76:MET:HE2	3:A:796:HOH:O	1.94	0.67
1:F:108:ARG:HD2	1:F:301:ALA:HB3	1.74	0.67
1:D:162:ASN:H	1:D:162:ASN:HD22	1.43	0.67
1:D:219:HIS:CD2	1:D:221:MET:H	2.09	0.66
1:E:73:ILE:CG2	1:E:86:MET:HE2	2.26	0.66
1:E:219:HIS:CD2	1:E:221:MET:H	2.07	0.66
1:D:73:ILE:CG2	1:D:86:MET:HE2	2.26	0.65
1:A:219:HIS:CD2	1:A:221:MET:H	2.10	0.65
1:D:151:LYS:HE2	1:D:153:GLN:HE21	1.62	0.65
1:B:151:LYS:HE2	1:B:153:GLN:HE21	1.62	0.65
1:A:158:LYS:HE3	1:A:223:PRO:HG3	1.79	0.64
1:D:28:HIS:CE1	1:F:22:LYS:HD2	2.33	0.64
1:E:242:ARG:HD3	3:E:831:HOH:O	1.97	0.64
1:F:44:ASN:ND2	1:F:51:LYS:H	1.94	0.64
1:A:173:VAL:O	1:A:219:HIS:HE1	1.80	0.64
1:D:151:LYS:HE2	1:D:153:GLN:NE2	2.13	0.64
1:F:159:LEU:HD23	1:F:221:MET:HE2	1.79	0.64
1:E:162:ASN:HD22	1:E:162:ASN:N	1.96	0.63
1:E:144:ASP:OD1	1:E:294:HIS:HD2	1.81	0.63
1:F:173:VAL:O	1:F:219:HIS:HE1	1.81	0.63
1:B:219:HIS:CD2	1:B:221:MET:H	2.08	0.63
1:B:112:GLU:HG2	3:B:796:HOH:O	1.99	0.62
1:B:173:VAL:O	1:B:219:HIS:HE1	1.82	0.62
1:C:173:VAL:O	1:C:219:HIS:HE1	1.81	0.62
1:C:162:ASN:HD22	1:C:162:ASN:N	1.96	0.62
1:F:151:LYS:HE2	1:F:153:GLN:HG2	1.82	0.62
1:F:44:ASN:ND2	1:F:51:LYS:HG3	2.15	0.62
1:B:144:ASP:OD1	1:B:294:HIS:HD2	1.83	0.62
1:D:159:LEU:HD23	1:D:221:MET:CE	2.31	0.61
1:D:162:ASN:ND2	1:D:168:VAL:H	1.96	0.61
1:D:242:ARG:HD3	3:D:691:HOH:O	2.00	0.61
1:D:242:ARG:HD2	3:D:707:HOH:O	1.99	0.61
1:F:108:ARG:NH1	1:F:139:GLY:O	2.32	0.61
1:B:45:ARG:NH1	1:B:114:GLU:OE1	2.34	0.61
1:A:162:ASN:HD22	1:A:162:ASN:N	1.99	0.61
1:B:291:GLU:CD	1:B:291:GLU:N	2.57	0.61
1:D:44:ASN:HD21	1:D:51:LYS:N	1.98	0.61
1:B:159:LEU:HD23	1:B:221:MET:CE	2.31	0.61
1:C:44:ASN:HD21	1:C:51:LYS:N	1.99	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:86:MET:HE3	1:E:106:PHE:HB2	1.82	0.61
1:F:219:HIS:CD2	1:F:221:MET:H	2.11	0.61
1:A:44:ASN:ND2	1:A:51:LYS:HG3	2.16	0.60
1:F:144:ASP:OD1	1:F:294:HIS:HD2	1.85	0.60
1:D:19:LEU:HD12	1:E:113:LEU:HD21	1.84	0.60
1:E:44:ASN:HD21	1:E:51:LYS:N	2.00	0.59
1:F:23:GLU:O	1:F:24:THR:O	2.20	0.59
1:E:153:GLN:CD	1:E:153:GLN:H	2.10	0.59
1:A:44:ASN:HD21	1:A:51:LYS:N	2.00	0.59
1:B:302:GLU:HG3	3:B:780:HOH:O	2.02	0.59
1:A:86:MET:HE3	1:A:106:PHE:HB2	1.84	0.59
1:B:51:LYS:NZ	3:B:505:HOH:O	2.36	0.58
1:C:159:LEU:HD23	1:C:221:MET:CE	2.32	0.58
1:C:242:ARG:HD2	3:C:934:HOH:O	2.04	0.58
1:E:242:ARG:HD2	3:E:830:HOH:O	2.04	0.58
