



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 12:36 AM UTC

PDB ID : 4BPT / pdb_00004bpt
Title : Structural and thermodynamic insight into phenylalanine hydroxylase from the human pathogen *Legionella pneumophila*
Authors : Leiros, H.-K.S.; Flydal, M.I.; Martinez, A.
Deposited on : 2013-05-28
Resolution : 2.50 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

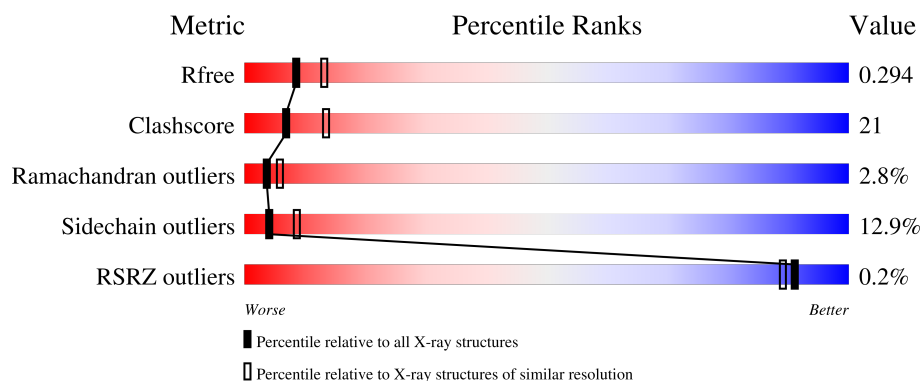
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	272	
1	B	272	
1	C	272	
1	D	272	

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	PEG	A	1260	-	-	X	-
2	PEG	A	1261	-	-	X	-
2	PEG	A	1262	-	-	X	-
2	PEG	B	1260	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8155 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 PHENYLALANINE-4-HYDROXYLASE (PAH) (PHE-4-MO NOOXYGENASE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	252	Total	C	N	O	S	5	1	0
			2062	1345	331	377	9			
1	B	252	Total	C	N	O	S	10	0	0
			2053	1340	330	374	9			
1	C	232	Total	C	N	O	S	193	0	0
			1900	1246	302	343	9			
1	D	237	Total	C	N	O	S	135	0	0
			1943	1272	311	351	9			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	60	THR	ILE	conflict	UNP I7HM43
B	60	THR	ILE	conflict	UNP I7HM43
C	60	THR	ILE	conflict	UNP I7HM43
D	60	THR	ILE	conflict	UNP I7HM43

- Molecule 2 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			7	4	3		
2	A	1	Total	C	O	0	0
			7	4	3		
2	A	1	Total	C	O	0	0
			7	4	3		
2	B	1	Total	C	O	0	0
			7	4	3		
2	B	1	Total	C	O	0	0
			7	4	3		
2	B	1	Total	C	O	0	0
			7	4	3		

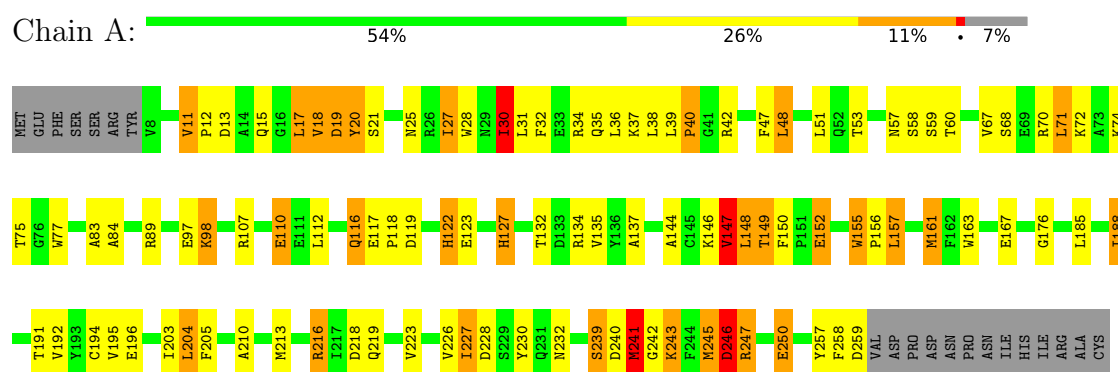
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	56	Total	O	0	0
			56	56		
3	B	51	Total	O	0	0
			51	51		
3	C	27	Total	O	0	0
			27	27		
3	D	21	Total	O	0	0
			21	21		

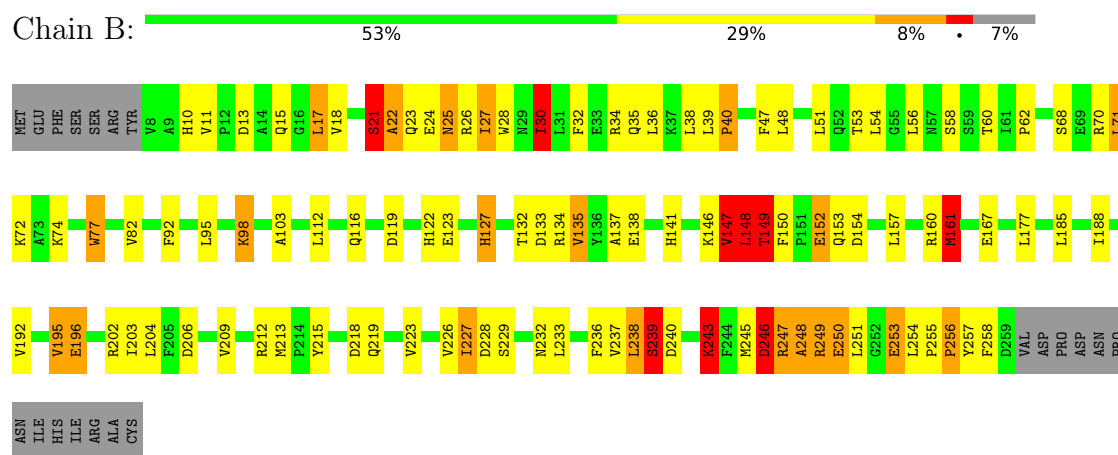
3 Residue-property plots

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.

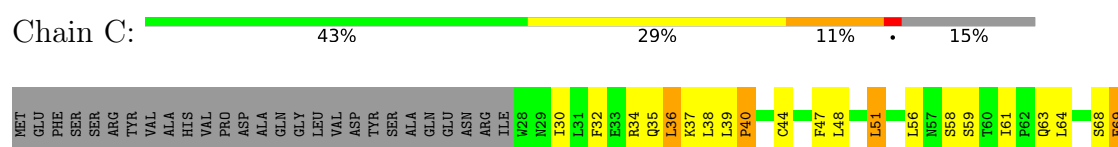
- Molecule 1: PHENYLALANINE-4-HYDROXYLASE (PAH) (PHE-4-MONOOXYGENASE)

