



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:05 PM UTC

PDB ID : 5OT0 / pdb_00005ot0
Title : The thermostable L-asparaginase from *Thermococcus kodakarensis*
Authors : Guo, J.; Coker, A.R.; Wood, S.P.; Cooper, J.B.; Rashid, N.; Chohan, S.M.; Akhtar, M.
Deposited on : 2017-08-18
Resolution : 2.18 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

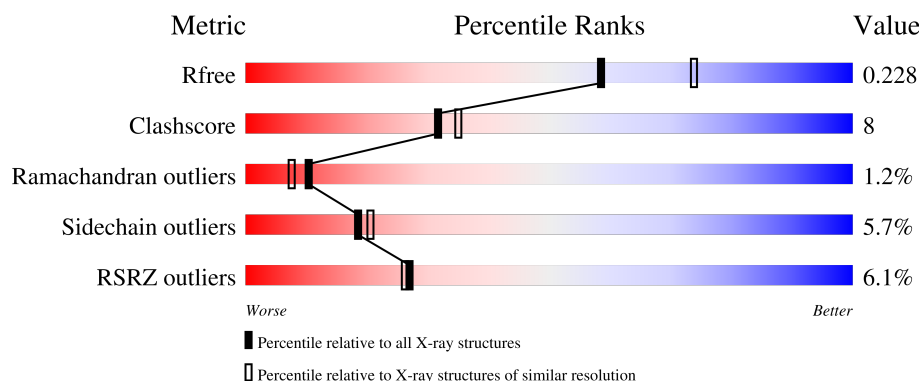
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.18 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	8975 (2.20-2.16)
Clashscore	190562	9786 (2.20-2.16)
Ramachandran outliers	187476	9664 (2.20-2.16)
Sidechain outliers	187428	9664 (2.20-2.16)
RSRZ outliers	180081	8979 (2.20-2.16)

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	328	84% 13% ..
1	B	328	86% 12% ..
1	C	328	84% 12% ..
1	D	328	89% 8% ..
1	E	328	7% 82% 14% ..

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Mol	Chain	Length	Quality of chain
1	F	328	28% 70% 21% 7%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PO4	B	401	-	X	-	-
2	PO4	C	401	-	X	-	-
2	PO4	D	401	-	X	-	-
2	PO4	E	401	-	X	-	-

2 Entry composition [i](#)

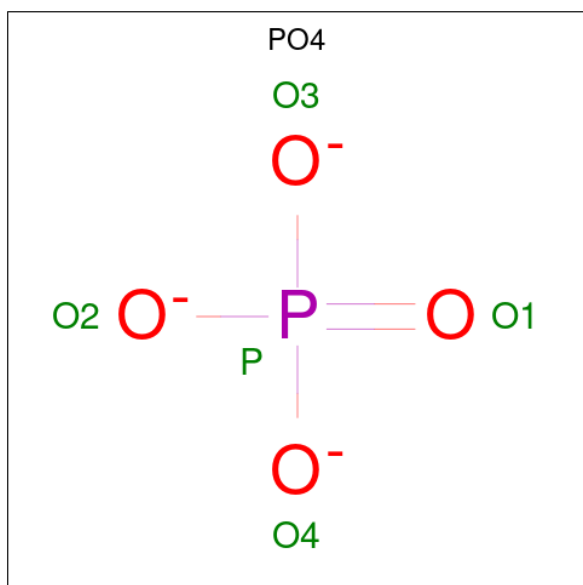
There are 5 unique types of molecules in this entry. The entry contains 15386 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 L-asparaginase.

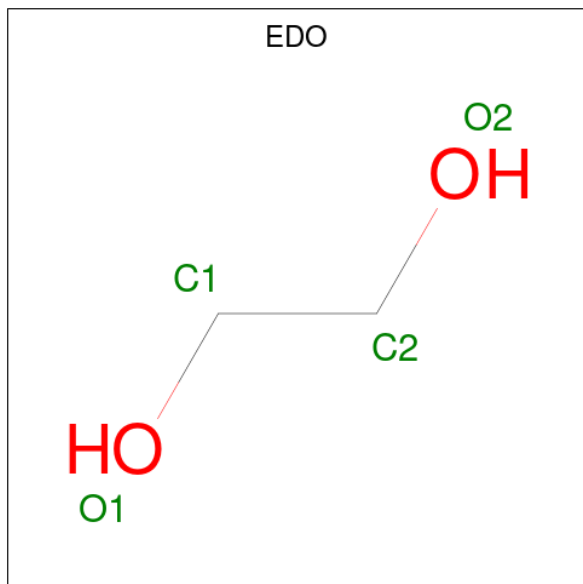
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	328	Total	C	N	O	S	0	2	0
			2520	1595	441	474	10			
1	B	328	Total	C	N	O	S	0	3	0
			2523	1598	438	477	10			
1	C	328	Total	C	N	O	S	0	3	0
			2525	1598	442	475	10			
1	D	328	Total	C	N	O	S	0	1	0
			2510	1589	436	475	10			
1	E	328	Total	C	N	O	S	0	0	0
			2507	1587	436	474	10			
1	F	328	Total	C	N	O	S	0	1	0
			2514	1592	438	474	10			

- Molecule 2 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



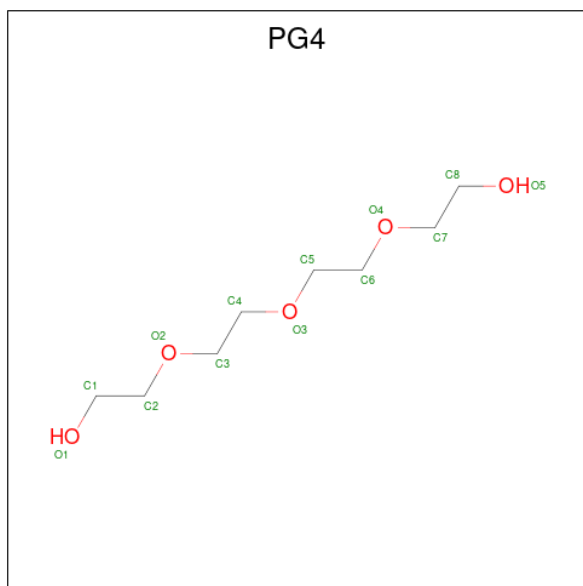
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O P 5 4 1	0	0
2	B	1	Total O P 5 4 1	0	0
2	C	1	Total O P 5 4 1	0	0
2	D	1	Total O P 5 4 1	0	0
2	E	1	Total O P 5 4 1	0	0
2	F	1	Total O P 5 4 1	0	0

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	D	1	Total C O 4 2 2	0	0
3	D	1	Total C O 4 2 2	0	0
3	F	1	Total C O 4 2 2	0	0