1:B:28:HIS:CD2	1:C:137:ASP:HB3	2.38	0.58
1:F:46:ASP:HB2	3:F:911:HOH:O	2.03	0.58
1:B:44:ASN:HD21	1:B:51:LYS:N	2.01	0.58
1:E:119:LYS:HE3	1:E:137:ASP:OD2	2.04	0.58
1:E:173:VAL:O	1:E:219:HIS:HE1	1.87	0.58
1:F:159:LEU:HD23	1:F:221:MET:CE	2.34	0.58
1:D:22:LYS:NZ	1:D:22:LYS:HB3	2.18	0.57
1:A:242:ARG:HD2	3:A:782:HOH:O	2.03	0.57
1:C:149:ILE:HD13	3:C:973:HOH:O	2.04	0.57
1:D:144:ASP:OD1	1:D:294:HIS:HD2	1.87	0.57
1:E:238:HIS:HE1	1:E:278:ASP:OD2	1.88	0.57
1:C:219:HIS:CD2	1:C:221:MET:H	2.10	0.57
1:B:151:LYS:HE3	1:B:165:GLU:HG2	1.87	0.56
1:D:115:ASN:ND2	1:D:117:GLN:OE1	2.38	0.56
1:D:18:PHE:CZ	1:D:22:LYS:HD2	2.41	0.56
1:D:86:MET:HE3	1:D:106:PHE:HB2	1.87	0.56
1:B:86:MET:HE3	1:B:106:PHE:HB2	1.88	0.56
1:D:44:ASN:ND2	1:D:51:LYS:H	2.03	0.56
1:C:86:MET:HE3	1:C:106:PHE:HD2	1.71	0.55
1:F:134:GLU:HG2	1:F:136:GLN:NE2	2.21	0.55
1:C:86:MET:HE3	1:C:106:PHE:HB2	1.88	0.55
1:D:173:VAL:O	1:D:219:HIS:HE1	1.90	0.55
1:C:76:MET:HB3	1:C:77:PRO:HD2	1.87	0.55
1:E:44:ASN:ND2	1:E:51:LYS:H	2.04	0.55
1:F:76:MET:HB3	1:F:77:PRO:HD2	1.88	0.55
1:F:73:ILE:CG2	1:F:86:MET:HE2	2.32	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:76:MET:HB3	1:D:77:PRO:HD2	1.88	0.55
1:A:86:MET:HE3	1:A:106:PHE:HD2	1.67	0.55
1:D:288:TRP:HE1	1:D:293:ASN:ND2	2.05	0.55
1:A:144:ASP:OD1	1:A:294:HIS:HD2	1.89	0.55
1:E:159:LEU:HD23	1:E:221:MET:HE2	1.89	0.54
1:F:225:ARG:HD3	3:F:854:HOH:O	2.07	0.54
1:B:44:ASN:ND2	1:B:51:LYS:H	2.04	0.54
1:C:208:ASN:HD22	1:C:210:PRO:HD2	1.73	0.54
1:E:134:GLU:HG2	1:E:136:GLN:NE2	2.23	0.54
1:C:44:ASN:ND2	1:C:51:LYS:HG3	2.23	0.53
1:D:44:ASN:ND2	1:D:51:LYS:HG3	2.23	0.53
1:D:219:HIS:HD2	1:D:221:MET:N	1.99	0.53
1:C:44:ASN:ND2	1:C:51:LYS:H	2.02	0.53
1:A:97:GLU:HG2	1:A:187:GLY:C	2.33	0.53
1:B:274:LYS:HG3	3:B:812:HOH:O	2.07	0.53
1:D:116:LEU:HD22	1:D:120:HIS:CE1	2.43	0.53
1:E:236:ARG:NH1	1:E:272:ASP:OD1	2.41	0.53
1:E:208:ASN:HD22	1:E:210:PRO:HD2	1.73	0.53
1:B:162:ASN:ND2	1:B:168:VAL:H	1.98	0.53
1:D:22:LYS:HD3	1:E:28:HIS:ND1	2.24	0.53
1:E:76:MET:HB3	1:E:77:PRO:HD2	1.91	0.53
1:E:86:MET:CE	1:E:106:PHE:HB2	2.39	0.53
1:F:242:ARG:HD2	3:F:870:HOH:O	2.07	0.52
1:D:119:LYS:HE3	1:D:137:ASP:OD2	2.10	0.52
1:F:162:ASN:HD22	1:F:162:ASN:N	1.96	0.52
1:D:208:ASN:HD22	1:D:210:PRO:HD2	1.75	0.52
1:B:288:TRP:HE1	1:B:293:ASN:ND2	2.08	0.52
1:C:51:LYS:NZ	3:C:953:HOH:O	2.28	0.52