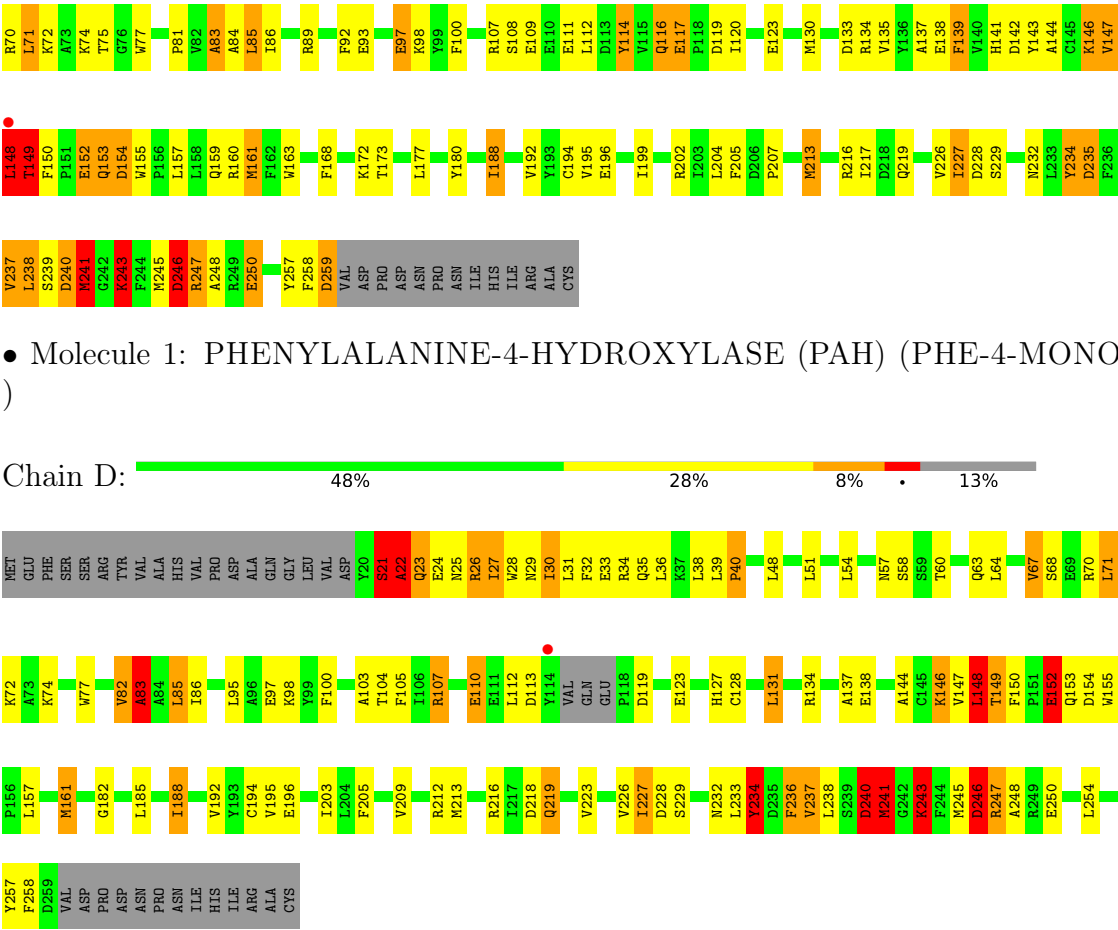


- Molecule 1: PHENYLALANINE-4-HYDROXYLASE (PAH) (PHE-4-MONOOXYGENASE)



- Molecule 1: PHENYLALANINE-4-HYDROXYLASE (PAH) (PHE-4-MONOOXYGENASE)





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	90.32Å 60.12Å 124.04Å 90.00° 94.07° 90.00°	Depositor
Resolution (Å)	10.00 – 2.50 10.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	90.4 (10.00-2.50) 90.5 (10.00-2.50)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.35 (at 2.50Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.264 , 0.302 (Not available) , 0.294	Depositor DCC
R_{free} test set	5871 reflections (12.63%)	wwPDB-VP
Wilson B-factor (Å ²)	38.6	Xtriage
Anisotropy	0.262	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 38.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	8155	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 18.43% 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: PEG

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	1.58	19/2121 (0.9%)	1.42	21/2885 (0.7%)
1	B	1.79	19/2112 (0.9%)	1.51	29/2873 (1.0%)
1	C	3.09	50/1956 (2.6%)	2.60	80/2659 (3.0%)
1	D	2.55	32/1999 (1.6%)	2.03	59/2714 (2.2%)
All	All	2.31	120/8188 (1.5%)	1.93	189/11131 (1.7%)

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	A	0	1
1	B	1	4
1	C	1	6
1	D	0	6
All	All	2	17

All (120) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	109	GLU	C-N	-49.39	0.67	1.34
1	C	81	PRO	C-N	-48.19	0.74	1.33
1	D	27	ILE	CA-CB	43.80	2.05	1.54
1	D	85	LEU	CB-CG	40.35	2.34	1.53
1	D	63	GLN	CG-CD	34.06	2.37	1.52
1	C	112	LEU	CB-CG	-34.06	0.85	1.53
1	B	21	SER	CA-CB	-33.17	1.10	1.53
1	D	104	THR	CA-CB	32.99	1.96	1.52
1	C	148	LEU	CB-CG	-32.48	0.88	1.53
1	C	108	SER	C-N	32.45	1.75	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	57	ASN	CA-CB	31.19	2.05	1.53
1	C	149	THR	CB-CG2	30.75	2.54	1.52
1	B	239	SER	CB-OG	-29.35	0.83	1.42
1	C	117	GLU	CG-CD	-28.90	0.79	1.52
1	C	146	LYS	CE-NZ	27.45	2.31	1.49
1	C	69	GLU	CA-CB	26.16	1.97	1.53
1	C	246	ASP	CB-CG	24.41	2.13	1.52
1	C	92	PHE	CB-CG	-24.00	0.95	1.50
1	A	110	GLU	CB-CG	23.96	2.24	1.52
1	D	82	VAL	C-N	23.37	1.66	1.33
1	D	74	LYS	CA-CB	-21.68	1.19	1.53
1	D	107	ARG	CD-NE	-20.94	1.17	1.46
1	C	134	ARG	CA-CB	18.76	1.83	1.53
1	D	21	SER	CA-CB	-18.49	1.21	1.53
1	D	26	ARG	CA-CB	17.90	1.81	1.53
1	D	97	GLU	CB-CG	17.84	2.06	1.52
1	D	64	LEU	CA-CB	16.71	1.77	1.53
1	C	83	ALA	C-N	16.50	1.56	1.33
1	C	74	LYS	CA-CB	-15.88	1.28	1.53
1	C	85	LEU	CB-CG	15.68	1.84	1.53
1	C	111	GLU	CB-CG	15.26	1.98	1.52
1	C	234	TYR	CZ-OH	15.24	1.70	1.38
1	C	72	LYS	CB-CG	15.17	1.98	1.52
1	C	86	ILE	CA-CB	14.59	1.74	1.54
1	C	234	TYR	CE2-CZ	-14.14	1.04	1.38
1	C	149	THR	CB-OG1	-14.02	1.21	1.43
1	D	218	ASP	CG-OD1	13.96	1.51	1.25
1	C	64	LEU	CA-CB	-13.07	1.35	1.53
1	D	241	MET	SD-CE	-12.74	1.47	1.79
1	C	36	LEU	CA-CB	-12.46	1.33	1.53
1	C	259	ASP	CA-CB	-12.11	1.29	1.53
1	B	253	GLU	CD-OE1	-11.97	1.02	1.25
1	D	110	GLU	CB-CG	11.84	1.88	1.52
1	C	139	PHE	CD1-CE1	-11.69	1.03	1.38
1	A	239	SER	CB-OG	-11.43	1.19	1.42
1	D	83	ALA	C-N	-11.42	1.17	1.33
1	C	89	ARG	CB-CG	-10.77	1.20	1.52
1	C	139	PHE	CG-CD2	-10.62	1.16	1.38
1	D	105	PHE	CB-CG	-10.39	1.26	1.50
1	D	54	LEU	CB-CG	-10.30	1.32	1.53
1	C	61	ILE	CB-CG2	-10.23	1.18	1.52
1	D	138	GLU	CG-CD	10.16	1.77	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	153	GLN	CG-CD	-10.07	1.26	1.52
1	C	146	LYS	CG-CD	-9.84	1.23	1.52
1	C	141	HIS	CA-CB	9.78	1.68	1.53
1	D	234	TYR	CD1-CE1	9.61	1.67	1.38
1	D	95	LEU	CB-CG	9.51	1.72	1.53
1	C	234	TYR	CB-CG	-9.46	1.30	1.51
1	D	218	ASP	CG-OD2	-9.07	1.08	1.25
1	A	30	ILE	CA-CB	8.92	1.66	1.54
1	D	234	TYR	CE2-CZ	8.77	1.59	1.38
1	C	116	GLN	CG-CD	-8.53	1.30	1.52
1	B	22	ALA	N-CA	8.49	1.57	1.46
1	C	56	LEU	CB-CG	8.32	1.70	1.53
1	B	149	THR	CB-OG1	8.29	1.57	1.43
1	A	148	LEU	CA-C	-8.26	1.42	1.53
1	D	243	LYS	CA-CB	8.24	1.66	1.53
1	C	37	LYS	CB-CG	-8.06	1.28	1.52
1	A	148	LEU	N-CA	8.04	1.55	1.45
1	D	134	ARG	CG-CD	7.86	1.76	1.52
1	B	127	HIS	CG-CD2	7.65	1.44	1.35
1	A	83	ALA	N-CA	7.53	1.55	1.45
1	A	122	HIS	CG-CD2	7.44	1.44	1.35
1	B	30	ILE	CA-CB	7.43	1.64	1.54
1	B	148	LEU	N-CA	7.39	1.54	1.46
1	C	100	PHE	CA-CB	-7.38	1.39	1.52
1	C	240	ASP	CG-OD2	7.38	1.39	1.25
1	D	22	ALA	C-N	7.35	1.43	1.33
1	D	146	LYS	CB-CG	-7.11	1.31	1.52
1	C	241	MET	SD-CE	-7.00	1.62	1.79
1	C	234	TYR	CG-CD2	-6.96	1.24	1.39
1	B	141	HIS	CG-ND1	-6.93	1.30	1.38
1	D	153	GLN	CG-CD	6.92	1.69	1.52
1	A	147	VAL	CA-C	6.85	1.61	1.52
1	B	147	VAL	CA-CB	6.77	1.63	1.54
1	A	122	HIS	CE1-NE2	6.42	1.39	1.32
1	D	71	LEU	CA-CB	6.36	1.63	1.53
1	C	51	LEU	CG-CD2	-6.25	1.31	1.52
1	B	127	HIS	ND1-CE1	6.11	1.38	1.32
1	C	120	ILE	CG1-CD1	6.01	1.75	1.51
1	C	239	SER	CB-OG	5.98	1.54	1.42
1	D	70	ARG	CB-CG	-5.92	1.34	1.52
1	A	210	ALA	C-O	-5.84	1.17	1.24
1	A	204	LEU	CA-C	-5.79	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	59	SER	CA-CB	5.79	1.63	1.53
1	A	19	ASP	C-O	-5.78	1.17	1.23
1	D	226	VAL	CA-CB	5.70	1.61	1.54
1	A	67	VAL	CA-CB	5.66	1.61	1.54
1	A	127	HIS	ND1-CE1	5.65	1.38	1.32
1	B	122	HIS	CE1-NE2	5.61	1.38	1.32
1	C	120	ILE	CB-CG2	-5.55	1.34	1.52
1	B	250	GLU	CA-CB	5.53	1.62	1.53
1	C	202	ARG	C-O	5.52	1.30	1.24
1	C	250	GLU	CB-CG	-5.52	1.35	1.52
1	A	132	THR	CA-C	5.48	1.60	1.52
1	C	217	ILE	CG1-CD1	-5.46	1.30	1.51
1	C	63	GLN	CA-CB	5.34	1.61	1.53
1	B	10	HIS	CG-ND1	-5.25	1.32	1.38
1	C	204	LEU	N-CA	5.19	1.52	1.46
1	A	127	HIS	CE1-NE2	5.16	1.37	1.32
1	B	122	HIS	CG-CD2	5.12	1.41	1.35
1	A	122	HIS	ND1-CE1	5.12	1.37	1.32
1	B	77	TRP	CD2-CE2	5.09	1.50	1.41
1	D	67	VAL	CB-CG2	-5.09	1.35	1.52
1	C	107	ARG	CB-CG	-5.07	1.37	1.52
1	A	30	ILE	C-O	-5.07	1.18	1.24
1	B	77	TRP	NE1-CE2	-5.06	1.31	1.37
1	A	191	THR	N-CA	5.05	1.52	1.46
1	B	127	HIS	CG-ND1	-5.02	1.32	1.38
1	B	132	THR	CA-C	5.00	1.59	1.52