- Molecule 4 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			10	6	4		

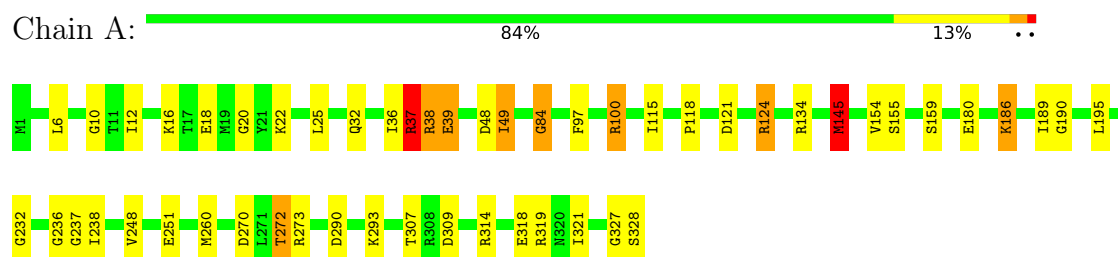
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	55	Total	O	0	0
			55	55		
5	B	49	Total	O	0	0
			49	49		
5	C	35	Total	O	0	0
			35	35		
5	D	46	Total	O	0	0
			46	46		
5	E	25	Total	O	0	0
			25	25		
5	F	13	Total	O	0	0
			13	13		

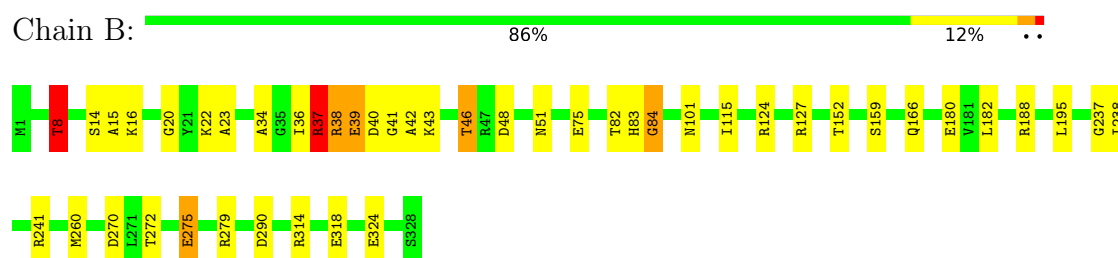
3 Residue-property plots

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.

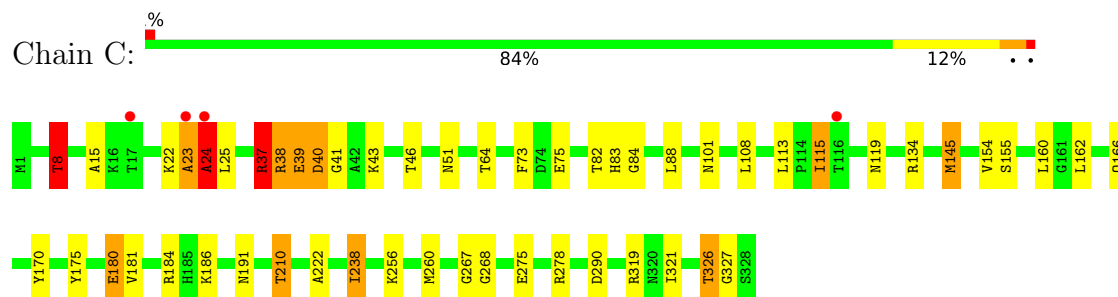
• Molecule 1: L-asparaginase



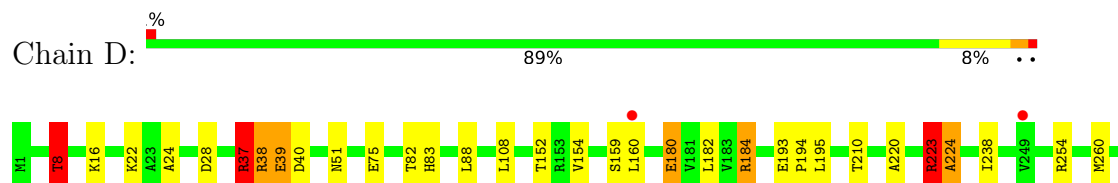
• Molecule 1: L-asparaginase

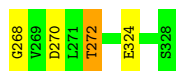


• Molecule 1: L-asparaginase

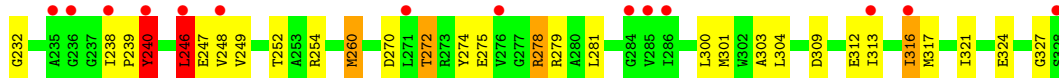
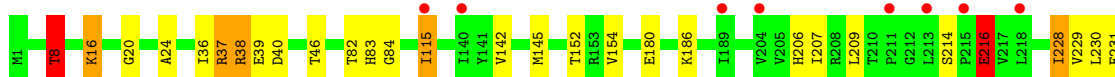
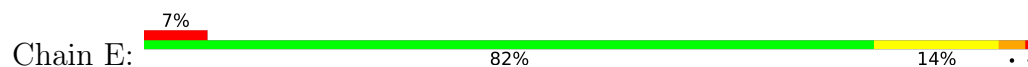


• Molecule 1: L-asparaginase

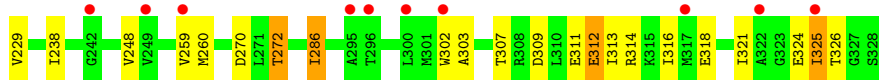
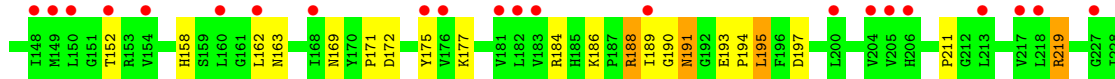
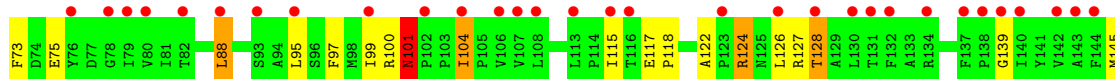




- Molecule 1: L-asparaginase



- Molecule 1: L-asparaginase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	70.74Å 70.96Å 107.73Å 72.13° 76.22° 87.83°	Depositor
Resolution (Å)	68.65 – 2.18 68.65 – 2.18	Depositor EDS
% Data completeness (in resolution range)	97.5 (68.65-2.18) 97.5 (68.65-2.18)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.70 (at 2.18Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.194 , 0.224 0.198 , 0.228	Depositor DCC
R_{free} test set	4896 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å ²)	49.6	Xtriage
Anisotropy	0.057	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 59.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.019 for -h,k,k-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	15386	wwPDB-VP
Average B, all atoms (Å ²)	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.20% 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: PO4, EDO, PG4

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.44	16/2573 (0.6%)	1.17	9/3491 (0.3%)
1	B	1.29	8/2581 (0.3%)	1.16	7/3503 (0.2%)
1	C	1.37	13/2582 (0.5%)	1.18	9/3503 (0.3%)
1	D	1.30	5/2557 (0.2%)	1.18	8/3470 (0.2%)
1	E	1.14	2/2551 (0.1%)	1.12	8/3462 (0.2%)
1	F	1.12	8/2562 (0.3%)	1.19	9/3477 (0.3%)
All	All	1.28	52/15406 (0.3%)	1.17	50/20906 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	C	0	2
1	D	0	1
1	E	0	1
1	F	0	2
All	All	0	7