1:B:44:ASN:ND2	1:B:51:LYS:HG3	2.24	0.52
1:B:208:ASN:HD22	1:B:210:PRO:HD2	1.74	0.52
1:B:76:MET:HB3	1:B:77:PRO:HD2	1.91	0.52
1:C:238:HIS:HE1	1:C:278:ASP:OD2	1.93	0.52
1:A:208:ASN:C	1:A:208:ASN:HD22	2.19	0.51
1:F:86:MET:HE3	1:F:106:PHE:HB2	1.91	0.51
1:A:242:ARG:HD3	3:A:655:HOH:O	2.10	0.51
1:B:75:ALA:HA	1:B:106:PHE:CE2	2.44	0.51
1:B:238:HIS:HE1	1:B:278:ASP:OD2	1.94	0.51
1:A:76:MET:HB3	1:A:77:PRO:HD2	1.91	0.51
1:A:162:ASN:ND2	1:A:168:VAL:H	1.95	0.51
1:D:116:LEU:HB3	1:D:120:HIS:CD2	2.45	0.51
1:A:44:ASN:ND2	1:A:51:LYS:H	2.06	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:238:HIS:HE1	1:A:278:ASP:OD2	1.93	0.51
1:E:97:GLU:HG2	1:E:187:GLY:C	2.35	0.51
1:E:44:ASN:ND2	1:E:51:LYS:HG3	2.26	0.51
1:B:97:GLU:HG2	1:B:187:GLY:C	2.36	0.51
1:D:238:HIS:HE1	1:D:278:ASP:OD2	1.92	0.51
1:F:122:PHE:O	1:F:133:PRO:HD2	2.11	0.51
1:C:97:GLU:HG2	1:C:187:GLY:C	2.36	0.50
1:E:86:MET:HE3	1:E:106:PHE:HD2	1.73	0.50
1:D:86:MET:HE3	1:D:106:PHE:HD2	1.69	0.50
1:F:208:ASN:HD22	1:F:210:PRO:HD2	1.75	0.50
1:E:238:HIS:CE1	1:E:278:ASP:OD2	2.64	0.50
1:B:238:HIS:HD2	3:B:810:HOH:O	1.95	0.50
1:F:242:ARG:HD3	3:F:871:HOH:O	2.12	0.50
1:B:236:ARG:NH1	1:B:272:ASP:OD1	2.46	0.49
1:A:219:HIS:HD2	1:A:221:MET:N	2.00	0.49
1:B:97:GLU:CG	1:B:187:GLY:O	2.61	0.49
1:A:310:LEU:HB2	3:A:833:HOH:O	2.13	0.49
1:B:165:GLU:N	1:B:165:GLU:CD	2.71	0.49
1:D:310:LEU:N	1:D:310:LEU:HD12	2.28	0.49
1:B:208:ASN:HD22	1:B:208:ASN:C	2.20	0.49
1:E:208:ASN:HD22	1:E:208:ASN:C	2.20	0.48
1:F:162:ASN:ND2	1:F:168:VAL:H	1.91	0.48
1:F:208:ASN:HD22	1:F:208:ASN:C	2.20	0.48
1:A:159:LEU:N	1:A:221:MET:HE3	2.28	0.48
1:A:236:ARG:NH1	1:A:272:ASP:OD1	2.46	0.48
1:B:162:ASN:HD22	1:B:162:ASN:N	2.02	0.48
1:C:97:GLU:CG	1:C:187:GLY:O	2.62	0.47
1:A:86:MET:CE	1:A:106:PHE:HB2	2.43	0.47
1:B:117:GLN:NE2	3:B:797:HOH:O	2.42	0.47
1:C:75:ALA:HA	1:C:106:PHE:CE2	2.49	0.47
1:C:208:ASN:HD22	1:C:208:ASN:C	2.21	0.47
1:E:163:LYS:HD3	1:E:168:VAL:HG21	1.97	0.47
1:F:86:MET:HE1	1:F:103:VAL:HA	1.96	0.47
1:A:75:ALA:HA	1:A:106:PHE:CE2	2.49	0.47
1:A:274:LYS:HG3	3:A:814:HOH:O	2.15	0.47
1:E:219:HIS:HD2	1:E:221:MET:N	1.98	0.47
1:A:208:ASN:HD22	1:A:210:PRO:HD2	1.78	0.47
1:C:117:GLN:HA	1:C:117:GLN:NE2	2.30	0.47
1:E:158:LYS:HE3	1:E:223:PRO:HG3	1.95	0.47
1:F:23:GLU:O	1:F:24:THR:C	2.57	0.47