All (189) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	83	ALA	O-C-N	-43.53	61.35	122.29
1	D	22	ALA	O-C-N	-33.86	77.56	122.59
1	C	109	GLU	O-C-N	30.78	155.27	122.03
1	D	107	ARG	CD-NE-CZ	-30.14	82.20	124.40
1	C	117	GLU	CG-CD-OE1	-27.76	54.55	118.40
1	C	97	GLU	CA-CB-CG	24.80	163.70	114.10
1	C	153	GLN	CG-CD-NE2	-22.15	83.18	116.40
1	D	234	TYR	CE1-CZ-CE2	-22.04	76.22	120.30
1	C	117	GLU	CB-CG-CD	-21.46	76.12	112.60
1	C	81	PRO	O-C-N	-21.28	96.88	123.06
1	D	107	ARG	CG-CD-NE	-20.75	66.34	112.00
1	C	97	GLU	CB-CG-CD	20.74	147.86	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	149	THR	OG1-CB-CG2	-19.70	69.91	109.30
1	D	153	GLN	CG-CD-NE2	-19.68	86.88	116.40
1	C	117	GLU	CG-CD-OE2	18.17	160.20	118.40
1	C	148	LEU	CA-CB-CG	17.74	178.40	116.30
1	C	154	ASP	CA-CB-CG	17.37	129.97	112.60
1	C	116	GLN	CB-CG-CD	-17.22	83.33	112.60
1	D	26	ARG	N-CA-CB	-16.80	85.30	110.16
1	C	81	PRO	CA-C-N	16.74	144.43	122.51
1	C	81	PRO	C-N-CA	16.74	144.43	122.51
1	C	146	LYS	CD-CE-NZ	-16.60	58.77	111.90
1	C	153	GLN	CG-CD-OE1	16.35	153.50	120.80
1	D	21	SER	CA-CB-OG	-16.11	78.89	111.10
1	B	21	SER	N-CA-CB	15.89	136.59	110.37
1	D	234	TYR	CG-CD1-CE1	-15.89	97.37	121.20
1	C	149	THR	CA-CB-CG2	-15.44	84.25	110.50
1	D	98	LYS	CA-CB-CG	-15.31	83.48	114.10
1	C	112	LEU	CB-CG-CD2	-14.95	65.86	110.70
1	A	110	GLU	CA-CB-CG	-14.45	85.21	114.10
1	C	148	LEU	CB-CG-CD2	14.07	152.92	110.70
1	C	234	TYR	CB-CG-CD2	14.05	141.88	120.80
1	C	259	ASP	CA-CB-CG	13.52	126.12	112.60
1	C	246	ASP	CA-CB-CG	-13.49	99.11	112.60
1	D	21	SER	CB-CA-C	-13.48	90.41	111.17
1	C	259	ASP	N-CA-CB	13.45	133.36	110.50
1	A	110	GLU	CB-CG-CD	13.38	135.35	112.60
1	B	238	LEU	N-CA-C	-13.31	93.69	110.19
1	D	153	GLN	CG-CD-OE1	13.26	147.32	120.80
1	C	112	LEU	CB-CG-CD1	13.21	150.34	110.70
1	B	256	PRO	N-CA-C	12.87	130.58	113.98
1	C	239	SER	CA-CB-OG	-12.85	85.41	111.10
1	C	238	LEU	N-CA-C	-12.73	93.73	110.53
1	C	108	SER	CA-C-N	-12.28	103.93	120.63
1	C	108	SER	C-N-CA	-12.28	103.93	120.63
1	D	110	GLU	CB-CG-CD	12.02	133.03	112.60
1	C	74	LYS	N-CA-CB	-11.89	92.54	110.26
1	D	86	ILE	CA-CB-CG2	-11.72	90.57	110.50
1	C	134	ARG	N-CA-CB	-11.66	92.90	110.16
1	D	86	ILE	CA-CB-CG1	-11.63	90.63	110.40
1	C	61	ILE	CG1-CB-CG2	11.54	145.32	110.70
1	C	139	PHE	CG-CD1-CE1	11.44	140.15	120.70
1	D	63	GLN	CB-CG-CD	-11.17	93.61	112.60
1	D	86	ILE	CB-CG1-CD1	-11.16	90.35	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	75	THR	CA-CB-CG2	-11.04	91.74	110.50
1	C	93	GLU	CB-CG-CD	10.75	130.87	112.60
1	C	59	SER	N-CA-CB	10.73	128.62	110.49
1	D	97	GLU	CB-CG-CD	10.61	130.64	112.60
1	D	83	ALA	CA-C-N	-10.51	101.46	121.54
1	D	83	ALA	C-N-CA	-10.51	101.46	121.54
1	C	70	ARG	CB-CG-CD	10.47	135.39	111.30
1	C	83	ALA	CA-C-N	10.11	140.84	121.54
1	C	83	ALA	C-N-CA	10.11	140.84	121.54
1	C	100	PHE	CA-CB-CG	-9.95	103.85	113.80
1	C	109	GLU	CA-C-N	-9.95	105.96	120.28
1	C	109	GLU	C-N-CA	-9.95	105.96	120.28
1	C	92	PHE	CA-CB-CG	-9.85	103.95	113.80
1	A	246	ASP	N-CA-C	-9.69	96.83	110.50
1	D	97	GLU	CA-CB-CG	9.68	133.47	114.10
1	D	218	ASP	CB-CG-OD2	9.23	139.62	118.40
1	C	243	LYS	CG-CD-CE	-9.18	90.18	111.30
1	C	241	MET	CG-SD-CE	9.18	121.09	100.90
1	D	26	ARG	CB-CA-C	9.07	126.27	110.85
1	C	234	TYR	CD1-CG-CD2	-8.75	104.98	118.10
1	B	21	SER	CA-CB-OG	8.69	128.48	111.10
1	C	139	PHE	CD1-CE1-CZ	-8.64	104.45	120.00
1	C	234	TYR	CA-CB-CG	8.60	129.37	113.90
1	B	246	ASP	N-CA-C	-8.56	98.42	110.50
1	D	27	ILE	CA-CB-CG2	-8.54	95.98	110.50
1	D	236	PHE	N-CA-C	-8.53	97.65	110.28
1	C	93	GLU	CA-CB-CG	8.50	131.10	114.10
1	C	246	ASP	N-CA-C	-8.49	98.52	110.50
1	C	234	TYR	CG-CD2-CE2	8.47	133.91	121.20
1	D	74	LYS	CA-CB-CG	-8.43	97.24	114.10
1	A	239	SER	CA-CB-OG	8.37	127.84	111.10
1	B	148	LEU	N-CA-C	8.26	122.88	109.59
1	D	246	ASP	N-CA-C	-8.24	98.88	110.50
1	C	85	LEU	CB-CG-CD2	-8.18	86.16	110.70
1	B	161	MET	CG-SD-CE	-8.03	83.23	100.90
1	D	27	ILE	N-CA-CB	-8.00	101.19	110.55
1	D	57	ASN	CB-CA-C	-8.00	94.82	109.54
1	D	54	LEU	CB-CG-CD1	-7.89	87.04	110.70
1	C	51	LEU	CD1-CG-CD2	7.88	128.15	110.80
