



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:35 PM UTC

PDB ID : 1L8L / pdb_00001181
Title : Molecular basis for the local conformational rearrangement of human phosphoserine phosphatase
Authors : Kim, H.Y.; Heo, Y.S.; Kim, J.H.; Park, M.H.; Moon, J.; Park, S.Y.; Lee, T.G.; Jeon, Y.H.; Ro, S.; Hwang, K.Y.
Deposited on : 2002-03-21
Resolution : 2.51 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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

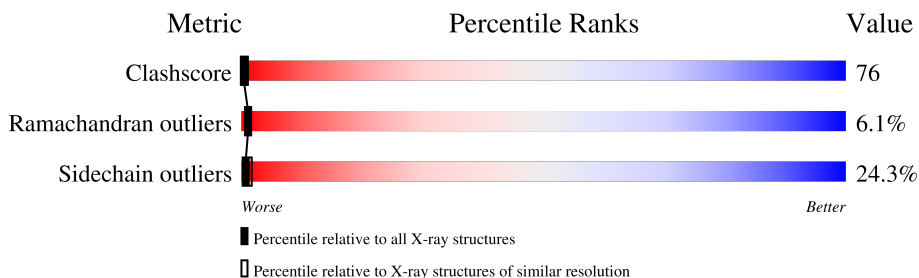
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.51 Å.

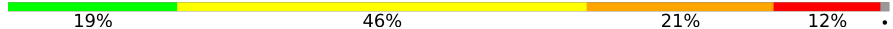
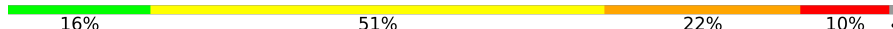
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	225	
1	B	225	

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 3493 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.

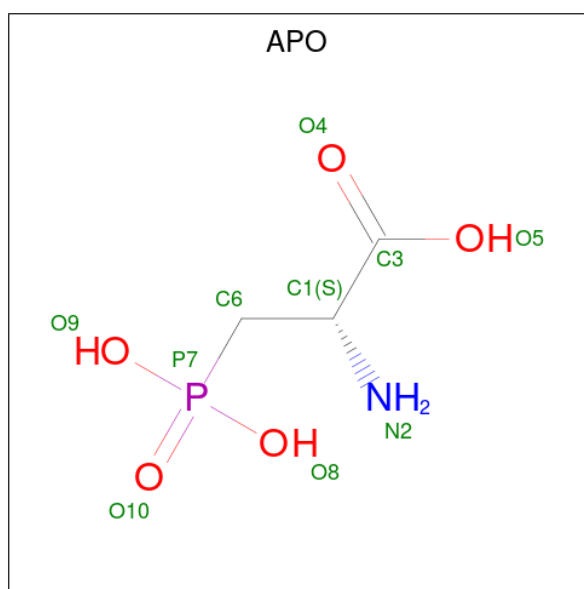
- Molecule 1 is a protein called L-3-phosphoserine phosphatase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	222	Total	C	N	O	S	0	0	0
			1732	1100	300	325	7			
1	B	222	Total	C	N	O	S	0	0	0
			1741	1109	300	325	7			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	164	PHE	LEU	engineered mutation	UNP P78330
B	164	PHE	LEU	engineered mutation	UNP P78330

- Molecule 2 is D-2-AMINO-3-PHOSPHONO-PROPIONIC ACID (CCD ID: APO) (formula: $C_3H_8NO_5P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			10	3	1	5	1		

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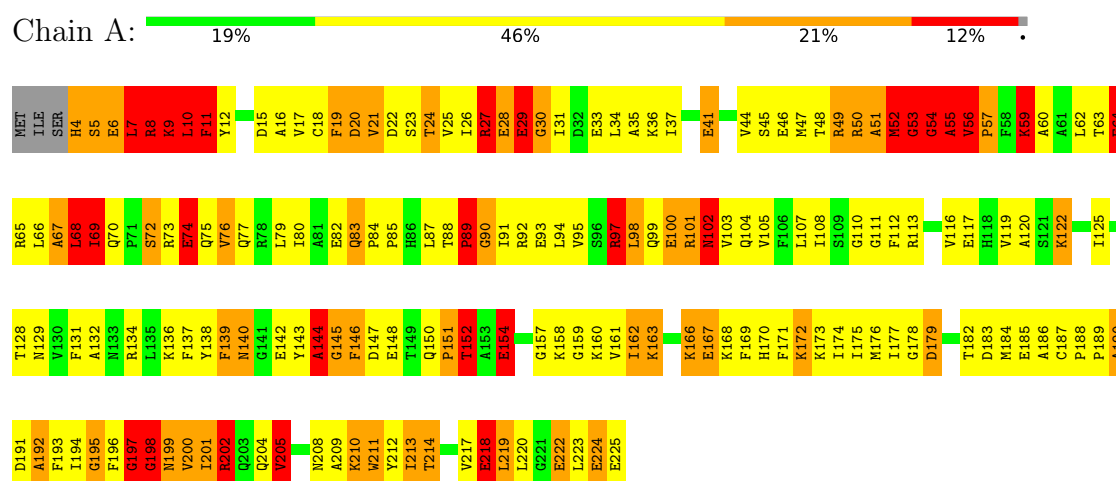
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	P	0	0
			10	3	1	5	1		

3 Residue-property plots

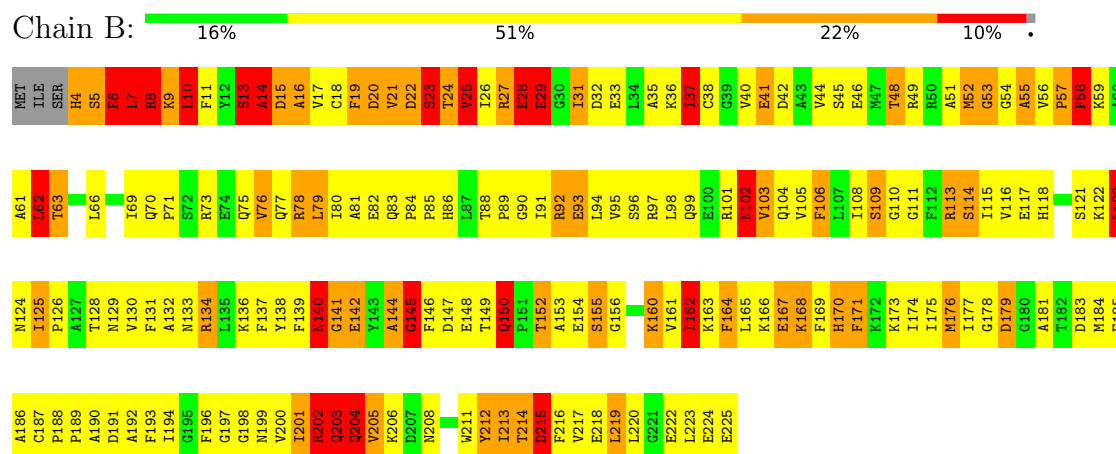
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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.

Note EDS was not executed.

• Molecule 1: L-3-phosphoserine phosphatase



• Molecule 1: L-3-phosphoserine phosphatase



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, α , β , γ	106.21 Å 106.21 Å 87.81 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.78 – 2.51	Depositor
% Data completeness (in resolution range)	89.9 (41.78-2.51)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.213 , 0.284	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3493	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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	2.29	29/1764 (1.6%)	3.01	129/2378 (5.4%)
1	B	2.62	24/1774 (1.4%)	2.62	121/2391 (5.1%)
All	All	2.46	53/3538 (1.5%)	2.82	250/4769 (5.2%)

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	A	1	14
1	B	0	7
All	All	1	21

All (53) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	7	LEU	C-N	-63.59	0.51	1.33
1	B	13	SER	C-N	-38.02	0.79	1.33
1	A	53	GLY	C-N	-37.12	0.79	1.33
1	A	198	GLY	CA-C	-33.97	1.03	1.51
1	A	30	GLY	C-N	32.97	1.75	1.33
1	B	6	GLU	C-N	-30.27	0.91	1.33
1	B	53	GLY	C-N	-28.84	0.91	1.33
1	A	10	LEU	C-N	-26.06	0.96	1.33
1	B	214	THR	C-N	-24.88	0.98	1.33
1	A	20	ASP	C-N	-24.32	1.03	1.33
1	B	4	HIS	C-N	22.55	1.65	1.33
1	A	145	GLY	C-N	22.13	1.61	1.33
1	B	57	PRO	C-N	-21.65	1.07	1.33
1	B	58	PHE	C-O	-19.68	1.00	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	67	ALA	C-N	18.77	1.59	1.33
1	B	14	ALA	C-N	-18.46	1.07	1.33
1	A	19	PHE	C-N	18.20	1.59	1.33
1	A	54	GLY	C-N	-17.91	1.11	1.33
1	A	144	ALA	C-N	-16.79	1.09	1.33
1	B	126	PRO	C-N	-16.09	1.12	1.33
1	A	56	VAL	C-N	15.87	1.71	1.33
1	A	55	ALA	C-N	-15.37	1.16	1.33
1	B	5	SER	C-N	14.95	1.54	1.33
1	B	215	ASP	C-N	12.53	1.50	1.34
1	B	125	ILE	C-N	-12.06	1.18	1.33
1	A	211	TRP	NE1-CE2	10.78	1.49	1.37
1	A	151	PRO	C-N	10.56	1.48	1.33
1	B	114	SER	N-CA	-10.53	1.34	1.46
1	B	144	ALA	N-CA	-9.86	1.34	1.46
1	A	4	HIS	C-N	9.59	1.47	1.33
1	A	54	GLY	CA-C	9.36	1.65	1.51
1	B	144	ALA	CA-C	-8.68	1.42	1.52
1	A	54	GLY	N-CA	8.50	1.57	1.45
1	A	29	GLU	C-N	-8.48	1.21	1.33
1	A	163	LYS	N-CA	8.45	1.57	1.46
1	A	163	LYS	CA-C	-8.42	1.40	1.52
1	B	103	VAL	N-CA	8.25	1.55	1.46
1	B	93	GLU	CA-C	7.77	1.63	1.52
1	A	140	ASN	CA-CB	7.21	1.65	1.53
1	B	62	LEU	N-CA	6.91	1.55	1.46
1	B	62	LEU	CA-C	-6.80	1.43	1.52
1	B	93	GLU	N-CA	-6.54	1.37	1.46
1	A	101	ARG	C-N	-6.14	1.25	1.33
1	B	76	VAL	N-CA	6.08	1.54	1.46
1	A	55	ALA	N-CA	-6.08	1.39	1.46
1	A	140	ASN	N-CA	5.99	1.53	1.46
1	B	103	VAL	CA-C	-5.67	1.45	1.52
1	B	23	SER	C-O	-5.62	1.16	1.23
1	A	166	LYS	N-CA	5.58	1.53	1.46
1	A	59	LYS	C-N	5.28	1.40	1.33
1	A	140	ASN	CB-CG	5.27	1.65	1.52
1	A	122	LYS	CA-C	5.12	1.59	1.52
1	A	55	ALA	CA-C	-5.10	1.46	1.52