1:F:22:LYS:HA	1:F:22:LYS:HD3	1.58	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:97:GLU:HG3	1:B:187:GLY:O	2.15	0.47
1:D:86:MET:CE	1:D:106:PHE:HB2	2.44	0.47
1:D:108:ARG:NH2	1:D:139:GLY:O	2.43	0.47
1:F:86:MET:CE	1:F:106:PHE:HB2	2.45	0.47
1:F:155:VAL:N	1:F:156:PRO:HA	2.30	0.46
1:A:155:VAL:N	1:A:156:PRO:HA	2.31	0.46
1:B:292:ASP:O	1:B:293:ASN:HB3	2.15	0.46
1:A:159:LEU:HD23	1:A:221:MET:CE	2.41	0.46
1:F:151:LYS:HE2	1:F:153:GLN:HE21	1.80	0.46
1:B:224:ALA:O	1:B:225:ARG:HB2	2.16	0.46
1:C:288:TRP:HE1	1:C:293:ASN:ND2	2.13	0.46
1:A:238:HIS:CE1	1:A:278:ASP:OD2	2.69	0.46
1:E:224:ALA:O	1:E:225:ARG:HB2	2.16	0.46
1:E:86:MET:HE1	1:E:103:VAL:HA	1.98	0.45
1:C:224:ALA:O	1:C:225:ARG:HB2	2.15	0.45
1:E:108:ARG:NH2	1:E:139:GLY:O	2.40	0.45
1:A:163:LYS:HD2	3:A:822:HOH:O	2.16	0.45
1:C:238:HIS:CE1	1:C:278:ASP:OD2	2.70	0.45
1:C:238:HIS:HD2	3:C:868:HOH:O	2.00	0.45
1:E:159:LEU:N	1:E:221:MET:HE3	2.30	0.45
1:F:236:ARG:NH1	1:F:272:ASP:OD1	2.50	0.45
1:F:274:LYS:HG2	1:F:287:GLU:HB2	1.98	0.45
1:B:114:GLU:CD	1:C:120:HIS:HE1	2.24	0.45
1:F:224:ALA:O	1:F:225:ARG:HB2	2.15	0.45
1:F:208:ASN:ND2	1:F:210:PRO:HD2	2.32	0.45
1:B:208:ASN:ND2	1:B:210:PRO:HD2	2.31	0.45
1:D:149:ILE:HB	1:D:185:SER:HB3	1.98	0.45
1:F:75:ALA:HA	1:F:106:PHE:CE2	2.52	0.45
1:B:219:HIS:HD2	1:B:221:MET:N	2.00	0.45
1:D:208:ASN:HD22	1:D:208:ASN:C	2.24	0.45
1:B:86:MET:HE3	1:B:106:PHE:HD2	1.76	0.45
1:A:159:LEU:HA	1:A:221:MET:CE	2.47	0.44
1:E:203:LYS:NZ	3:E:829:HOH:O	2.50	0.44
1:A:97:GLU:CG	1:A:187:GLY:O	2.66	0.44
1:D:162:ASN:HD22	1:D:162:ASN:N	2.07	0.44
1:E:115:ASN:ND2	1:E:117:GLN:OE1	2.50	0.44
1:D:18:PHE:CE2	1:D:22:LYS:HD2	2.53	0.44
1:D:86:MET:HE1	1:D:103:VAL:HA	1.99	0.44
1:D:236:ARG:NH1	1:D:272:ASP:OD1	2.50	0.44
1:E:208:ASN:ND2	1:E:210:PRO:HD2	2.32	0.44
1:C:304:VAL:O	1:D:310:LEU:HD13	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:208:ASN:ND2	1:D:210:PRO:HD2	2.33	0.43
1:C:180:ASN:HD22	1:C:180:ASN:HA	1.62	0.43
1:C:208:ASN:ND2	1:C:210:PRO:HD2	2.32	0.43
1:E:97:GLU:CG	1:E:187:GLY:O	2.66	0.43
1:F:219:HIS:HD2	1:F:221:MET:N	2.03	0.43
1:F:238:HIS:HE1	1:F:278:ASP:OD2	2.02	0.43
1:D:238:HIS:HD2	3:D:687:HOH:O	2.00	0.43
1:F:288:TRP:HE1	1:F:293:ASN:ND2	2.16	0.43
1:B:155:VAL:N	1:B:156:PRO:HA	2.34	0.43
1:F:114:GLU:OE1	1:F:114:GLU:HA	2.18	0.43
1:A:192:ILE:HG12	1:A:261:LEU:HA	2.01	0.43
1:C:302:GLU:HG3	3:C:783:HOH:O	2.19	0.43