1	D	54	LEU	CA-CB-CG	-7.86	88.79	116.30
1	C	72	LYS	CB-CG-CD	7.72	129.06	111.30
1	C	120	ILE	CA-CB-CG2	7.63	123.47	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	72	LYS	CA-CB-CG	7.59	129.27	114.10
1	D	67	VAL	CG1-CB-CG2	7.58	127.47	110.80
1	B	255	PRO	CA-C-N	7.56	127.23	119.82
1	B	255	PRO	C-N-CA	7.56	127.23	119.82
1	A	148	LEU	N-CA-CB	7.48	121.93	110.49
1	C	92	PHE	CB-CG-CD2	-7.48	107.99	120.70
1	D	234	TYR	CD1-CE1-CZ	7.46	133.03	119.60
1	C	70	ARG	CG-CD-NE	7.29	128.03	112.00
1	C	74	LYS	CB-CA-C	7.29	123.88	110.11
1	A	155	TRP	CA-C-N	-7.25	110.94	118.85
1	A	155	TRP	C-N-CA	-7.25	110.94	118.85
1	D	23	GLN	O-C-N	-7.24	111.42	123.00
1	B	226	VAL	N-CA-C	7.20	118.25	108.17
1	D	104	THR	CB-CA-C	-7.16	102.26	111.50
1	D	74	LYS	CB-CA-C	-7.14	96.62	110.11
1	B	253	GLU	CG-CD-OE1	-7.08	102.11	118.40
1	B	148	LEU	CA-C-O	7.07	128.21	120.71
1	D	218	ASP	CB-CG-OD1	-7.05	102.18	118.40
1	D	67	VAL	CA-CB-CG2	6.79	121.94	110.40
1	C	250	GLU	CB-CG-CD	-6.79	101.06	112.60
1	D	57	ASN	CA-CB-CG	-6.72	105.88	112.60
1	B	196	GLU	CB-CA-C	-6.61	99.09	109.34
1	C	61	ILE	CA-CB-CG1	-6.51	99.34	110.40
1	C	92	PHE	CB-CG-CD1	6.49	131.73	120.70
1	B	135	VAL	N-CA-C	-6.38	104.27	110.72
1	D	71	LEU	N-CA-CB	-6.35	100.81	110.01
1	B	249	ARG	CB-CA-C	6.31	122.79	110.67
1	C	75	THR	OG1-CB-CG2	6.27	121.83	109.30
1	D	85	LEU	CB-CG-CD2	-6.16	92.22	110.70
1	D	29	ASN	CB-CA-C	-6.15	100.97	110.81
1	C	148	LEU	CB-CG-CD1	-6.06	92.53	110.70
1	D	71	LEU	CB-CA-C	-6.00	101.46	110.88
1	D	152	GLU	CG-CD-OE1	-5.97	104.67	118.40
1	D	209	VAL	N-CA-C	-5.92	104.55	111.00
1	B	149	THR	N-CA-C	-5.92	98.20	110.80
1	B	25	ASN	N-CA-C	5.89	117.70	111.28
1	A	167	GLU	N-CA-C	5.88	118.57	111.40
1	A	67	VAL	N-CA-C	-5.88	105.00	110.53
1	A	149	THR	N-CA-C	-5.87	98.30	110.80
1	A	226	VAL	N-CA-C	5.83	116.33	108.17
1	C	240	ASP	OD1-CG-OD2	-5.78	109.03	122.90
1	D	64	LEU	CB-CA-C	-5.76	101.06	112.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	148	LEU	N-CA-C	-5.74	101.46	110.36
1	B	243	LYS	N-CA-C	5.71	117.18	111.07
1	C	155	TRP	CA-C-N	-5.68	112.65	118.85
1	C	155	TRP	C-N-CA	-5.68	112.65	118.85
1	B	27	ILE	CB-CA-C	-5.68	104.70	111.97
1	D	234	TYR	CZ-CE2-CD2	-5.68	109.38	119.60
1	C	36	LEU	CB-CA-C	5.67	120.32	110.68
1	A	97	GLU	CA-CB-CG	5.65	125.40	114.10
1	C	234	TYR	CB-CG-CD1	-5.65	112.33	120.80
1	D	134	ARG	CB-CG-CD	-5.62	98.38	111.30
1	D	155	TRP	CA-C-N	-5.60	112.74	118.85
1	D	155	TRP	C-N-CA	-5.60	112.74	118.85
1	C	56	LEU	CB-CG-CD2	5.54	127.32	110.70
1	A	241	MET	O-C-N	-5.50	115.28	122.59
1	D	98	LYS	CB-CG-CD	-5.48	98.71	111.30
1	B	98	LYS	N-CA-C	5.43	119.19	112.24
1	D	74	LYS	N-CA-CB	-5.43	102.17	110.26
1	C	37	LYS	CB-CG-CD	5.39	123.70	111.30
1	C	86	ILE	N-CA-CB	-5.36	102.39	111.23
1	C	192	VAL	CB-CA-C	-5.36	104.87	111.94
1	B	215	TYR	N-CA-C	5.34	116.96	108.79
1	B	10	HIS	CA-C-N	-5.33	118.14	123.04
1	B	10	HIS	C-N-CA	-5.33	118.14	123.04
1	B	21	SER	CA-C-N	5.33	131.72	121.54
1	B	21	SER	C-N-CA	5.33	131.72	121.54
1	D	153	GLN	CB-CG-CD	-5.31	103.57	112.60
1	C	74	LYS	CA-CB-CG	5.30	124.71	114.10
1	D	243	LYS	CB-CA-C	-5.30	102.52	110.90
1	D	57	ASN	N-CA-CB	-5.30	102.54	110.17
1	D	105	PHE	CB-CG-CD1	5.30	129.70	120.70
1	D	63	GLN	CG-CD-NE2	-5.29	108.47	116.40
1	A	176	GLY	N-CA-C	5.27	118.17	111.85
1	D	105	PHE	CB-CG-CD2	-5.27	111.74	120.70
1	C	226	VAL	N-CA-C	5.26	115.54	108.17
1	A	98	LYS	N-CA-C	5.24	118.94	112.24
1	C	217	ILE	CB-CG1-CD1	-5.21	102.85	113.80
1	D	250	GLU	CB-CA-C	-5.16	103.01	110.96
1	B	249	ARG	CA-CB-CG	5.13	124.36	114.10
1	D	70	ARG	CA-CB-CG	5.11	124.33	114.10
1	A	20	TYR	CA-C-N	-5.10	113.92	123.05
1	A	20	TYR	C-N-CA	-5.10	113.92	123.05
1	C	107	ARG	CB-CG-CD	-5.09	99.58	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	64	LEU	CB-CA-C	-5.08	102.34	112.05
1	C	120	ILE	CG1-CB-CG2	-5.08	95.48	110.70
1	C	100	PHE	CB-CA-C	-5.06	102.10	109.38
1	B	248	ALA	N-CA-C	-5.05	105.67	111.07
1	B	238	LEU	CA-C-O	-5.04	116.71	122.01
1	A	84	ALA	CA-C-N	-5.04	115.47	123.24
1	A	84	ALA	C-N-CA	-5.04	115.47	123.24
1	B	250	GLU	CB-CA-C	-5.03	102.96	110.90
1	A	27	ILE	CB-CA-C	-5.01	105.56	111.97