All (250) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	53	GLY	O-C-N	-55.48	50.58	122.70
1	A	56	VAL	O-C-N	32.11	157.71	121.10
1	B	121	SER	CA-C-N	-31.72	70.20	122.54
1	B	121	SER	C-N-CA	-31.72	70.20	122.54
1	A	144	ALA	O-C-N	-27.77	85.28	122.49
1	A	144	ALA	CA-C-N	26.68	169.73	121.70
1	A	144	ALA	C-N-CA	26.68	169.73	121.70
1	B	7	LEU	O-C-N	-23.93	90.76	122.59
1	A	56	VAL	N-CA-CB	-20.16	82.99	111.21
1	B	55	ALA	N-CA-CB	-19.50	83.67	110.38
1	A	145	GLY	CA-C-N	-19.31	88.79	121.80
1	A	145	GLY	C-N-CA	-19.31	88.79	121.80
1	B	58	PHE	CA-CB-CG	-18.41	95.39	113.80
1	A	146	PHE	O-C-N	-17.55	104.83	123.26
1	A	89	PRO	N-CA-C	17.37	148.24	112.47
1	B	11	PHE	N-CA-C	16.93	131.46	111.82
1	B	140	ASN	CA-CB-CG	-16.85	95.75	112.60
1	B	7	LEU	CA-C-N	16.71	150.74	123.33
1	B	7	LEU	C-N-CA	16.71	150.74	123.33
1	A	67	ALA	CA-C-N	-16.31	93.10	122.46
1	A	67	ALA	C-N-CA	-16.31	93.10	122.46
1	A	56	VAL	CA-C-N	-16.07	99.76	119.84
1	A	56	VAL	C-N-CA	-16.07	99.76	119.84
1	A	151	PRO	CB-CA-C	15.89	137.78	111.56
1	B	125	ILE	CA-C-N	15.42	136.42	119.92
1	B	125	ILE	C-N-CA	15.42	136.42	119.92
1	B	23	SER	CA-C-O	-15.42	103.99	122.03
1	A	198	GLY	N-CA-C	15.25	149.31	113.18
1	B	103	VAL	O-C-N	15.18	139.21	122.97
1	A	7	LEU	N-CA-C	-15.14	76.05	107.70
1	A	200	VAL	N-CA-CB	-14.97	92.18	111.64
1	A	19	PHE	CA-C-N	14.92	143.35	121.72
1	A	19	PHE	C-N-CA	14.92	143.35	121.72
1	B	125	ILE	O-C-N	-14.28	104.82	121.10
1	B	57	PRO	O-C-N	14.25	140.68	123.01
1	B	10	LEU	CB-CA-C	14.20	138.68	110.42
1	B	126	PRO	O-C-N	14.10	139.97	122.91
1	B	14	ALA	N-CA-C	13.57	131.33	109.76
1	A	55	ALA	CA-C-N	-13.45	97.25	122.13
1	A	55	ALA	C-N-CA	-13.45	97.25	122.13
1	A	145	GLY	O-C-N	13.40	144.44	123.00
1	B	126	PRO	CA-C-N	-13.38	101.29	120.29
1	B	126	PRO	C-N-CA	-13.38	101.29	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	168	LYS	N-CA-C	13.21	127.51	111.40
1	B	114	SER	N-CA-C	-13.11	96.68	110.97
1	A	49	ARG	O-C-N	-13.09	106.90	122.22
1	A	191	ASP	N-CA-C	12.96	126.67	111.11
1	A	8	ARG	N-CA-C	12.69	146.54	111.00
1	A	48	THR	N-CA-C	12.53	128.02	112.23
1	A	224	GLU	CB-CA-C	12.52	130.53	110.88
1	B	144	ALA	N-CA-C	-12.32	88.12	108.32
1	B	93	GLU	N-CA-CB	-12.15	91.38	110.46
1	A	152	THR	N-CA-CB	-12.15	89.96	110.49
1	A	30	GLY	O-C-N	12.13	138.47	122.70
1	A	225	GLU	N-CA-CB	-12.12	89.90	110.50
1	B	11	PHE	N-CA-CB	-12.11	91.52	110.28
1	A	20	ASP	CA-C-N	-11.76	106.54	120.88
1	A	20	ASP	C-N-CA	-11.76	106.54	120.88
1	B	7	LEU	N-CA-CB	11.63	130.15	110.49
1	B	155	SER	CB-CA-C	-11.61	87.33	110.42
1	B	79	LEU	N-CA-C	-11.46	97.41	111.40
1	A	67	ALA	O-C-N	11.36	137.54	122.43
1	B	155	SER	N-CA-C	11.13	134.52	110.80
1	B	14	ALA	CB-CA-C	-10.63	92.50	109.84
1	A	59	LYS	O-C-N	-10.58	111.03	122.03
1	A	8	ARG	N-CA-CB	-10.44	92.75	110.50
1	A	55	ALA	N-CA-C	-10.39	99.65	110.97
1	A	51	ALA	N-CA-C	-10.38	94.20	109.15
1	B	4	HIS	CA-C-N	-10.20	105.01	122.56
1	B	4	HIS	C-N-CA	-10.20	105.01	122.56
1	B	217	VAL	CB-CA-C	10.21	124.94	111.88
1	B	8	ARG	O-C-N	10.18	137.93	122.87
1	B	22	ASP	CA-C-N	10.13	136.75	122.46
1	B	22	ASP	C-N-CA	10.13	136.75	122.46
1	B	52	MET	CB-CA-C	-10.02	92.92	110.95
1	B	53	GLY	CA-C-N	9.99	141.00	121.41
1	B	53	GLY	C-N-CA	9.99	141.00	121.41
1	B	152	THR	CA-CB-CG2	-9.92	93.64	110.50
1	A	132	ALA	N-CA-CB	-9.73	95.06	111.31
1	B	22	ASP	N-CA-C	9.70	131.45	110.80
1	A	29	GLU	CA-C-N	-9.69	102.42	121.41
1	A	29	GLU	C-N-CA	-9.69	102.42	121.41
1	A	53	GLY	CA-C-N	9.64	140.31	121.41
1	A	53	GLY	C-N-CA	9.64	140.31	121.41
1	A	218	GLU	CB-CA-C	9.59	129.06	110.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	48	THR	CB-CA-C	-9.55	90.90	110.38
1	A	192	ALA	N-CA-CB	-9.54	94.06	111.13
1	B	37	ILE	CA-CB-CG2	-9.50	94.36	110.50
1	A	101	ARG	O-C-N	9.48	134.61	122.39
1	B	53	GLY	O-C-N	-9.46	110.40	122.70
1	B	208	ASN	N-CA-C	9.46	125.02	113.38
1	A	190	ALA	CB-CA-C	-9.32	92.31	109.37
1	B	6	GLU	CB-CG-CD	-9.24	96.89	112.60
1	B	61	ALA	CA-C-N	-9.09	105.14	122.06
1	B	61	ALA	C-N-CA	-9.09	105.14	122.06
1	A	57	PRO	O-C-N	-8.99	110.50	122.64
1	A	10	LEU	O-C-N	8.84	132.28	122.20
1	A	205	VAL	CA-CB-CG2	-8.84	95.37	110.40
1	B	103	VAL	CB-CA-C	-8.80	98.23	110.90
1	B	92	ARG	CA-C-N	-8.61	106.04	122.06
1	B	92	ARG	C-N-CA	-8.61	106.04	122.06
1	A	100	GLU	CA-C-N	-8.59	107.78	122.56
1	A	100	GLU	C-N-CA	-8.59	107.78	122.56
1	A	140	ASN	CA-CB-CG	8.38	120.98	112.60
1	A	152	THR	N-CA-C	8.31	128.51	110.80
1	B	15	ASP	CB-CA-C	8.27	124.68	110.79
1	B	13	SER	O-C-N	-8.24	110.20	122.39
1	A	200	VAL	N-CA-C	8.15	119.65	107.75
1	A	219	LEU	N-CA-CB	-8.03	99.48	110.56
1	B	167	GLU	CB-CA-C	8.03	124.11	110.79
1	B	28	GLU	CB-CA-C	-7.99	95.33	109.71
1	B	192	ALA	N-CA-CB	-7.99	98.94	111.56
1	B	203	GLN	CA-C-N	-7.96	106.33	121.54
1	B	203	GLN	C-N-CA	-7.96	106.33	121.54
1	A	162	ILE	CA-C-N	-7.95	107.99	122.38
1	A	162	ILE	C-N-CA	-7.95	107.99	122.38
1	B	205	VAL	N-CA-C	7.93	123.53	112.50
1	A	179	ASP	N-CA-C	7.91	123.04	113.23
1	B	6	GLU	N-CA-C	7.75	127.32	110.80
1	B	13	SER	CA-C-N	7.74	132.56	121.50
1	B	13	SER	C-N-CA	7.74	132.56	121.50
1	A	191	ASP	CB-CA-C	7.73	123.18	110.81
1	A	69	ILE	O-C-N	7.66	132.14	122.57
1	B	150	GLN	N-CA-C	7.64	119.28	109.65
1	B	191	ASP	CB-CA-C	7.54	122.72	110.88