1:D:294:HIS:HE1	3:D:695:HOH:O	2.01	0.43
1:A:86:MET:HE1	1:A:103:VAL:HA	2.01	0.43
1:F:180:ASN:HD22	1:F:180:ASN:HA	1.64	0.43
1:A:76:MET:HB3	1:A:76:MET:HE3	1.93	0.42
1:D:22:LYS:H	1:D:22:LYS:HG2	1.41	0.42
1:E:86:MET:HE3	1:E:106:PHE:CB	2.47	0.42
1:E:153:GLN:CD	1:E:153:GLN:N	2.75	0.42
1:E:180:ASN:HD22	1:E:180:ASN:HA	1.63	0.42
1:C:84:TYR:OH	1:C:114:GLU:OE2	2.22	0.42
1:D:238:HIS:CE1	1:D:278:ASP:OD2	2.71	0.42
1:B:180:ASN:HD22	1:B:180:ASN:HA	1.63	0.42
1:C:86:MET:HE1	1:C:103:VAL:HA	2.00	0.42
1:D:310:LEU:N	1:D:310:LEU:CD1	2.83	0.42
1:E:75:ALA:HA	1:E:106:PHE:CE2	2.55	0.42
1:E:149:ILE:HB	1:E:185:SER:HB3	2.01	0.42
1:A:208:ASN:ND2	1:A:210:PRO:HD2	2.34	0.42
1:E:162:ASN:ND2	1:E:168:VAL:H	1.93	0.42
1:C:86:MET:CE	1:C:106:PHE:HB2	2.48	0.42
1:F:274:LYS:HB3	1:F:274:LYS:HE2	1.87	0.42
1:C:292:ASP:O	1:C:293:ASN:HB3	2.20	0.42
1:B:86:MET:HE1	1:B:103:VAL:HA	2.00	0.42
1:B:159:LEU:N	1:B:221:MET:HE3	2.35	0.42
1:C:97:GLU:HG3	1:C:187:GLY:O	2.20	0.42
1:C:119:LYS:HE3	1:C:137:ASP:CG	2.45	0.42
1:D:269:GLY:HA2	3:D:706:HOH:O	2.20	0.42
1:D:180:ASN:HD22	1:D:180:ASN:HA	1.62	0.41
1:D:153:GLN:HG2	3:D:726:HOH:O	2.20	0.41
1:D:289:LYS:NZ	3:D:746:HOH:O	2.52	0.41
1:D:75:ALA:HA	1:D:106:PHE:CE2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:238:HIS:CE1	1:B:278:ASP:OD2	2.72	0.41
1:A:108:ARG:CD	1:A:301:ALA:HB3	2.51	0.41
1:A:140:GLN:NE2	3:A:780:HOH:O	2.54	0.41
1:C:192:ILE:HG12	1:C:261:LEU:HA	2.03	0.41
1:A:179:TRP:HA	1:A:196:LYS:HA	2.02	0.40
1:D:18:PHE:O	1:D:22:LYS:HG2	2.21	0.40
1:E:179:TRP:HA	1:E:196:LYS:HA	2.04	0.40
1:F:114:GLU:O	1:F:115:ASN:C	2.63	0.40
1:A:97:GLU:HG2	1:A:187:GLY:O	2.21	0.40
1:B:159:LEU:HA	1:B:221:MET:CE	2.51	0.40
1:D:76:MET:HB3	1:D:76:MET:HE3	1.98	0.40
1:F:19:LEU:HD12	1:F:19:LEU:HA	1.84	0.40
1:F:20:ASP:C	1:F:22:LYS:H	2.29	0.40
1:C:165:GLU:HG2	3:C:861:HOH:O	2.21	0.40
1:C:219:HIS:HD2	1:C:221:MET:N	2.01	0.40
1:C:117:GLN:HA	1:C:117:GLN:HE21	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	285/317 (90%)	279 (98%)	6 (2%)	0	100	100
1	B	286/317 (90%)	279 (98%)	7 (2%)	0	100	100
1	C	285/317 (90%)	277 (97%)	8 (3%)	0	100	100
1	D	299/317 (94%)	287 (96%)	11 (4%)	1 (0%)	36	28
1	E	285/317 (90%)	281 (99%)	4 (1%)	0	100	100
1	F	299/317 (94%)	290 (97%)	6 (2%)	3 (1%)	12	5
All	All	1739/1902 (91%)	1693 (97%)	42 (2%)	4 (0%)	43	36