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	B	21	SER	CA
1	C	259	ASP	CA

All (17) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	147	VAL	Peptide
1	B	147	VAL	Peptide
1	B	148	LEU	Peptide
1	B	21	SER	Peptide
1	B	253	GLU	Sidechain
1	C	148	LEU	Peptide
1	C	240	ASP	Sidechain
1	C	241	MET	Peptide
1	C	246	ASP	Sidechain
1	C	83	ALA	Mainchain,Peptide
1	D	148	LEU	Peptide
1	D	22	ALA	Mainchain
1	D	23	GLN	Peptide
1	D	234	TYR	Sidechain
1	D	240	ASP	Peptide
1	D	83	ALA	Mainchain

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	2062	0	2010	88	0
1	B	2053	0	2005	96	0
1	C	1900	0	1857	58	0
1	D	1943	0	1900	66	0
2	A	21	0	30	14	0
2	B	21	0	30	8	0
3	A	56	0	0	5	0
3	B	51	0	0	14	0
3	C	27	0	0	3	0
3	D	21	0	0	0	0
All	All	8155	0	7832	319	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 21.

All (319) 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:44:CYS:SG	1:C:130:MET:HE1	1.26	1.68
1:C:44:CYS:SG	1:C:130:MET:CE	2.13	1.34
1:B:26:ARG:N	3:B:2006:HOH:O	1.71	1.21
1:B:27:ILE:N	3:B:2006:HOH:O	1.73	1.19
1:A:127:HIS:NE2	3:A:2032:HOH:O	1.76	1.12
1:B:177:LEU:HD23	1:B:195:VAL:HG12	1.32	1.11
1:A:30:ILE:HD11	1:A:112:LEU:HD21	1.25	1.07
1:B:30:ILE:HD11	1:B:112:LEU:HD21	1.08	1.06
1:D:194:CYS:SG	1:D:195:VAL:HG13	1.96	1.04
1:A:148:LEU:O	1:A:149:THR:HB	1.49	1.04
1:C:142:ASP:CG	1:C:237:VAL:HG11	1.84	1.02
1:B:161:MET:HE3	1:B:161:MET:C	1.86	1.00
1:C:142:ASP:OD2	1:C:237:VAL:HG11	1.62	0.99
1:D:236:PHE:O	1:D:237:VAL:HG22	1.60	0.99
2:A:1262:PEG:H11	2:A:1262:PEG:H42	1.42	0.98
1:C:154:ASP:HB3	1:C:245:MET:HE1	1.44	0.98
1:A:25:ASN:ND2	1:A:60:THR:HG22	1.79	0.97
1:D:212:ARG:HB3	1:D:254:LEU:HD13	1.46	0.96
2:A:1262:PEG:H42	2:A:1262:PEG:C1	1.93	0.96
1:D:154:ASP:HB3	1:D:245:MET:HE1	1.49	0.95
1:B:30:ILE:CD1	1:B:112:LEU:HD21	1.96	0.93
1:C:47:PHE:HB2	1:C:130:MET:HE2	1.50	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:44:CYS:HG	1:C:130:MET:HE1	1.27	0.90
1:B:25:ASN:HD22	1:B:60:THR:HA	1.37	0.90
1:A:149:THR:HG21	3:A:2036:HOH:O	1.73	0.89
1:B:212:ARG:HB3	1:B:254:LEU:HD13	1.55	0.88
1:A:163:TRP:HZ3	2:A:1261:PEG:H22	1.41	0.86
1:A:148:LEU:O	1:A:149:THR:CB	2.19	0.85
1:B:202:ARG:HD2	3:B:2040:HOH:O	1.75	0.85
2:B:1260:PEG:H42	2:B:1260:PEG:O1	1.76	0.85
1:B:148:LEU:O	1:B:149:THR:HG22	1.77	0.84
1:C:142:ASP:OD2	1:C:237:VAL:CG1	2.25	0.84
1:A:161:MET:C	1:A:161:MET:HE3	2.02	0.84
1:B:153:GLN:HG3	3:B:2033:HOH:O	1.77	0.82
1:B:25:ASN:ND2	1:B:60:THR:HA	1.93	0.82
1:A:30:ILE:CD1	1:A:112:LEU:HD21	2.10	0.81
1:B:240:ASP:OD2	1:B:243:LYS:HB2	1.80	0.80
1:D:25:ASN:ND2	1:D:60:THR:HG22	1.97	0.79
1:A:25:ASN:HD22	1:A:60:THR:HG22	1.46	0.79
1:B:148:LEU:C	1:B:149:THR:HG22	2.07	0.79
1:D:128:CYS:HA	1:D:131:LEU:HD22	1.62	0.79
1:D:25:ASN:HD22	1:D:60:THR:HG22	1.49	0.78
1:B:71:LEU:HD13	1:B:77:TRP:HB3	1.65	0.77
1:A:127:HIS:CE1	3:A:2032:HOH:O	2.28	0.77
1:B:154:ASP:HB3	1:B:245:MET:HE1	1.67	0.77
1:D:31:LEU:HD11	1:D:107:ARG:HD2	1.65	0.77
1:D:234:TYR:O	1:D:238:LEU:HD13	1.85	0.76
1:C:243:LYS:O	1:C:246:ASP:O	2.04	0.76
1:A:247:ARG:HA	1:A:250[B]:GLU:HG2	1.67	0.76
1:D:243:LYS:O	1:D:246:ASP:O	2.05	0.74
1:B:25:ASN:ND2	1:B:60:THR:HG22	2.03	0.73
1:A:148:LEU:C	1:A:150:PHE:H	1.95	0.72
1:A:146:LYS:O	1:A:148:LEU:O	2.08	0.72
1:B:243:LYS:O	1:B:246:ASP:O	2.07	0.72
2:A:1261:PEG:H11	2:A:1262:PEG:H12	1.72	0.71
1:B:213:MET:HE1	1:C:257:TYR:OH	1.91	0.71
2:A:1260:PEG:H22	2:A:1262:PEG:O4	1.90	0.71
1:D:154:ASP:CB	1:D:245:MET:HE1	2.20	0.70
1:A:194:CYS:SG	1:A:195:VAL:HG13	2.31	0.70
1:A:243:LYS:O	1:A:246:ASP:O	2.08	0.70
1:A:57:ASN:ND2	1:A:59:SER:HB3	2.07	0.69
1:A:163:TRP:CZ3	2:A:1261:PEG:H22	2.26	0.69
1:B:153:GLN:CB	3:B:2033:HOH:O	2.41	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:228:ASP:H	1:C:232:ASN:ND2	1.91	0.69
1:C:228:ASP:H	1:C:232:ASN:HD21	1.41	0.69
1:C:138:GLU:OE1	3:C:2014:HOH:O	2.11	0.68
1:A:150:PHE:CE1	1:A:245:MET:HE1	2.29	0.68
1:D:212:ARG:HB3	1:D:254:LEU:CD1	2.23	0.68
1:D:212:ARG:CZ	1:D:254:LEU:HD11	2.24	0.67
1:B:177:LEU:HD23	1:B:195:VAL:CG1	2.20	0.66
2:A:1261:PEG:H11	2:A:1262:PEG:C1	2.25	0.66
1:B:177:LEU:CD2	1:B:195:VAL:HG12	2.20	0.66
1:C:142:ASP:OD1	1:C:237:VAL:HG11	1.95	0.65
2:B:1260:PEG:O4	2:B:1262:PEG:H22	1.96	0.65
1:D:203:ILE:HD12	1:D:223:VAL:HG13	1.76	0.65
1:B:25:ASN:ND2	1:B:60:THR:CA	2.59	0.65
1:D:236:PHE:O	1:D:237:VAL:CG2	2.42	0.65
1:C:154:ASP:CB	1:C:245:MET:HE1	2.25	0.65
1:C:235:ASP:CG	3:C:2021:HOH:O	2.39	0.65
1:C:130:MET:HE3	1:C:180:TYR:HB2	1.79	0.64
1:B:25:ASN:HD22	1:B:60:THR:HG22	1.62	0.64
2:B:1260:PEG:C1	2:B:1260:PEG:C4	2.73	0.64
1:A:213:MET:HE1	1:D:257:TYR:OH	1.98	0.64
1:A:246:ASP:O	1:A:247:ARG:CB	2.46	0.64
2:B:1260:PEG:H42	2:B:1260:PEG:C1	2.28	0.63
1:D:227:ILE:HG23	1:D:229:SER:H	1.63	0.63
1:A:228:ASP:H	1:A:232:ASN:HD21	1.47	0.62
1:B:238:LEU:O	1:B:239:SER:CB	2.44	0.62
1:B:212:ARG:CB	1:B:254:LEU:HD13	2.28	0.62
1:B:228:ASP:H	1:B:232:ASN:ND2	1.98	0.62
1:B:246:ASP:O	1:B:247:ARG:CB	2.48	0.62
1:A:228:ASP:H	1:A:232:ASN:ND2	1.98	0.61
1:B:18:VAL:HG23	3:B:2003:HOH:O	1.99	0.61
1:B:25:ASN:HD22	1:B:60:THR:CA	2.12	0.61
