Full wwPDB X-ray Structure Validation Report ⓘ

May 17, 2020 – 01:54 am BST

PDB ID	:	1NOI
Title	:	COMPLEX OF GLYCOGEN PHOSPHORYLASE WITH A TRANSITION STATE ANALOGUE NOJIRIMYCIN TETRAZOLE AND PHOSPHATE IN THE T AND R STATES
Authors	:	Johnson, L.N.; Mitchell, E.P.
Deposited on	:	1996-03-12
Resolution	:	2.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

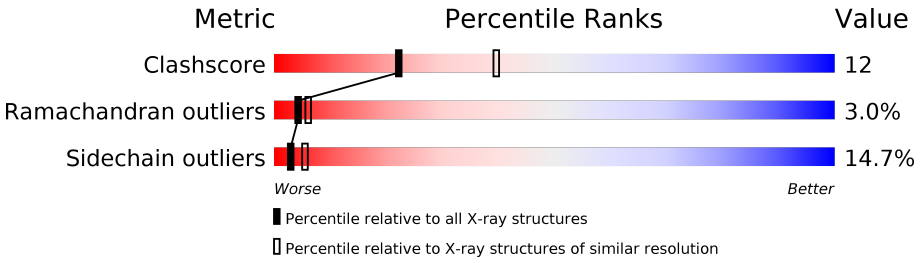
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (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 >=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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	842	59% 28% 7%
1	B	842	59% 29% 8%
1	C	842	60% 27% 8%
1	D	842	61% 26% 9%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PO4	A	997	-	X	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PO4	B	997	-	X	-	-
2	PO4	C	997	-	X	-	-
2	PO4	D	997	-	X	-	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 27788 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.

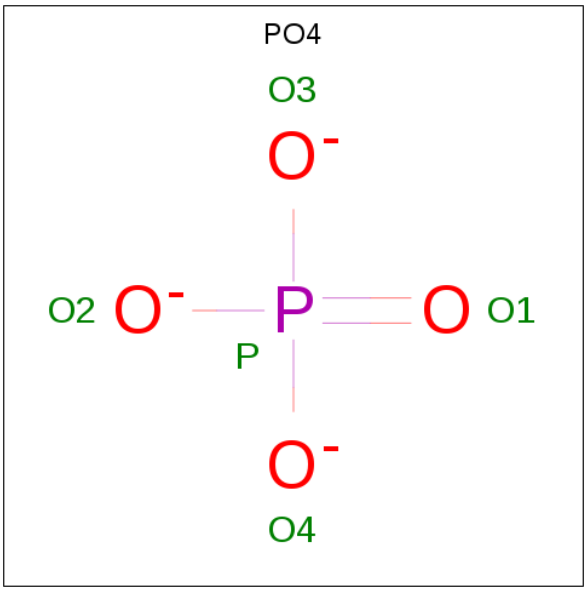
- Molecule 1 is a protein called GLYCOGEN PHOSPHORYLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	824	Total	C	N	O	S	0	0	1
			6692	4264	1185	1213	30			
1	B	824	Total	C	N	O	S	0	0	1
			6692	4264	1185	1213	30			
1	C	824	Total	C	N	O	S	0	0	1
			6692	4264	1185	1213	30			
1	D	824	Total	C	N	O	S	0	0	1
			6692	4264	1185	1213	30			

There are 8 discrepancies between the modelled and reference sequences:

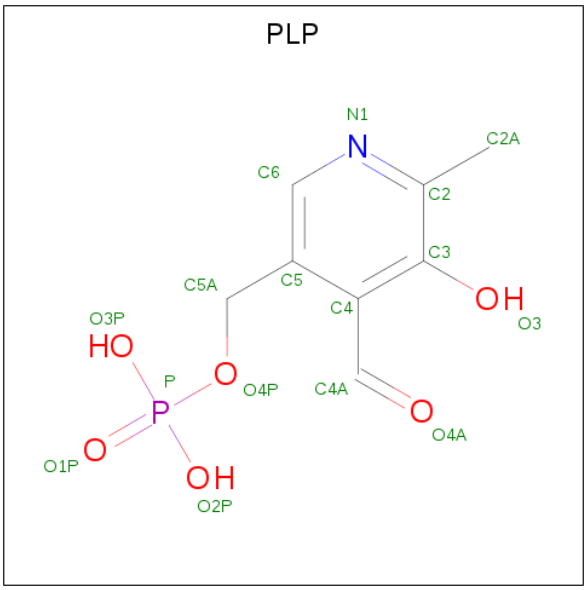
Chain	Residue	Modelled	Actual	Comment	Reference
A	380	ILE	LEU	CONFLICT	UNP P00489
A	609	PRO	ALA	CONFLICT	UNP P00489
B	380	ILE	LEU	CONFLICT	UNP P00489
B	609	PRO	ALA	CONFLICT	UNP P00489
C	380	ILE	LEU	CONFLICT	UNP P00489
C	609	PRO	ALA	CONFLICT	UNP P00489
D	380	ILE	LEU	CONFLICT	UNP P00489
D	609	PRO	ALA	CONFLICT	UNP P00489

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



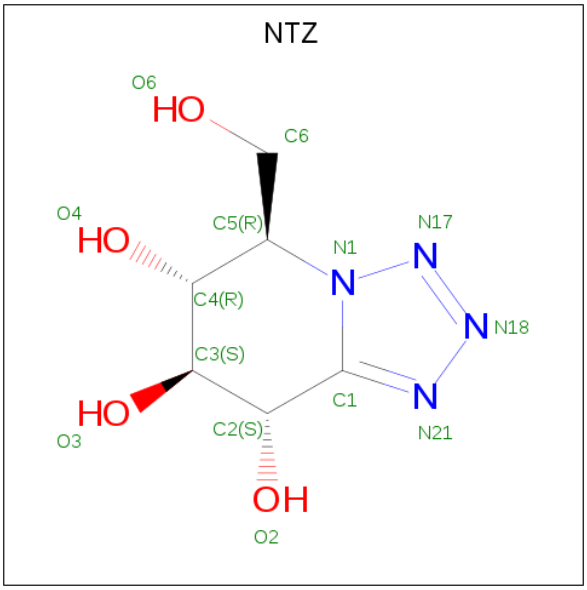
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O P 5 4 1	0	0
2	B	1	Total O P 5 4 1	0	0
2	C	1	Total O P 5 4 1	0	0
2	D	1	Total O P 5 4 1	0	0

- Molecule 3 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: $C_8H_{10}NO_6P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
3	B	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
3	C	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
3	D	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

- Molecule 4 is NOJIRIMYCINE TETRAZOLE (three-letter code: NTZ) (formula: $C_6H_{10}N_4O_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	6	4	4		
4	B	1	Total	C	N	O	0	0
			14	6	4	4		
4	C	1	Total	C	N	O	0	0
			14	6	4	4		
4	D	1	Total	C	N	O	0	0
			14	6	4	4		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	223	Total	O	0	0
			223	223		
5	B	222	Total	O	0	0
			222	222		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	218	Total O 218 218	0	0
5	D	221	Total O 221 221	0	0