1	A	139	PHE	CA-C-N	7.48	131.29	120.38
1	A	139	PHE	C-N-CA	7.48	131.29	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	103	VAL	CA-C-N	-7.47	111.66	122.19
1	B	103	VAL	C-N-CA	-7.47	111.66	122.19
1	B	115	ILE	N-CA-C	7.44	118.04	110.82
1	A	10	LEU	CB-CA-C	7.39	124.81	110.46
1	A	68	LEU	N-CA-C	7.36	122.14	112.72
1	A	219	LEU	N-CA-C	7.34	121.15	112.93
1	A	110	GLY	N-CA-C	-7.31	104.25	115.66
1	A	97	ARG	O-C-N	-7.28	112.93	122.39
1	A	131	PHE	O-C-N	-7.25	113.20	123.06
1	B	114	SER	CA-C-N	7.23	131.08	120.74
1	B	114	SER	C-N-CA	7.23	131.08	120.74
1	B	6	GLU	CG-CD-OE2	-7.22	101.78	118.40
1	B	76	VAL	CB-CA-C	-7.21	100.58	112.26
1	B	62	LEU	O-C-N	-7.20	112.19	122.41
1	A	7	LEU	CB-CA-C	7.14	122.17	111.17
1	A	30	GLY	CA-C-N	7.13	129.68	120.56
1	A	30	GLY	C-N-CA	7.13	129.68	120.56
1	B	204	GLN	CB-CA-C	7.09	124.53	110.42
1	A	167	GLU	CB-CA-C	7.08	122.50	110.74
1	B	93	GLU	O-C-N	-7.08	112.35	122.41
1	A	218	GLU	CA-CB-CG	7.06	128.21	114.10
1	B	167	GLU	N-CA-C	-7.03	103.61	111.28
1	A	19	PHE	O-C-N	-6.99	114.36	123.16
1	A	98	LEU	N-CA-C	6.95	120.20	111.24
1	A	11	PHE	CA-C-N	-6.93	110.63	122.56
1	A	11	PHE	C-N-CA	-6.93	110.63	122.56
1	A	69	ILE	CA-C-N	-6.92	104.92	121.80
1	A	69	ILE	C-N-CA	-6.92	104.92	121.80
1	A	197	GLY	CA-C-N	-6.84	108.00	121.41
1	A	197	GLY	C-N-CA	-6.84	108.00	121.41
1	B	215	ASP	O-C-N	-6.83	113.51	122.59
1	B	57	PRO	CA-C-N	-6.75	110.46	121.19
1	B	57	PRO	C-N-CA	-6.75	110.46	121.19
1	A	218	GLU	CB-CG-CD	6.74	124.06	112.60
1	B	118	HIS	N-CA-C	-6.71	104.04	111.82
1	A	163	LYS	CA-CB-CG	6.68	127.45	114.10
1	A	54	GLY	O-C-N	6.66	131.36	122.70
1	B	6	GLU	CG-CD-OE1	6.55	133.47	118.40
1	A	163	LYS	CB-CG-CD	6.46	126.14	111.30
1	A	89	PRO	CB-CA-C	-6.40	101.00	111.56
1	B	23	SER	N-CA-C	6.38	119.98	111.30
1	A	163	LYS	CG-CD-CE	-6.35	96.69	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	142	GLU	CB-CA-C	6.30	125.40	111.09
1	B	22	ASP	CB-CA-C	-6.28	97.92	110.42
1	A	64	GLU	N-CA-CB	-6.28	100.46	110.19
1	A	213	ILE	CB-CA-C	-6.25	104.72	111.59
1	A	57	PRO	CA-C-N	6.23	131.11	120.71
1	A	57	PRO	C-N-CA	6.23	131.11	120.71
1	A	146	PHE	N-CA-C	6.22	117.69	108.60
1	A	73	ARG	N-CA-C	-6.19	104.45	111.14
1	B	16	ALA	N-CA-CB	-6.19	100.38	110.59
1	A	208	ASN	N-CA-C	6.18	120.82	113.16
1	B	114	SER	N-CA-CB	-6.16	100.92	109.91
1	A	102	ASN	CA-C-N	6.14	131.53	122.99
1	A	102	ASN	C-N-CA	6.14	131.53	122.99
1	B	102	ASN	CA-C-N	-6.14	112.44	122.57
1	B	102	ASN	C-N-CA	-6.14	112.44	122.57
1	B	21	VAL	N-CA-C	6.13	116.32	110.74
1	A	122	LYS	CA-CB-CG	6.06	126.22	114.10
1	B	145	GLY	N-CA-C	6.04	127.50	113.18
1	A	218	GLU	CG-CD-OE2	-6.04	104.52	118.40
1	A	154	GLU	O-C-N	-6.01	115.87	122.84
1	B	24	THR	N-CA-CB	6.00	120.64	110.49
1	B	123	LEU	O-C-N	5.96	130.52	122.59
1	A	56	VAL	C-N-CD	5.96	149.42	125.00
1	A	102	ASN	O-C-N	-5.96	114.67	122.59
1	A	122	LYS	N-CA-C	-5.95	105.98	113.18
1	B	202	ARG	N-CA-C	5.93	123.43	110.80
1	B	142	GLU	N-CA-C	-5.92	100.14	108.96
1	A	21	VAL	CA-CB-CG1	5.88	120.40	110.40
1	B	93	GLU	CB-CA-C	5.87	120.99	109.72
1	B	5	SER	O-C-N	-5.83	114.86	122.39
1	B	156	GLY	N-CA-C	-5.83	99.35	113.18
1	B	58	PHE	CB-CG-CD2	-5.82	110.80	120.70
1	B	114	SER	CB-CA-C	5.81	119.91	110.96
1	B	86	HIS	O-C-N	-5.75	116.50	123.29
1	A	191	ASP	N-CA-CB	-5.74	101.38	109.94
1	B	4	HIS	O-C-N	5.74	132.18	123.00
1	B	106	PHE	CB-CA-C	-5.72	96.86	109.56
1	A	152	THR	O-C-N	5.67	130.14	122.59
1	A	88	THR	CA-C-N	5.66	126.92	119.84
1	A	88	THR	C-N-CA	5.66	126.92	119.84
1	A	11	PHE	N-CA-C	5.65	118.64	111.69
1	B	212	TYR	N-CA-C	-5.62	96.55	107.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	214	THR	O-C-N	5.60	131.89	122.93
1	B	58	PHE	CA-C-N	-5.59	112.79	120.28
1	B	58	PHE	C-N-CA	-5.59	112.79	120.28
1	B	29	GLU	N-CA-C	5.59	118.64	109.76
1	B	106	PHE	N-CA-C	5.55	117.84	109.23
1	B	202	ARG	N-CA-CB	-5.46	101.26	110.49
1	B	15	ASP	N-CA-CB	-5.46	102.05	110.13
1	A	101	ARG	CA-C-N	-5.45	111.14	121.54
1	A	101	ARG	C-N-CA	-5.45	111.14	121.54
1	B	57	PRO	N-CA-CB	5.43	108.08	103.35
1	B	162	ILE	CA-CB-CG2	-5.42	101.29	110.50
1	B	54	GLY	O-C-N	-5.40	115.67	122.70
1	A	74	GLU	O-C-N	5.39	129.76	122.59
1	A	163	LYS	CD-CE-NZ	-5.38	94.68	111.90
1	B	192	ALA	N-CA-C	5.33	116.90	108.96
1	B	205	VAL	N-CA-CB	-5.33	99.67	111.50
1	B	208	ASN	N-CA-CB	-5.32	102.60	110.53
1	B	214	THR	CA-C-N	-5.32	111.39	121.54
1	B	214	THR	C-N-CA	-5.32	111.39	121.54
1	A	166	LYS	N-CA-CB	5.29	118.40	110.19
1	A	195	GLY	N-CA-C	-5.26	104.45	112.51
1	B	171	PHE	N-CA-CB	-5.26	102.75	110.85
1	B	25	VAL	CA-CB-CG2	5.22	119.27	110.40
1	A	218	GLU	CG-CD-OE1	5.20	130.36	118.40
1	A	50	ARG	CD-NE-CZ	-5.13	117.21	124.40
1	A	4	HIS	O-C-N	-5.12	114.81	123.00
1	B	37	ILE	CB-CG1-CD1	-5.11	103.06	113.80
1	B	202	ARG	CD-NE-CZ	-5.11	117.25	124.40
1	A	97	ARG	CD-NE-CZ	-5.10	117.26	124.40
1	A	54	GLY	N-CA-C	5.10	125.26	113.18
1	A	8	ARG	CD-NE-CZ	-5.07	117.30	124.40
1	B	78	ARG	CD-NE-CZ	-5.07	117.30	124.40
1	A	27	ARG	CD-NE-CZ	-5.07	117.31	124.40
1	A	152	THR	CA-C-N	-5.06	112.64	122.06
1	A	152	THR	C-N-CA	-5.06	112.64	122.06
1	B	27	ARG	N-CA-C	5.04	116.62	111.03
1	A	68	LEU	CB-CA-C	-5.03	102.11	110.37
1	A	101	ARG	CD-NE-CZ	-5.03	117.35	124.40
1	A	90	GLY	N-CA-C	-5.01	101.31	113.18