1:B:148:LEU:O	1:B:149:THR:CG2	2.48	0.61
1:B:212:ARG:HB3	1:B:254:LEU:CD1	2.28	0.61
2:B:1260:PEG:O1	2:B:1260:PEG:C4	2.49	0.61
1:B:246:ASP:O	1:B:247:ARG:HB3	2.02	0.60
1:A:246:ASP:O	1:A:247:ARG:HB3	2.01	0.60
1:D:246:ASP:O	1:D:247:ARG:CB	2.48	0.60
1:C:227:ILE:HG23	1:C:229:SER:H	1.67	0.60
1:B:206:ASP:OD2	1:B:209:VAL:HG23	2.02	0.59
1:D:246:ASP:O	1:D:247:ARG:HB3	2.02	0.59
1:A:18:VAL:HG21	1:A:20:TYR:CZ	2.38	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:148:LEU:C	1:B:149:THR:CG2	2.75	0.59
1:C:246:ASP:O	1:C:247:ARG:CB	2.49	0.59
1:D:21:SER:O	1:D:22:ALA:C	2.45	0.59
1:B:25:ASN:ND2	1:B:60:THR:CB	2.66	0.58
1:B:25:ASN:C	3:B:2006:HOH:O	2.24	0.58
1:A:242:GLY:H	1:A:245:MET:HE2	1.69	0.58
1:C:246:ASP:O	1:C:247:ARG:HB3	2.04	0.57
1:B:71:LEU:HD13	1:B:77:TRP:CB	2.34	0.57
1:B:154:ASP:CB	1:B:245:MET:HE1	2.34	0.57
2:A:1260:PEG:O4	2:A:1261:PEG:C1	2.53	0.57
1:B:153:GLN:HB2	3:B:2033:HOH:O	2.01	0.57
1:C:142:ASP:OD1	1:C:143:TYR:N	2.38	0.57
1:C:119:ASP:O	1:C:123:GLU:HG2	2.05	0.56
1:C:130:MET:HE3	1:C:180:TYR:CB	2.34	0.56
1:C:133:ASP:OD1	1:C:135:VAL:HG22	2.05	0.56
1:D:119:ASP:O	1:D:123:GLU:HG2	2.05	0.56
1:A:34:ARG:O	1:A:38:LEU:HD13	2.05	0.56
1:C:71:LEU:HD13	1:C:77:TRP:HB3	1.85	0.56
1:B:138:GLU:HG2	3:B:2031:HOH:O	2.05	0.56
1:B:161:MET:HE3	1:B:161:MET:CA	2.01	0.56
1:A:25:ASN:HD21	1:A:60:THR:HG22	1.65	0.56
1:A:122:HIS:NE2	3:A:2032:HOH:O	2.26	0.56
1:B:149:THR:HG23	1:B:150:PHE:CD2	2.41	0.56
1:A:240:ASP:C	1:A:241:MET:O	2.46	0.55
1:C:194:CYS:SG	1:C:195:VAL:HG13	2.47	0.55
1:B:119:ASP:O	1:B:123:GLU:HG2	2.07	0.55
1:A:119:ASP:O	1:A:123:GLU:HG2	2.07	0.55
1:D:203:ILE:HD12	1:D:223:VAL:CG1	2.37	0.55
1:C:36:LEU:HA	1:C:39:LEU:HD12	1.89	0.55
1:B:238:LEU:O	1:B:239:SER:HB3	2.06	0.54
1:D:127:HIS:ND1	1:D:182:GLY:HA3	2.22	0.54
1:A:157:LEU:HD23	1:A:245:MET:HG2	1.90	0.54
1:D:236:PHE:CD2	1:D:237:VAL:HG13	2.43	0.54
1:A:161:MET:HE3	1:A:161:MET:O	2.08	0.54
1:B:228:ASP:OD2	1:C:172:LYS:NZ	2.36	0.54
1:A:75:THR:HG22	1:A:134:ARG:HD2	1.90	0.54
1:A:75:THR:HG22	1:A:134:ARG:CD	2.38	0.53
1:D:254:LEU:CD1	1:D:254:LEU:N	2.71	0.53
1:A:257:TYR:OH	1:D:213:MET:HE1	2.09	0.53
1:A:32:PHE:CD1	1:A:58:SER:HB2	2.44	0.53
1:B:25:ASN:ND2	1:B:60:THR:CG2	2.71	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:245:MET:O	1:D:248:ALA:HB3	2.09	0.53
1:B:127:HIS:HE1	1:B:167:GLU:OE2	1.92	0.52
1:B:148:LEU:N	1:B:148:LEU:HD12	2.25	0.52
1:B:32:PHE:CD1	1:B:58:SER:HB2	2.43	0.52
1:B:153:GLN:CG	3:B:2033:HOH:O	2.40	0.52
1:B:237:VAL:C	1:B:238:LEU:O	2.48	0.52
1:A:57:ASN:CG	1:A:59:SER:HB3	2.34	0.52
1:A:240:ASP:OD1	1:A:241:MET:O	2.27	0.52
1:A:205:PHE:CD2	1:A:227:ILE:HD11	2.45	0.52
1:D:34:ARG:O	1:D:38:LEU:HD13	2.10	0.52
1:B:133:ASP:OD1	1:B:135:VAL:HG22	2.09	0.52
1:D:228:ASP:H	1:D:232:ASN:ND2	2.08	0.52
1:D:240:ASP:OD1	1:D:241:MET:O	2.28	0.52
1:D:144:ALA:O	1:D:147:VAL:HG22	2.10	0.52
1:B:23:GLN:O	3:B:2006:HOH:O	2.19	0.51
1:D:35:GLN:NE2	1:D:188:ILE:HG22	2.25	0.51
1:C:44:CYS:SG	1:C:130:MET:HE2	2.38	0.51
1:B:148:LEU:HA	1:B:150:PHE:H	1.76	0.51
1:C:35:GLN:NE2	1:C:188:ILE:HG22	2.25	0.51
1:C:173:THR:HA	3:C:2016:HOH:O	2.10	0.51
1:D:233:LEU:O	1:D:236:PHE:O	2.28	0.51
1:A:47:PHE:CG	1:A:185:LEU:HD13	2.46	0.51
1:A:13:ASP:OD1	1:A:17:LEU:N	2.44	0.51
1:B:148:LEU:O	1:B:149:THR:CB	2.59	0.50
2:B:1260:PEG:H32	3:B:2049:HOH:O	2.11	0.50
1:B:13:ASP:OD1	1:B:17:LEU:N	2.45	0.50
1:B:161:MET:HE3	1:B:161:MET:O	2.08	0.50
1:C:144:ALA:O	1:C:147:VAL:HG22	2.12	0.50
1:A:15:GLN:HG3	1:A:17:LEU:HD22	1.93	0.50
1:B:39:LEU:N	1:B:40:PRO:CD	2.75	0.50
1:B:34:ARG:O	1:B:38:LEU:HD13	2.11	0.50
1:C:32:PHE:CD1	1:C:58:SER:HB2	2.47	0.50
1:B:39:LEU:N	1:B:40:PRO:HD2	2.26	0.49
1:A:144:ALA:O	1:A:147:VAL:HG22	2.12	0.49
2:A:1261:PEG:H42	2:A:1262:PEG:O4	2.12	0.49
1:B:256:PRO:O	1:B:258:PHE:N	2.43	0.49
1:D:32:PHE:CD1	1:D:58:SER:HB2	2.47	0.49
1:A:25:ASN:ND2	1:A:60:THR:CG2	2.64	0.49
1:C:142:ASP:CG	1:C:237:VAL:CG1	2.70	0.49
1:B:212:ARG:CZ	1:B:254:LEU:HD11	2.43	0.49
1:D:26:ARG:O	1:D:30:ILE:HG22	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:254:LEU:N	1:D:254:LEU:HD12	2.28	0.49
1:C:161:MET:C	1:C:161:MET:HE3	2.38	0.49
1:A:19:ASP:CG	1:A:19:ASP:O	2.53	0.49
1:A:227:ILE:HG13	1:A:232:ASN:HD22	1.78	0.48
1:D:212:ARG:NE	1:D:254:LEU:HD11	2.28	0.48
1:B:77:TRP:CD1	1:B:137:ALA:HB1	2.48	0.48
1:B:228:ASP:H	1:B:232:ASN:HD21	1.59	0.48
1:A:203:ILE:HD12	1:A:223:VAL:HG13	1.96	0.48
1:B:227:ILE:HG23	1:B:229:SER:H	1.79	0.48
2:A:1260:PEG:C2	2:A:1262:PEG:O4	2.61	0.48
1:A:205:PHE:CG	1:A:227:ILE:HD12	2.48	0.48
1:C:237:VAL:C	1:C:238:LEU:O	2.48	0.48
1:D:112:LEU:HD23	1:D:113:ASP:H	1.78	0.48
1:A:47:PHE:CD2	1:A:185:LEU:HD13	2.48	0.48
2:A:1261:PEG:C4	2:A:1262:PEG:HO4	2.26	0.48
1:B:154:ASP:CG	1:B:245:MET:HE1	2.39	0.48
1:A:18:VAL:CG2	1:A:20:TYR:CZ	2.96	0.47
1:A:163:TRP:HE3	2:A:1262:PEG:HO1	1.59	0.47
1:C:139:PHE:O	1:C:142:ASP:OD1	2.32	0.47
1:A:146:LYS:O	1:A:150:PHE:HD2	1.98	0.47
1:B:177:LEU:HD21	1:B:202:ARG:HD3	1.95	0.47
1:D:205:PHE:CB	1:D:227:ILE:HD12	2.43	0.47
1:B:15:GLN:HG3	1:B:17:LEU:HD22	1.96	0.47
1:A:216:ARG:HG2	1:A:258:PHE:CE1	2.49	0.47