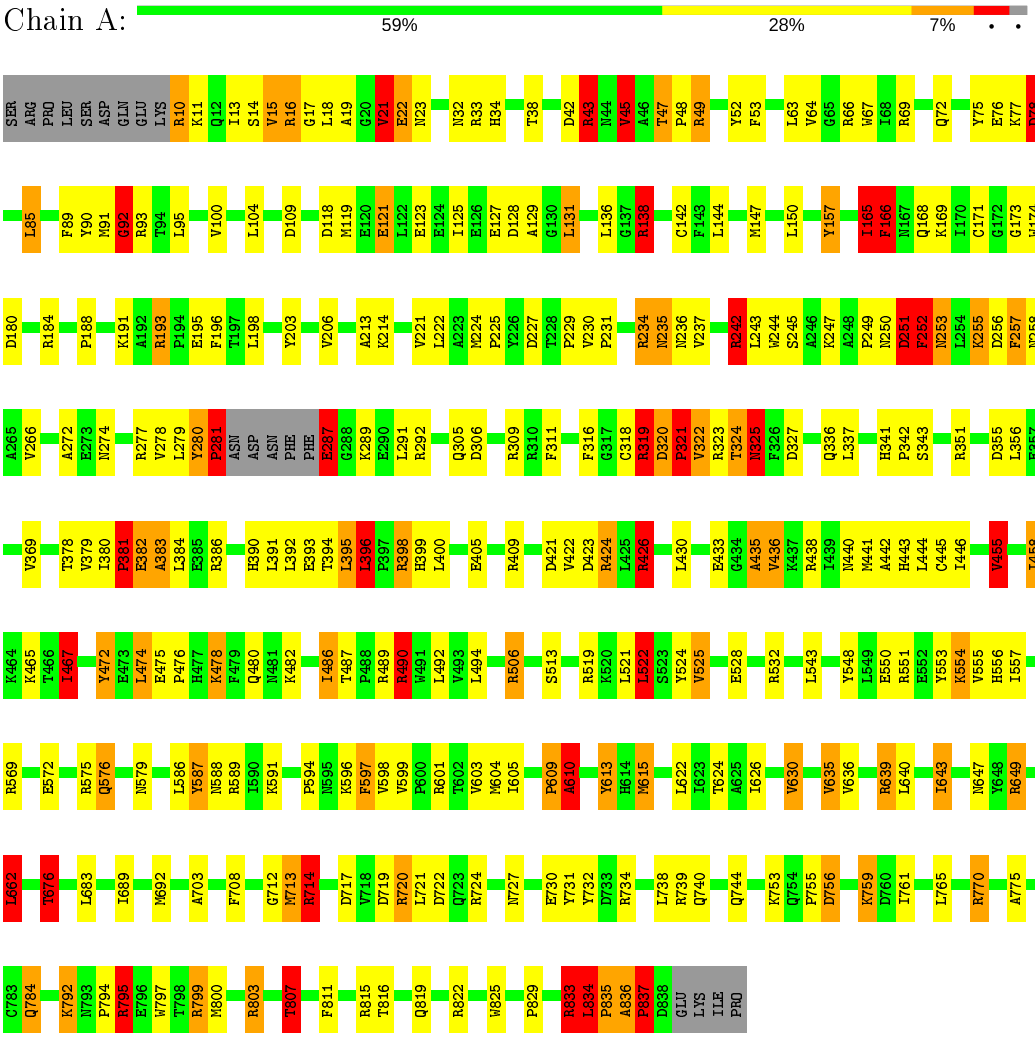
3 Residue-property plots (i)

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. 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.

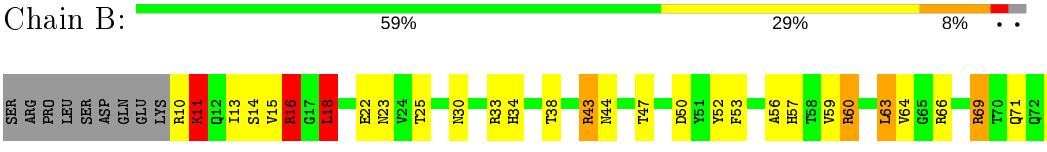
- Molecule 1: GLYCOGEN PHOSPHORYLASE

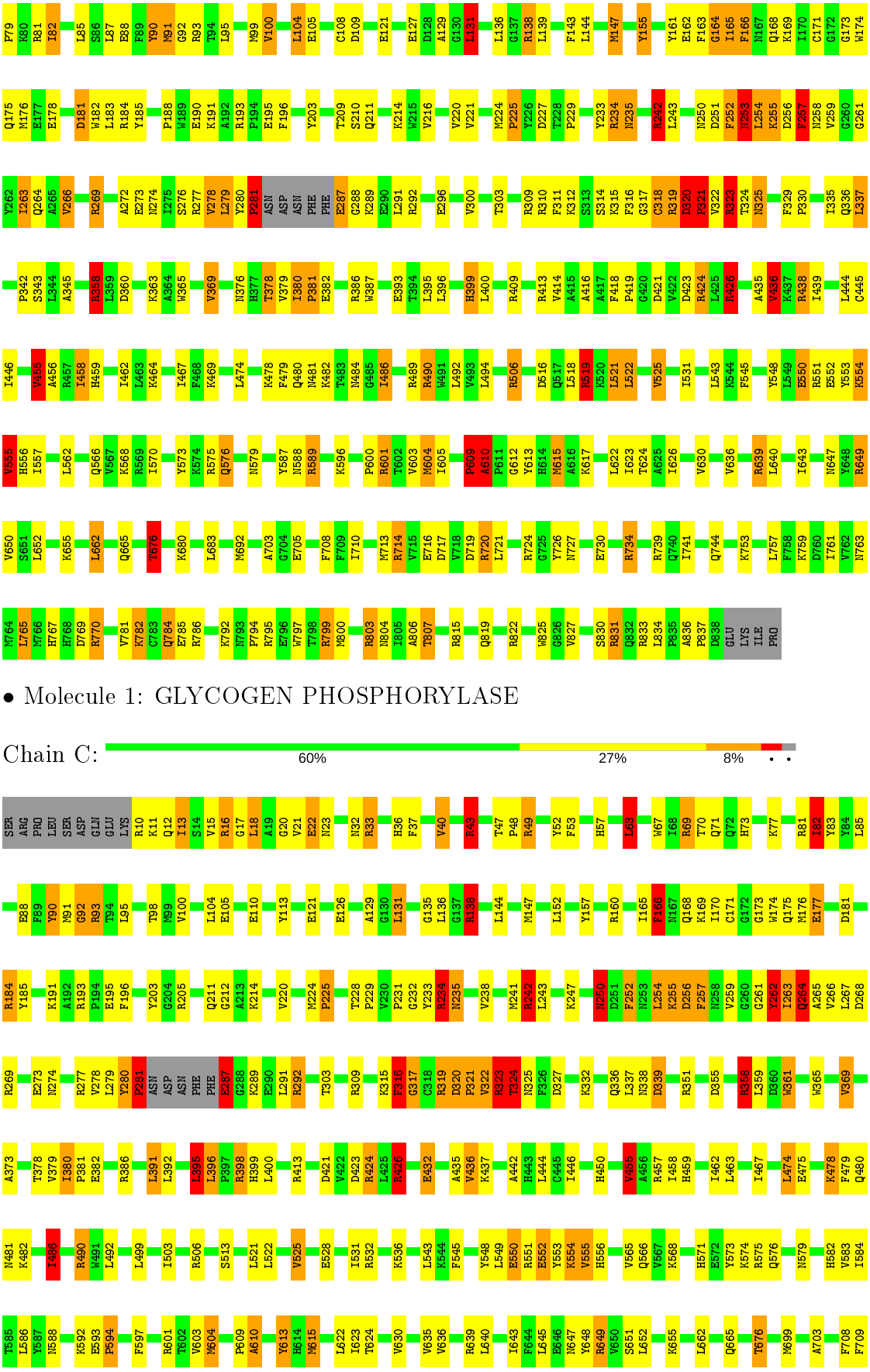
Chain A:



- Molecule 1: GLYCOGEN PHOSPHORYLASE

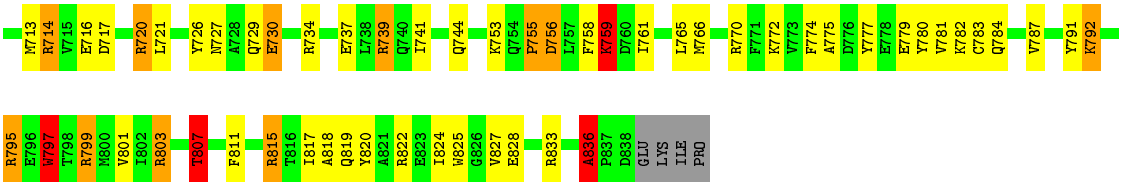
Chain B:





