



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 07:51 am GMT

PDB ID : 1L8L  
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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

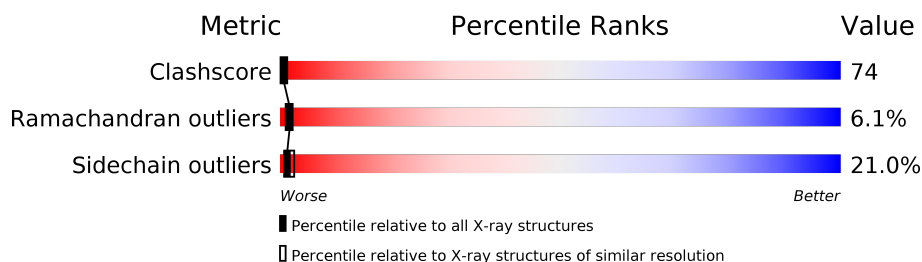
# 1 Overall quality at a glance

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	112137	4554 (2.50-2.50)
Ramachandran outliers	110173	4463 (2.50-2.50)
Sidechain outliers	110143	4465 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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.

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.

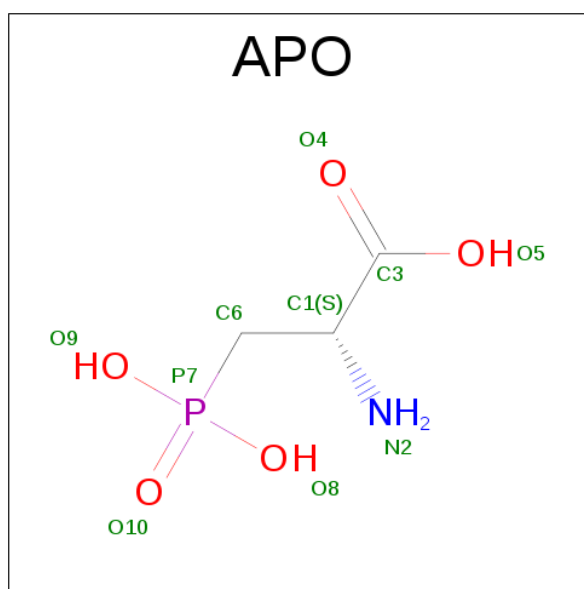
- Molecule 1 is a protein called L-3-phosphoserine phosphatase.

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	UNP P78330
B	164	PHE	LEU	ENGINEERED	UNP P78330

- Molecule 2 is D-2-AMINO-3-PHOSPHONO-PROPIONIC ACID (three-letter code: 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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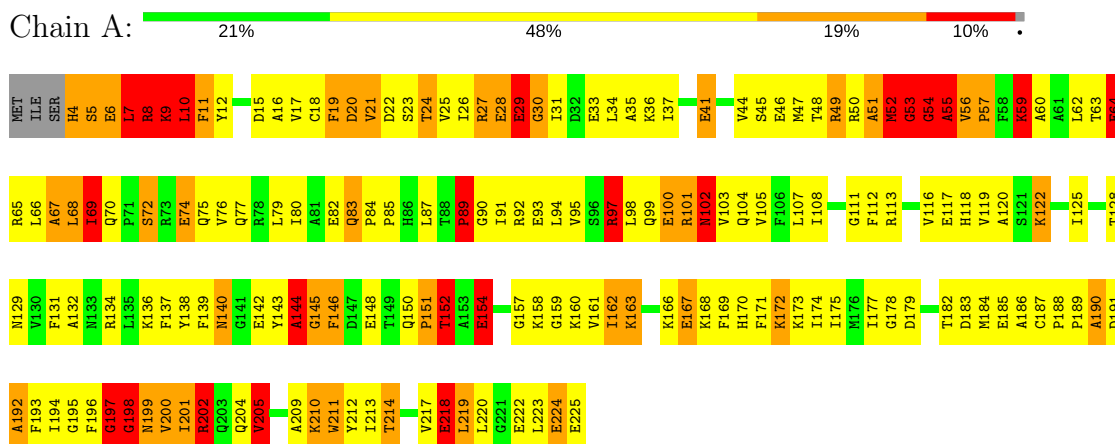
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	P	0	0
			10	3	1	5	1		

### 3 Residue-property plots

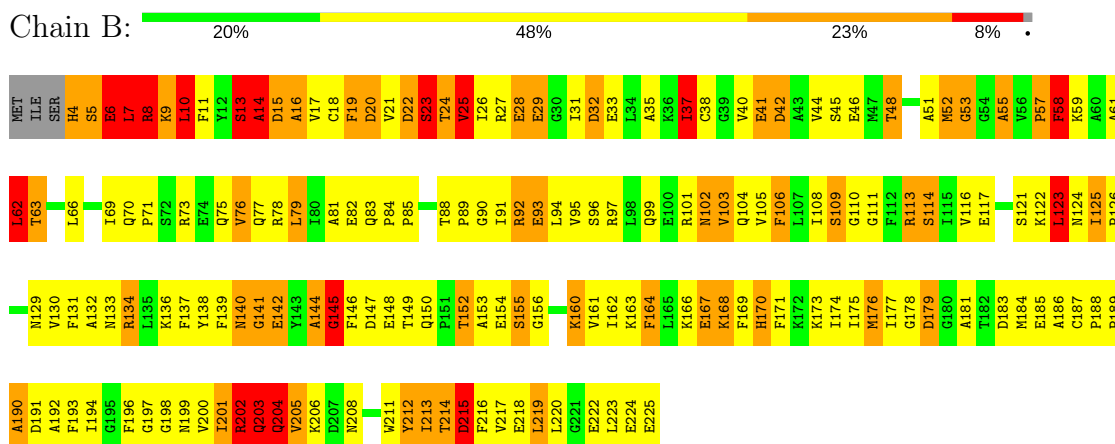
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