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	52	MET	CA

All (21) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	10	LEU	Mainchain
1	A	144	ALA	Peptide
1	A	154	GLU	Mainchain
1	A	197	GLY	Peptide
1	A	198	GLY	Mainchain
1	A	29	GLU	Peptide
1	A	49	ARG	Mainchain
1	A	52	MET	Peptide
1	A	53	GLY	Mainchain,Peptide
1	A	54	GLY	Mainchain
1	A	55	ALA	Mainchain
1	A	59	LYS	Mainchain
1	A	97	ARG	Mainchain
1	B	13	SER	Mainchain
1	B	14	ALA	Mainchain
1	B	23	SER	Mainchain
1	B	5	SER	Mainchain
1	B	58	PHE	Sidechain
1	B	7	LEU	Mainchain,Peptide

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	1732	0	1717	257	0
1	B	1741	0	1733	281	1
2	A	10	0	6	3	0
2	B	10	0	6	3	0
All	All	3493	0	3462	531	1

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 76.

All (531) 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:A:7:LEU:CA	1:A:8:ARG:HB3	1.34	1.49
1:A:56:VAL:C	1:A:57:PRO:N	1.71	1.49
1:A:30:GLY:C	1:A:31:ILE:N	1.75	1.41
1:B:62:LEU:HD21	1:B:66:LEU:CD1	1.59	1.32
1:B:7:LEU:CD2	1:B:225:GLU:OE1	1.78	1.31
1:B:62:LEU:CD2	1:B:66:LEU:HD12	1.60	1.31
1:A:7:LEU:CA	1:A:8:ARG:CB	2.00	1.29
1:B:28:GLU:CB	1:B:33:GLU:OE1	1.83	1.26
1:B:13:SER:C	1:B:14:ALA:CA	2.08	1.25
1:A:20:ASP:O	1:A:25:VAL:HG23	1.28	1.25
1:B:28:GLU:HB2	1:B:33:GLU:OE1	1.09	1.22
1:A:7:LEU:N	1:A:8:ARG:CB	2.01	1.20
1:B:15:ASP:O	1:B:103:VAL:HG13	1.36	1.20
1:B:13:SER:O	1:B:14:ALA:N	1.68	1.19
1:A:56:VAL:CA	1:A:57:PRO:N	2.06	1.17
1:B:13:SER:CA	1:B:14:ALA:N	2.10	1.14
1:B:113:ARG:HA	1:B:116:VAL:HG22	1.27	1.14
1:B:136:LYS:NZ	1:B:146:PHE:C	2.06	1.14
1:B:140:ASN:OD1	1:B:140:ASN:C	1.91	1.12
1:A:68:LEU:HD23	1:A:68:LEU:H	1.14	1.11
1:B:136:LYS:HZ1	1:B:147:ASP:HA	0.94	1.11
1:A:4:HIS:O	1:A:7:LEU:O	1.69	1.10
1:A:51:ALA:O	1:A:52:MET:CG	2.01	1.09
1:A:51:ALA:O	1:A:52:MET:HG3	1.53	1.08
1:A:56:VAL:HA	1:A:57:PRO:N	1.64	1.08
1:B:37:ILE:HD11	1:B:79:LEU:HD13	1.37	1.07
1:B:136:LYS:HZ2	1:B:147:ASP:N	1.52	1.05
1:A:6:GLU:O	1:A:7:LEU:HD22	1.58	1.04
1:B:136:LYS:NZ	1:B:147:ASP:HA	1.71	1.04
1:A:27:ARG:NH1	1:A:28:GLU:OE2	1.91	1.03
1:B:7:LEU:HD21	1:B:225:GLU:OE1	0.88	1.03
1:A:5:SER:O	1:A:8:ARG:HB2	1.57	1.03
1:A:10:LEU:C	1:A:10:LEU:HD23	1.83	1.03
1:B:136:LYS:HZ1	1:B:147:ASP:CA	1.71	1.03
1:B:62:LEU:HD23	1:B:62:LEU:O	1.59	1.02
1:B:136:LYS:NZ	1:B:147:ASP:CA	2.21	1.02
1:A:68:LEU:O	1:A:70:GLN:HG2	1.59	1.02
1:B:140:ASN:OD1	1:B:142:GLU:HG2	1.59	1.01
1:A:7:LEU:HA	1:A:8:ARG:HB3	1.05	1.01
1:B:188:PRO:HG2	1:B:189:PRO:HD3	1.41	1.01
1:B:52:MET:O	1:B:55:ALA:HB2	1.59	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:187:CYS:O	1:A:190:ALA:O	1.80	1.00
1:B:122:LYS:C	1:B:124:ASN:H	1.60	0.99
1:B:103:VAL:HG12	1:B:104:GLN:N	1.76	0.99
1:A:184:MET:SD	1:A:205:VAL:HG23	2.03	0.99
1:B:136:LYS:HZ2	1:B:146:PHE:C	1.67	0.99
1:A:56:VAL:HA	1:A:57:PRO:CD	1.93	0.98
1:B:186:ALA:O	1:B:189:PRO:HD2	1.62	0.98
1:B:4:HIS:O	1:B:4:HIS:ND1	1.95	0.98
1:B:103:VAL:CG1	1:B:104:GLN:N	2.23	0.98
1:B:136:LYS:NZ	1:B:147:ASP:N	2.10	0.97
1:A:20:ASP:HB3	1:A:24:THR:HG21	1.47	0.97
1:B:29:GLU:O	1:B:33:GLU:HG3	1.65	0.96
1:A:10:LEU:HD23	1:A:11:PHE:N	1.80	0.96
1:A:143:TYR:CZ	1:A:145:GLY:HA2	2.00	0.95
1:A:10:LEU:CD2	1:A:11:PHE:N	2.30	0.95
1:B:203:GLN:O	1:B:204:GLN:C	2.05	0.95
1:B:122:LYS:C	1:B:124:ASN:N	2.22	0.95
1:A:68:LEU:H	1:A:68:LEU:CD2	1.79	0.94
1:B:134:ARG:HB3	1:B:134:ARG:HH21	1.32	0.93
1:A:52:MET:H	1:A:53:GLY:C	1.76	0.93
1:B:62:LEU:CD2	1:B:62:LEU:O	2.16	0.93
1:A:68:LEU:O	1:A:70:GLN:CG	2.16	0.92
1:B:133:ASN:OD1	1:B:150:GLN:HB3	1.69	0.92
1:B:214:THR:O	1:B:215:ASP:HB2	1.67	0.92
1:B:52:MET:H	1:B:55:ALA:HB2	1.31	0.92
1:A:20:ASP:O	1:A:25:VAL:CG2	2.16	0.92
1:B:16:ALA:HA	1:B:103:VAL:CG1	2.00	0.91
1:A:56:VAL:C	1:A:57:PRO:CA	2.43	0.91
1:A:44:VAL:HA	1:A:47:MET:HG3	1.51	0.91
1:A:8:ARG:O	1:A:10:LEU:N	2.03	0.90
1:B:13:SER:C	1:B:14:ALA:N	0.79	0.89
1:A:68:LEU:HD23	1:A:68:LEU:N	1.83	0.89
1:A:33:GLU:HG3	1:A:79:LEU:HD21	1.54	0.89
1:A:68:LEU:CD2	1:A:68:LEU:N	2.35	0.89
1:B:17:VAL:HG23	1:B:175:ILE:HB	1.55	0.88
1:A:63:THR:O	1:A:67:ALA:HB2	1.73	0.88
1:B:7:LEU:HD21	1:B:225:GLU:CD	1.99	0.88
1:B:93:GLU:HA	1:B:96:SER:HB3	1.54	0.87
1:A:51:ALA:C	1:A:52:MET:HG2	1.95	0.87
1:B:88:THR:HG22	1:B:199:ASN:HD21	1.39	0.87
1:A:51:ALA:C	1:A:52:MET:CG	2.43	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:GLY:O	1:A:94:LEU:HB2	1.75	0.85
1:B:84:PRO:HD2	1:B:85:PRO:HD3	1.58	0.85
1:A:6:GLU:HA	1:A:6:GLU:OE1	1.76	0.85
1:B:213:ILE:HD12	1:B:219:LEU:HD13	1.58	0.84
1:B:21:VAL:HG23	1:B:109:SER:HB3	1.58	0.84
1:B:62:LEU:CD2	1:B:62:LEU:C	2.50	0.84
1:B:136:LYS:NZ	1:B:146:PHE:O	2.02	0.84
1:A:202:ARG:HH11	1:A:202:ARG:HA	1.43	0.84
1:B:122:LYS:O	1:B:124:ASN:N	2.10	0.84
1:B:90:GLY:HA3	1:B:220:LEU:HD11	1.61	0.83
1:A:7:LEU:N	1:A:8:ARG:HB2	1.39	0.83
1:B:37:ILE:CD1	1:B:79:LEU:HD13	2.07	0.83
1:A:6:GLU:C	1:A:7:LEU:CD2	2.52	0.82
1:B:103:VAL:CG1	1:B:104:GLN:H	1.92	0.82
1:B:198:GLY:HA2	1:B:215:ASP:OD1	1.80	0.81
1:B:136:LYS:HZ3	1:B:146:PHE:C	1.78	0.81
1:A:5:SER:O	1:A:8:ARG:CB	2.27	0.81
1:B:52:MET:H	1:B:55:ALA:CB	1.93	0.81
1:A:6:GLU:O	1:A:7:LEU:CD2	2.28	0.81
1:A:68:LEU:O	1:A:69:ILE:C	2.24	0.81
1:B:97:ARG:HH21	1:B:224:GLU:HA	1.47	0.79
1:A:8:ARG:O	1:A:8:ARG:HG3	1.80	0.79
1:B:23:SER:HA	1:B:26:ILE:O	1.81	0.79
1:B:8:ARG:C	1:B:10:LEU:N	2.33	0.79
1:B:62:LEU:HD21	1:B:66:LEU:HD12	0.81	0.79
1:A:6:GLU:C	1:A:7:LEU:HD23	2.07	0.79
1:B:8:ARG:C	1:B:10:LEU:H	1.91	0.79
1:B:28:GLU:OE1	1:B:28:GLU:N	2.16	0.79
1:B:13:SER:C	1:B:14:ALA:HA	2.08	0.78
1:B:40:VAL:HG21	1:B:69:ILE:HA	1.64	0.78
1:B:214:THR:O	1:B:215:ASP:CB	2.24	0.78
1:B:213:ILE:HD11	1:B:216:PHE:HA	1.66	0.78
1:A:20:ASP:CB	1:A:24:THR:HG21	2.15	0.77
1:A:72:SER:OG	1:A:74:GLU:HG3	1.84	0.77
1:B:15:ASP:C	1:B:103:VAL:HG13	2.08	0.77
1:A:4:HIS:O	1:A:7:LEU:N	2.12	0.77
1:A:162:ILE:HD13	1:A:190:ALA:HB2	1.66	0.77
1:A:186:ALA:C	1:A:189:PRO:HD2	2.10	0.77