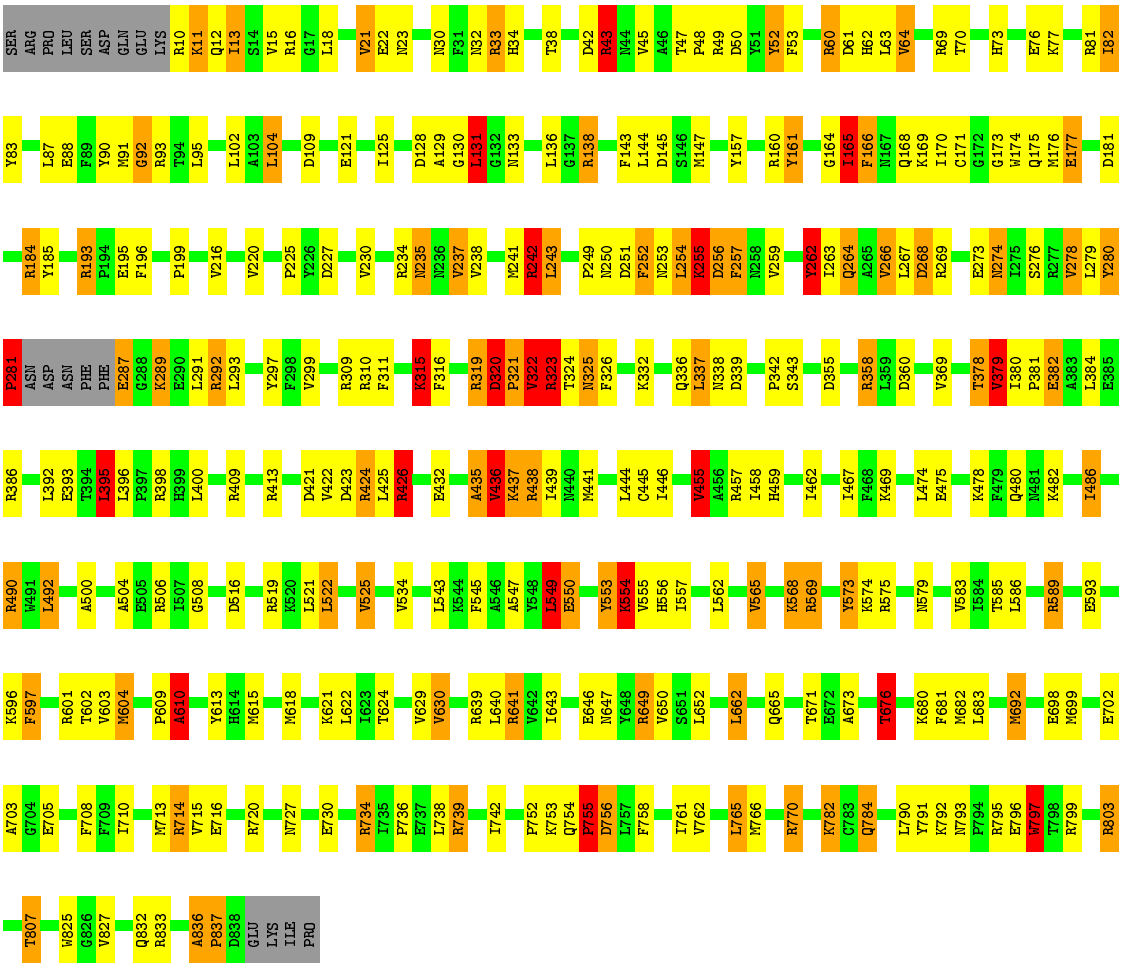
• Molecule 1: GLYCOGEN PHOSPHORYLASE

Chain C:



- Molecule 1: GLYCOGEN PHOSPHORYLASE

Chain D:



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	119.00Å 190.00Å 88.20Å 90.00° 109.35° 90.00°	Depositor
Resolution (Å)	8.00 – 2.50	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-2.50)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.171 , 0.273	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	27788	wwPDB-VP
Average B, all atoms (Å^2)	34.0	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: PO4, NTZ, PLP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.91	4/6843 (0.1%)	1.80	148/9261 (1.6%)
1	B	0.89	2/6843 (0.0%)	1.77	154/9261 (1.7%)
1	C	0.88	2/6843 (0.0%)	1.71	120/9261 (1.3%)
1	D	0.91	6/6843 (0.1%)	1.83	151/9261 (1.6%)
All	All	0.90	14/27372 (0.1%)	1.78	573/37044 (1.5%)

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	0	9
1	B	0	4
1	C	0	7
1	D	0	6
All	All	0	26

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	322	VAL	CA-CB	7.96	1.71	1.54
1	A	78	ASP	CA-CB	6.40	1.68	1.53
1	B	100	VAL	CA-CB	6.23	1.67	1.54
1	D	237	VAL	CA-CB	5.88	1.67	1.54
1	C	82	ILE	CA-CB	5.81	1.68	1.54
1	B	379	VAL	CA-CB	5.52	1.66	1.54
1	D	565	VAL	CA-CB	5.51	1.66	1.54
1	C	263	ILE	CA-CB	5.47	1.67	1.54
1	D	630	VAL	CA-CB	5.41	1.66	1.54
1	D	827	VAL	CA-CB	5.21	1.65	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	436	VAL	CA-CB	5.12	1.65	1.54
1	A	121	GLU	CG-CD	5.05	1.59	1.51
1	A	121	GLU	CB-CG	5.03	1.61	1.52
1	A	78	ASP	CB-CG	5.03	1.62	1.51