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, $\alpha$ , $\beta$ , $\gamma$	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 1.1	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 <sup>2</sup> )	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	1.66	20/1764 (1.1%)	2.30	84/2378 (3.5%)
1	B	1.66	16/1774 (0.9%)	1.92	83/2391 (3.5%)
All	All	1.66	36/3538 (1.0%)	2.12	167/4769 (3.5%)

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 (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	7	LEU	C-N	-35.91	0.51	1.34
1	A	198	GLY	CA-C	-29.91	1.03	1.51
1	A	53	GLY	C-N	-29.86	0.79	1.33
1	B	13	SER	C-N	-23.54	0.79	1.34
1	B	53	GLY	C-N	-23.14	0.91	1.33
1	A	56	VAL	C-N	19.32	1.71	1.34
1	B	6	GLU	C-N	-18.58	0.91	1.34
1	A	30	GLY	C-N	17.96	1.75	1.34
1	A	10	LEU	C-N	-16.28	0.96	1.34
1	B	214	THR	C-N	-15.30	0.98	1.34
1	B	4	HIS	C-N	13.80	1.65	1.34
1	A	20	ASP	C-N	-13.08	1.03	1.34
1	A	144	ALA	C-N	-12.89	1.09	1.33
1	B	58	PHE	C-O	-12.15	1.00	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	145	GLY	C-N	11.87	1.61	1.34
1	B	14	ALA	C-N	-11.41	1.07	1.34
1	B	57	PRO	C-N	-11.37	1.07	1.34
1	A	67	ALA	C-N	11.22	1.59	1.34
1	A	19	PHE	C-N	11.01	1.59	1.34
1	A	54	GLY	C-N	-9.67	1.11	1.34
1	B	126	PRO	C-N	-9.56	1.12	1.34
1	A	211	TRP	NE1-CE2	9.05	1.49	1.37
1	B	5	SER	C-N	8.95	1.54	1.34
1	B	125	ILE	C-N	-8.33	1.18	1.34
1	A	54	GLY	CA-C	8.27	1.65	1.51
1	A	55	ALA	C-N	-7.85	1.16	1.34
1	A	54	GLY	N-CA	7.76	1.57	1.46
1	B	215	ASP	C-N	7.16	1.50	1.34
1	B	114	SER	CB-OG	6.64	1.50	1.42
1	A	29	GLU	C-N	-6.63	1.21	1.33
1	A	151	PRO	C-N	6.27	1.48	1.34
1	A	140	ASN	CB-CG	6.17	1.65	1.51
1	B	114	SER	N-CA	-6.16	1.34	1.46
1	B	144	ALA	N-CA	-5.79	1.34	1.46
1	A	4	HIS	C-N	5.68	1.47	1.34
1	A	163	LYS	N-CA	5.43	1.57	1.46