All (52) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	16	LYS	C-O	-9.50	1.12	1.24
1	A	84	GLY	CA-C	7.40	1.60	1.52
1	A	12	ILE	CA-C	7.21	1.62	1.52
1	A	154	VAL	C-O	-7.20	1.15	1.24
1	A	49	ILE	C-O	-7.19	1.17	1.24
1	B	84	GLY	CA-C	7.16	1.59	1.52
1	B	101	ASN	C-O	-6.97	1.20	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	223	ARG	C-N	-6.61	1.24	1.33
1	C	180	GLU	CA-C	6.57	1.60	1.52
1	B	159	SER	C-O	-6.40	1.15	1.24
1	A	186	LYS	C-O	-6.26	1.16	1.24
1	A	155	SER	CA-C	-6.11	1.45	1.52
1	A	290	ASP	CA-C	6.06	1.61	1.52
1	A	37	ARG	CA-C	-6.02	1.44	1.52
1	D	159	SER	C-O	-5.99	1.16	1.24
1	B	241	ARG	CZ-NH1	5.94	1.41	1.32
1	F	34	ALA	C-O	5.93	1.30	1.23
1	F	35	GLY	CA-C	5.81	1.60	1.51
1	B	15	ALA	C-O	-5.68	1.16	1.23
1	B	23	ALA	CA-C	-5.68	1.46	1.52
1	E	16	LYS	C-O	-5.67	1.17	1.24
1	A	49	ILE	N-CA	5.63	1.52	1.45
1	F	101	ASN	CA-CB	5.47	1.57	1.52
1	F	17	THR	C-O	-5.44	1.17	1.24
1	C	321	ILE	C-O	-5.42	1.18	1.24
1	C	154	VAL	C-O	-5.41	1.17	1.24
1	C	181	VAL	N-CA	-5.38	1.39	1.46
1	C	170	TYR	CE1-CZ	5.37	1.51	1.38
1	A	10	GLY	CA-C	-5.32	1.45	1.52
1	C	37	ARG	C-O	-5.31	1.17	1.24
1	A	22	LYS	C-O	-5.27	1.17	1.23
1	C	155	SER	CA-C	-5.27	1.46	1.52
1	F	16	LYS	CA-CB	5.26	1.62	1.53
1	C	113	LEU	CA-C	5.25	1.60	1.52
1	C	73	PHE	C-N	-5.25	1.27	1.33
1	F	101	ASN	CG-ND2	5.23	1.44	1.33
1	C	166[A]	GLN	CA-C	-5.18	1.46	1.52
1	C	166[B]	GLN	CA-C	-5.18	1.46	1.52
1	E	186	LYS	C-O	-5.17	1.17	1.24
1	A	159	SER	C-O	-5.14	1.17	1.24
1	D	194	PRO	C-O	-5.13	1.17	1.23
1	A	18	GLU	C-O	-5.12	1.17	1.24
1	C	186	LYS	C-O	-5.11	1.17	1.24
1	B	290	ASP	CA-C	5.09	1.60	1.52
1	F	190	GLY	C-O	-5.09	1.17	1.23
1	B	37	ARG	CA-C	-5.08	1.46	1.52
1	D	38	ARG	N-CA	5.07	1.52	1.46
1	A	25	LEU	C-O	-5.06	1.17	1.23
1	F	21	TYR	C-O	-5.06	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	101	ASN	C-O	-5.04	1.21	1.23
1	D	24	ALA	CA-C	5.03	1.59	1.53
1	A	48	ASP	CA-C	-5.02	1.46	1.52

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	223	ARG	N-CA-C	-11.49	89.92	108.41
1	F	128	THR	CB-CA-C	10.97	129.50	110.85
1	F	36	ILE	CB-CA-C	8.76	125.65	111.29
1	F	39	GLU	O-C-N	-8.48	115.29	123.26
1	F	57	ILE	CB-CG1-CD1	8.18	130.98	113.80
1	F	99	ILE	CB-CG1-CD1	7.90	130.40	113.80
1	E	246	LEU	CB-CG-CD2	6.81	131.12	110.70
1	A	134	ARG	CG-CD-NE	-6.59	97.49	112.00
1	E	40	ASP	N-CA-C	6.42	124.48	110.80
1	B	41	GLY	N-CA-C	-6.22	98.44	113.18
1	B	22	LYS	N-CA-C	6.21	118.41	108.41
1	F	101	ASN	CB-CG-ND2	6.01	125.42	116.40
1	F	24	ALA	N-CA-C	5.97	119.88	112.59
1	F	191	ASN	N-CA-C	5.95	123.48	110.80
1	C	327	GLY	N-CA-C	-5.94	99.10	113.18
1	A	145	MET	CG-SD-CE	5.93	113.94	100.90
1	D	24	ALA	N-CA-C	-5.91	95.81	107.69
1	E	38	ARG	N-CA-C	5.89	123.34	110.80
1	B	8	THR	N-CA-CB	-5.85	102.53	110.95
1	D	8	THR	N-CA-CB	-5.83	102.56	110.95
1	D	223	ARG	N-CA-CB	5.80	119.44	110.21
1	F	101	ASN	CB-CG-OD1	-5.80	109.21	120.80
1	E	240	TYR	CA-CB-CG	5.72	124.20	113.90
1	E	8	THR	N-CA-CB	-5.61	103.58	110.98
1	E	216	GLU	CA-CB-CG	5.58	125.26	114.10
1	E	20	GLY	CA-C-O	-5.56	116.84	122.56
1	C	267	GLY	N-CA-C	5.44	121.55	115.08
1	A	124	ARG	CG-CD-NE	-5.42	100.08	112.00
1	D	180	GLU	CA-CB-CG	-5.41	103.28	114.10
1	E	24	ALA	N-CA-C	5.41	119.88	113.28
1	A	37	ARG	N-CA-C	-5.39	99.31	110.80
1	B	38	ARG	N-CA-C	5.39	122.28	110.80
1	C	8	THR	N-CA-CB	-5.34	103.93	110.98
1	C	115	ILE	CB-CA-C	-5.31	105.08	112.04
1	C	210	THR	CA-CB-CG2	5.30	119.51	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	238	ILE	CA-C-N	5.25	125.50	119.83
1	C	238	ILE	C-N-CA	5.25	125.50	119.83
1	B	237	GLY	CA-C-N	-5.24	118.77	123.33
1	B	237	GLY	C-N-CA	-5.24	118.77	123.33
1	C	210	THR	OG1-CB-CG2	5.23	119.75	109.30
1	D	224	ALA	N-CA-CB	5.15	119.20	110.49
1	A	38	ARG	N-CA-C	5.15	121.77	110.80
1	C	41	GLY	N-CA-C	-5.14	101.00	113.18
1	A	20	GLY	CA-C-O	-5.11	116.65	122.78
1	A	238	ILE	CA-C-N	5.07	125.31	119.83
1	A	238	ILE	C-N-CA	5.07	125.31	119.83
1	B	46	THR	CA-CB-OG1	5.05	117.18	109.60
1	A	118	PRO	N-CA-C	5.05	120.19	113.57
1	D	22	LYS	N-CA-C	5.04	116.53	108.41
1	D	16	LYS	CB-CA-C	5.00	118.72	109.71

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	40	ASP	Peptide
1	C	24	ALA	Peptide
1	C	326	THR	Peptide
1	D	37	ARG	Peptide
1	E	309	ASP	Mainchain
1	F	35	GLY	Peptide
1	F	39	GLU	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2520	0	2577	27	0
1	B	2523	0	2580	26	1
1	C	2525	0	2581	22	0
1	D	2510	0	2566	16	1
1	E	2507	0	2561	59	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	2514	0	2568	100	0
2	A	5	0	0	1	0
2	B	5	0	0	0	0
2	C	5	0	0	1	0
2	D	5	0	0	0	0
2	E	5	0	0	1	0
2	F	5	0	0	0	0
3	A	4	0	6	0	0
3	B	8	0	12	0	0
3	D	8	0	12	1	0
3	F	4	0	6	1	0
4	B	10	0	13	2	0
5	A	55	0	0	1	0
5	B	49	0	0	2	1
5	C	35	0	0	1	0
5	D	46	0	0	0	1
5	E	25	0	0	2	0
5	F	13	0	0	2	0
All	All	15386	0	15482	248	2

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 8.