1:C:216:ARG:HG2	1:C:258:PHE:CE1	2.49	0.47
1:B:203:ILE:HD12	1:B:223:VAL:HG13	1.96	0.47
1:A:247:ARG:CA	1:A:250[B]:GLU:HG2	2.41	0.47
1:C:35:GLN:HE22	1:C:188:ILE:CG2	2.28	0.47
1:B:53:THR:HG21	1:B:74:LYS:HG3	1.96	0.46
1:A:31:LEU:HD11	1:A:107:ARG:HD2	1.97	0.46
1:A:204:LEU:HD23	1:A:204:LEU:HA	1.64	0.46
1:A:116:GLN:HE22	1:A:218:ASP:HB3	1.79	0.46
1:B:77:TRP:NE1	1:B:137:ALA:HB1	2.31	0.46
1:C:245:MET:O	1:C:248:ALA:HB3	2.16	0.46
1:D:148:LEU:O	1:D:149:THR:CB	2.63	0.46
2:B:1260:PEG:C3	3:B:2049:HOH:O	2.64	0.46
1:C:205:PHE:CD2	1:C:227:ILE:HD11	2.51	0.46
1:A:240:ASP:CG	1:A:241:MET:O	2.59	0.46
1:D:205:PHE:HB2	1:D:227:ILE:HD12	1.97	0.46
1:B:146:LYS:O	1:B:150:PHE:HD2	1.97	0.46
1:B:236:PHE:CD2	1:B:237:VAL:HG23	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:27:ILE:HA	1:D:30:ILE:HG23	1.97	0.46
1:A:163:TRP:HE3	2:A:1262:PEG:O1	2.00	0.45
1:D:205:PHE:CD2	1:D:227:ILE:HD11	2.51	0.45
1:A:39:LEU:N	1:A:40:PRO:HD2	2.31	0.45
2:A:1260:PEG:O4	2:A:1261:PEG:H12	2.16	0.45
1:C:77:TRP:CD1	1:C:137:ALA:HB1	2.52	0.45
1:D:82:VAL:O	1:D:103:ALA:HA	2.16	0.45
1:D:240:ASP:C	1:D:241:MET:O	2.59	0.45
2:B:1260:PEG:O4	2:B:1261:PEG:H31	2.17	0.45
1:B:218:ASP:OD1	1:B:218:ASP:N	2.49	0.45
1:A:30:ILE:HD13	1:A:112:LEU:HD11	1.98	0.45
1:D:39:LEU:N	1:D:40:PRO:HD2	2.32	0.45
1:D:146:LYS:O	1:D:150:PHE:HD2	2.00	0.45
1:A:11:VAL:HA	1:A:12:PRO:HD3	1.82	0.45
1:B:227:ILE:HD13	1:B:233:LEU:HD21	1.99	0.45
1:B:251:LEU:HD21	1:C:199:ILE:HD11	1.99	0.44
1:A:35:GLN:O	1:A:36:LEU:C	2.59	0.44
1:D:216:ARG:HG2	1:D:258:PHE:CE1	2.51	0.44
1:C:146:LYS:O	1:C:150:PHE:HD2	1.99	0.44
1:B:38:LEU:HD23	1:B:192:VAL:HG23	2.00	0.44
1:C:34:ARG:CZ	1:C:188:ILE:CD1	2.95	0.44
1:C:205:PHE:CG	1:C:227:ILE:HD12	2.53	0.44
1:B:25:ASN:HD22	1:B:60:THR:CG2	2.27	0.43
1:A:27:ILE:HA	1:A:30:ILE:HG23	2.00	0.43
1:A:48:LEU:HD12	1:A:48:LEU:HA	1.63	0.43
1:B:248:ALA:O	1:B:251:LEU:O	2.36	0.43
1:C:34:ARG:O	1:C:38:LEU:HD13	2.17	0.43
1:D:195:VAL:O	1:D:195:VAL:HG23	2.17	0.43
1:C:35:GLN:NE2	1:C:188:ILE:CG2	2.81	0.43
1:A:39:LEU:N	1:A:40:PRO:CD	2.81	0.43
1:D:148:LEU:HD12	1:D:148:LEU:N	2.33	0.43
1:B:25:ASN:HD21	1:B:60:THR:HB	1.82	0.43
1:B:32:PHE:CE1	1:B:58:SER:HB2	2.54	0.43
1:A:38:LEU:HD23	1:A:192:VAL:HG23	2.01	0.42
1:A:74:LYS:O	1:A:134:ARG:HD3	2.19	0.42
1:A:135:VAL:CG2	1:A:230:TYR:HB2	2.49	0.42
1:C:227:ILE:HG13	1:C:232:ASN:HD22	1.84	0.42
1:D:35:GLN:HE22	1:D:188:ILE:HG22	1.83	0.42
1:D:35:GLN:HE22	1:D:188:ILE:CG2	2.31	0.42
1:B:251:LEU:HD21	1:C:199:ILE:CD1	2.50	0.42
1:A:205:PHE:CB	1:A:227:ILE:HD12	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:24:GLU:C	3:B:2006:HOH:O	2.63	0.42
1:B:92:PHE:CG	1:B:147:VAL:HG21	2.54	0.42
1:C:195:VAL:HG23	1:C:196:GLU:HG3	2.01	0.42
1:D:39:LEU:N	1:D:40:PRO:CD	2.83	0.42
1:A:37:LYS:NZ	3:A:2007:HOH:O	1.90	0.42
1:A:71:LEU:HD13	1:A:77:TRP:HB3	2.00	0.42
1:B:27:ILE:O	1:B:28:TRP:C	2.58	0.42
1:D:100:PHE:HZ	1:D:127:HIS:HD2	1.68	0.42
1:A:34:ARG:CZ	1:A:188:ILE:CD1	2.97	0.42
1:A:148:LEU:C	1:A:150:PHE:N	2.58	0.42
1:A:213:MET:CE	1:D:257:TYR:OH	2.68	0.42
1:D:77:TRP:CD1	1:D:137:ALA:HB1	2.55	0.42
1:D:31:LEU:HD11	1:D:107:ARG:CD	2.43	0.42
1:B:47:PHE:CG	1:B:185:LEU:HD13	2.54	0.41
1:C:39:LEU:N	1:C:40:PRO:HD2	2.35	0.41
1:C:114:TYR:HD1	1:C:114:TYR:H	1.68	0.41
1:D:234:TYR:CD1	1:D:238:LEU:HD11	2.55	0.41
1:A:25:ASN:ND2	1:A:60:THR:HA	2.35	0.41
1:C:71:LEU:HD13	1:C:77:TRP:CB	2.49	0.41
1:B:56:LEU:HD22	1:B:62:PRO:CG	2.50	0.41
1:B:160:ARG:HD3	1:B:213:MET:O	2.21	0.41
1:D:161:MET:HE3	1:D:161:MET:C	2.45	0.41
1:D:185:LEU:HD23	1:D:185:LEU:HA	1.89	0.41
1:A:117:GLU:HA	1:A:118:PRO:HD2	1.89	0.41
1:A:18:VAL:CG2	1:A:20:TYR:CE2	3.04	0.41
1:A:32:PHE:CE1	1:A:58:SER:HB2	2.56	0.41
1:D:25:ASN:ND2	1:D:60:THR:HA	2.36	0.41
1:A:218:ASP:N	1:A:218:ASP:OD1	2.52	0.41
1:C:163:TRP:CZ2	1:C:168:PHE:CE2	3.08	0.41
1:D:161:MET:HE2	1:D:236:PHE:CE2	2.56	0.41
1:A:42:ARG:NE	1:A:196:GLU:OE2	2.54	0.41
1:A:57:ASN:HD21	1:A:59:SER:HB3	1.84	0.41
1:B:54:LEU:HD23	1:B:54:LEU:HA	1.90	0.41
1:B:134:ARG:NH1	1:B:134:ARG:HG2	2.35	0.41
1:D:38:LEU:HD23	1:D:192:VAL:CG2	2.50	0.41
1:A:27:ILE:O	1:A:28:TRP:C	2.62	0.41
1:C:130:MET:HE3	1:C:180:TYR:HA	2.03	0.41
1:A:53:THR:HG21	1:A:74:LYS:HG3	2.02	0.41
1:B:35:GLN:O	1:B:36:LEU:C	2.61	0.41
1:B:82:VAL:O	1:B:103:ALA:HA	2.21	0.41
1:A:77:TRP:CD1	1:A:137:ALA:HB1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:56:LEU:HD22	1:B:62:PRO:HG2	2.03	0.41
1:A:38:LEU:HD23	1:A:192:VAL:CG2	2.51	0.40
1:A:155:TRP:N	1:A:156:PRO:CD	2.84	0.40
1:C:160:ARG:HD3	1:C:213:MET:O	2.22	0.40
1:B:47:PHE:CD2	1:B:185:LEU:HD13	2.56	0.40
1:D:27:ILE:O	1:D:28:TRP:C	2.62	0.40
1:D:35:GLN:O	1:D:36:LEU:C	2.64	0.40
1:C:172:LYS:HD3	1:C:177:LEU:HD13	2.04	0.40
1:D:219:GLN:HE22	1:D:258:PHE:CB	2.35	0.40
1:B:134:ARG:HG2	1:B:134:ARG:HH11	1.86	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	251/272 (92%)	227 (90%)	20 (8%)	4 (2%)	7	14
1	B	250/272 (92%)	223 (89%)	21 (8%)	6 (2%)	4	8
1	C	230/272 (85%)	203 (88%)	21 (9%)	6 (3%)	4	7
1	D	202/272 (74%)	176 (87%)	16 (8%)	10 (5%)	1	2
All	All	933/1088 (86%)	829 (89%)	78 (8%)	26 (3%)	4	6