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	23	GLU
1	F	24	THR
1	D	82	THR
1	F	21	LYS

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	231/255 (91%)	220 (95%)	11 (5%)	23	12
1	B	232/255 (91%)	221 (95%)	11 (5%)	23	12
1	C	231/255 (91%)	217 (94%)	14 (6%)	17	7
1	D	242/255 (95%)	234 (97%)	8 (3%)	33	24
1	E	231/255 (91%)	219 (95%)	12 (5%)	21	9
1	F	242/255 (95%)	230 (95%)	12 (5%)	22	11
All	All	1409/1530 (92%)	1341 (95%)	68 (5%)	23	12

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	42	VAL
1	A	76	MET
1	A	97	GLU
1	A	98	MET
1	A	162	ASN
1	A	172	LEU
1	A	180	ASN
1	A	184	VAL
1	A	203	LYS
1	A	208	ASN
1	A	283	PRO
1	B	42	VAL
1	B	76	MET

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Mol	Chain	Res	Type
1	B	97	GLU
1	B	98	MET
1	B	112	GLU
1	B	156	PRO
1	B	162	ASN
1	B	172	LEU
1	B	180	ASN
1	B	184	VAL
1	B	203	LYS
1	C	42	VAL
1	C	76	MET
1	C	88	ILE
1	C	97	GLU
1	C	98	MET
1	C	156	PRO
1	C	162	ASN
1	C	165	GLU
1	C	172	LEU
1	C	180	ASN
1	C	184	VAL
1	C	203	LYS
1	C	208	ASN
1	C	283	PRO
1	D	22	LYS
1	D	42	VAL
1	D	76	MET
1	D	98	MET
1	D	162	ASN
1	D	172	LEU
1	D	184	VAL
1	D	203	LYS
1	E	42	VAL
1	E	76	MET
1	E	88	ILE
1	E	97	GLU
1	E	98	MET
1	E	112	GLU
1	E	162	ASN
1	E	165	GLU
1	E	172	LEU
1	E	184	VAL
1	E	203	LYS