All (248) 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:15:ALA:HB2	1:C:25:LEU:HD11	1.30	1.08
1:F:101:ASN:OD1	1:F:194:PRO:HA	1.61	1.00
1:F:65:ILE:HD11	1:F:95:LEU:HD21	1.45	0.98
1:F:24:ALA:HA	1:F:51:ASN:HD21	1.30	0.97
1:F:12:ILE:HD11	1:F:126:LEU:HD21	1.47	0.94
1:F:62:TRP:O	1:F:65:ILE:HD13	1.69	0.93
1:E:274:TYR:O	1:E:278:ARG:HD3	1.71	0.90
1:F:122:ALA:O	1:F:126:LEU:HD23	1.73	0.89
1:B:166:GLN:HG3	5:B:501:HOH:O	1.70	0.89
1:E:240:TYR:CE1	1:E:246:LEU:HB2	2.07	0.88
1:F:15:ALA:HB3	1:F:20:GLY:O	1.74	0.88
1:F:54:SER:HA	1:F:57:ILE:HD13	1.54	0.87
1:F:172:ASP:O	1:F:184:ARG:HD3	1.75	0.86
1:F:25:LEU:HB3	1:F:29:ASP:OD1	1.78	0.83
1:F:62:TRP:HA	1:F:65:ILE:HD12	1.61	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:97:PHE:O	1:F:100:ARG:NH1	2.12	0.81
1:F:65:ILE:CD1	1:F:95:LEU:HD21	2.11	0.80
1:F:23:ALA:O	1:F:51:ASN:ND2	2.15	0.80
1:E:240:TYR:CE2	1:E:246:LEU:HG	2.16	0.80
1:A:307:THR:HG22	1:A:309:ASP:H	1.46	0.80
1:C:15:ALA:HB2	1:C:25:LEU:CD1	2.08	0.80
1:E:313:ILE:O	1:E:316:ILE:HD13	1.82	0.80
1:A:6:LEU:HD22	1:A:49:ILE:HD11	1.63	0.79
1:E:240:TYR:OH	1:E:279:ARG:CB	2.31	0.79
1:F:303:ALA:HB1	1:F:316:ILE:HD11	1.65	0.78
1:B:275:GLU:HG2	1:B:279:ARG:NH1	1.99	0.78
1:F:229:VAL:HG22	1:F:259:VAL:CG1	2.14	0.78
1:F:62:TRP:HA	1:F:65:ILE:CD1	2.15	0.77
1:E:312:GLU:O	1:E:316:ILE:HG23	1.84	0.76
1:E:246:LEU:HD13	1:E:247:GLU:N	2.01	0.76
1:F:101:ASN:CG	1:F:101:ASN:O	2.29	0.76
1:F:188:ARG:O	1:F:189:ILE:HG13	1.87	0.75
1:F:101:ASN:HD21	1:F:194:PRO:CD	2.02	0.73
1:C:23:ALA:O	1:C:24:ALA:HB3	1.86	0.73
1:E:206:HIS:CE1	1:E:231:GLU:OE1	2.41	0.73
1:F:219:ARG:HD2	1:F:248:VAL:HG13	1.69	0.73
1:F:35:GLY:O	1:F:36:ILE:HG13	1.88	0.73
1:A:6:LEU:HD22	1:A:49:ILE:CD1	2.19	0.72
1:F:101:ASN:HD21	1:F:194:PRO:N	1.87	0.72
1:A:237:GLY:H	1:A:260:MET:HE1	1.53	0.72
1:F:101:ASN:OD1	1:F:194:PRO:CA	2.38	0.71
1:E:232:GLY:HA3	1:E:260:MET:CE	2.20	0.71
1:F:101:ASN:O	1:F:101:ASN:ND2	2.23	0.71
1:E:240:TYR:OH	1:E:279:ARG:HB3	1.90	0.71
1:F:219:ARG:CD	1:F:248:VAL:HG13	2.21	0.70
1:E:303:ALA:HB2	1:E:316:ILE:HD11	1.72	0.70
1:E:8:THR:HG22	1:E:83:HIS:HA	1.76	0.68
1:A:237:GLY:H	1:A:260:MET:CE	2.06	0.67
1:C:8:THR:HG22	1:C:83:HIS:HA	1.76	0.67
1:E:240:TYR:OH	1:E:279:ARG:HB2	1.95	0.66
1:F:307:THR:HG21	1:F:312:GLU:HG3	1.76	0.66
1:F:259:VAL:HG23	1:F:286:ILE:HG23	1.77	0.66
1:D:8:THR:HG22	1:D:83:HIS:HA	1.78	0.65
1:F:24:ALA:HA	1:F:51:ASN:ND2	2.08	0.65
1:B:8:THR:HG22	1:B:83:HIS:HA	1.79	0.64
1:F:309:ASP:HB3	1:F:312:GLU:CD	2.22	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:100:ARG:O	1:F:101:ASN:OD1	2.15	0.64
1:A:32:GLN:NE2	1:D:182:LEU:HD13	2.14	0.62
1:C:37:ARG:O	1:C:39:GLU:N	2.33	0.62
1:E:228:ILE:HD11	1:E:230:LEU:HD23	1.81	0.61
1:F:145:MET:HE3	1:F:162:LEU:C	2.25	0.61
1:F:37:ARG:O	1:F:39:GLU:N	2.34	0.61
1:F:158[A]:HIS:CE1	5:F:504:HOH:O	2.52	0.61
1:A:236:GLY:HA2	1:A:260:MET:CE	2.31	0.61
1:F:172:ASP:O	1:F:184:ARG:CD	2.49	0.61
1:A:236:GLY:CA	1:A:260:MET:HE2	2.31	0.60
1:F:101:ASN:ND2	1:F:194:PRO:N	2.49	0.60
1:B:34:ALA:CB	1:B:36:ILE:HD13	2.31	0.60
1:F:101:ASN:OD1	1:F:193:GLU:O	2.18	0.60
1:A:37:ARG:O	1:A:39:GLU:N	2.33	0.60
1:E:37:ARG:O	1:E:39:GLU:N	2.33	0.60
1:E:303:ALA:CB	1:E:316:ILE:HD11	2.31	0.60
1:B:37:ARG:O	1:B:39:GLU:N	2.34	0.60
1:F:61:ASP:O	1:F:65:ILE:HG23	2.01	0.60
1:C:23:ALA:O	1:C:24:ALA:CB	2.50	0.60
1:F:39:GLU:O	1:F:40:ASP:CG	2.44	0.60
1:B:124:ARG:NH1	1:B:127:ARG:HH11	2.01	0.58
1:F:35:GLY:O	1:F:36:ILE:CG1	2.50	0.58
1:B:16:LYS:HE3	1:B:20:GLY:HA2	1.86	0.58
1:B:83:HIS:HD2	1:B:84:GLY:O	1.87	0.58
1:D:37:ARG:O	1:D:39:GLU:N	2.37	0.58