All (167) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	53	GLY	O-C-N	-42.72	50.58	123.20
1	A	53	GLY	CA-C-N	23.39	162.98	116.20
1	A	144	ALA	C-N-CA	22.58	169.73	122.30
1	A	144	ALA	O-C-N	-22.31	85.28	123.20
1	B	121	SER	C-N-CA	-20.60	70.20	121.70
1	B	7	LEU	O-C-N	-19.96	90.76	122.70
1	A	56	VAL	O-C-N	19.27	157.71	121.10
1	A	144	ALA	CA-C-N	19.12	154.44	116.20
1	B	55	ALA	N-CA-CB	-18.88	83.67	110.10
1	B	10	LEU	CB-CA-C	14.99	138.68	110.20
1	A	198	GLY	CA-C-N	-14.85	84.53	117.20
1	A	198	GLY	N-CA-C	14.49	149.31	113.10
1	B	58	PHE	CB-CG-CD2	-14.28	110.80	120.80
1	A	89	PRO	N-CA-C	13.90	148.24	112.10
1	A	145	GLY	O-C-N	13.59	144.44	122.70
1	A	56	VAL	CA-C-N	-13.50	79.29	117.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	152	THR	CA-CB-CG2	-13.40	93.64	112.40
1	A	145	GLY	C-N-CA	-13.17	88.79	121.70
1	A	8	ARG	N-CA-C	13.16	146.54	111.00
1	A	56	VAL	N-CA-CB	-12.96	82.99	111.50
1	A	7	LEU	N-CA-C	-12.95	76.05	111.00
1	B	155	SER	CB-CA-C	-11.99	87.33	110.10
1	A	190	ALA	CB-CA-C	-11.86	92.31	110.10
1	A	145	GLY	CA-C-N	-11.75	91.34	117.20
1	B	14	ALA	CB-CA-C	-11.73	92.50	110.10
1	B	7	LEU	C-N-CA	11.61	150.74	121.70
1	A	225	GLU	N-CA-CB	-11.50	89.90	110.60
1	A	192	ALA	N-CA-CB	-11.46	94.06	110.10
1	A	67	ALA	C-N-CA	-11.44	93.10	121.70
1	B	57	PRO	O-C-N	11.24	140.68	122.70
1	A	146	PHE	O-C-N	-11.17	104.83	122.70
1	B	57	PRO	CA-C-N	-11.15	92.68	117.20
1	B	7	LEU	CA-C-N	11.05	141.51	117.20
1	B	126	PRO	O-C-N	10.79	139.97	122.70
1	A	132	ALA	N-CA-CB	-10.74	95.06	110.10
1	A	152	THR	N-CA-CB	-10.71	89.96	110.30
1	B	93	GLU	N-CA-CB	-10.68	91.38	110.60
1	B	11	PHE	N-CA-CB	-10.60	91.52	110.60
1	A	205	VAL	CA-CB-CG2	-10.35	95.37	110.90
1	B	103	VAL	O-C-N	10.32	139.21	122.70
1	A	151	PRO	CB-CA-C	10.31	137.78	112.00
1	A	224	GLU	CB-CA-C	10.06	130.53	110.40
1	A	56	VAL	C-N-CD	10.01	149.42	128.40
1	A	8	ARG	N-CA-CB	-9.91	92.75	110.60
1	B	7	LEU	N-CA-CB	9.88	130.15	110.40
1	A	49	ARG	O-C-N	-9.88	106.90	122.70
1	A	30	GLY	O-C-N	9.86	138.47	122.70
1	A	55	ALA	C-N-CA	-9.78	97.25	121.70
1	A	10	LEU	CA-C-N	-9.52	96.25	117.20
1	B	8	ARG	O-C-N	9.52	137.93	122.70
1	A	29	GLU	C-N-CA	-9.46	102.42	122.30
1	A	218	GLU	CB-CA-C	9.33	129.06	110.40
1	A	67	ALA	O-C-N	9.27	137.54	122.70
1	A	54	GLY	CA-C-N	-9.09	97.21	117.20
1	B	53	GLY	C-N-CA	8.90	141.00	122.30
1	A	200	VAL	N-CA-CB	-8.78	92.18	111.50
1	B	52	MET	CB-CA-C	-8.74	92.92	110.40
1	B	155	SER	N-CA-C	8.71	134.52	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	19	PHE	C-N-CA	8.66	143.35	121.70
1	B	4	HIS	CA-C-N	-8.59	98.31	117.20
1	A	53	GLY	C-N-CA	8.57	140.31	122.30
1	B	125	ILE	O-C-N	-8.57	104.82	121.10
1	B	144	ALA	N-CA-C	-8.47	88.12	111.00
1	B	126	PRO	CA-C-N	-8.40	98.72	117.20
1	B	37	ILE	CA-CB-CG2	-8.27	94.36	110.90
1	B	6	GLU	CG-CD-OE2	-8.26	101.78	118.30
1	B	103	VAL	CA-C-N	-8.24	99.06	117.20
1	B	126	PRO	C-N-CA	-8.16	101.29	121.70
1	B	140	ASN	CA-CB-CG	-8.02	95.75	113.40
1	B	192	ALA	N-CA-CB	-7.97	98.94	110.10
1	B	58	PHE	CB-CG-CD1	7.95	126.36	120.80
1	B	13	SER	O-C-N	-7.81	110.20	122.70
1	A	30	GLY	CA-C-N	-7.71	100.23	117.20
1	B	58	PHE	CA-CB-CG	-7.71	95.39	113.90
1	A	10	LEU	CB-CA-C	7.69	124.81	110.20
1	B	23	SER	CA-C-O	-7.67	103.99	120.10
1	A	48	THR	CB-CA-C	-7.67	90.90	111.60
1	A	57	PRO	O-C-N	-7.63	110.50	122.70
1	B	6	GLU	CG-CD-OE1	7.59	133.47	118.30
1	B	11	PHE	N-CA-C	7.58	131.46	111.00
1	B	22	ASP	N-CA-C	7.58	131.45	111.00
1	B	28	GLU	CB-CA-C	-7.54	95.33	110.40
1	B	53	GLY	O-C-N	-7.53	110.40	123.20