1:A:20:ASP:HB3	1:A:24:THR:CG2	2.15	0.76
1:A:128:THR:HG23	1:A:129:ASN:ND2	2.00	0.76
1:B:91:ILE:O	1:B:95:VAL:HG12	1.85	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:94:LEU:HB2	1:B:220:LEU:HD21	1.65	0.76
1:B:52:MET:N	1:B:55:ALA:HB2	2.01	0.76
1:A:36:LYS:HA	1:A:41:GLU:HG3	1.68	0.75
1:A:184:MET:SD	1:A:205:VAL:CG2	2.75	0.75
1:B:22:ASP:HB2	2:B:801:APO:O9	1.86	0.75
1:A:68:LEU:O	1:A:70:GLN:N	2.20	0.75
1:B:62:LEU:C	1:B:62:LEU:HD22	2.12	0.75
1:B:133:ASN:OD1	1:B:153:ALA:HB2	1.87	0.75
1:B:188:PRO:CG	1:B:189:PRO:HD3	2.16	0.74
1:A:5:SER:O	1:A:8:ARG:N	2.20	0.74
1:A:210:LYS:O	1:A:211:TRP:HB2	1.87	0.74
1:A:30:GLY:CA	1:A:31:ILE:N	2.50	0.74
1:A:157:GLY:HA2	1:A:160:LYS:HD2	1.69	0.74
1:B:94:LEU:C	1:B:94:LEU:HD23	2.12	0.74
1:A:4:HIS:O	1:A:7:LEU:C	2.31	0.73
1:A:34:LEU:HD12	1:A:112:PHE:HE1	1.51	0.73
1:B:13:SER:O	1:B:14:ALA:CA	2.25	0.73
1:A:72:SER:OG	1:A:74:GLU:CG	2.37	0.73
1:B:213:ILE:HD12	1:B:219:LEU:HB3	1.70	0.73
1:B:84:PRO:CD	1:B:85:PRO:HD3	2.18	0.73
1:B:7:LEU:HD11	1:B:225:GLU:CB	2.19	0.73
1:B:194:ILE:HG22	1:B:213:ILE:HG22	1.70	0.73
1:A:8:ARG:C	1:A:10:LEU:N	2.45	0.72
1:B:18:CYS:HB3	1:B:106:PHE:HB2	1.71	0.72
1:A:184:MET:SD	1:A:209:ALA:HB2	2.28	0.72
1:B:84:PRO:HD2	1:B:85:PRO:CD	2.19	0.72
1:B:7:LEU:HD11	1:B:225:GLU:HB2	1.69	0.72
1:B:28:GLU:CG	1:B:33:GLU:OE1	2.37	0.72
1:B:8:ARG:HE	1:B:10:LEU:H	1.35	0.72
1:B:220:LEU:HD23	1:B:223:LEU:HD13	1.71	0.72
1:B:95:VAL:HG23	1:B:105:VAL:HG21	1.70	0.72
1:B:133:ASN:ND2	1:B:147:ASP:O	2.19	0.72
1:B:18:CYS:CB	1:B:106:PHE:HB2	2.20	0.71
1:B:186:ALA:C	1:B:189:PRO:HD2	2.15	0.71
1:A:169:PHE:HB2	1:A:171:PHE:CE1	2.25	0.71
1:B:24:THR:HG21	1:B:178:GLY:HA2	1.72	0.71
1:A:34:LEU:HD12	1:A:112:PHE:CE1	2.26	0.70
1:A:220:LEU:O	1:A:224:GLU:HG2	1.91	0.70
1:A:22:ASP:HB3	1:A:29:GLU:HG2	1.73	0.70
1:A:140:ASN:ND2	1:A:142:GLU:OE2	2.17	0.70
1:A:93:GLU:O	1:A:97:ARG:HG2	1.92	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:84:PRO:N	1:B:85:PRO:CD	2.53	0.70
1:A:8:ARG:C	1:A:10:LEU:H	1.99	0.69
1:A:72:SER:H	1:A:75:GLN:HE21	1.38	0.69
1:B:22:ASP:OD1	1:B:29:GLU:HA	1.92	0.69
1:A:10:LEU:HD22	1:A:11:PHE:N	2.07	0.69
1:B:71:PRO:HA	1:B:75:GLN:NE2	2.09	0.68
1:B:52:MET:O	1:B:55:ALA:N	2.26	0.68
1:A:52:MET:N	1:A:53:GLY:C	2.52	0.68
1:A:6:GLU:OE1	1:A:8:ARG:NE	2.27	0.68
1:B:162:ILE:HD11	1:B:176:MET:HG2	1.75	0.68
1:A:175:ILE:HG13	1:A:192:ALA:HB3	1.75	0.68
1:A:51:ALA:O	1:A:52:MET:CB	2.42	0.67
1:A:171:PHE:O	1:A:172:LYS:HB3	1.93	0.67
1:B:17:VAL:O	1:B:105:VAL:HA	1.93	0.67
1:A:21:VAL:HA	1:A:25:VAL:CG2	2.24	0.67
1:A:83:GLN:N	1:A:84:PRO:HD3	2.10	0.67
1:A:74:GLU:O	1:A:77:GLN:HB3	1.95	0.67
1:B:52:MET:N	1:B:55:ALA:CB	2.58	0.67
1:B:78:ARG:CG	1:B:78:ARG:O	2.43	0.66
1:B:8:ARG:NE	1:B:10:LEU:HB2	2.10	0.66
1:B:140:ASN:OD1	1:B:142:GLU:CG	2.37	0.66
1:B:84:PRO:CD	1:B:85:PRO:CD	2.73	0.66
1:B:35:ALA:HB1	1:B:40:VAL:HG23	1.77	0.66
1:A:27:ARG:HD3	1:A:28:GLU:OE2	1.96	0.66
1:B:15:ASP:O	1:B:103:VAL:CG1	2.29	0.66
1:B:147:ASP:OD2	1:B:149:THR:HG22	1.95	0.65
1:B:187:CYS:O	1:B:190:ALA:O	2.14	0.65
1:A:65:ARG:O	1:A:68:LEU:HD23	1.96	0.65
1:B:134:ARG:HH21	1:B:134:ARG:CB	2.06	0.65
1:A:199:ASN:N	1:A:199:ASN:ND2	2.45	0.65
1:A:95:VAL:HG23	1:A:105:VAL:HG11	1.78	0.65
1:B:78:ARG:O	1:B:78:ARG:HG2	1.97	0.64
1:A:217:VAL:HG13	1:A:220:LEU:HD12	1.78	0.64
1:B:82:GLU:O	1:B:83:GLN:C	2.38	0.64
1:A:63:THR:HG22	1:A:146:PHE:CZ	2.32	0.64
1:B:52:MET:O	1:B:55:ALA:CB	2.39	0.64
1:B:16:ALA:HA	1:B:103:VAL:HG13	1.78	0.64
1:B:103:VAL:HG13	1:B:104:GLN:H	1.61	0.64
1:B:13:SER:O	1:B:14:ALA:HA	1.96	0.64
1:B:160:LYS:O	1:B:164:PHE:HB2	1.98	0.64
1:A:19:PHE:CE2	1:A:177:ILE:HG13	2.33	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:206:LYS:HA	1:B:212:TYR:CE2	2.33	0.64
1:A:59:LYS:O	1:A:60:ALA:C	2.40	0.63
1:A:68:LEU:C	1:A:70:GLN:N	2.54	0.63
1:A:213:ILE:HG22	1:A:214:THR:N	2.13	0.63
1:A:8:ARG:O	1:A:9:LYS:C	2.40	0.63
1:A:95:VAL:HG21	1:A:125:ILE:HD11	1.81	0.63
1:B:20:ASP:O	1:B:25:VAL:HG13	1.98	0.62
1:B:113:ARG:O	1:B:114:SER:C	2.42	0.62
1:A:20:ASP:OD1	1:A:24:THR:CG2	2.47	0.62
1:A:35:ALA:HB2	1:A:69:ILE:HD13	1.82	0.62
1:B:84:PRO:N	1:B:85:PRO:HD2	2.14	0.62
1:B:88:THR:O	1:B:91:ILE:HG22	1.99	0.62
1:A:59:LYS:O	1:A:63:THR:HG23	2.00	0.62
1:A:113:ARG:HA	1:A:116:VAL:HG22	1.81	0.62
1:A:56:VAL:HG13	1:A:56:VAL:O	2.00	0.62
1:B:166:LYS:O	1:B:170:HIS:HA	2.00	0.61
1:A:65:ARG:O	1:A:69:ILE:HG13	2.00	0.61
1:B:44:VAL:HG13	1:B:45:SER:N	2.14	0.61
1:B:160:LYS:HB2	1:B:160:LYS:NZ	2.16	0.61
1:A:16:ALA:O	1:A:174:ILE:HG13	2.01	0.61
1:B:16:ALA:O	1:B:174:ILE:HA	1.99	0.61
1:B:110:GLY:N	2:B:801:APO:O8	2.31	0.61
1:B:88:THR:CG2	1:B:199:ASN:HD21	2.12	0.60
1:B:6:GLU:CG	1:B:6:GLU:O	2.49	0.60
1:B:213:ILE:CD1	1:B:219:LEU:HB3	2.30	0.60
1:A:177:ILE:HD13	1:A:194:ILE:HB	1.84	0.60
1:B:28:GLU:HB2	1:B:33:GLU:CD	2.13	0.60
1:A:21:VAL:HA	1:A:25:VAL:HB	1.84	0.60
1:A:36:LYS:HA	1:A:41:GLU:CG	2.30	0.60
1:B:14:ALA:HA	1:B:173:LYS:HB3	1.83	0.60
1:A:27:ARG:HA	1:A:199:ASN:OD1	2.02	0.60
1:B:79:LEU:O	1:B:83:GLN:N	2.36	0.59
1:A:100:GLU:C	1:A:102:ASN:H	2.07	0.59
1:A:199:ASN:HD22	1:A:200:VAL:HG12	1.67	0.59
1:B:213:ILE:HD12	1:B:219:LEU:CB	2.31	0.59
1:A:56:VAL:HA	1:A:57:PRO:HD2	1.83	0.59
1:A:222:GLU:CD	1:A:222:GLU:H	2.11	0.59
1:B:59:LYS:NZ	1:B:154:GLU:HB3	2.17	0.59
1:B:78:ARG:O	1:B:81:ALA:HB3	2.03	0.59
1:A:91:ILE:HG23	1:A:92:ARG:N	2.17	0.59
1:B:8:ARG:HE	1:B:10:LEU:HB2	1.66	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:213:ILE:HD12	1:B:219:LEU:CD1	2.31	0.59
1:B:6:GLU:O	1:B:6:GLU:HG3	1.99	0.59
1:A:27:ARG:CD	1:A:28:GLU:OE2	2.50	0.59
1:A:99:GLN:HA	1:A:103:VAL:O	2.03	0.59
1:B:140:ASN:OD1	1:B:141:GLY:N	2.36	0.59
1:B:206:LYS:HA	1:B:212:TYR:CD2	2.39	0.58
1:A:16:ALA:C	1:A:174:ILE:HG13	2.28	0.58
1:A:63:THR:HG22	1:A:146:PHE:HZ	1.68	0.58
1:B:62:LEU:O	1:B:62:LEU:HD22	1.99	0.58
1:B:37:ILE:CD1	1:B:79:LEU:CD1	2.81	0.57