All (573) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	490	ARG	NE-CZ-NH2	-23.04	108.78	120.30
1	A	490	ARG	NE-CZ-NH1	19.12	129.86	120.30
1	D	490	ARG	NE-CZ-NH2	-17.23	111.69	120.30
1	D	575	ARG	NE-CZ-NH1	15.58	128.09	120.30
1	D	575	ARG	NE-CZ-NH2	-14.13	113.23	120.30
1	D	138	ARG	NE-CZ-NH1	14.04	127.32	120.30
1	A	615	MET	CG-SD-CE	-13.41	78.74	100.20
1	D	770	ARG	NE-CZ-NH1	12.80	126.70	120.30
1	D	242	ARG	NE-CZ-NH1	12.70	126.65	120.30
1	D	490	ARG	NE-CZ-NH1	12.65	126.62	120.30
1	B	506	ARG	NE-CZ-NH1	12.37	126.49	120.30
1	C	138	ARG	NE-CZ-NH2	-12.26	114.17	120.30
1	D	60	ARG	NE-CZ-NH2	-11.98	114.31	120.30
1	C	234	ARG	NE-CZ-NH1	11.97	126.29	120.30
1	D	193	ARG	NE-CZ-NH2	-11.86	114.37	120.30
1	B	734	ARG	NE-CZ-NH1	11.70	126.15	120.30
1	D	604	MET	CG-SD-CE	-11.37	82.01	100.20
1	D	639	ARG	NE-CZ-NH2	-11.17	114.72	120.30
1	B	93	ARG	NE-CZ-NH1	11.13	125.86	120.30
1	C	490	ARG	NE-CZ-NH2	-11.10	114.75	120.30
1	C	424	ARG	NE-CZ-NH1	11.06	125.83	120.30
1	A	424	ARG	NE-CZ-NH2	-11.02	114.79	120.30
1	B	234	ARG	NE-CZ-NH2	-10.96	114.82	120.30
1	B	506	ARG	NE-CZ-NH2	-10.94	114.83	120.30
1	C	424	ARG	NE-CZ-NH2	-10.84	114.88	120.30
1	D	424	ARG	NE-CZ-NH1	10.81	125.71	120.30
1	B	234	ARG	NE-CZ-NH1	10.79	125.69	120.30
1	B	615	MET	CG-SD-CE	-10.66	83.15	100.20
1	B	242	ARG	NE-CZ-NH1	10.62	125.61	120.30
1	B	138	ARG	NE-CZ-NH1	10.61	125.60	120.30
1	C	184	ARG	NE-CZ-NH1	10.57	125.58	120.30
1	C	241	MET	CG-SD-CE	10.47	116.96	100.20
1	D	325	ASN	CA-C-N	-10.42	94.28	117.20
1	D	60	ARG	NE-CZ-NH1	10.35	125.48	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	325	ASN	CA-C-N	-10.25	94.64	117.20
1	B	575	ARG	NE-CZ-NH2	-10.19	115.21	120.30
1	A	309	ARG	NE-CZ-NH2	-10.11	115.25	120.30
1	B	714	ARG	NE-CZ-NH1	10.08	125.34	120.30
1	C	815	ARG	NE-CZ-NH2	-10.08	115.26	120.30
1	D	457	ARG	NE-CZ-NH2	-10.07	115.27	120.30
1	C	615	MET	CG-SD-CE	-9.99	84.22	100.20
1	D	378	THR	CA-C-N	-9.76	95.74	117.20
1	A	639	ARG	NE-CZ-NH1	9.71	125.16	120.30
1	D	378	THR	O-C-N	9.62	138.09	122.70
1	B	604	MET	CG-SD-CE	-9.61	84.83	100.20
1	A	21	VAL	CG1-CB-CG2	-9.61	95.53	110.90
1	A	799	ARG	NE-CZ-NH1	9.53	125.06	120.30
1	D	615	MET	CG-SD-CE	-9.41	85.14	100.20
1	D	325	ASN	O-C-N	9.36	137.67	122.70
1	D	193	ARG	NE-CZ-NH1	9.30	124.95	120.30
1	A	424	ARG	NE-CZ-NH1	9.26	124.93	120.30
1	D	413	ARG	NE-CZ-NH2	-9.05	115.77	120.30
1	A	177	GLU	CA-CB-CG	9.04	133.29	113.40
1	C	242	ARG	NE-CZ-NH1	8.81	124.70	120.30
1	D	138	ARG	NE-CZ-NH2	-8.74	115.93	120.30
1	C	398	ARG	NE-CZ-NH1	8.71	124.66	120.30
1	D	184	ARG	NE-CZ-NH1	8.67	124.63	120.30
1	A	455	VAL	N-CA-CB	-8.61	92.57	111.50
1	B	831	ARG	NE-CZ-NH1	8.60	124.60	120.30
1	A	486	ILE	CA-CB-CG1	-8.60	94.67	111.00
1	D	797	TRP	CG-CD2-CE3	-8.56	126.19	133.90
1	D	310	ARG	NE-CZ-NH1	8.53	124.56	120.30
1	A	242	ARG	NE-CZ-NH1	8.52	124.56	120.30
1	D	639	ARG	NE-CZ-NH1	8.52	124.56	120.30
1	D	393	GLU	CA-CB-CG	8.51	132.11	113.40
1	A	692	MET	CG-SD-CE	-8.50	86.61	100.20
1	D	676	THR	N-CA-CB	-8.48	94.18	110.30
1	A	724	ARG	NE-CZ-NH2	-8.44	116.08	120.30
1	A	395	LEU	CA-CB-CG	8.43	134.69	115.30
1	D	177	GLU	CA-CB-CG	8.43	131.94	113.40
1	C	730	GLU	CA-CB-CG	8.42	131.93	113.40
1	A	252	PHE	N-CA-C	-8.40	88.33	111.00
1	A	426	ARG	NE-CZ-NH1	8.38	124.49	120.30
1	D	649	ARG	NE-CZ-NH2	-8.32	116.14	120.30
1	D	395	LEU	CA-CB-CG	8.30	134.39	115.30
1	D	256	ASP	N-CA-C	-8.28	88.64	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	604	MET	CG-SD-CE	-8.28	86.96	100.20
1	B	69	ARG	NE-CZ-NH2	-8.25	116.17	120.30
1	C	309	ARG	NE-CZ-NH1	8.25	124.42	120.30
1	A	649	ARG	NE-CZ-NH1	-8.24	116.18	120.30
1	C	455	VAL	N-CA-CB	-8.19	93.48	111.50
1	B	93	ARG	NE-CZ-NH2	-8.15	116.22	120.30
1	C	40	VAL	CG1-CB-CG2	-8.15	97.86	110.90
1	C	604	MET	CG-SD-CE	-8.13	87.19	100.20
1	D	281	PRO	N-CA-C	8.13	133.23	112.10
1	A	309	ARG	NE-CZ-NH1	8.11	124.36	120.30
1	C	797	TRP	CG-CD2-CE3	-8.09	126.62	133.90
1	A	78	ASP	CB-CG-OD2	8.09	125.58	118.30
1	A	639	ARG	NE-CZ-NH2	-8.05	116.28	120.30
1	D	242	ARG	NE-CZ-NH2	-8.04	116.28	120.30
1	C	81	ARG	NE-CZ-NH1	7.98	124.29	120.30
1	A	797	TRP	CG-CD2-CE3	-7.96	126.74	133.90
1	C	770	ARG	NE-CZ-NH1	7.94	124.27	120.30
1	A	770	ARG	NE-CZ-NH1	7.91	124.26	120.30
1	A	242	ARG	NE-CZ-NH2	-7.84	116.38	120.30
1	B	378	THR	O-C-N	7.79	135.17	122.70
1	D	181	ASP	CA-C-N	-7.78	100.09	117.20
1	A	184	ARG	NE-CZ-NH1	7.77	124.19	120.30
1	B	713	MET	CG-SD-CE	-7.74	87.82	100.20
1	D	455	VAL	N-CA-CB	-7.74	94.47	111.50
1	B	519	ARG	NE-CZ-NH2	-7.73	116.43	120.30
1	D	184	ARG	NE-CZ-NH2	-7.71	116.44	120.30
1	A	234	ARG	NE-CZ-NH2	-7.70	116.45	120.30
1	D	161	TYR	CB-CG-CD2	-7.69	116.39	121.00
1	C	413	ARG	NE-CZ-NH2	-7.68	116.46	120.30
1	D	629	VAL	CG1-CB-CG2	-7.68	98.61	110.90
1	A	138	ARG	NE-CZ-NH2	-7.68	116.46	120.30
1	D	426	ARG	NE-CZ-NH1	7.67	124.13	120.30
1	D	69	ARG	NE-CZ-NH1	7.63	124.11	120.30
1	A	486	ILE	CA-CB-CG2	7.61	126.12	110.90
1	D	81	ARG	NE-CZ-NH2	-7.59	116.51	120.30
1	C	138	ARG	NE-CZ-NH1	7.57	124.08	120.30
1	A	321	PRO	N-CA-C	7.57	131.77	112.10
1	C	720	ARG	CA-CB-CG	7.57	130.04	113.40
1	B	575	ARG	CB-CG-CD	-7.54	92.01	111.60
1	B	786	ARG	NE-CZ-NH1	7.53	124.06	120.30
1	B	734	ARG	NE-CZ-NH2	-7.51	116.54	120.30
1	A	575	ARG	CB-CG-CD	-7.51	92.08	111.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	309	ARG	CA-CB-CG	7.50	129.90	113.40
1	C	262	TYR	CB-CG-CD2	-7.50	116.50	121.00
1	C	281	PRO	CA-N-CD	-7.48	101.02	111.50
1	C	815	ARG	NE-CZ-NH1	7.48	124.04	120.30
1	A	713	MET	CG-SD-CE	-7.48	88.24	100.20
1	A	18	LEU	CA-CB-CG	7.44	132.41	115.30
1	D	649	ARG	NE-CZ-NH1	7.42	124.01	120.30
1	A	731	TYR	CB-CG-CD1	-7.39	116.56	121.00
1	D	262	TYR	CA-C-N	-7.37	100.98	117.20
1	B	257	PHE	CA-C-N	-7.36	101.01	117.20
1	C	458	ILE	CA-CB-CG2	-7.34	96.22	110.90
1	C	649	ARG	NE-CZ-NH2	-7.31	116.64	120.30
1	B	639	ARG	NE-CZ-NH2	-7.30	116.65	120.30
1	B	575	ARG	NE-CZ-NH1	7.29	123.94	120.30
1	D	321	PRO	CA-C-N	7.28	133.22	117.20
1	D	692	MET	CG-SD-CE	-7.25	88.59	100.20
1	A	255	LYS	CA-C-N	-7.25	101.24	117.20
1	B	378	THR	CA-C-N	-7.25	101.25	117.20
1	D	320	ASP	N-CA-C	7.24	130.55	111.00
1	A	64	VAL	CG1-CB-CG2	-7.23	99.34	110.90
1	A	281	PRO	CA-N-CD	-7.22	101.40	111.50
1	A	490	ARG	CD-NE-CZ	7.20	133.68	123.60
1	B	609	PRO	N-CA-CB	7.19	111.93	103.30
1	B	797	TRP	CG-CD2-CE3	-7.18	127.44	133.90
1	B	455	VAL	N-CA-CB	-7.17	95.71	111.50
1	B	589	ARG	CA-CB-CG	7.17	129.19	113.40
1	B	713	MET	CA-CB-CG	7.17	125.49	113.30
1	D	457	ARG	NE-CZ-NH1	7.15	123.88	120.30
1	D	10	ARG	NE-CZ-NH2	-7.15	116.72	120.30
1	B	108	CYS	CA-CB-SG	-7.14	101.16	114.00
1	A	109	ASP	CB-CG-OD2	-7.13	111.88	118.30
1	A	43	ARG	NE-CZ-NH2	7.09	123.84	120.30
1	C	361	TRP	CG-CD2-CE3	-7.08	127.52	133.90
1	D	165	ILE	N-CA-C	-7.07	91.92	111.00
1	B	649	ARG	NE-CZ-NH2	-7.05	116.77	120.30
1	B	181	ASP	CA-C-N	-7.05	101.69	117.20
1	C	234	ARG	NE-CZ-NH2	-7.05	116.78	120.30
1	A	109	ASP	CB-CG-OD1	7.03	124.62	118.30
1	D	315	LYS	CA-C-N	7.02	132.65	117.20
1	A	21	VAL	CA-CB-CG1	7.02	121.43	110.90
1	B	234	ARG	CD-NE-CZ	6.97	133.35	123.60
1	C	165	ILE	N-CA-C	-6.97	92.19	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	90	TYR	CB-CG-CD2	-6.94	116.84	121.00
1	A	203	TYR	CB-CG-CD2	-6.92	116.85	121.00
1	A	165	ILE	N-CA-C	-6.92	92.31	111.00
1	A	649	ARG	CG-CD-NE	-6.92	97.27	111.80
1	B	281	PRO	CA-N-CD	-6.92	101.81	111.50
1	B	720	ARG	NE-CZ-NH1	6.92	123.76	120.30
1	D	455	VAL	CG1-CB-CG2	6.91	121.95	110.90
1	A	318	CYS	CA-C-N	6.88	132.33	117.20
1	C	575	ARG	NE-CZ-NH2	-6.87	116.86	120.30
1	A	251	ASP	CA-C-N	-6.87	102.08	117.20
1	A	92	GLY	CA-C-N	6.87	132.31	117.20
1	D	255	LYS	O-C-N	6.85	133.66	122.70
1	B	18	LEU	CA-CB-CG	6.81	130.96	115.30
1	D	321	PRO	N-CA-C	6.80	129.79	112.10
1	B	325	ASN	O-C-N	6.79	133.57	122.70
1	B	589	ARG	NE-CZ-NH2	-6.77	116.92	120.30
1	C	759	LYS	CA-CB-CG	6.77	128.29	113.40
1	B	438	ARG	NE-CZ-NH2	-6.76	116.92	120.30
1	C	699	MET	CG-SD-CE	6.76	111.01	100.20
1	C	486	ILE	CA-CB-CG1	-6.74	98.20	111.00
1	D	426	ARG	CA-CB-CG	6.74	128.22	113.40
1	A	325	ASN	CA-C-N	-6.73	102.39	117.20
1	A	610	ALA	N-CA-CB	6.73	119.52	110.10
1	A	393	GLU	CA-CB-CG	6.73	128.20	113.40
1	B	378	THR	C-N-CA	6.71	138.48	121.70
1	D	490	ARG	CG-CD-NE	-6.71	97.72	111.80
1	B	321	PRO	CA-N-CD	-6.71	102.11	111.50
1	B	309	ARG	NE-CZ-NH1	6.70	123.65	120.30
1	C	770	ARG	CD-NE-CZ	6.67	132.94	123.60