1	B	14	ALA	N-CA-C	7.53	131.33	111.00
1	B	142	GLU	CB-CA-C	7.50	125.40	110.40
1	A	101	ARG	O-C-N	7.45	134.61	122.70
1	A	163	LYS	CD-CE-NZ	-7.40	94.68	111.70
1	A	59	LYS	O-C-N	-7.29	111.03	122.70
1	A	146	PHE	CA-C-N	7.29	133.25	117.20
1	B	8	ARG	CA-C-N	-7.27	101.21	117.20
1	A	55	ALA	CA-C-N	-7.23	101.29	117.20
1	B	15	ASP	CB-CA-C	7.14	124.68	110.40
1	B	217	VAL	CB-CA-C	7.13	124.94	111.40
1	B	204	GLN	CB-CA-C	7.07	124.53	110.40
1	A	101	ARG	CA-C-N	-6.99	101.82	117.20
1	B	16	ALA	N-CA-CB	-6.94	100.38	110.10
1	B	103	VAL	CB-CA-C	-6.93	98.23	111.40
1	A	218	GLU	CG-CD-OE2	-6.89	104.52	118.30
1	B	167	GLU	CB-CA-C	6.86	124.11	110.40
1	A	197	GLY	C-N-CA	-6.81	108.00	122.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	106	PHE	CB-CA-C	-6.77	96.86	110.40
1	A	218	GLU	CA-CB-CG	6.73	128.21	113.40
1	A	67	ALA	CA-C-N	-6.72	102.41	117.20
1	A	69	ILE	C-N-CA	-6.71	104.92	121.70
1	B	4	HIS	C-N-CA	-6.68	105.01	121.70
1	B	190	ALA	CB-CA-C	-6.66	100.11	110.10
1	B	61	ALA	C-N-CA	-6.62	105.14	121.70
1	B	62	LEU	O-C-N	-6.57	112.19	122.70
1	A	152	THR	N-CA-C	6.48	128.51	111.00
1	B	93	GLU	O-C-N	-6.47	112.35	122.70
1	B	6	GLU	CB-CG-CD	-6.41	96.89	114.20
1	A	163	LYS	CA-CB-CG	6.39	127.45	113.40
1	A	191	ASP	CB-CA-C	6.39	123.18	110.40
1	B	114	SER	N-CA-CB	-6.39	100.92	110.50
1	A	21	VAL	CA-CB-CG1	6.33	120.40	110.90
1	A	7	LEU	CB-CA-C	6.30	122.17	110.20
1	A	48	THR	N-CA-C	6.30	128.02	111.00
1	B	92	ARG	C-N-CA	-6.26	106.04	121.70
1	B	22	ASP	CB-CA-C	-6.24	97.92	110.40
1	A	51	ALA	N-CA-C	-6.22	94.20	111.00
1	B	191	ASP	CB-CA-C	6.16	122.72	110.40
1	B	203	GLN	C-N-CA	-6.15	106.33	121.70
1	A	168	LYS	N-CA-C	6.12	127.51	111.00
1	A	97	ARG	O-C-N	-6.11	112.93	122.70
1	A	20	ASP	C-N-CA	-6.07	106.54	121.70
1	A	167	GLU	CB-CA-C	6.05	122.50	110.40
1	B	6	GLU	N-CA-C	6.04	127.32	111.00
1	A	218	GLU	CG-CD-OE1	6.03	130.36	118.30
1	B	22	ASP	C-N-CA	6.02	136.75	121.70
1	B	125	ILE	CA-C-N	6.01	133.94	117.10
1	A	10	LEU	O-C-N	5.99	132.28	122.70
1	A	131	PHE	O-C-N	-5.94	113.20	122.70
1	B	4	HIS	O-C-N	5.92	132.18	122.70
1	A	69	ILE	O-C-N	5.90	132.14	122.70
1	A	122	LYS	CA-CB-CG	5.83	126.22	113.40
1	B	62	LEU	CA-CB-CG	5.82	128.69	115.30
1	A	191	ASP	N-CA-C	5.80	126.67	111.00
1	B	145	GLY	N-CA-C	5.76	127.50	113.10
1	B	215	ASP	O-C-N	-5.75	113.51	122.70
1	B	214	THR	O-C-N	5.74	131.89	122.70
1	B	76	VAL	CB-CA-C	-5.70	100.58	111.40
1	A	122	LYS	CD-CE-NZ	5.64	124.67	111.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	64	GLU	N-CA-CB	-5.63	100.46	110.60
1	B	53	GLY	CA-C-N	5.61	127.41	116.20
1	A	163	LYS	CB-CG-CD	5.59	126.14	111.60
1	B	25	VAL	CA-CB-CG2	5.58	119.27	110.90
1	A	100	GLU	C-N-CA	-5.57	107.78	121.70
1	B	156	GLY	N-CA-C	-5.50	99.35	113.10
1	A	162	ILE	C-N-CA	-5.48	107.99	121.70
1	A	219	LEU	N-CA-CB	-5.46	99.48	110.40
1	B	24	THR	N-CA-CB	5.44	120.64	110.30
1	A	54	GLY	O-C-N	5.41	131.36	122.70
1	B	205	VAL	N-CA-CB	-5.38	99.67	111.50
1	B	212	TYR	N-CA-C	-5.35	96.55	111.00
1	A	69	ILE	CA-C-N	-5.33	105.48	117.20
1	B	114	SER	N-CA-C	-5.30	96.68	111.00
1	A	56	VAL	C-N-CA	-5.30	99.76	122.00
1	B	93	GLU	CB-CA-C	5.30	120.99	110.40
1	A	19	PHE	O-C-N	-5.21	114.36	122.70
1	B	208	ASN	N-CA-C	5.19	125.02	111.00
1	B	202	ARG	N-CA-CB	-5.19	101.26	110.60
1	B	114	SER	CB-CA-C	5.16	119.91	110.10
1	B	62	LEU	CB-CG-CD2	-5.14	102.25	111.00
1	A	191	ASP	N-CA-CB	-5.12	101.38	110.60
1	A	163	LYS	CG-CD-CE	-5.07	96.69	111.90
1	B	79	LEU	N-CA-C	-5.03	97.41	111.00
1	A	102	ASN	O-C-N	-5.02	114.67	122.70