1:A:10:LEU:HD23	1:A:11:PHE:CA	2.34	0.57
1:A:5:SER:C	1:A:7:LEU:N	2.62	0.57
1:B:82:GLU:O	1:B:82:GLU:HG2	2.04	0.57
1:A:113:ARG:HA	1:A:116:VAL:CG2	2.34	0.57
1:B:194:ILE:HG22	1:B:213:ILE:CG2	2.35	0.57
1:A:17:VAL:HG13	1:A:17:VAL:O	2.04	0.57
1:A:201:ILE:HD13	1:A:201:ILE:N	2.20	0.57
1:A:79:LEU:O	1:A:84:PRO:HD3	2.05	0.57
1:A:91:ILE:HG23	1:A:92:ARG:H	1.70	0.56
1:B:83:GLN:C	1:B:85:PRO:HD2	2.30	0.56
1:A:5:SER:O	1:A:6:GLU:C	2.48	0.56
1:A:79:LEU:HD13	1:A:84:PRO:HD2	1.87	0.56
1:A:188:PRO:HB2	1:A:189:PRO:HD3	1.88	0.56
1:B:133:ASN:OD1	1:B:150:GLN:CB	2.47	0.56
1:B:184:MET:HG3	1:B:193:PHE:CD2	2.41	0.56
1:A:20:ASP:OD1	1:A:22:ASP:O	2.23	0.56
1:A:72:SER:CB	1:A:75:GLN:HG3	2.34	0.56
1:A:20:ASP:OD2	2:A:800:APO:HC61	2.06	0.56
1:B:7:LEU:HD11	1:B:225:GLU:OE1	2.05	0.56
1:B:52:MET:C	1:B:55:ALA:HB2	2.31	0.56
1:B:82:GLU:OE2	1:B:84:PRO:HG3	2.06	0.56
1:A:25:VAL:C	1:A:26:ILE:HG23	2.31	0.55
1:B:220:LEU:HA	1:B:223:LEU:HB3	1.88	0.55
1:A:23:SER:HB3	1:A:200:VAL:HG11	1.88	0.55
1:A:60:ALA:O	1:A:64:GLU:HB2	2.06	0.55
1:B:197:GLY:HA2	1:B:200:VAL:O	2.05	0.55
1:A:65:ARG:O	1:A:68:LEU:CD2	2.54	0.55
1:B:9:LYS:O	1:B:10:LEU:C	2.50	0.55
1:A:79:LEU:O	1:A:84:PRO:CD	2.55	0.55
1:B:8:ARG:O	1:B:10:LEU:N	2.40	0.55
1:B:216:PHE:O	1:B:220:LEU:HG	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:72:SER:OG	1:A:75:GLN:HG3	2.06	0.55
1:A:100:GLU:C	1:A:102:ASN:N	2.61	0.55
1:A:166:LYS:O	1:A:167:GLU:C	2.50	0.55
1:B:214:THR:HB	1:B:215:ASP:OD2	2.07	0.54
1:A:44:VAL:C	1:A:46:GLU:H	2.14	0.54
1:A:117:GLU:O	1:A:120:ALA:HB3	2.07	0.54
1:A:5:SER:O	1:A:8:ARG:CA	2.54	0.54
1:A:134:ARG:NH2	1:B:138:TYR:CD1	2.76	0.54
1:B:113:ARG:HD2	1:B:134:ARG:HG2	1.90	0.54
1:A:7:LEU:HD11	1:A:10:LEU:HG	1.74	0.54
1:A:12:TYR:CG	1:A:12:TYR:O	2.60	0.54
1:A:30:GLY:N	1:A:31:ILE:N	2.55	0.54
1:A:33:GLU:CG	1:A:79:LEU:HD21	2.33	0.54
1:A:158:LYS:O	1:A:161:VAL:HG12	2.08	0.54
1:B:201:ILE:HD12	1:B:202:ARG:H	1.71	0.54
1:B:203:GLN:O	1:B:205:VAL:N	2.41	0.54
1:A:187:CYS:HB3	1:A:188:PRO:HD3	1.88	0.54
1:A:6:GLU:C	1:A:7:LEU:HD22	2.18	0.54
1:A:146:PHE:CD1	1:A:146:PHE:C	2.86	0.54
1:A:143:TYR:OH	1:A:145:GLY:HA2	2.08	0.54
1:A:219:LEU:O	1:A:223:LEU:HB2	2.08	0.54
1:B:18:CYS:HB2	1:B:106:PHE:HB2	1.89	0.53
1:B:93:GLU:OE1	1:B:93:GLU:N	2.33	0.53
1:A:218:GLU:O	1:A:222:GLU:OE2	2.27	0.53
1:B:21:VAL:CG2	1:B:109:SER:HB3	2.36	0.53
1:A:62:LEU:O	1:A:66:LEU:HB2	2.08	0.53
1:A:174:ILE:C	1:A:175:ILE:HD12	2.33	0.53
1:B:7:LEU:O	1:B:9:LYS:N	2.41	0.53
1:B:111:GLY:O	1:B:132:ALA:HB1	2.08	0.53
1:B:4:HIS:ND1	1:B:4:HIS:C	2.67	0.53
1:A:5:SER:O	1:A:8:ARG:HD3	2.08	0.53
1:A:25:VAL:C	1:A:26:ILE:CG2	2.82	0.53
1:B:205:VAL:HG13	1:B:212:TYR:HE2	1.73	0.53
1:B:7:LEU:CG	1:B:225:GLU:OE1	2.55	0.53
1:B:213:ILE:CD1	1:B:219:LEU:HD13	2.37	0.53
1:A:5:SER:C	1:A:8:ARG:HB2	2.31	0.53
1:A:161:VAL:HG13	1:A:162:ILE:N	2.24	0.53
1:A:186:ALA:O	1:A:189:PRO:HD2	2.07	0.53
1:A:52:MET:H	1:A:54:GLY:N	1.97	0.52
1:B:19:PHE:CD1	1:B:19:PHE:N	2.76	0.52
1:A:20:ASP:CG	1:A:24:THR:HG21	2.33	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:217:VAL:O	1:A:220:LEU:HG	2.09	0.52
1:B:81:ALA:C	1:B:83:GLN:H	2.15	0.52
1:B:187:CYS:N	1:B:188:PRO:HD2	2.24	0.52
1:B:194:ILE:CG2	1:B:213:ILE:HG22	2.37	0.52
1:A:59:LYS:C	1:A:63:THR:HG23	2.34	0.52
1:B:48:THR:O	1:B:51:ALA:HB3	2.09	0.52
1:B:41:GLU:O	1:B:44:VAL:HG12	2.10	0.52
1:B:214:THR:O	1:B:218:GLU:HG3	2.10	0.52
1:B:44:VAL:CG1	1:B:45:SER:N	2.72	0.52
1:A:64:GLU:HA	1:A:67:ALA:HB3	1.91	0.52
1:A:200:VAL:O	1:A:200:VAL:HG13	2.08	0.52
1:B:31:ILE:HG23	1:B:32:ASP:N	2.24	0.52
1:A:9:LYS:HG3	1:A:9:LYS:O	2.11	0.51
1:B:27:ARG:HB3	1:B:28:GLU:OE1	2.10	0.51
1:B:19:PHE:HB2	1:B:25:VAL:HG11	1.92	0.51
1:B:91:ILE:HG13	1:B:123:LEU:HD21	1.93	0.51
1:B:196:PHE:HA	1:B:213:ILE:O	2.10	0.51
1:A:4:HIS:O	1:A:5:SER:C	2.54	0.51
1:B:18:CYS:HB3	1:B:106:PHE:HD2	1.76	0.51
1:B:81:ALA:C	1:B:83:GLN:N	2.68	0.51
1:B:134:ARG:O	1:B:146:PHE:HB2	2.11	0.51
1:B:144:ALA:O	1:B:145:GLY:O	2.28	0.51
1:A:9:LYS:C	1:A:11:PHE:N	2.58	0.51
1:A:175:ILE:HD12	1:A:175:ILE:N	2.25	0.51
1:B:97:ARG:NH2	1:B:224:GLU:HA	2.23	0.51
1:A:8:ARG:O	1:A:8:ARG:CG	2.54	0.51
1:B:133:ASN:ND2	1:B:146:PHE:HD1	2.09	0.51
1:B:6:GLU:O	1:B:7:LEU:C	2.46	0.50
1:B:108:ILE:HD12	1:B:176:MET:HE3	1.93	0.50
1:B:101:ARG:O	1:B:102:ASN:HB2	2.11	0.50
1:A:21:VAL:HA	1:A:25:VAL:CB	2.40	0.50
1:B:24:THR:HG23	1:B:179:ASP:HB3	1.92	0.50
1:A:182:THR:HB	2:A:800:APO:HN21	1.75	0.50
1:B:20:ASP:O	1:B:24:THR:OG1	2.28	0.50
1:B:116:VAL:HG23	1:B:130:VAL:HG11	1.93	0.50
1:A:178:GLY:HA3	1:A:183:ASP:HB3	1.93	0.50
1:A:21:VAL:HG13	1:A:26:ILE:HD13	1.94	0.50
1:A:82:GLU:C	1:A:84:PRO:HD3	2.37	0.50
1:B:103:VAL:HG12	1:B:104:GLN:O	2.11	0.50
1:A:11:PHE:HZ	1:A:177:ILE:HD11	1.76	0.50
1:A:159:GLY:O	1:A:162:ILE:HG22	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:220:LEU:O	1:B:224:GLU:N	2.38	0.49
1:B:219:LEU:C	1:B:219:LEU:HD23	2.37	0.49
1:B:222:GLU:HA	1:B:225:GLU:HG3	1.94	0.49
1:A:28:GLU:OE1	1:A:84:PRO:O	2.30	0.49
1:B:8:ARG:NE	1:B:8:ARG:HA	2.26	0.49
1:B:38:CYS:SG	1:B:75:GLN:NE2	2.85	0.49
1:B:7:LEU:CD1	1:B:225:GLU:OE1	2.60	0.49
1:B:94:LEU:HG	1:B:223:LEU:HD11	1.95	0.49
1:B:176:MET:HB3	1:B:193:PHE:HD1	1.78	0.49
1:B:62:LEU:CD2	1:B:66:LEU:CD1	2.47	0.49
1:A:197:GLY:HA3	1:A:212:TYR:OH	2.12	0.49
1:A:44:VAL:C	1:A:46:GLU:N	2.71	0.48
1:A:163:LYS:HZ3	1:A:163:LYS:HG3	0.80	0.48
1:A:7:LEU:N	1:A:7:LEU:CD2	2.73	0.48
1:B:24:THR:CG2	1:B:179:ASP:HB3	2.44	0.48
1:A:83:GLN:N	1:A:84:PRO:CD	2.76	0.48
1:B:18:CYS:O	1:B:176:MET:HE2	2.13	0.48
1:B:41:GLU:OE1	1:B:42:ASP:OD1	2.31	0.48
1:A:20:ASP:OD1	1:A:24:THR:HG23	2.13	0.48
1:B:62:LEU:HD21	1:B:66:LEU:HD11	1.79	0.48
1:A:56:VAL:C	1:A:57:PRO:C	2.82	0.48
1:B:16:ALA:CA	1:B:103:VAL:CG1	2.84	0.48
1:B:16:ALA:CA	1:B:103:VAL:HG13	2.44	0.48
1:B:57:PRO:O	1:B:58:PHE:C	2.57	0.48
1:B:205:VAL:HG13	1:B:212:TYR:CE2	2.49	0.48