1	D	280	TYR	CB-CG-CD2	-6.67	117.00	121.00
1	D	292	ARG	NE-CZ-NH2	-6.66	116.97	120.30
1	B	16	ARG	CA-CB-CG	6.64	128.01	113.40
1	B	252	PHE	CA-C-N	-6.59	102.69	117.20
1	C	324	THR	N-CA-C	-6.59	93.21	111.00
1	C	799	ARG	NE-CZ-NH1	6.59	123.59	120.30
1	A	257	PHE	CA-C-N	-6.59	102.71	117.20
1	B	66	ARG	NE-CZ-NH1	6.59	123.59	120.30
1	B	255	LYS	CA-C-N	-6.58	102.73	117.20
1	C	474	LEU	CA-CB-CG	6.57	130.41	115.30
1	D	234	ARG	NE-CZ-NH1	6.57	123.58	120.30
1	A	180	ASP	CA-C-N	6.55	131.62	117.20
1	B	831	ARG	CA-CB-CG	6.55	127.81	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	469	LYS	CA-CB-CG	6.54	127.78	113.40
1	C	770	ARG	CG-CD-NE	6.54	125.52	111.80
1	D	426	ARG	NE-CZ-NH2	-6.52	117.04	120.30
1	C	205	ARG	NE-CZ-NH1	6.52	123.56	120.30
1	C	177	GLU	CA-CB-CG	6.52	127.74	113.40
1	A	613	TYR	CB-CG-CD2	-6.51	117.09	121.00
1	C	575	ARG	CB-CG-CD	-6.50	94.71	111.60
1	B	458	ILE	CB-CG1-CD1	-6.49	95.72	113.90
1	D	569	ARG	NE-CZ-NH2	6.49	123.54	120.30
1	A	833	ARG	CB-CG-CD	6.48	128.45	111.60
1	A	251	ASP	CA-CB-CG	-6.48	99.15	113.40
1	D	424	ARG	NE-CZ-NH2	-6.48	117.06	120.30
1	A	438	ARG	NE-CZ-NH1	6.47	123.53	120.30
1	A	458	ILE	CA-CB-CG2	-6.47	97.96	110.90
1	B	421	ASP	CA-C-N	-6.47	102.97	117.20
1	A	720	ARG	NE-CZ-NH2	-6.46	117.07	120.30
1	B	827	VAL	CG1-CB-CG2	-6.46	100.56	110.90
1	B	358	ARG	NE-CZ-NH1	6.46	123.53	120.30
1	A	489	ARG	NE-CZ-NH2	-6.46	117.07	120.30
1	B	587	TYR	CB-CG-CD2	-6.46	117.13	121.00
1	B	424	ARG	CA-CB-CG	6.45	127.58	113.40
1	D	323	ARG	CA-CB-CG	6.45	127.58	113.40
1	D	714	ARG	NE-CZ-NH2	-6.45	117.08	120.30
1	D	33	ARG	CB-CG-CD	-6.43	94.89	111.60
1	A	255	LYS	O-C-N	6.41	132.96	122.70
1	B	309	ARG	CD-NE-CZ	6.41	132.57	123.60
1	C	458	ILE	CA-CB-CG1	6.40	123.16	111.00
1	B	255	LYS	O-C-N	6.39	132.92	122.70
1	A	250	ASN	CA-C-N	-6.38	103.16	117.20
1	A	351	ARG	NE-CZ-NH1	6.38	123.49	120.30
1	C	737	GLU	N-CA-CB	6.37	122.07	110.60
1	D	713	MET	CA-CB-CG	6.37	124.13	113.30
1	A	166	PHE	N-CA-C	6.37	128.19	111.00
1	B	601	ARG	NE-CZ-NH1	6.34	123.47	120.30
1	D	525	VAL	CG1-CB-CG2	-6.34	100.75	110.90
1	D	92	GLY	CA-C-N	6.33	131.13	117.20
1	D	252	PHE	CA-C-N	-6.32	103.29	117.20
1	A	426	ARG	CA-CB-CG	6.31	127.29	113.40
1	C	426	ARG	CA-CB-CG	6.30	127.26	113.40
1	A	383	ALA	N-CA-CB	-6.30	101.29	110.10
1	D	323	ARG	NE-CZ-NH1	6.30	123.45	120.30
1	C	323	ARG	N-CA-C	6.29	128.00	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	81	ARG	NE-CZ-NH1	6.27	123.44	120.30
1	B	486	ILE	CA-CB-CG1	-6.26	99.11	111.00
1	B	69	ARG	NE-CZ-NH1	6.25	123.43	120.30
1	C	281	PRO	N-CA-C	6.25	128.35	112.10
1	A	33	ARG	CA-CB-CG	6.25	127.14	113.40
1	D	378	THR	C-N-CA	6.24	137.31	121.70
1	D	641	ARG	NE-CZ-NH2	-6.23	117.18	120.30
1	C	281	PRO	CA-C-N	6.23	130.90	117.20
1	A	613	TYR	CB-CG-CD1	6.22	124.73	121.00
1	A	351	ARG	NE-CZ-NH2	-6.20	117.20	120.30
1	B	309	ARG	NE-CZ-NH2	-6.20	117.20	120.30
1	D	575	ARG	CB-CG-CD	-6.19	95.52	111.60
1	B	81	ARG	NE-CZ-NH2	-6.18	117.21	120.30
1	D	33	ARG	CA-CB-CG	6.18	127.01	113.40
1	A	478	LYS	CA-CB-CG	6.18	127.00	113.40
1	D	255	LYS	CA-C-N	-6.18	103.60	117.20
1	C	43	ARG	CA-CB-CG	6.18	127.00	113.40
1	B	759	LYS	CA-CB-CG	6.17	126.98	113.40
1	D	325	ASN	CA-CB-CG	6.17	126.97	113.40
1	D	321	PRO	N-CA-CB	-6.16	95.82	102.60
1	A	714	ARG	NE-CZ-NH2	-6.15	117.22	120.30
1	A	724	ARG	NE-CZ-NH1	6.15	123.37	120.30
1	C	69	ARG	NE-CZ-NH1	6.14	123.37	120.30
1	A	361	TRP	CG-CD2-CE3	-6.13	128.38	133.90
1	D	64	VAL	CG1-CB-CG2	-6.13	101.09	110.90
1	B	242	ARG	NE-CZ-NH2	-6.13	117.23	120.30
1	C	795	ARG	NE-CZ-NH1	6.13	123.36	120.30
1	A	770	ARG	CD-NE-CZ	6.12	132.17	123.60
1	C	280	TYR	CB-CG-CD2	-6.12	117.33	121.00
1	C	435	ALA	N-CA-C	-6.12	94.49	111.00
1	B	714	ARG	CB-CG-CD	6.11	127.49	111.60
1	C	250	ASN	N-CA-C	6.11	127.50	111.00
1	C	160	ARG	NE-CZ-NH2	6.09	123.34	120.30
1	B	325	ASN	N-CA-C	6.08	127.42	111.00
1	A	799	ARG	NE-CZ-NH2	-6.08	117.26	120.30
1	B	224	MET	CG-SD-CE	-6.07	90.48	100.20
1	C	83	TYR	CB-CG-CD2	6.07	124.64	121.00
1	D	281	PRO	CA-N-CD	-6.07	103.00	111.50
1	D	455	VAL	CA-CB-CG2	-6.06	101.81	110.90
1	D	827	VAL	CG1-CB-CG2	-6.06	101.21	110.90
1	D	43	ARG	NE-CZ-NH1	6.05	123.32	120.30
1	D	610	ALA	N-CA-C	-6.04	94.68	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	834	LEU	CA-CB-CG	6.04	129.19	115.30
1	B	831	ARG	CD-NE-CZ	6.04	132.05	123.60
1	B	379	VAL	O-C-N	6.04	132.35	122.70
1	C	184	ARG	CD-NE-CZ	6.03	132.05	123.60
1	C	234	ARG	CG-CD-NE	-6.03	99.14	111.80
1	B	155	TYR	CB-CG-CD1	-6.01	117.39	121.00
1	D	714	ARG	NE-CZ-NH1	6.01	123.31	120.30
1	A	822	ARG	NE-CZ-NH1	6.01	123.30	120.30
1	C	797	TRP	CD1-CG-CD2	-6.00	101.50	106.30
1	D	438	ARG	NE-CZ-NH1	6.00	123.30	120.30
1	D	770	ARG	CD-NE-CZ	6.00	131.99	123.60
1	D	486	ILE	CA-CB-CG1	-5.99	99.62	111.00
1	B	164	GLY	O-C-N	5.99	132.28	122.70
1	B	379	VAL	CA-C-N	-5.98	104.05	117.20
1	B	91	MET	CG-SD-CE	-5.97	90.65	100.20
1	B	250	ASN	CA-C-N	-5.97	104.06	117.20
1	B	376	ASN	CA-C-N	5.97	130.33	117.20
1	C	739	ARG	CG-CD-NE	5.97	124.33	111.80
1	D	797	TRP	CD1-CG-CD2	-5.96	101.53	106.30
1	A	426	ARG	CG-CD-NE	5.96	124.31	111.80
1	A	318	CYS	O-C-N	-5.95	113.17	122.70
1	D	714	ARG	CA-CB-CG	-5.95	100.31	113.40
1	A	807	THR	N-CA-CB	-5.95	99.00	110.30
1	B	310	ARG	NE-CZ-NH2	-5.95	117.33	120.30
1	C	351	ARG	NE-CZ-NH2	-5.94	117.33	120.30
1	A	321	PRO	CA-N-CD	-5.94	103.19	111.50
1	C	737	GLU	CA-CB-CG	5.94	126.46	113.40
1	C	92	GLY	CA-C-N	5.92	130.23	117.20
1	B	726	TYR	CB-CG-CD1	-5.92	117.45	121.00
1	C	655	LYS	CA-CB-CG	5.92	126.42	113.40
1	B	555	VAL	CG1-CB-CG2	-5.92	101.44	110.90
1	D	720	ARG	CA-CB-CG	5.92	126.41	113.40
1	B	99	MET	CG-SD-CE	5.90	109.65	100.20
1	D	322	VAL	CA-C-N	-5.90	104.22	117.20
1	C	309	ARG	NE-CZ-NH2	-5.89	117.35	120.30
1	D	409	ARG	NE-CZ-NH1	5.89	123.25	120.30
1	B	610	ALA	N-CA-C	-5.89	95.11	111.00
1	C	238	VAL	CG1-CB-CG2	-5.88	101.49	110.90
1	B	770	ARG	NE-CZ-NH1	5.88	123.24	120.30
1	A	193	ARG	NE-CZ-NH1	5.87	123.24	120.30
1	C	184	ARG	CA-CB-CG	5.87	126.31	113.40
1	B	525	VAL	CG1-CB-CG2	-5.87	101.51	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	795	ARG	NE-CZ-NH1	5.85	123.22	120.30
1	A	525	VAL	CG1-CB-CG2	-5.84	101.56	110.90
1	B	720	ARG	CA-CB-CG	5.83	126.23	113.40
1	D	739	ARG	CG-CD-NE	5.83	124.04	111.80
1	A	458	ILE	CA-CB-CG1	5.82	122.05	111.00
1	B	393	GLU	CA-CB-CG	5.81	126.19	113.40
1	B	782	LYS	CA-CB-CG	5.81	126.18	113.40
1	B	486	ILE	CA-CB-CG2	5.81	122.51	110.90
1	B	289	LYS	CA-CB-CG	5.80	126.16	113.40
1	B	164	GLY	CA-C-N	-5.79	104.45	117.20
1	D	88	GLU	CB-CA-C	-5.79	98.81	110.40
1	C	807	THR	N-CA-CB	-5.78	99.32	110.30
1	B	320	ASP	CA-CB-CG	5.78	126.11	113.40
1	C	490	ARG	CG-CD-NE	-5.77	99.68	111.80
1	B	195	GLU	CB-CA-C	-5.76	98.89	110.40
1	A	712	GLY	CA-C-N	-5.75	104.54	117.20
1	A	85	LEU	CA-CB-CG	5.75	128.52	115.30
1	C	613	TYR	CB-CG-CD1	5.75	124.45	121.00
1	D	274	ASN	CA-CB-CG	5.75	126.04	113.40
1	B	220	VAL	CA-CB-CG2	-5.74	102.29	110.90
1	B	11	LYS	CA-CB-CG	5.74	126.03	113.40
1	B	88	GLU	CA-CB-CG	5.74	126.03	113.40
1	D	782	LYS	CB-CG-CD	5.74	126.52	111.60
1	B	490	ARG	CG-CD-NE	-5.73	99.78	111.80
1	D	220	VAL	CG1-CB-CG2	-5.72	101.75	110.90
1	A	435	ALA	N-CA-C	-5.72	95.56	111.00
1	A	138	ARG	NE-CZ-NH1	5.71	123.16	120.30
1	A	441	MET	CG-SD-CE	5.71	109.33	100.20
1	B	650	VAL	CG1-CB-CG2	-5.70	101.78	110.90
1	B	23	ASN	N-CA-C	5.69	126.37	111.00
1	B	676	THR	N-CA-CB	-5.69	99.49	110.30
1	D	166	PHE	N-CA-C	5.69	126.35	111.00
1	C	292	ARG	NE-CZ-NH1	5.69	123.14	120.30
1	C	395	LEU	CA-CB-CG	5.68	128.37	115.30
1	A	398	ARG	NE-CZ-NH1	5.68	123.14	120.30
1	D	278	VAL	CA-CB-CG2	-5.68	102.38	110.90
1	D	63	LEU	CA-CB-CG	5.68	128.37	115.30
1	B	436	VAL	CA-CB-CG2	-5.67	102.40	110.90
1	D	69	ARG	NE-CZ-NH2	-5.66	117.47	120.30
1	B	786	ARG	NE-CZ-NH2	-5.66	117.47	120.30
1	D	264	GLN	CA-CB-CG	5.65	125.83	113.40
1	B	464	LYS	CA-CB-CG	5.65	125.83	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	10	ARG	NE-CZ-NH1	5.65	123.12	120.30
1	B	409	ARG	NE-CZ-NH1	5.65	123.12	120.30
1	B	822	ARG	NE-CZ-NH1	5.64	123.12	120.30
1	B	555	VAL	CB-CA-C	-5.64	100.68	111.40
1	B	436	VAL	CA-CB-CG1	5.64	119.35	110.90
1	A	280	TYR	CB-CG-CD2	-5.63	117.62	121.00
1	C	33	ARG	CB-CA-C	-5.63	99.14	110.40
1	D	337	LEU	CB-CG-CD2	-5.63	101.44	111.00
1	C	486	ILE	CA-CB-CG2	5.62	122.14	110.90
1	A	474	LEU	CA-CB-CG	5.61	128.21	115.30
1	A	33	ARG	N-CA-CB	5.60	120.69	110.60