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

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Mol	Chain	Res	Type	Group
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	248	0
1	B	1741	0	1733	276	1
2	A	10	0	6	3	0
2	B	10	0	6	3	0
All	All	3493	0	3462	517	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 74.

All (517) 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	1.44
1:A:30:GLY:C	1:A:31:ILE:N	1.75	1.36
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:13:SER:C	1:B:14:ALA:CA	2.08	1.21
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: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:B:136:LYS:NZ	1:B:146:PHE:C	2.06	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:140:ASN:C	1:B:140:ASN:OD1	1.91	1.07
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: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
1:A:187:CYS:O	1:A:190:ALA:O	1.80	1.00
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:122:LYS:C	1:B:124:ASN:H	1.60	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:103:VAL:CG1	1:B:104:GLN:N	2.23	0.98
1:B:4:HIS:ND1	1:B:4:HIS:O	1.95	0.98
1:B:136:LYS:NZ	1:B:147:ASP:N	2.10	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:20:ASP:HB3	1:A:24:THR:HG21	1.47	0.97
1:A:10:LEU:HD23	1:A:11:PHE:N	1.80	0.97
1:A:7:LEU:N	1:A:8:ARG:HB2	1.39	0.96
1:A:10:LEU:C	1:A:10:LEU:HD23	1.83	0.96
1:B:29:GLU:O	1:B:33:GLU:HG3	1.65	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:A:68:LEU:CD2	1:A:68:LEU:H	1.79	0.94
1:B:136:LYS:HZ2	1:B:146:PHE:C	1.67	0.94
1:B:134:ARG:HH21	1:B:134:ARG:HB3	1.32	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:136:LYS:NZ	1:B:146:PHE:O	2.02	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: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:122:LYS:C	1:B:124:ASN:N	2.22	0.90
1:B:203:GLN:O	1:B:204:GLN:C	2.05	0.90
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:52:MET:H	1:A:53:GLY:C	1.76	0.88
1:A:63:THR:O	1:A:67:ALA:HB2	1.73	0.88
1:B:93:GLU:HA	1:B:96:SER:HB3	1.54	0.87
1:B:88:THR:HG22	1:B:199:ASN:HD21	1.39	0.87
1:A:56:VAL:C	1:A:57:PRO:CA	2.43	0.86
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:OE1	1:A:6:GLU:HA	1.76	0.85
1:B:213:ILE:HD12	1:B:219:LEU:HD13	1.58	0.84
1:B:13:SER:C	1:B:14:ALA:N	0.79	0.84
1:B:21:VAL:HG23	1:B:109:SER:HB3	1.58	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:B:37:ILE:CD1	1:B:79:LEU:HD13	2.07	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:51:ALA:C	1:A:52:MET:HG2	1.95	0.83
1:A:51:ALA:C	1:A:52:MET:CG	2.43	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:52:MET:H	1:B:55:ALA:CB	1.93	0.81
1:A:5:SER:O	1:A:8:ARG:CB	2.27	0.81
1:A:6:GLU:O	1:A:7:LEU:CD2	2.28	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:13:SER:O	1:B:14:ALA:CA	2.25	0.79
1:B:23:SER:HA	1:B:26:ILE:O	1.81	0.79
1:B:62:LEU:HD21	1:B:66:LEU:HD12	0.81	0.79
1:B:28:GLU:OE1	1:B:28:GLU:N	2.16	0.79
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:B:7:LEU:HD21	1:B:225:GLU:CD	1.99	0.78
1:A:6:GLU:C	1:A:7:LEU:CD2	2.52	0.77
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:62:LEU:CD2	1:B:62:LEU:C	2.50	0.77
1:A:162:ILE:HD13	1:A:190:ALA:HB2	1.66	0.77
1:A:4:HIS:O	1:A:7:LEU:N	2.12	0.77
1:B:136:LYS:HZ3	1:B:146:PHE:C	1.78	0.77
1:A:128:THR:HG23	1:A:129:ASN:ND2	2.00	0.76
1:A:20:ASP:HB3	1:A:24:THR:CG2	2.15	0.76
1:B:91:ILE:O	1:B:95:VAL:HG12	1.85	0.76
1:A:68:LEU:O	1:A:69:ILE:C	2.24	0.76
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:8:ARG:C	1:B:10:LEU:N	2.33	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: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:6:GLU:C	1:A:7:LEU:HD23	2.07	0.74
1:A:30:GLY:CA	1:A:31:ILE:N	2.50	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:8:ARG:C	1:B:10:LEU:H	1.91	0.74
1:A:157:GLY:HA2	1:A:160:LYS:HD2	1.69	0.74
1:B:13:SER:C	1:B:14:ALA:HA	2.08	0.74
1:A:34:LEU:HD12	1:A:112:PHE:HE1	1.51	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: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:15:ASP:C	1:B:103:VAL:HG13	2.08	0.72
1:B:84:PRO:HD2	1:B:85:PRO:CD	2.19	0.72
1:A:186:ALA:C	1:A:189:PRO:HD2	2.10	0.72
1:B:28:GLU:CG	1:B:33:GLU:OE1	2.37	0.72
1:B:7:LEU:HD11	1:B:225:GLU:HB2	1.69	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: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:B:62:LEU:HD22	1:B:62:LEU:C	2.12	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
1:B:84:PRO:N	1:B:85:PRO:CD	2.53	0.70
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:B:94:LEU:C	1:B:94:LEU:HD23	2.12	0.69
1:A:4:HIS:O	1:A:7:LEU:C	2.31	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:A:8:ARG:C	1:A:10:LEU:N	2.45	0.68
1:B:52:MET:O	1:B:55:ALA:N	2.26	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:186:ALA:C	1:B:189:PRO:HD2	2.15	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:O	1:B:78:ARG:CG	2.43	0.66
1:B:140:ASN:OD1	1:B:142:GLU:CG	2.37	0.66
1:B:8:ARG:NE	1:B:10:LEU:HB2	2.10	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:8:ARG:C	1:A:10:LEU:H	1.99	0.65