1:A:34:LEU:O	1:A:37:ILE:HG22	2.15	0.47
1:A:35:ALA:HB2	1:A:69:ILE:CD1	2.42	0.47
1:A:18:CYS:O	1:A:176:MET:HE3	2.14	0.47
1:B:18:CYS:HB3	1:B:106:PHE:CD2	2.49	0.47
1:A:7:LEU:HA	1:A:8:ARG:CB	1.93	0.47
1:A:162:ILE:CD1	1:A:190:ALA:HB2	2.42	0.47
1:B:203:GLN:HE21	1:B:203:GLN:HB3	1.58	0.47
1:B:219:LEU:HD23	1:B:219:LEU:O	2.13	0.47
1:A:18:CYS:SG	1:A:108:ILE:HD11	2.55	0.47
1:B:7:LEU:HA	1:B:7:LEU:HD22	1.64	0.47
1:B:214:THR:C	1:B:215:ASP:CG	2.81	0.47
1:B:223:LEU:HD23	1:B:223:LEU:C	2.40	0.47
1:A:5:SER:O	1:A:7:LEU:N	2.48	0.47
1:A:19:PHE:HB3	1:A:25:VAL:HG22	1.96	0.47
1:A:83:GLN:HE21	1:A:83:GLN:HB2	1.54	0.47
1:B:10:LEU:HG	1:B:211:TRP:CH2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:29:GLU:H	1:B:29:GLU:HG3	1.29	0.47
1:A:137:PHE:O	1:B:137:PHE:N	2.46	0.47
1:B:79:LEU:O	1:B:84:PRO:HD3	2.15	0.47
1:A:22:ASP:O	1:A:23:SER:HB2	2.15	0.47
1:B:28:GLU:OE2	1:B:84:PRO:O	2.33	0.46
1:A:150:GLN:O	1:A:151:PRO:C	2.58	0.46
1:B:16:ALA:HA	1:B:103:VAL:HG12	1.93	0.46
1:B:19:PHE:CE2	1:B:177:ILE:HD12	2.50	0.46
1:B:125:ILE:HG22	1:B:129:ASN:HB2	1.98	0.46
1:B:213:ILE:HG12	1:B:214:THR:N	2.29	0.46
1:B:202:ARG:O	1:B:203:GLN:C	2.57	0.46
1:A:11:PHE:CE2	1:A:194:ILE:HD12	2.51	0.46
1:A:82:GLU:O	1:A:82:GLU:HG2	2.16	0.46
1:A:76:VAL:O	1:A:80:ILE:HG13	2.16	0.46
1:B:93:GLU:HA	1:B:96:SER:CB	2.38	0.46
1:B:140:ASN:OD1	1:B:140:ASN:O	2.26	0.46
1:B:169:PHE:HB2	1:B:171:PHE:CE2	2.51	0.46
1:A:167:GLU:O	1:A:170:HIS:CE1	2.69	0.45
1:B:116:VAL:HG21	1:B:132:ALA:HB2	1.98	0.45
1:B:59:LYS:HZ3	1:B:154:GLU:HB3	1.81	0.45
1:A:23:SER:C	1:A:24:THR:HG22	2.41	0.45
1:A:138:TYR:O	1:A:139:PHE:C	2.60	0.45
1:A:152:THR:H	1:A:152:THR:HG22	1.00	0.45
1:B:25:VAL:HB	1:B:91:ILE:HG12	1.99	0.45
1:B:92:ARG:HB3	1:B:93:GLU:HG3	1.98	0.45
1:B:14:ALA:O	1:B:103:VAL:CG2	2.64	0.45
1:A:11:PHE:CZ	1:A:177:ILE:HD11	2.52	0.45
1:B:219:LEU:O	1:B:223:LEU:HB2	2.15	0.45
1:A:87:LEU:HD23	1:A:91:ILE:HG23	1.99	0.45
1:B:76:VAL:O	1:B:76:VAL:HG12	2.16	0.45
1:B:103:VAL:HG12	1:B:104:GLN:C	2.42	0.45
1:B:223:LEU:HD23	1:B:223:LEU:O	2.16	0.45
1:B:10:LEU:HD13	1:B:173:LYS:CE	2.47	0.45
1:B:216:PHE:O	1:B:220:LEU:N	2.50	0.45
1:A:22:ASP:HB2	2:A:800:APO:O10	2.17	0.44
1:A:72:SER:HG	1:A:74:GLU:HG3	1.80	0.44
1:A:113:ARG:O	1:A:117:GLU:HB2	2.17	0.44
1:B:93:GLU:O	1:B:94:LEU:C	2.56	0.44
1:B:13:SER:N	1:B:14:ALA:N	2.62	0.44
1:B:62:LEU:HD23	1:B:62:LEU:C	2.21	0.44
1:B:131:PHE:CG	1:B:161:VAL:HG21	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:56:VAL:H	1:A:56:VAL:HG12	1.04	0.44
1:B:10:LEU:HD13	1:B:10:LEU:HA	1.72	0.44
1:B:20:ASP:OD1	2:B:801:APO:O10	2.35	0.44
1:B:35:ALA:HB3	1:B:44:VAL:HG11	1.99	0.44
1:B:215:ASP:HB2	1:B:218:GLU:HG3	2.00	0.44
1:A:7:LEU:N	1:A:7:LEU:HD23	2.33	0.44
1:A:12:TYR:O	1:A:12:TYR:CD1	2.70	0.44
1:B:122:LYS:O	1:B:124:ASN:OD1	2.35	0.44
1:B:17:VAL:HG23	1:B:175:ILE:CB	2.38	0.43
1:B:90:GLY:HA3	1:B:220:LEU:CD1	2.39	0.43
1:A:69:ILE:O	1:A:70:GLN:C	2.56	0.43
1:A:101:ARG:HH11	1:A:101:ARG:HD3	1.61	0.43
1:A:19:PHE:CD2	1:A:177:ILE:HB	2.53	0.43
1:A:136:LYS:CD	1:B:144:ALA:HB1	2.48	0.43
1:B:160:LYS:HB2	1:B:160:LYS:HZ3	1.81	0.43
1:A:94:LEU:O	1:A:98:LEU:HD12	2.18	0.43
1:B:40:VAL:HG21	1:B:69:ILE:CA	2.43	0.43
1:A:21:VAL:CG1	1:A:26:ILE:HD13	2.48	0.43
1:A:218:GLU:O	1:A:222:GLU:CD	2.62	0.43
1:A:213:ILE:CG2	1:A:214:THR:N	2.81	0.43
1:A:79:LEU:HD13	1:A:79:LEU:C	2.44	0.42
1:A:146:PHE:O	1:A:147:ASP:C	2.57	0.42
1:B:91:ILE:HG23	1:B:92:ARG:N	2.34	0.42
1:B:92:ARG:HB3	1:B:93:GLU:CD	2.44	0.42
1:B:122:LYS:O	1:B:123:LEU:C	2.60	0.42
1:A:27:ARG:O	1:A:27:ARG:HG2	2.18	0.42
1:A:66:LEU:HD12	1:A:66:LEU:HA	1.81	0.42
1:A:79:LEU:HD22	1:A:84:PRO:HG2	2.01	0.42
1:B:162:ILE:HG22	1:B:163:LYS:N	2.29	0.42
1:B:71:PRO:HA	1:B:75:GLN:HE22	1.82	0.42
1:A:24:THR:HA	1:A:196:PHE:CD2	2.55	0.42
1:A:146:PHE:CE1	1:A:148:GLU:HG2	2.54	0.42
1:A:24:THR:OG1	1:A:25:VAL:N	2.51	0.42
1:A:64:GLU:O	1:A:67:ALA:HB3	2.20	0.42
1:A:137:PHE:HE2	1:B:139:PHE:HB2	1.84	0.42
1:A:154:GLU:H	1:A:154:GLU:HG2	1.52	0.42
1:B:167:GLU:O	1:B:170:HIS:CD2	2.72	0.42
1:A:4:HIS:ND1	1:A:5:SER:N	2.67	0.42
1:A:52:MET:HE2	1:A:52:MET:O	2.20	0.41
1:A:6:GLU:OE1	1:A:8:ARG:CZ	2.69	0.41
1:A:6:GLU:OE1	1:A:8:ARG:NH2	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:164:PHE:O	1:B:168:LYS:HB2	2.20	0.41
1:A:136:LYS:HE2	1:A:146:PHE:C	2.44	0.41
1:B:33:GLU:OE2	1:B:84:PRO:HB2	2.21	0.41
1:B:108:ILE:HG23	1:B:161:VAL:HG11	2.02	0.41
1:B:171:PHE:HD2	1:B:174:ILE:HD11	1.85	0.41
1:B:134:ARG:HH21	1:B:134:ARG:CG	2.33	0.41
1:A:193:PHE:CZ	1:A:195:GLY:HA2	2.55	0.41
1:A:55:ALA:O	1:A:57:PRO:N	2.53	0.41
1:A:138:TYR:HB3	1:B:134:ARG:NH2	2.35	0.41
1:B:24:THR:HG21	1:B:178:GLY:CA	2.46	0.41
1:A:138:TYR:HB3	1:B:134:ARG:HH22	1.86	0.41
1:A:214:THR:HG21	1:A:218:GLU:OE2	2.20	0.41
1:A:44:VAL:O	1:A:47:MET:HB2	2.21	0.41
1:A:84:PRO:N	1:A:85:PRO:CD	2.84	0.41
1:B:88:THR:OG1	1:B:91:ILE:HB	2.21	0.41
1:A:7:LEU:HD22	1:A:8:ARG:HB3	2.03	0.41
1:A:116:VAL:O	1:A:119:VAL:HB	2.20	0.41
1:A:144:ALA:HB1	1:B:136:LYS:HG2	2.02	0.41
1:B:59:LYS:O	1:B:63:THR:OG1	2.38	0.41
1:B:184:MET:HG3	1:B:193:PHE:CE2	2.56	0.41
1:B:187:CYS:HB2	1:B:193:PHE:HB2	2.02	0.41
1:A:10:LEU:CD2	1:A:11:PHE:CA	2.96	0.40
1:A:56:VAL:O	1:A:56:VAL:CG1	2.69	0.40
1:B:84:PRO:CD	1:B:85:PRO:HD2	2.48	0.40
1:B:113:ARG:O	1:B:114:SER:O	2.38	0.40
1:A:68:LEU:C	1:A:70:GLN:HG2	2.40	0.40
1:B:94:LEU:C	1:B:94:LEU:CD2	2.84	0.40
1:A:145:GLY:O	1:A:146:PHE:HB3	2.21	0.40
1:A:16:ALA:HB2	1:A:171:PHE:CD2	2.57	0.40
1:A:94:LEU:HD12	1:A:94:LEU:HA	1.85	0.40
1:A:213:ILE:HG22	1:A:214:THR:H	1.84	0.40
1:A:20:ASP:CG	1:A:24:THR:CG2	2.95	0.40
1:A:63:THR:HG22	1:A:146:PHE:CE2	2.57	0.40
1:A:66:LEU:C	1:A:68:LEU:N	2.79	0.40
1:A:72:SER:OG	1:A:74:GLU:CB	2.69	0.40
1:B:31:ILE:CG2	1:B:32:ASP:N	2.84	0.40
1:B:76:VAL:O	1:B:76:VAL:CG1	2.67	0.40
1:B:95:VAL:CG2	1:B:105:VAL:HG11	2.51	0.40
1:B:181:ALA:O	1:B:185:GLU:HG2	2.22	0.40