1	A	490	ARG	CG-CD-NE	-5.60	100.03	111.80
1	D	384	LEU	CA-CB-CG	5.60	128.18	115.30
1	C	552	GLU	N-CA-C	-5.59	95.89	111.00
1	A	635	VAL	CA-CB-CG2	-5.59	102.52	110.90
1	C	49	ARG	NE-CZ-NH2	-5.59	117.50	120.30
1	B	409	ARG	NE-CZ-NH2	-5.59	117.51	120.30
1	D	88	GLU	CA-CB-CG	5.59	125.69	113.40
1	C	13	ILE	N-CA-C	-5.58	95.92	111.00
1	C	93	ARG	CB-CA-C	-5.58	99.23	110.40
1	D	13	ILE	N-CA-C	-5.58	95.92	111.00
1	C	455	VAL	CB-CA-C	5.58	122.00	111.40
1	A	713	MET	CA-CB-CG	5.57	122.78	113.30
1	B	323	ARG	CA-C-N	-5.56	104.96	117.20
1	D	441	MET	CG-SD-CE	5.56	109.10	100.20
1	A	47	THR	N-CA-CB	-5.56	99.74	110.30
1	B	278	VAL	CA-CB-CG2	-5.56	102.56	110.90
1	A	609	PRO	C-N-CA	5.54	135.55	121.70
1	B	734	ARG	CD-NE-CZ	5.54	131.35	123.60
1	C	478	LYS	CA-CB-CG	5.53	125.57	113.40
1	B	147	MET	CG-SD-CE	5.53	109.05	100.20
1	C	359	LEU	CA-CB-CG	5.53	128.02	115.30
1	D	602	THR	N-CA-C	-5.53	96.07	111.00
1	A	15	VAL	CG1-CB-CG2	-5.53	102.05	110.90
1	B	399	HIS	CA-C-N	5.52	129.34	117.20
1	B	719	ASP	CB-CG-OD1	5.52	123.27	118.30
1	A	21	VAL	CA-CB-CG2	-5.52	102.63	110.90
1	A	147	MET	CA-CB-CG	-5.51	103.93	113.30
1	A	655	LYS	CA-CB-CG	5.51	125.53	113.40
1	D	268	ASP	CB-CG-OD1	5.50	123.25	118.30
1	D	30	ASN	CA-CB-CG	-5.50	101.30	113.40
1	C	309	ARG	CD-NE-CZ	5.50	131.29	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	127	GLU	CB-CA-C	-5.50	99.41	110.40
1	B	378	THR	OG1-CB-CG2	-5.49	97.37	110.00
1	C	90	TYR	CB-CG-CD2	-5.49	117.71	121.00
1	D	299	VAL	CG1-CB-CG2	-5.48	102.13	110.90
1	B	138	ARG	NE-CZ-NH2	-5.48	117.56	120.30
1	D	413	ARG	NE-CZ-NH1	5.48	123.04	120.30
1	C	88	GLU	CA-CB-CG	5.47	125.44	113.40
1	B	680	LYS	CD-CE-NZ	-5.47	99.12	111.70
1	B	325	ASN	CA-C-O	5.46	131.57	120.10
1	C	801	VAL	CG1-CB-CG2	-5.46	102.16	110.90
1	C	203	TYR	CB-CG-CD2	-5.45	117.73	121.00
1	A	281	PRO	N-CA-C	5.45	126.26	112.10
1	C	255	LYS	CA-C-N	-5.45	105.22	117.20
1	C	287	GLU	CA-CB-CG	5.44	125.37	113.40
1	D	421	ASP	CB-CG-OD1	5.44	123.19	118.30
1	D	455	VAL	CB-CA-C	5.44	121.73	111.40
1	B	414	VAL	CA-CB-CG2	-5.43	102.75	110.90
1	D	649	ARG	CD-NE-CZ	5.43	131.21	123.60
1	D	833	ARG	NE-CZ-NH1	5.43	123.02	120.30
1	D	435	ALA	N-CA-C	-5.42	96.35	111.00
1	A	587	TYR	CB-CG-CD2	-5.42	117.75	121.00
1	C	820	TYR	CB-CG-CD2	5.42	124.25	121.00
1	C	649	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	B	216	VAL	CG1-CB-CG2	-5.41	102.25	110.90
1	A	770	ARG	CG-CD-NE	5.41	123.15	111.80
1	B	799	ARG	NE-CZ-NH1	5.41	123.00	120.30
1	A	455	VAL	CB-CA-C	5.40	121.67	111.40
1	D	755	PRO	CA-N-CD	-5.40	103.94	111.50
1	B	64	VAL	CG1-CB-CG2	-5.40	102.26	110.90
1	A	203	TYR	CB-CG-CD1	5.40	124.24	121.00
1	A	277	ARG	CA-CB-CG	-5.39	101.54	113.40
1	B	739	ARG	CG-CD-NE	5.39	123.12	111.80
1	A	193	ARG	NE-CZ-NH2	-5.38	117.61	120.30
1	B	438	ARG	CB-CG-CD	-5.38	97.60	111.60
1	B	799	ARG	NE-CZ-NH2	-5.38	117.61	120.30
1	D	184	ARG	CA-CB-CG	5.38	125.24	113.40
1	C	16	ARG	CA-CB-CG	5.38	125.23	113.40
1	C	358	ARG	NE-CZ-NH1	5.37	122.98	120.30
1	B	424	ARG	NE-CZ-NH2	-5.36	117.62	120.30
1	A	253	ASN	CA-CB-CG	5.36	125.19	113.40
1	B	210	SER	N-CA-CB	-5.35	102.48	110.50
1	D	467	ILE	CG1-CB-CG2	-5.35	99.64	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	636	VAL	CG1-CB-CG2	-5.34	102.35	110.90
1	A	569	ARG	NE-CZ-NH2	5.34	122.97	120.30
1	A	572	GLU	CA-C-N	5.34	128.94	117.20
1	B	60	ARG	CA-CB-CG	-5.34	101.66	113.40
1	C	737	GLU	CB-CA-C	-5.33	99.74	110.40
1	B	25	THR	CA-CB-CG2	-5.33	104.94	112.40
1	A	224	MET	CA-CB-CG	-5.33	104.24	113.30
1	C	714	ARG	NE-CZ-NH2	-5.33	117.64	120.30
1	D	650	VAL	CA-C-N	5.33	128.92	117.20
1	B	589	ARG	NE-CZ-NH1	5.33	122.96	120.30
1	A	465	LYS	CA-CB-CG	5.32	125.11	113.40
1	B	131	LEU	CA-CB-CG	5.32	127.54	115.30
1	C	386	ARG	O-C-N	5.32	131.21	122.70
1	C	811	PHE	N-CA-CB	-5.32	101.03	110.60
1	A	390	HIS	CA-CB-CG	5.31	122.64	113.60
1	C	212	GLY	CA-C-N	-5.31	105.52	117.20
1	C	358	ARG	CA-CB-CG	5.30	125.07	113.40
1	D	310	ARG	NE-CZ-NH2	-5.30	117.65	120.30
1	A	45	VAL	N-CA-CB	-5.30	99.85	111.50
1	B	203	TYR	CB-CG-CD1	5.28	124.17	121.00
1	D	262	TYR	O-C-N	5.28	131.14	122.70
1	C	181	ASP	CA-C-N	-5.27	105.60	117.20
1	C	166	PHE	N-CA-C	5.27	125.23	111.00
1	C	255	LYS	O-C-N	5.27	131.13	122.70
1	A	176	MET	CG-SD-CE	5.26	108.62	100.20
1	B	181	ASP	CB-CG-OD2	-5.26	113.56	118.30
1	A	521	LEU	N-CA-CB	-5.26	99.89	110.40
1	D	549	LEU	CA-CB-CG	5.26	127.39	115.30
1	D	42	ASP	CB-CG-OD1	5.25	123.03	118.30
1	A	643	ILE	CB-CG1-CD1	-5.24	99.22	113.90
1	A	731	TYR	CB-CG-CD2	5.24	124.14	121.00
1	B	266	VAL	N-CA-C	-5.24	96.85	111.00
1	B	319	ARG	NE-CZ-NH1	5.24	122.92	120.30
1	B	424	ARG	NE-CZ-NH1	5.24	122.92	120.30
1	B	800	MET	CG-SD-CE	-5.23	91.84	100.20
1	A	521	LEU	CB-CG-CD2	-5.22	102.12	111.00
1	B	165	ILE	N-CA-C	-5.22	96.90	111.00
1	D	425	LEU	CA-CB-CG	5.22	127.30	115.30
1	D	109	ASP	CB-CG-OD1	5.21	122.99	118.30
1	A	263	ILE	CA-C-N	-5.21	105.74	117.20
1	B	769	ASP	CB-CG-OD1	5.21	122.99	118.30
1	D	378	THR	CA-CB-CG2	-5.21	105.11	112.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	33	ARG	CB-CA-C	-5.21	99.98	110.40
1	A	467	ILE	CG1-CB-CG2	-5.21	99.95	111.40
1	D	181	ASP	CA-C-O	5.20	131.02	120.10
1	C	316	PHE	CA-CB-CG	-5.20	101.43	113.90
1	A	712	GLY	O-C-N	5.19	131.01	122.70
1	B	253	ASN	N-CA-C	-5.19	96.98	111.00
1	D	145	ASP	CB-CG-OD2	5.19	122.97	118.30
1	A	49	ARG	NE-CZ-NH2	-5.19	117.70	120.30
1	B	769	ASP	CB-CG-OD2	-5.19	113.63	118.30
1	C	63	LEU	CA-CB-CG	5.19	127.24	115.30
1	C	212	GLY	O-C-N	5.19	131.01	122.70
1	A	599	VAL	CG1-CB-CG2	-5.18	102.61	110.90
1	A	396	LEU	CB-CG-CD2	-5.17	102.20	111.00
1	C	10	ARG	NE-CZ-NH1	5.17	122.89	120.30
1	B	269	ARG	N-CA-CB	5.17	119.91	110.60
1	C	77	LYS	CB-CG-CD	5.17	125.04	111.60
1	D	438	ARG	NE-CZ-NH2	-5.17	117.72	120.30
1	B	455	VAL	CB-CA-C	5.16	121.21	111.40
1	B	44	ASN	CB-CA-C	-5.15	100.09	110.40
1	D	216	VAL	CG1-CB-CG2	-5.15	102.65	110.90
1	A	610	ALA	N-CA-C	-5.15	97.09	111.00
1	D	409	ARG	NE-CZ-NH2	-5.15	117.72	120.30
1	D	554	LYS	CA-CB-CG	5.15	124.73	113.40
1	B	720	ARG	NE-CZ-NH2	-5.14	117.73	120.30
1	C	195	GLU	CB-CA-C	-5.13	100.13	110.40
1	C	277	ARG	CA-CB-CG	-5.13	102.11	113.40
1	B	400	LEU	CB-CA-C	-5.13	100.46	110.20
1	D	547	ALA	CA-C-N	5.12	128.47	117.20
1	D	516	ASP	CB-CG-OD2	-5.12	113.69	118.30
1	D	534	VAL	CG1-CB-CG2	-5.12	102.71	110.90
1	D	131	LEU	N-CA-CB	-5.11	100.19	110.40
1	C	432	GLU	CA-CB-CG	5.11	124.63	113.40
1	C	220	VAL	CG1-CB-CG2	-5.10	102.73	110.90
1	A	519	ARG	NE-CZ-NH2	5.10	122.85	120.30
1	D	573	TYR	CA-CB-CG	5.10	123.09	113.40
1	A	770	ARG	CA-CB-CG	5.09	124.61	113.40
1	A	16	ARG	N-CA-C	5.09	124.75	111.00
1	C	322	VAL	CB-CA-C	5.09	121.07	111.40
1	D	281	PRO	CA-C-N	5.09	128.40	117.20
1	A	662	LEU	CB-CG-CD1	-5.09	102.35	111.00
1	C	396	LEU	CB-CG-CD2	-5.08	102.36	111.00
1	B	269	ARG	CB-CA-C	-5.08	100.25	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	15	VAL	CB-CA-C	-5.08	101.76	111.40
1	B	263	ILE	CA-CB-CG2	-5.07	100.75	110.90
1	C	234	ARG	O-C-N	-5.07	114.58	122.70
1	B	426	ARG	NE-CZ-NH1	5.07	122.83	120.30
1	D	52	TYR	CB-CG-CD2	-5.07	117.96	121.00
1	D	490	ARG	CD-NE-CZ	5.07	130.69	123.60
1	C	770	ARG	NE-CZ-NH2	-5.06	117.77	120.30
1	D	734	ARG	CA-CB-CG	5.06	124.53	113.40
1	A	422	VAL	CA-CB-CG2	-5.06	103.32	110.90
1	D	138	ARG	CD-NE-CZ	5.05	130.67	123.60
1	D	238	VAL	CG1-CB-CG2	-5.05	102.83	110.90
1	D	379	VAL	N-CA-CB	-5.04	100.40	111.50
1	C	242	ARG	CB-CG-CD	-5.04	98.49	111.60
1	D	266	VAL	CG1-CB-CG2	-5.04	102.83	110.90
1	A	522	LEU	CA-CB-CG	5.04	126.89	115.30
1	A	797	TRP	CB-CG-CD1	5.04	133.55	127.00
1	C	18	LEU	CA-CB-CG	5.04	126.89	115.30
1	B	277	ARG	NE-CZ-NH2	-5.04	117.78	120.30
1	B	834	LEU	N-CA-C	-5.04	97.40	111.00
1	A	287	GLU	CA-CB-CG	5.04	124.48	113.40
1	C	81	ARG	NE-CZ-NH2	-5.03	117.78	120.30
1	C	457	ARG	NE-CZ-NH2	-5.03	117.79	120.30
1	D	280	TYR	N-CA-C	5.03	124.58	111.00
1	D	797	TRP	CG-CD1-NE1	5.03	115.13	110.10
1	A	730	GLU	CA-CB-CG	5.03	124.45	113.40
1	A	195	GLU	CB-CA-C	-5.02	100.36	110.40
1	B	770	ARG	CG-CD-NE	5.02	122.34	111.80
1	C	799	ARG	NE-CZ-NH2	-5.02	117.79	120.30
1	A	359	LEU	CA-CB-CG	5.02	126.84	115.30
1	B	376	ASN	O-C-N	-5.02	114.67	122.70
1	A	118	ASP	CB-CG-OD1	5.01	122.81	118.30
1	A	816	THR	CA-CB-CG2	-5.01	105.38	112.40
1	A	319	ARG	NE-CZ-NH1	5.01	122.80	120.30
1	D	326	PHE	CA-C-N	5.00	128.21	117.20
1	A	424	ARG	CD-NE-CZ	5.00	130.61	123.60