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	241	MET
1	A	247	ARG
1	B	22	ALA
1	B	247	ARG
1	C	84	ALA

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Mol	Chain	Res	Type
1	C	247	ARG
1	D	22	ALA
1	D	83	ALA
1	D	237	VAL
1	D	247	ARG
1	A	152	GLU
1	B	149	THR
1	B	257	TYR
1	C	149	THR
1	C	152	GLU
1	C	241	MET
1	D	24	GLU
1	D	149	THR
1	D	152	GLU
1	D	240	ASP
1	B	152	GLU
1	B	219	GLN
1	C	219	GLN
1	D	219	GLN
1	D	241	MET
1	A	219	GLN

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	223/241 (92%)	194 (87%)	29 (13%)	4	8
1	B	222/241 (92%)	194 (87%)	28 (13%)	4	9
1	C	206/241 (86%)	175 (85%)	31 (15%)	3	6
1	D	210/241 (87%)	186 (89%)	24 (11%)	5	12
All	All	861/964 (89%)	749 (87%)	112 (13%)	4	8

All (112) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	VAL
1	A	17	LEU
1	A	18	VAL
1	A	21	SER
1	A	30	ILE
1	A	40	PRO
1	A	48	LEU
1	A	51	LEU
1	A	68	SER
1	A	70	ARG
1	A	71	LEU
1	A	72	LYS
1	A	89	ARG
1	A	98	LYS
1	A	110	GLU
1	A	116	GLN
1	A	152	GLU
1	A	157	LEU
1	A	161	MET
1	A	188	ILE
1	A	216	ARG
1	A	227	ILE
1	A	239	SER
1	A	243	LYS
1	A	245	MET
1	A	246	ASP
1	A	250[A]	GLU
1	A	250[B]	GLU
1	A	259	ASP
1	B	11	VAL
1	B	17	LEU
1	B	21	SER
1	B	30	ILE
1	B	40	PRO
1	B	48	LEU
1	B	51	LEU
1	B	68	SER
1	B	70	ARG
1	B	71	LEU
1	B	72	LYS
1	B	95	LEU
1	B	98	LYS
1	B	116	GLN

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Mol	Chain	Res	Type
1	B	148	LEU
1	B	152	GLU
1	B	157	LEU
1	B	161	MET
1	B	188	ILE
1	B	195	VAL
1	B	196	GLU
1	B	204	LEU
1	B	227	ILE
1	B	239	SER
1	B	243	LYS
1	B	246	ASP
1	B	249	ARG
1	B	250	GLU
1	C	30	ILE
1	C	40	PRO
1	C	48	LEU
1	C	51	LEU
1	C	68	SER
1	C	69	GLU
1	C	71	LEU
1	C	85	LEU
1	C	97	GLU
1	C	98	LYS
1	C	114	TYR
1	C	116	GLN
1	C	117	GLU
1	C	147	VAL
1	C	148	LEU
1	C	149	THR
1	C	152	GLU
1	C	153	GLN
1	C	157	LEU
1	C	159	GLN
1	C	161	MET
1	C	188	ILE
1	C	207	PRO
1	C	213	MET
1	C	227	ILE
1	C	234	TYR
1	C	235	ASP
1	C	237	VAL

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Mol	Chain	Res	Type
1	C	243	LYS
1	C	250	GLU
1	C	259	ASP
1	D	21	SER
1	D	30	ILE
1	D	33	GLU
1	D	40	PRO
1	D	48	LEU
1	D	51	LEU
1	D	67	VAL
1	D	68	SER
1	D	71	LEU
1	D	72	LYS
1	D	85	LEU
1	D	110	GLU
1	D	131	LEU
1	D	148	LEU
1	D	152	GLU
1	D	157	LEU
1	D	161	MET
1	D	188	ILE
1	D	196	GLU
1	D	227	ILE
1	D	234	TYR
1	D	241	MET
1	D	243	LYS
1	D	246	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	25	ASN
1	A	35	GLN
1	A	57	ASN
1	A	116	GLN
1	A	219	GLN
1	A	232	ASN
1	B	23	GLN
1	B	25	ASN
1	B	35	GLN
1	B	219	GLN
1	B	232	ASN

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Mol	Chain	Res	Type
1	C	35	GLN
1	C	219	GLN
1	C	232	ASN
1	D	25	ASN
1	D	35	GLN
1	D	219	GLN
1	D	232	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 ⓘ

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	PEG	B	1261	-	6,6,6	0.47	0	5,5,5	0.89	0
2	PEG	A	1262	-	6,6,6	1.42	2 (33%)	5,5,5	0.60	0
2	PEG	A	1261	-	6,6,6	0.67	0	5,5,5	0.56	0
2	PEG	B	1260	-	6,6,6	1.02	0	5,5,5	0.72	0
2	PEG	A	1260	-	6,6,6	0.76	0	5,5,5	0.99	0
2	PEG	B	1262	-	6,6,6	0.75	0	5,5,5	1.30	1 (20%)

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	PEG	B	1261	-	-	3/4/4/4	-
2	PEG	A	1262	-	-	3/4/4/4	-
2	PEG	A	1261	-	-	3/4/4/4	-
2	PEG	B	1260	-	-	4/4/4/4	-
2	PEG	A	1260	-	-	3/4/4/4	-
2	PEG	B	1262	-	-	3/4/4/4	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1262	PEG	C3-C4	2.57	1.63	1.49
2	A	1262	PEG	O2-C3	2.20	1.51	1.42

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1262	PEG	C3-O2-C2	2.18	122.79	113.26

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1260	PEG	C4-C3-O2-C2
2	B	1262	PEG	C4-C3-O2-C2
2	A	1262	PEG	C4-C3-O2-C2
2	B	1262	PEG	O2-C3-C4-O4
2	B	1260	PEG	C1-C2-O2-C3
2	A	1260	PEG	O2-C3-C4-O4
2	A	1261	PEG	O1-C1-C2-O2
2	A	1262	PEG	O2-C3-C4-O4
2	B	1260	PEG	O1-C1-C2-O2
2	A	1260	PEG	C4-C3-O2-C2
2	A	1262	PEG	O1-C1-C2-O2
2	B	1260	PEG	O2-C3-C4-O4
2	A	1260	PEG	O1-C1-C2-O2
2	B	1261	PEG	C4-C3-O2-C2

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Mol	Chain	Res	Type	Atoms
2	B	1261	PEG	C1-C2-O2-C3
2	B	1262	PEG	C1-C2-O2-C3
2	A	1261	PEG	C1-C2-O2-C3
2	B	1261	PEG	O2-C3-C4-O4
2	A	1261	PEG	C4-C3-O2-C2

There are no ring outliers.

6 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1261	PEG	1	0
2	A	1262	PEG	10	0
2	A	1261	PEG	8	0
2	B	1260	PEG	8	0
2	A	1260	PEG	4	0
2	B	1262	PEG	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	C	3
1	D	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	108:SER	C	109:GLU	N	1.75
1	D	82:VAL	C	83:ALA	N	1.66
1	D	83:ALA	C	84:ALA	N	1.17
1	C	81:PRO	C	82:VAL	N	0.74
1	C	109:GLU	C	110:GLU	N	0.67

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	252/272 (92%)	-1.41	0 100 100	15, 26, 49, 84	5 (1%)
1	B	252/272 (92%)	-1.38	0 100 100	16, 29, 54, 90	5 (1%)
1	C	229/272 (84%)	-0.97	1 (0%) 88 86	9, 54, 105, 130	56 (24%)
1	D	235/272 (86%)	-0.93	1 (0%) 88 86	13, 54, 91, 115	40 (17%)
All	All	968/1088 (88%)	-1.18	2 (0%) 91 89	9, 36, 90, 130	106 (10%)

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	148	LEU	2.2
1	D	114	TYR	2.1

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($\text{\AA}^2$)	Q<0.9
2	PEG	A	1261	7/7	0.98	0.05	27,29,34,36	0
2	PEG	A	1262	7/7	0.98	0.06	13,23,27,33	0
2	PEG	A	1260	7/7	0.99	0.04	12,14,17,20	0
2	PEG	B	1261	7/7	0.99	0.03	24,28,34,36	0
2	PEG	B	1262	7/7	0.99	0.04	36,39,46,47	0
2	PEG	B	1260	7/7	1.00	0.02	12,12,14,15	0

6.5 Other polymers [i](#)

There are no such residues in this entry.