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Mol	Chain	Res	Type
1	E	208	ASN
1	F	19	LEU
1	F	42	VAL
1	F	76	MET
1	F	88	ILE
1	F	97	GLU
1	F	98	MET
1	F	156	PRO
1	F	162	ASN
1	F	172	LEU
1	F	180	ASN
1	F	184	VAL
1	F	203	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (74) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	44	ASN
1	A	54	GLN
1	A	115	ASN
1	A	117	GLN
1	A	162	ASN
1	A	180	ASN
1	A	208	ASN
1	A	219	HIS
1	A	238	HIS
1	A	293	ASN
1	A	294	HIS
1	B	44	ASN
1	B	115	ASN
1	B	117	GLN
1	B	125	HIS
1	B	153	GLN
1	B	162	ASN
1	B	180	ASN
1	B	208	ASN
1	B	219	HIS
1	B	238	HIS
1	B	290	GLN
1	B	293	ASN
1	B	294	HIS
1	C	44	ASN

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Mol	Chain	Res	Type
1	C	54	GLN
1	C	115	ASN
1	C	117	GLN
1	C	162	ASN
1	C	180	ASN
1	C	208	ASN
1	C	219	HIS
1	C	238	HIS
1	C	293	ASN
1	C	294	HIS
1	D	44	ASN
1	D	115	ASN
1	D	117	GLN
1	D	120	HIS
1	D	153	GLN
1	D	162	ASN
1	D	180	ASN
1	D	208	ASN
1	D	219	HIS
1	D	238	HIS
1	D	290	GLN
1	D	293	ASN
1	D	294	HIS
1	E	44	ASN
1	E	54	GLN
1	E	80	ASN
1	E	115	ASN
1	E	117	GLN
1	E	125	HIS
1	E	162	ASN
1	E	180	ASN
1	E	208	ASN
1	E	219	HIS
1	E	238	HIS
1	E	293	ASN
1	E	294	HIS
1	F	44	ASN
1	F	115	ASN
1	F	117	GLN
1	F	153	GLN
1	F	162	ASN
1	F	180	ASN

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Mol	Chain	Res	Type
1	F	208	ASN
1	F	218	HIS
1	F	219	HIS
1	F	238	HIS
1	F	290	GLN
1	F	293	ASN
1	F	294	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

6 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	ZDP	F	500	-	9,13,13	1.24	1 (11%)	10,18,18	0.67	0
2	ZDP	B	500	-	9,13,13	1.14	0	10,18,18	0.68	0
2	ZDP	A	500	-	9,13,13	1.17	1 (11%)	10,18,18	0.69	0
2	ZDP	E	500	-	9,13,13	1.16	0	10,18,18	0.64	0
2	ZDP	C	500	-	9,13,13	1.25	1 (11%)	10,18,18	0.65	0
2	ZDP	D	500	-	9,13,13	1.22	1 (11%)	10,18,18	0.61	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ZDP	F	500	-	-	7/17/17/17	-
2	ZDP	B	500	-	-	6/17/17/17	-
2	ZDP	A	500	-	-	6/17/17/17	-
2	ZDP	E	500	-	-	7/17/17/17	-
2	ZDP	C	500	-	-	6/17/17/17	-
2	ZDP	D	500	-	-	6/17/17/17	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	500	ZDP	OAF-CAQ	2.28	1.29	1.22
2	C	500	ZDP	OAF-CAQ	2.23	1.29	1.22
2	A	500	ZDP	OAF-CAQ	2.15	1.28	1.22
2	D	500	ZDP	OAF-CAQ	2.09	1.28	1.22

There are no bond angle outliers.

There are no chirality outliers.

All (38) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	500	ZDP	OAF-CAQ-CAT-CAM
2	A	500	ZDP	OAH-CAQ-CAT-NAC
2	B	500	ZDP	OAF-CAQ-CAT-CAM
2	B	500	ZDP	OAH-CAQ-CAT-NAC
2	C	500	ZDP	OAF-CAQ-CAT-CAM
2	C	500	ZDP	OAH-CAQ-CAT-NAC
2	D	500	ZDP	OAF-CAQ-CAT-CAM
2	D	500	ZDP	OAH-CAQ-CAT-NAC
2	E	500	ZDP	OAF-CAQ-CAT-CAM
2	E	500	ZDP	OAH-CAQ-CAT-NAC
2	F	500	ZDP	OAF-CAQ-CAT-CAM
2	F	500	ZDP	OAH-CAQ-CAT-NAC
2	B	500	ZDP	CAM-CAJ-CAK-CAS
2	A	500	ZDP	OAH-CAQ-CAT-CAM
2	B	500	ZDP	OAH-CAQ-CAT-CAM
2	C	500	ZDP	OAH-CAQ-CAT-CAM

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Mol	Chain	Res	Type	Atoms
2	D	500	ZDP	OAH-CAQ-CAT-CAM
2	E	500	ZDP	OAH-CAQ-CAT-CAM
2	F	500	ZDP	OAH-CAQ-CAT-CAM
2	C	500	ZDP	CAM-CAJ-CAK-CAS
2	A	500	ZDP	CAM-CAJ-CAK-CAS
2	E	500	ZDP	CAJ-CAM-CAT-CAN
2	F	500	ZDP	CAJ-CAM-CAT-CAN
2	D	500	ZDP	CAM-CAJ-CAK-CAS
2	F	500	ZDP	CAM-CAJ-CAK-CAS
2	C	500	ZDP	OAF-CAQ-CAT-CAN
2	D	500	ZDP	OAF-CAQ-CAT-CAN
2	E	500	ZDP	OAF-CAQ-CAT-CAN
2	F	500	ZDP	OAF-CAQ-CAT-CAN
2	E	500	ZDP	CAM-CAJ-CAK-CAS
2	A	500	ZDP	OAF-CAQ-CAT-CAN
2	B	500	ZDP	OAF-CAQ-CAT-CAN
2	C	500	ZDP	OAH-CAQ-CAT-CAN
2	D	500	ZDP	OAH-CAQ-CAT-CAN
2	E	500	ZDP	OAH-CAQ-CAT-CAN
2	F	500	ZDP	OAH-CAQ-CAT-CAN
2	A	500	ZDP	OAH-CAQ-CAT-CAN
2	B	500	ZDP	OAH-CAQ-CAT-CAN