1:F:229:VAL:HG22	1:F:259:VAL:HG11	1.84	0.58
1:E:274:TYR:O	1:E:278:ARG:CD	2.47	0.58
1:F:238:ILE:HG13	1:F:260:MET:HE1	1.84	0.58
1:E:209:LEU:HD11	1:E:238:ILE:CD1	2.34	0.57
1:D:220:ALA:O	1:D:223:ARG:O	2.22	0.57
1:F:259:VAL:HA	1:F:286:ILE:HG22	1.86	0.57
1:F:172:ASP:HB2	1:F:184:ARG:HD2	1.87	0.56
1:E:240:TYR:CD1	1:E:246:LEU:CB	2.89	0.56
1:C:145:MET:HE1	1:C:162:LEU:HB3	1.87	0.55
1:F:313:ILE:O	1:F:316:ILE:HG12	2.06	0.55
1:F:325:ILE:HD13	1:F:326:THR:O	2.07	0.55
1:E:313:ILE:O	1:E:316:ILE:CD1	2.55	0.55
1:F:65:ILE:HD11	1:F:95:LEU:CD2	2.26	0.55
1:A:270:ASP:OD1	1:A:272:THR:HB	2.07	0.54
1:F:15:ALA:CB	1:F:20:GLY:O	2.51	0.54
1:C:24:ALA:HB2	1:C:51:ASN:HD21	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:240:TYR:CD1	1:E:246:LEU:HB3	2.42	0.54
1:B:46:THR:OG1	4:B:404:PG4:H41	2.08	0.54
1:E:240:TYR:CZ	1:E:246:LEU:HB2	2.43	0.54
1:F:6:LEU:HD13	1:F:47:ARG:HB3	1.89	0.54
1:E:270:ASP:OD1	1:E:272:THR:HB	2.08	0.53
1:F:270:ASP:OD1	1:F:272:THR:HB	2.07	0.53
1:B:270:ASP:OD1	1:B:272:THR:HB	2.08	0.53
1:A:236:GLY:CA	1:A:260:MET:CE	2.86	0.53
1:D:238:ILE:HG13	1:D:260:MET:HE1	1.89	0.53
1:D:270:ASP:OD1	1:D:272:THR:HB	2.08	0.53
1:E:316:ILE:HD13	1:E:317:MET:N	2.23	0.53
1:F:6:LEU:HD11	1:F:49:ILE:HG13	1.89	0.53
1:E:249:VAL:HA	1:E:252:THR:HG22	1.89	0.53
1:E:238:ILE:O	1:E:240:TYR:CD1	2.61	0.53
1:C:238:ILE:HG13	1:C:260:MET:HE1	1.91	0.53
1:F:286:ILE:HD11	1:F:318:GLU:HG3	1.91	0.53
1:C:22:LYS:C	1:C:23:ALA:O	2.48	0.52
1:F:35:GLY:C	1:F:36:ILE:HG13	2.34	0.52
1:E:84:GLY:HA3	2:E:401:PO4:O4	2.09	0.52
1:E:214:SER:OG	1:E:216:GLU:HG2	2.10	0.52
1:F:17:THR:HA	1:F:21:TYR:CE2	2.45	0.52
1:F:5:VAL:HG23	1:F:44:ILE:HD11	1.91	0.52
1:E:232:GLY:HA3	1:E:260:MET:HE2	1.91	0.52
1:E:300:LEU:O	1:E:304:LEU:HD23	2.10	0.52
1:B:238:ILE:HG13	1:B:260:MET:HE1	1.92	0.52
1:B:34:ALA:HB3	1:B:36:ILE:HD13	1.92	0.51
1:E:313:ILE:HA	1:E:316:ILE:HD12	1.91	0.51
1:F:23:ALA:O	1:F:51:ASN:CG	2.52	0.51
1:F:145:MET:HE3	1:F:163:ASN:N	2.25	0.51
1:E:8:THR:CG2	1:E:83:HIS:HA	2.41	0.51
1:B:124:ARG:NH1	1:B:127:ARG:NH1	2.57	0.51
1:C:275:GLU:HG3	1:C:278:ARG:NH2	2.26	0.51
1:E:115:ILE:HG22	5:E:511:HOH:O	2.11	0.51
1:A:248:VAL:O	1:A:251:GLU:HG2	2.11	0.50
1:F:12:ILE:CD1	1:F:126:LEU:HD21	2.31	0.50
1:F:17:THR:HG23	1:F:18:GLU:OE1	2.12	0.50
1:A:237:GLY:N	1:A:260:MET:HE2	2.26	0.50
1:E:316:ILE:HD13	1:E:317:MET:H	1.77	0.50
1:A:327:GLY:O	1:A:328:SER:C	2.54	0.50
1:F:88:LEU:HD23	1:F:88:LEU:O	2.11	0.50
1:E:240:TYR:CZ	1:E:246:LEU:HG	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:219:ARG:HD3	1:F:248:VAL:HG22	1.94	0.50
1:E:275:GLU:CD	1:E:275:GLU:H	2.20	0.50
1:F:44:ILE:C	1:F:44:ILE:HD13	2.37	0.50
1:E:206:HIS:HE1	1:E:231:GLU:OE1	1.93	0.49
1:F:5:VAL:CG2	1:F:44:ILE:HD11	2.42	0.49
1:F:309:ASP:HB3	1:F:312:GLU:HG2	1.93	0.49
1:F:313:ILE:HA	1:F:316:ILE:CD1	2.42	0.49
1:A:36:ILE:HG22	1:A:37:ARG:N	2.27	0.49
1:B:48:ASP:OD2	4:B:404:PG4:H62	2.13	0.49
1:E:240:TYR:CD2	1:E:246:LEU:HG	2.48	0.49
1:F:62:TRP:C	1:F:65:ILE:HD13	2.34	0.49
1:F:313:ILE:HA	1:F:316:ILE:HD11	1.95	0.49
1:A:237:GLY:N	1:A:260:MET:CE	2.73	0.48
1:B:275:GLU:CG	1:B:279:ARG:NH1	2.72	0.48
1:B:34:ALA:HB1	1:B:36:ILE:HD13	1.95	0.48
1:C:8:THR:CG2	1:C:83:HIS:HA	2.42	0.48
1:F:101:ASN:HD21	1:F:194:PRO:CG	2.27	0.48
1:D:184:ARG:C	1:D:184:ARG:CD	2.86	0.48
1:D:51:ASN:CG	1:D:51:ASN:O	2.56	0.48
1:E:240:TYR:CD1	1:E:246:LEU:HB2	2.46	0.48
1:F:40:ASP:OD1	1:F:42:ALA:O	2.31	0.48
1:E:249:VAL:HA	1:E:252:THR:CG2	2.44	0.48
1:F:127:ARG:HG3	1:F:128:THR:HG23	1.96	0.47
1:F:44:ILE:HG23	1:F:44:ILE:O	2.14	0.47
1:D:254:ARG:HB3	1:D:254:ARG:NH1	2.28	0.47
1:A:270:ASP:HB3	1:A:273:ARG:HD3	1.97	0.47