1:A:199:ASN:ND2	1:A:199:ASN:N	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: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:A:213:ILE:HG22	1:A:214:THR:N	2.13	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
1:B:206:LYS:HA	1:B:212:TYR:CE2	2.33	0.64
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:6:GLU:O	1:B:6:GLU:HG3	1.99	0.62
1:A:20:ASP:OD1	1:A:24:THR:CG2	2.47	0.62
1:A:52:MET:N	1:A:53:GLY:C	2.52	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:NZ	1:B:160:LYS:HB2	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:A:52:MET:H	1:A:54:GLY:N	1.97	0.60
1:B:88:THR:CG2	1:B:199:ASN:HD21	2.12	0.60
1:B:6:GLU:O	1:B:6:GLU:CG	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: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:82:GLU:O	1:B:83:GLN:C	2.38	0.59
1:B:79:LEU:O	1:B:83:GLN:N	2.36	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: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
1:B:213:ILE:HD12	1:B:219:LEU:CD1	2.31	0.59
1:A:27:ARG:CD	1:A:28:GLU:OE2	2.50	0.59
1:A:59:LYS:O	1:A:60:ALA:C	2.40	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:A:68:LEU:C	1:A:70:GLN:N	2.54	0.58
1:B:206:LYS:HA	1:B:212:TYR:CD2	2.39	0.58
1:A:63:THR:HG22	1:A:146:PHE:HZ	1.68	0.58
1:A:8:ARG:O	1:A:9:LYS:C	2.40	0.58
1:A:17:VAL:HG13	1:A:17:VAL:O	2.04	0.58
1:B:62:LEU:HD22	1:B:62:LEU:O	1.99	0.58
1:B:113:ARG:O	1:B:114:SER:C	2.42	0.58
1:B:37:ILE:CD1	1:B:79:LEU:CD1	2.81	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:10:LEU:HD23	1:A:11:PHE:CA	2.34	0.57
1:B:82:GLU:HG2	1:B:82:GLU:O	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: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:A:188:PRO:HB2	1:A:189:PRO:HD3	1.88	0.56
1:A:79:LEU:HD13	1:A:84:PRO:HD2	1.87	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:82:GLU:OE2	1:B:84:PRO:HG3	2.06	0.56
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:100:GLU:C	1:A:102:ASN:H	2.07	0.55
1:A:65:ARG:O	1:A:68:LEU:CD2	2.54	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
1:A:72:SER:OG	1:A:75:GLN:HG3	2.06	0.55
1:B:214:THR:HB	1:B:215:ASP:OD2	2.07	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:B:113:ARG:HD2	1:B:134:ARG:HG2	1.90	0.54
1:A:134:ARG:NH2	1:B:138:TYR:CD1	2.76	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:158:LYS:O	1:A:161:VAL:HG12	2.08	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: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:16:ALA:C	1:A:174:ILE:HG13	2.28	0.54
1:A:143:TYR:OH	1:A:145:GLY:HA2	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:N	1:B:93:GLU:OE1	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:B:111:GLY:O	1:B:132:ALA:HB1	2.08	0.53
1:B:7:LEU:O	1:B:9:LYS:N	2.41	0.53
1:A:5:SER:O	1:A:8:ARG:HD3	2.08	0.53
1:B:205:VAL:HG13	1:B:212:TYR:HE2	1.73	0.53
1:B:213:ILE:CD1	1:B:219:LEU:HD13	2.37	0.53
1:B:7:LEU:CG	1:B:225:GLU:OE1	2.55	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:B:19:PHE:CD1	1:B:19:PHE:N	2.76	0.52
1:A:217:VAL:O	1:A:220:LEU:HG	2.09	0.52
1:A:5:SER:C	1:A:7:LEU:N	2.62	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:B:48:THR:O	1:B:51:ALA:HB3	2.09	0.52
1:B:214:THR:O	1:B:218:GLU:HG3	2.10	0.52
1:B:41:GLU:O	1:B:44:VAL:HG12	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:B:31:ILE:HG23	1:B:32:ASP:N	2.24	0.52
1:A:200:VAL:HG13	1:A:200:VAL:O	2.08	0.52
1:A:5:SER:O	1:A:6:GLU:C	2.48	0.52
1:A:7:LEU:CD2	1:A:7:LEU:N	2.73	0.52
1:B:83:GLN:C	1:B:85:PRO:HD2	2.30	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:222:GLU:CD	1:A:222:GLU:H	2.11	0.51
1:B:52:MET:C	1:B:55:ALA:HB2	2.31	0.51
1:A:25:VAL:C	1:A:26:ILE:HG23	2.31	0.51
1:A:44:VAL:C	1:A:46:GLU:H	2.14	0.51
1:B:18:CYS:HB3	1:B:106:PHE:HD2	1.76	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:175:ILE:N	1:A:175:ILE:HD12	2.25	0.51
1:B:97:ARG:NH2	1:B:224:GLU:HA	2.23	0.51
1:A:8:ARG:CG	1:A:8:ARG:O	2.54	0.51
1:B:133:ASN:ND2	1:B:146:PHE:HD1	2.09	0.51
1:B:140:ASN:O	1:B:140:ASN:OD1	2.26	0.51
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:9:LYS:O	1:B:10:LEU:C	2.50	0.50
1:B:20:ASP:O	1:B:24:THR:OG1	2.28	0.50
1:A:100:GLU:C	1:A:102:ASN:N	2.61	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:166:LYS:O	1:A:167:GLU:C	2.50	0.50
1:A:21:VAL:HG13	1:A:26:ILE:HD13	1.94	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
1:B:220:LEU:O	1:B:224:GLU:N	2.38	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:28:GLU:HB2	1:B:33:GLU:CD	2.13	0.49
1:B:38:CYS:SG	1:B:75:GLN:NE2	2.85	0.49
1:B:8:ARG:HA	1:B:8:ARG:NE	2.26	0.49
1:A:146:PHE:C	1:A:146:PHE:CD1	2.86	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:6:GLU:C	1:A:7:LEU:HD22	2.18	0.49
1:A:197:GLY:HA3	1:A:212:TYR:OH	2.12	0.49
1:A:163:LYS:HZ3	1:A:163:LYS:HG3	0.80	0.48
1:A:174:ILE:C	1:A:175:ILE:HD12	2.33	0.48
1:B:24:THR:CG2	1:B:179:ASP:HB3	2.44	0.48
1:B:4:HIS:ND1	1:B:4:HIS:C	2.67	0.48
1:A:83:GLN:N	1:A:84:PRO:CD	2.76	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:A:25:VAL:C	1:A:26:ILE:CG2	2.82	0.48