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	287/317 (90%)	-0.20	4 (1%)	73 79	14, 19, 33, 42	0
1	B	288/317 (90%)	-0.14	6 (2%)	63 70	14, 21, 35, 48	0
1	C	287/317 (90%)	-0.05	7 (2%)	59 66	15, 21, 36, 46	0
1	D	301/317 (94%)	0.20	12 (3%)	42 49	16, 24, 44, 62	2 (0%)
1	E	287/317 (90%)	0.09	8 (2%)	55 62	16, 23, 44, 50	0
1	F	301/317 (94%)	0.58	27 (8%)	15 17	17, 28, 54, 64	2 (0%)
All	All	1751/1902 (92%)	0.09	64 (3%)	45 52	14, 23, 42, 64	4 (0%)

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	81	GLY	6.4
1	D	24	THR	5.2
1	F	79	VAL	4.1
1	F	24	THR	3.9
1	D	21	LYS	3.9
1	F	21	LYS	3.8
1	B	291	GLU	3.5
1	F	23	GLU	3.5
1	F	139	GLY	3.5
1	F	116	LEU	3.3
1	E	46	ASP	3.2
1	F	80	ASN	3.2
1	F	113	LEU	3.2
1	F	48	SER	3.1
1	D	23	GLU	3.1
1	C	137	ASP	3.1
1	E	25	GLY	3.1
1	F	46	ASP	3.0
1	F	135	ILE	3.0

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Mol	Chain	Res	Type	RSRZ
1	F	138	ASP	2.9
1	B	48	SER	2.9
1	C	48	SER	2.9
1	B	49	GLU	2.9
1	B	306	TYR	2.8
1	F	289	LYS	2.8
1	A	80	ASN	2.8
1	F	136	GLN	2.8
1	F	306	TYR	2.8
1	C	113	LEU	2.8
1	A	306	TYR	2.7
1	E	80	ASN	2.7
1	C	306	TYR	2.7
1	E	311	LEU	2.7
1	E	49	GLU	2.6
1	F	22	LYS	2.6
1	F	311	LEU	2.6
1	C	49	GLU	2.6
1	B	312	HIS	2.5
1	D	137	ASP	2.5
1	F	108	ARG	2.5
1	F	137	ASP	2.5
1	E	122	PHE	2.5
1	F	122	PHE	2.5
1	B	46	ASP	2.4
1	D	49	GLU	2.4
1	A	115	ASN	2.3
1	F	165	GLU	2.3
1	D	22	LYS	2.3
1	F	49	GLU	2.3
1	C	120	HIS	2.3
1	A	117	GLN	2.2
1	F	132	VAL	2.2
1	F	140	GLN	2.2
1	D	122	PHE	2.2
1	D	121	SER	2.2
1	D	25	GLY	2.2
1	F	291	GLU	2.1
1	E	42	VAL	2.1
1	E	157	THR	2.1
1	F	123	THR	2.1
1	F	117	GLN	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	16	ALA	2.0
1	C	291	GLU	2.0
1	D	48	SER	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	ZDP	E	500	14/14	0.96	0.06	18,19,21,21	0
2	ZDP	F	500	14/14	0.96	0.07	20,21,24,24	0
2	ZDP	C	500	14/14	0.97	0.06	14,16,18,19	0
2	ZDP	D	500	14/14	0.97	0.06	16,18,19,19	0
2	ZDP	A	500	14/14	0.97	0.06	12,15,16,17	0
2	ZDP	B	500	14/14	0.97	0.06	14,14,17,17	0

6.5 Other polymers [i](#)

There are no such residues in this entry.