1:D:8:THR:CG2	1:D:83:HIS:HA	2.44	0.47
1:F:309:ASP:HB3	1:F:312:GLU:CG	2.44	0.47
1:B:314:ARG:NH1	1:B:318:GLU:OE1	2.48	0.47
1:F:101:ASN:CG	1:F:193:GLU:C	2.83	0.47
1:F:259:VAL:HA	1:F:286:ILE:CG2	2.45	0.47
1:E:303:ALA:HB2	1:E:316:ILE:CD1	2.43	0.46
1:F:171:PRO:CB	1:F:184:ARG:HE	2.28	0.46
1:F:158[A]:HIS:HE1	5:F:504:HOH:O	1.94	0.46
1:A:121:ASP:HB2	1:A:124:ARG:NH2	2.30	0.46
1:A:84:GLY:HA3	2:A:401:PO4:O1	2.16	0.46
1:E:239:PRO:C	1:E:240:TYR:HD1	2.23	0.46
1:B:51:ASN:O	1:B:51:ASN:CG	2.58	0.46
1:F:122:ALA:O	1:F:126:LEU:CD2	2.54	0.45
1:B:124:ARG:HA	1:B:127:ARG:NH1	2.31	0.45
1:F:100:ARG:NH2	1:F:302:TRP:CH2	2.83	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:8:THR:HG23	5:B:532:HOH:O	2.17	0.45
1:E:206:HIS:NE2	1:E:231:GLU:OE1	2.48	0.45
1:E:238:ILE:O	1:E:240:TYR:CE1	2.70	0.45
1:E:228:ILE:HD13	1:E:229:VAL:C	2.41	0.45
1:F:44:ILE:HD13	1:F:45:GLU:N	2.32	0.45
1:B:182:LEU:N	1:B:182:LEU:HD12	2.32	0.44
1:E:240:TYR:CE1	1:E:246:LEU:CB	2.87	0.44
1:F:303:ALA:HB1	1:F:316:ILE:CD1	2.39	0.44
1:C:22:LYS:O	1:C:23:ALA:O	2.34	0.44
1:E:228:ILE:CD1	1:E:230:LEU:CD2	2.96	0.44
1:F:117:GLU:CD	1:F:118:PRO:HD2	2.41	0.44
1:B:37:ARG:NH1	1:B:42:ALA:O	2.50	0.44
1:F:169:ASN:HD21	3:F:402:EDO:C1	2.30	0.44
1:D:8:THR:HG22	1:D:82:THR:O	2.17	0.44
1:E:8:THR:HG22	1:E:82:THR:O	2.18	0.44
1:F:152:THR:OG1	1:F:324:GLU:HB3	2.17	0.44
1:F:62:TRP:CA	1:F:65:ILE:CD1	2.93	0.44
1:D:88:LEU:HD11	1:D:108:LEU:HB3	2.00	0.43
1:D:184:ARG:HD3	1:D:184:ARG:O	2.18	0.43
1:D:268:GLY:HA2	3:D:403:EDO:H22	2.00	0.43
1:A:314:ARG:NH1	1:A:318:GLU:OE1	2.51	0.43
1:D:152:THR:OG1	1:D:324:GLU:HB3	2.19	0.43
1:F:73:PHE:HD1	1:F:104:ILE:HD11	1.84	0.43
1:C:84:GLY:HA3	2:C:401:PO4:O4	2.18	0.43
1:C:290:ASP:OD2	1:C:326:THR:OG1	2.36	0.43
1:E:152:THR:OG1	1:E:324:GLU:HB3	2.18	0.43
1:F:54:SER:HA	1:F:57:ILE:CD1	2.37	0.43
1:F:101:ASN:CG	1:F:194:PRO:HA	2.37	0.43
1:A:97:PHE:O	1:A:100:ARG:NH2	2.52	0.43
1:A:232:GLY:HA3	1:A:260:MET:CE	2.49	0.42
1:B:152[A]:THR:OG1	1:B:324:GLU:HB3	2.18	0.42
1:E:248:VAL:O	1:E:252:THR:HG22	2.19	0.42
1:E:303:ALA:CB	1:E:316:ILE:CD1	2.96	0.42
1:A:6:LEU:HD22	1:A:49:ILE:HD12	2.00	0.42
1:F:25:LEU:HB3	1:F:29:ASP:CG	2.43	0.42
1:B:8:THR:HG22	1:B:82:THR:O	2.19	0.42
1:A:124:ARG:NE	1:A:145:MET:HA	2.34	0.42
1:C:88:LEU:HD11	1:C:108:LEU:HB3	2.02	0.42
1:F:303:ALA:CB	1:F:316:ILE:CD1	2.97	0.42
1:F:311:GLU:OE1	1:F:314:ARG:NH1	2.50	0.42
1:A:190:GLY:HA2	5:A:549:HOH:O	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:272:THR:O	1:E:278:ARG:NH1	2.42	0.42
1:C:8:THR:HG23	5:C:520:HOH:O	2.20	0.41
1:E:8:THR:HG23	5:E:512:HOH:O	2.20	0.41
1:E:240:TYR:CZ	1:E:279:ARG:CB	3.03	0.41
1:F:101:ASN:ND2	1:F:193:GLU:C	2.78	0.41
1:C:8:THR:HG22	1:C:82:THR:O	2.20	0.41
1:F:15:ALA:N	1:F:20:GLY:O	2.53	0.41
1:F:139:GLY:HA3	1:F:189:ILE:HD13	2.01	0.41
1:D:184:ARG:CD	1:D:184:ARG:O	2.68	0.41
1:E:301:MET:HE1	1:F:211:PRO:O	2.21	0.41
1:F:101:ASN:OD1	1:F:193:GLU:C	2.63	0.41
1:E:142:VAL:HG21	1:E:154:VAL:HG21	2.02	0.41
1:E:240:TYR:CG	1:E:246:LEU:HB3	2.56	0.41
1:F:195:LEU:HD13	1:F:197:ASP:HB2	2.03	0.41
1:F:303:ALA:CB	1:F:316:ILE:HD11	2.45	0.41
1:F:175:TYR:OH	1:F:184:ARG:NH1	2.54	0.41
1:F:124:ARG:HD3	1:F:124:ARG:H	1.85	0.40
1:A:121:ASP:HB2	1:A:124:ARG:HH22	1.86	0.40
1:C:222:ALA:O	1:C:256:LYS:NZ	2.48	0.40
1:A:186:LYS:HE2	1:A:189:ILE:HD12	2.04	0.40
1:C:119:ASN:HD22	1:C:119:ASN:HA	1.73	0.40
1:C:175:TYR:OH	1:C:184[B]:ARG:NH1	2.54	0.40
1:E:36:ILE:HG22	1:E:37:ARG:N	2.37	0.40
1:E:246:LEU:HD13	1:E:246:LEU:C	2.46	0.40
1:C:268:GLY:HA3	1:C:290:ASP:HA	2.03	0.40
1:F:124:ARG:O	1:F:127:ARG:HG2	2.22	0.40