There are no chirality outliers.

All (26) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	157	TYR	Sidechain
1	A	252	PHE	Sidechain

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Mol	Chain	Res	Type	Group
1	A	262	TYR	Sidechain
1	A	472	TYR	Sidechain
1	A	52	TYR	Sidechain
1	A	597	PHE	Sidechain
1	A	811	PHE	Sidechain
1	A	836	ALA	Mainchain,Peptide
1	B	155	TYR	Sidechain
1	B	320	ASP	Peptide
1	B	380	ILE	Peptide
1	B	52	TYR	Sidechain
1	C	262	TYR	Sidechain
1	C	280	TYR	Peptide
1	C	316	PHE	Sidechain
1	C	320	ASP	Peptide
1	C	324	THR	Peptide
1	C	52	TYR	Sidechain
1	C	836	ALA	Peptide
1	D	262	TYR	Sidechain
1	D	297	TYR	Sidechain
1	D	320	ASP	Peptide
1	D	52	TYR	Sidechain
1	D	597	PHE	Sidechain
1	D	836	ALA	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	6692	0	6650	150	0
1	B	6692	0	6650	162	1
1	C	6692	0	6650	181	0
1	D	6692	0	6650	158	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	1	0
2	D	5	0	0	0	0
3	A	15	0	7	0	0
3	B	15	0	6	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	15	0	7	1	0
3	D	15	0	6	0	0
4	A	14	0	10	0	0
4	B	14	0	10	0	0
4	C	14	0	10	0	0
4	D	14	0	10	0	0
5	A	223	0	0	14	1
5	B	222	0	0	18	0
5	C	218	0	0	16	1
5	D	221	0	0	16	1
All	All	27788	0	26666	625	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