1:B:62:LEU:HD21	1:B:66:LEU:HD11	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:81:ALA:C	1:B:83:GLN:H	2.15	0.48
1:A:59:LYS:C	1:A:63:THR:HG23	2.34	0.48
1:A:5:SER:C	1:A:8:ARG:HB2	2.31	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:A:20:ASP:CG	1:A:24:THR:HG21	2.33	0.48
1:B:205:VAL:HG13	1:B:212:TYR:CE2	2.49	0.48
1:A:35:ALA:HB2	1:A:69:ILE:CD1	2.42	0.47
1:A:34:LEU:O	1:A:37:ILE:HG22	2.15	0.47
1:B:18:CYS:HB3	1:B:106:PHE:CD2	2.49	0.47
1:A:162:ILE:CD1	1:A:190:ALA:HB2	2.42	0.47
1:A:7:LEU:HA	1:A:8:ARG:CB	1.93	0.47
1:B:203:GLN:HB3	1:B:203:GLN:HE21	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:HD22	1:B:7:LEU:HA	1.64	0.47
1:A:19:PHE:HB3	1:A:25:VAL:HG22	1.96	0.47
1:A:83:GLN:HB2	1:A:83:GLN:HE21	1.54	0.47
1:A:5:SER:O	1:A:7:LEU:N	2.48	0.47
1:B:10:LEU:HG	1:B:211:TRP:CH2	2.50	0.47
1:B:29:GLU:H	1:B:29:GLU:HG3	1.29	0.47
1:A:22:ASP:O	1:A:23:SER:HB2	2.15	0.47
1:A:9:LYS:C	1:A:11:PHE:N	2.58	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:B:160:LYS:HB2	1:B:160:LYS:HZ2	1.80	0.47
1:B:28:GLU:OE2	1:B:84:PRO:O	2.33	0.46
1:B:6:GLU:O	1:B:7:LEU:C	2.46	0.46
1:B:16:ALA:HA	1:B:103:VAL:HG12	1.93	0.46
1:B:81:ALA:C	1:B:83:GLN:N	2.68	0.46
1:A:4:HIS:O	1:A:5:SER:C	2.54	0.46
1:B:125:ILE:HG22	1:B:129:ASN:HB2	1.98	0.46
1:B:19:PHE:CE2	1:B:177:ILE:HD12	2.50	0.46
1:B:213:ILE:HG12	1:B:214:THR:N	2.29	0.46
1:A:11:PHE:CE2	1:A:194:ILE:HD12	2.51	0.46
1:A:82:GLU:HG2	1:A:82:GLU:O	2.16	0.46
1:A:76:VAL:O	1:A:80:ILE:HG13	2.16	0.46
1:B:169:PHE:HB2	1:B:171:PHE:CE2	2.51	0.46
1:B:93:GLU:HA	1:B:96:SER:CB	2.38	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:59:LYS:HZ3	1:B:154:GLU:HB3	1.81	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:A:82:GLU:C	1:A:84:PRO:HD3	2.37	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:HG12	1:B:76:VAL:O	2.16	0.45
1:B:219:LEU:HD23	1:B:219:LEU:C	2.37	0.45
1:B:223:LEU:HD23	1:B:223:LEU:O	2.16	0.45
1:A:44:VAL:C	1:A:46:GLU:N	2.71	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:113:ARG:O	1:A:117:GLU:HB2	2.17	0.44
1:A:72:SER:HG	1:A:74:GLU:HG3	1.80	0.44
1:A:22:ASP:HB2	2:A:800:APO:O10	2.17	0.44
1:B:13:SER:N	1:B:14:ALA:N	2.62	0.44
1:B:131:PHE:CG	1:B:161:VAL:HG21	2.53	0.44
1:A:56:VAL:HG12	1:A:56:VAL:H	1.04	0.44
1:B:10:LEU:HA	1:B:10:LEU:HD13	1.72	0.44
1:B:215:ASP:HB2	1:B:218:GLU:HG3	2.00	0.44
1:B:35:ALA:HB3	1:B:44:VAL:HG11	1.99	0.44
1:B:20:ASP:OD1	2:B:801:APO:O10	2.35	0.44
1:A:12:TYR:O	1:A:12:TYR:CD1	2.70	0.44
1:A:7:LEU:HD23	1:A:7:LEU:N	2.33	0.44
1:B:122:LYS:O	1:B:124:ASN:OD1	2.35	0.44
1:B:93:GLU:O	1:B:94:LEU:C	2.56	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:101:ARG:HH11	1:A:101:ARG:HD3	1.61	0.43
1:A:136:LYS:CD	1:B:144:ALA:HB1	2.48	0.43
1:A:19:PHE:CD2	1:A:177:ILE:HB	2.53	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:B:57:PRO:O	1:B:58:PHE:C	2.57	0.43
1:A:21:VAL:CG1	1:A:26:ILE:HD13	2.48	0.43
1:A:213:ILE:CG2	1:A:214:THR:N	2.81	0.43
1:B:91:ILE:HG23	1:B:92:ARG:N	2.34	0.42
1:A:27:ARG:HG2	1:A:27:ARG:O	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:66:LEU:HA	1:A:66:LEU:HD12	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:18:CYS:SG	1:B:176:MET:HE2	2.59	0.42
1:B:223:LEU:C	1:B:223:LEU:HD23	2.40	0.42
1:B:71:PRO:HA	1:B:75:GLN:HE22	1.82	0.42
1:A:146:PHE:CE1	1:A:148:GLU:HG2	2.54	0.42
1:A:24:THR:HA	1:A:196:PHE:CD2	2.55	0.42
1:A:137:PHE:HE2	1:B:139:PHE:HB2	1.84	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:154:GLU:HG2	1:A:154:GLU:H	1.52	0.42
1:B:167:GLU:O	1:B:170:HIS:CD2	2.72	0.42
1:A:150:GLN:O	1:A:151:PRO:C	2.58	0.42
1:A:4:HIS:ND1	1:A:5:SER:N	2.67	0.42
1:A:69:ILE:O	1:A:70:GLN:C	2.56	0.42
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
1:B:164:PHE:O	1:B:168:LYS:HB2	2.20	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:33:GLU:OE2	1:B:84:PRO:HB2	2.21	0.41
1:B:94:LEU:C	1:B:94:LEU:CD2	2.84	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:B:202:ARG:O	1:B:203:GLN:C	2.57	0.41
1:A:116:VAL:HG23	1:A:117:GLU:N	2.36	0.41
1:A:138:TYR:HB3	1:B:134:ARG:NH2	2.35	0.41
1:A:55:ALA:O	1:A:57:PRO:N	2.53	0.41
1:B:24:THR:HG21	1:B:178:GLY:CA	2.46	0.41
1:A:214:THR:HG21	1:A:218:GLU:OE2	2.20	0.41
1:A:138:TYR:HB3	1:B:134:ARG:HH22	1.86	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:B:94:LEU:O	1:B:94:LEU:HD23	2.21	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:A:23:SER:C	1:A:24:THR:HG22	2.41	0.41
1:A:7:LEU:HD22	1:A:8:ARG:HB3	2.03	0.41
1:B:184:MET:HG3	1:B:193:PHE:CE2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:187:CYS:HB2	1:B:193:PHE:HB2	2.02	0.41
1:B:59:LYS:O	1:B:63:THR:OG1	2.38	0.41
1:A:10:LEU:CD2	1:A:11:PHE:CA	2.96	0.40
1:A:138:TYR:O	1:A:139:PHE:C	2.60	0.40
1:A:56:VAL:CG1	1:A:56:VAL:O	2.69	0.40
1:B:113:ARG:O	1:B:114:SER:O	2.38	0.40
1:B:84:PRO:CD	1:B:85:PRO:HD2	2.48	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:213:ILE:HG22	1:A:214:THR:H	1.84	0.40
1:A:94:LEU:HD12	1:A:94:LEU:HA	1.85	0.40
1:A:63:THR:HG22	1:A:146:PHE:CE2	2.57	0.40
1:A:72:SER:OG	1:A:74:GLU:CB	2.69	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
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