All (2) 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)
5:B:504:HOH:O	5:D:502:HOH:O[1_445]	1.05	1.15
1:B:51:ASN:OD1	1:D:28:ASP:OD2[1_445]	2.14	0.06

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	328/328 (100%)	321 (98%)	5 (2%)	2 (1%)	21	20
1	B	330/328 (101%)	319 (97%)	9 (3%)	2 (1%)	21	20
1	C	329/328 (100%)	315 (96%)	9 (3%)	5 (2%)	8	5
1	D	327/328 (100%)	316 (97%)	7 (2%)	4 (1%)	10	7
1	E	326/328 (99%)	315 (97%)	8 (2%)	3 (1%)	14	12
1	F	327/328 (100%)	306 (94%)	14 (4%)	7 (2%)	5	3
All	All	1967/1968 (100%)	1892 (96%)	52 (3%)	23 (1%)	10	7

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	37	ARG
1	A	38	ARG
1	B	37	ARG
1	B	38	ARG
1	C	37	ARG
1	C	38	ARG
1	D	37	ARG
1	D	38	ARG
1	D	224	ALA
1	E	37	ARG
1	E	38	ARG
1	F	15	ALA
1	F	36	ILE
1	F	37	ARG
1	F	38	ARG
1	F	40	ASP
1	F	191	ASN
1	C	23	ALA
1	C	24	ALA
1	F	22	LYS
1	C	40	ASP
1	D	40	ASP
1	E	327	GLY

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	269/267 (101%)	259 (96%)	10 (4%)	30	38
1	B	271/267 (102%)	262 (97%)	9 (3%)	33	42
1	C	270/267 (101%)	254 (94%)	16 (6%)	18	19
1	D	268/267 (100%)	256 (96%)	12 (4%)	24	30
1	E	267/267 (100%)	249 (93%)	18 (7%)	15	15
1	F	268/267 (100%)	242 (90%)	26 (10%)	8	7
All	All	1613/1602 (101%)	1522 (94%)	91 (6%)	18	21

All (91) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	GLU
1	A	100	ARG
1	A	115	ILE
1	A	145	MET
1	A	180	GLU
1	A	195	LEU
1	A	272	THR
1	A	293	LYS
1	A	319	ARG
1	A	321	ILE
1	B	8	THR
1	B	39	GLU
1	B	43	LYS
1	B	75	GLU
1	B	115	ILE
1	B	180	GLU
1	B	188	ARG
1	B	195	LEU
1	B	275	GLU
1	C	8	THR
1	C	38	ARG
1	C	39	GLU

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Mol	Chain	Res	Type
1	C	40	ASP
1	C	43	LYS
1	C	46	THR
1	C	64	THR
1	C	75	GLU
1	C	115	ILE
1	C	134	ARG
1	C	145	MET
1	C	160	LEU
1	C	180	GLU
1	C	191	ASN
1	C	210	THR
1	C	319	ARG
1	D	8	THR
1	D	39	GLU
1	D	75	GLU
1	D	154	VAL
1	D	160	LEU
1	D	180	GLU
1	D	184	ARG
1	D	193	GLU
1	D	195	LEU
1	D	210	THR
1	D	223	ARG
1	D	272	THR
1	E	8	THR
1	E	16	LYS
1	E	46	THR
1	E	115	ILE
1	E	145	MET
1	E	180	GLU
1	E	207	ILE
1	E	216	GLU
1	E	228	ILE
1	E	240	TYR
1	E	246	LEU
1	E	254	ARG
1	E	260	MET
1	E	272	THR
1	E	278	ARG
1	E	281	LEU
1	E	316	ILE

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Mol	Chain	Res	Type
1	E	321	ILE
1	F	6	LEU
1	F	19	MET
1	F	33	LEU
1	F	36	ILE
1	F	44	ILE
1	F	46	THR
1	F	47	ARG
1	F	49	ILE
1	F	57	ILE
1	F	65	ILE
1	F	75	GLU
1	F	88	LEU
1	F	101	ASN
1	F	104	ILE
1	F	115	ILE
1	F	124	ARG
1	F	177	LYS
1	F	186	LYS
1	F	188	ARG
1	F	195	LEU
1	F	219	ARG
1	F	272	THR
1	F	286	ILE
1	F	312	GLU
1	F	321	ILE
1	F	325	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	GLN
1	A	163	ASN
1	B	83	HIS
1	B	163	ASN
1	B	166	GLN
1	C	119	ASN
1	E	163	ASN
1	E	203	ASN
1	E	206	HIS
1	F	51	ASN

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 ⓘ

13 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	C	401	-	4,4,4	1.72	1 (25%)	6,6,6	3.35	5 (83%)
3	EDO	D	402	-	3,3,3	0.46	0	2,2,2	0.84	0
2	PO4	B	401	-	4,4,4	2.17	1 (25%)	6,6,6	3.26	3 (50%)
3	EDO	B	402	-	3,3,3	0.67	0	2,2,2	0.55	0
3	EDO	A	402	-	3,3,3	1.06	0	2,2,2	0.41	0
2	PO4	E	401	-	4,4,4	2.00	2 (50%)	6,6,6	1.93	3 (50%)
2	PO4	F	401	-	4,4,4	2.22	1 (25%)	6,6,6	1.31	1 (16%)
2	PO4	A	401	-	4,4,4	2.17	1 (25%)	6,6,6	2.48	2 (33%)
3	EDO	F	402	-	3,3,3	0.59	0	2,2,2	0.18	0
4	PG4	B	404	-	9,9,12	0.44	0	8,8,11	1.06	1 (12%)
3	EDO	B	403	-	3,3,3	0.54	0	2,2,2	0.80	0
3	EDO	D	403	-	3,3,3	0.68	0	2,2,2	0.46	0
2	PO4	D	401	-	4,4,4	2.56	2 (50%)	6,6,6	4.07	5 (83%)

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	EDO	D	402	-	-	1/1/1/1	-
3	EDO	B	402	-	-	0/1/1/1	-
3	EDO	A	402	-	-	0/1/1/1	-
3	EDO	F	402	-	-	1/1/1/1	-
4	PG4	B	404	-	-	5/7/7/10	-
3	EDO	B	403	-	-	1/1/1/1	-
3	EDO	D	403	-	-	1/1/1/1	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	401	PO4	P-O4	-4.02	1.42	1.54
2	F	401	PO4	P-O1	4.02	1.59	1.50
2	A	401	PO4	P-O2	-3.59	1.44	1.54
2	B	401	PO4	P-O4	-3.04	1.45	1.54
2	D	401	PO4	P-O2	-3.00	1.45	1.54
2	C	401	PO4	P-O3	-2.93	1.46	1.54
2	E	401	PO4	P-O4	-2.91	1.46	1.54
2	E	401	PO4	P-O1	2.04	1.55	1.50

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	401	PO4	O4-P-O1	-6.23	88.92	110.95
2	B	401	PO4	O2-P-O1	-5.92	90.00	110.95
2	C	401	PO4	O4-P-O3	5.25	124.26	107.91
2	D	401	PO4	O3-P-O2	-4.65	93.43	107.91
2	B	401	PO4	O3-P-O2	4.07	120.56	107.91
2	D	401	PO4	O4-P-O3	4.04	120.50	107.91
2	A	401	PO4	O2-P-O1	3.93	124.86	110.95
2	A	401	PO4	O4-P-O2	-3.66	96.51	107.91
2	C	401	PO4	O3-P-O1	-3.54	98.44	110.95
2	C	401	PO4	O3-P-O2	3.49	118.79	107.91
2	D	401	PO4	O2-P-O1	3.49	123.29	110.95
2	B	401	PO4	O4-P-O2	3.35	118.35	107.91
2	C	401	PO4	O4-P-O2	-3.19	98.00	107.91
2	E	401	PO4	O4-P-O3	2.79	116.61	107.91
2	E	401	PO4	O4-P-O1	-2.66	101.54	110.95
2	D	401	PO4	O4-P-O2	2.61	116.05	107.91
2	F	401	PO4	O3-P-O2	2.47	115.60	107.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	401	PO4	O3-P-O2	-2.30	100.77	107.91
2	C	401	PO4	O2-P-O1	-2.12	103.46	110.95
4	B	404	PG4	O1-C1-C2	-2.05	99.78	111.82

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	404	PG4	O1-C1-C2-O2
4	B	404	PG4	O2-C3-C4-O3
4	B	404	PG4	C6-C5-O3-C4
4	B	404	PG4	C1-C2-O2-C3
3	F	402	EDO	O1-C1-C2-O2
4	B	404	PG4	O3-C5-C6-O4
3	B	403	EDO	O1-C1-C2-O2
3	D	403	EDO	O1-C1-C2-O2
3	D	402	EDO	O1-C1-C2-O2

There are no ring outliers.