All (1) 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)
1:B:78:ARG:NH1	1:B:225:GLU:O[6_455]	1.63	0.57

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	220/225 (98%)	183 (83%)	22 (10%)	15 (7%)	1	1
1	B	220/225 (98%)	175 (80%)	33 (15%)	12 (6%)	1	1
All	All	440/450 (98%)	358 (81%)	55 (12%)	27 (6%)	1	1

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	9	LYS
1	A	54	GLY
1	A	69	ILE
1	A	89	PRO
1	A	102	ASN
1	B	53	GLY
1	B	145	GLY
1	B	204	GLN
1	A	6	GLU
1	A	8	ARG
1	A	41	GLU
1	A	198	GLY
1	B	9	LYS
1	B	123	LEU
1	B	102	ASN
1	B	202	ARG
1	B	215	ASP
1	B	170	HIS
1	A	172	LYS
1	A	173	LYS

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Mol	Chain	Res	Type
1	A	5	SER
1	A	52	MET
1	A	202	ARG
1	B	155	SER
1	B	168	LYS
1	A	111	GLY
1	B	141	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	182/187 (97%)	143 (79%)	39 (21%)	1	2
1	B	184/187 (98%)	134 (73%)	50 (27%)	0	1
All	All	366/374 (98%)	277 (76%)	89 (24%)	1	1

All (89) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	LEU
1	A	8	ARG
1	A	9	LYS
1	A	10	LEU
1	A	11	PHE
1	A	15	ASP
1	A	24	THR
1	A	27	ARG
1	A	28	GLU
1	A	29	GLU
1	A	45	SER
1	A	50	ARG
1	A	52	MET
1	A	56	VAL
1	A	64	GLU
1	A	68	LEU

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Mol	Chain	Res	Type
1	A	69	ILE
1	A	72	SER
1	A	74	GLU
1	A	76	VAL
1	A	83	GLN
1	A	89	PRO
1	A	102	ASN
1	A	104	GLN
1	A	107	LEU
1	A	122	LYS
1	A	152	THR
1	A	154	GLU
1	A	179	ASP
1	A	185	GLU
1	A	199	ASN
1	A	201	ILE
1	A	202	ARG
1	A	204	GLN
1	A	205	VAL
1	A	210	LYS
1	A	214	THR
1	A	218	GLU
1	A	222	GLU
1	B	6	GLU
1	B	7	LEU
1	B	8	ARG
1	B	10	LEU
1	B	19	PHE
1	B	20	ASP
1	B	23	SER
1	B	25	VAL
1	B	28	GLU
1	B	29	GLU
1	B	31	ILE
1	B	36	LYS
1	B	37	ILE
1	B	41	GLU
1	B	46	GLU
1	B	48	THR
1	B	49	ARG
1	B	56	VAL
1	B	58	PHE

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Mol	Chain	Res	Type
1	B	62	LEU
1	B	63	THR
1	B	70	GLN
1	B	73	ARG
1	B	77	GLN
1	B	80	ILE
1	B	89	PRO
1	B	98	LEU
1	B	99	GLN
1	B	109	SER
1	B	113	ARG
1	B	117	GLU
1	B	123	LEU
1	B	128	THR
1	B	134	ARG
1	B	140	ASN
1	B	148	GLU
1	B	150	GLN
1	B	152	THR
1	B	160	LYS
1	B	162	ILE
1	B	164	PHE
1	B	165	LEU
1	B	176	MET
1	B	179	ASP
1	B	183	ASP
1	B	201	ILE
1	B	203	GLN
1	B	204	GLN
1	B	213	ILE
1	B	219	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	75	GLN
1	A	104	GLN
1	A	129	ASN
1	A	150	GLN
1	A	170	HIS
1	A	199	ASN
1	B	70	GLN

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Mol	Chain	Res	Type
1	B	75	GLN
1	B	77	GLN
1	B	99	GLN
1	B	129	ASN
1	B	150	GLN
1	B	170	HIS
1	B	199	ASN
1	B	203	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 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	APO	B	801	-	7,9,9	2.36	3 (42%)	5,13,13	1.23	1 (20%)
2	APO	A	800	-	7,9,9	2.94	4 (57%)	5,13,13	1.33	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	APO	B	801	-	-	2/8/9/9	-
2	APO	A	800	-	-	2/8/9/9	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	800	APO	P7-O10	5.77	1.61	1.50
2	B	801	APO	P7-O10	4.93	1.60	1.50
2	A	800	APO	P7-O9	3.55	1.62	1.55
2	A	800	APO	P7-O8	2.97	1.61	1.55
2	B	801	APO	O5-C3	2.53	1.38	1.30
2	A	800	APO	O5-C3	2.40	1.38	1.30
2	B	801	APO	P7-O9	2.09	1.59	1.55

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	800	APO	O8-P7-O10	-2.80	105.15	112.39
2	B	801	APO	O8-P7-O10	-2.61	105.63	112.39

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	801	APO	N2-C1-C3-O4
2	B	801	APO	N2-C1-C3-O5
2	A	800	APO	C6-C1-C3-O4
2	A	800	APO	C6-C1-C3-O5

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	801	APO	3	0
2	A	800	APO	3	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	B	10
1	A	9

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	30:GLY	C	31:ILE	N	1.75
1	A	56:VAL	C	57:PRO	N	1.71
1	B	4:HIS	C	5:SER	N	1.65
1	A	145:GLY	C	146:PHE	N	1.61
1	B	125:ILE	C	126:PRO	N	1.18
1	A	55:ALA	C	56:VAL	N	1.16
1	B	126:PRO	C	127:ALA	N	1.12
1	A	54:GLY	C	55:ALA	N	1.11
1	A	144:ALA	C	145:GLY	N	1.09
1	B	14:ALA	C	15:ASP	N	1.07
1	B	57:PRO	C	58:PHE	N	1.07
1	A	20:ASP	C	21:VAL	N	1.04
1	B	214:THR	C	215:ASP	N	0.98
1	A	10:LEU	C	11:PHE	N	0.96
1	B	6:GLU	C	7:LEU	N	0.91
1	B	53:GLY	C	54:GLY	N	0.91
1	A	53:GLY	C	54:GLY	N	0.79
1	B	13:SER	C	14:ALA	N	0.79
1	B	7:LEU	C	8:ARG	N	0.51

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.