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 [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	220/225 (98%)	183 (83%)	22 (10%)	15 (7%)	1	1
1	B	220/225 (98%)	175 (80%)	33 (15%)	12 (6%)	2	2
All	All	440/450 (98%)	358 (81%)	55 (12%)	27 (6%)	2	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
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%)	145 (80%)	37 (20%)	1	2
1	B	184/187 (98%)	144 (78%)	40 (22%)	1	2
All	All	366/374 (98%)	289 (79%)	77 (21%)	1	2

All (77) 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	64	GLU
1	A	68	LEU
1	A	69	ILE
1	A	72	SER
1	A	74	GLU
1	A	83	GLN
1	A	89	PRO
1	A	102	ASN
1	A	104	GLN
1	A	107	LEU
1	A	118	HIS
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	B	6	GLU
1	B	7	LEU
1	B	8	ARG
1	B	10	LEU
1	B	19	PHE

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Mol	Chain	Res	Type
1	B	20	ASP
1	B	23	SER
1	B	25	VAL
1	B	29	GLU
1	B	32	ASP
1	B	37	ILE
1	B	41	GLU
1	B	42	ASP
1	B	46	GLU
1	B	48	THR
1	B	58	PHE
1	B	62	LEU
1	B	63	THR
1	B	70	GLN
1	B	73	ARG
1	B	77	GLN
1	B	89	PRO
1	B	99	GLN
1	B	109	SER
1	B	113	ARG
1	B	117	GLU
1	B	123	LEU
1	B	134	ARG
1	B	148	GLU
1	B	152	THR
1	B	160	LYS
1	B	164	PHE
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

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	75	GLN
1	A	83	GLN
1	A	99	GLN

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Mol	Chain	Res	Type
1	A	104	GLN
1	A	129	ASN
1	A	133	ASN
1	A	170	HIS
1	A	199	ASN
1	B	70	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 carbohydrates 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	A	800	-	4,9,9	3.49	3 (75%)	6,13,13	1.39	1 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	APO	B	801	-	4,9,9	2.63	2 (50%)	6,13,13	1.52	2 (33%)

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	A	800	-	-	0/4/9/9	0/0/0/0
2	APO	B	801	-	-	0/4/9/9	0/0/0/0

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	801	APO	P7-O9	2.01	1.59	1.54
2	A	800	APO	P7-O8	2.84	1.61	1.54
2	A	800	APO	P7-O9	3.40	1.62	1.54
2	B	801	APO	P7-O10	4.60	1.60	1.50
2	A	800	APO	P7-O10	5.39	1.61	1.50

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	800	APO	O8-P7-O10	-2.68	105.15	112.32
2	B	801	APO	O8-P7-O10	-2.49	105.63	112.32
2	B	801	APO	O9-P7-C6	2.64	113.05	106.88

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 6 short contacts:

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

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.



## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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.