6 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	401	PO4	1	0
2	E	401	PO4	1	0
2	A	401	PO4	1	0
3	F	402	EDO	1	0
4	B	404	PG4	2	0
3	D	403	EDO	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	328/328 (100%)	0.06	0	100	100	22, 56, 96, 147	2 (0%)
1	B	328/328 (100%)	0.08	0	100	100	24, 64, 107, 150	3 (0%)
1	C	328/328 (100%)	0.19	4 (1%)	76	76	25, 61, 105, 145	3 (0%)
1	D	328/328 (100%)	0.21	2 (0%)	85	84	34, 64, 106, 165	1 (0%)
1	E	328/328 (100%)	0.63	22 (6%)	24	23	44, 78, 146, 180	0
1	F	328/328 (100%)	1.52	93 (28%)	1	1	46, 115, 167, 205	1 (0%)
All	All	1968/1968 (100%)	0.45	121 (6%)	27	26	22, 69, 140, 205	10 (0%)

All (121) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	106	VAL	6.0
1	F	143	ALA	5.5
1	F	130	LEU	4.5
1	F	36	ILE	4.2
1	F	20	GLY	4.1
1	F	5	VAL	4.0
1	F	183	VAL	3.9
1	F	107	VAL	3.9
1	F	139	GLY	3.9
1	E	240	TYR	3.8
1	F	57	ILE	3.7
1	F	182	LEU	3.6
1	F	204	VAL	3.6
1	F	126	LEU	3.5
1	F	108	LEU	3.4
1	F	49	ILE	3.4
1	F	68	ALA	3.4
1	F	16	LYS	3.3
1	F	78	GLY	3.3

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Mol	Chain	Res	Type	RSRZ
1	F	25	LEU	3.3
1	F	88	LEU	3.3
1	F	175	TYR	3.2
1	F	115	ILE	3.2
1	F	137	PHE	3.2
1	F	79	ILE	3.2
1	F	42	ALA	3.2
1	F	35	GLY	3.2
1	F	24	ALA	3.1
1	E	189	ILE	3.1
1	F	23	ALA	3.1
1	F	296	THR	3.0
1	F	132	PHE	3.0
1	F	33	LEU	2.9
1	F	95	LEU	2.9
1	F	300	LEU	2.9
1	F	154	VAL	2.9
1	F	205	VAL	2.9
1	F	82	THR	2.9
1	C	23	ALA	2.9
1	F	138	PRO	2.8
1	F	12	ILE	2.8
1	F	123	PRO	2.8
1	F	189	ILE	2.8
1	F	4	LEU	2.8
1	E	246	LEU	2.8
1	F	31	LEU	2.8
1	F	181	VAL	2.8
1	F	69	VAL	2.7
1	F	3	LEU	2.7
1	F	56	LEU	2.7
1	F	150	LEU	2.7
1	F	104	ILE	2.7
1	F	15	ALA	2.7
1	F	17	THR	2.7
1	F	249	VAL	2.7
1	E	238	ILE	2.6
1	F	140	ILE	2.6
1	D	160	LEU	2.6
1	F	200	LEU	2.6
1	F	213	LEU	2.6
1	F	21	TYR	2.6

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Mol	Chain	Res	Type	RSRZ
1	E	313	ILE	2.6
1	F	142	VAL	2.6
1	F	168	ILE	2.6
1	F	162	LEU	2.6
1	F	113	LEU	2.5
1	F	160	LEU	2.5
1	F	99	ILE	2.5
1	F	148	ILE	2.5
1	F	176	VAL	2.4
1	C	17	THR	2.4
1	F	116	THR	2.4
1	F	19	MET	2.4
1	F	22	LYS	2.4
1	E	328	SER	2.4
1	F	134	ARG	2.4
1	E	286	ILE	2.4
1	F	128	THR	2.4
1	E	271	LEU	2.3
1	E	248	VAL	2.3
1	F	322	ALA	2.3
1	E	316	ILE	2.3
1	F	18	GLU	2.3
1	F	259	VAL	2.3
1	F	149	MET	2.3
1	F	295	ALA	2.3
1	E	236	GLY	2.3
1	F	30	ILE	2.2
1	D	249	VAL	2.2
1	F	102	PRO	2.2
1	F	218	LEU	2.2
1	F	93	SER	2.2
1	F	144	PHE	2.2
1	E	204	VAL	2.2
1	E	285	VAL	2.2
1	F	317	MET	2.2
1	F	227	GLY	2.2
1	C	24	ALA	2.2
1	E	218	LEU	2.2
1	E	115	ILE	2.2
1	F	50	LEU	2.2
1	F	131	THR	2.2
1	F	152	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	235	ALA	2.1
1	E	213	LEU	2.1
1	F	76	TYR	2.1
1	F	302	TRP	2.1
1	F	65	ILE	2.1
1	F	325	ILE	2.1
1	F	80	VAL	2.1
1	F	217	VAL	2.1
1	F	242	GLY	2.1
1	E	140	ILE	2.1
1	F	206	HIS	2.0
1	C	116	THR	2.0
1	E	215	PRO	2.0
1	F	11	THR	2.0
1	E	276	VAL	2.0
1	F	70	PHE	2.0
1	E	211	PRO	2.0
1	E	284	GLY	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	F	401	5/5	0.79	0.12	98,99,103,106	0
4	PG4	B	404	10/13	0.90	0.11	73,79,89,90	0
3	EDO	D	402	4/4	0.95	0.07	59,60,63,65	0
3	EDO	F	402	4/4	0.95	0.09	68,72,72,75	0
3	EDO	B	403	4/4	0.95	0.10	60,61,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	EDO	A	402	4/4	0.96	0.07	42,43,44,45	0
3	EDO	D	403	4/4	0.96	0.08	58,61,62,65	0
3	EDO	B	402	4/4	0.96	0.08	48,51,52,53	0
2	PO4	C	401	5/5	0.96	0.08	62,63,69,71	0
2	PO4	B	401	5/5	0.98	0.06	49,49,54,57	0
2	PO4	A	401	5/5	0.98	0.05	41,45,48,48	0
2	PO4	D	401	5/5	0.98	0.05	46,48,55,56	0
2	PO4	E	401	5/5	0.98	0.05	50,53,54,55	0

6.5 Other polymers [i](#)

There are no such residues in this entry.