All (625) 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:D:322:VAL:HG13	1:D:325:ASN:HB3	1.43	0.98
1:C:171:CYS:SG	1:C:176:MET:HG3	2.09	0.92
1:B:85:LEU:HD21	1:B:303:THR:HG21	1.54	0.90
1:D:225:PRO:HB2	1:D:242:ARG:HD2	1.58	0.86
1:C:325:ASN:HB3	1:C:327:ASP:HB2	1.58	0.84
1:A:676:THR:HG21	5:A:1022:HOH:O	1.78	0.84
1:B:144:LEU:HD12	5:B:1135:HOH:O	1.79	0.82
1:A:381:PRO:HA	1:A:384:LEU:HD13	1.60	0.82
1:D:82:ILE:HB	5:D:1150:HOH:O	1.79	0.81
1:C:254:LEU:HA	1:C:259:VAL:HG21	1.62	0.81
1:B:692:MET:SD	1:B:710:ILE:HD12	2.20	0.80
1:C:173:GLY:HA3	1:C:624:THR:HG21	1.63	0.79
1:B:168:GLN:HE21	1:B:647:ASN:H	1.28	0.79
1:B:676:THR:HG21	5:B:1031:HOH:O	1.83	0.78
1:B:10:ARG:HG3	1:B:13:ILE:HD12	1.66	0.78
1:D:703:ALA:HA	1:D:807:THR:HG21	1.66	0.78
1:C:676:THR:HG21	5:C:1022:HOH:O	1.82	0.77
1:C:381:PRO:HG3	1:C:467:ILE:HG12	1.64	0.77
1:C:85:LEU:HD21	1:C:303:THR:HG21	1.66	0.77
1:B:703:ALA:HA	1:B:807:THR:HG21	1.66	0.77
1:A:225:PRO:HB2	1:A:242:ARG:HD2	1.67	0.76
1:A:455:VAL:H	1:A:459:HIS:HD2	1.32	0.76
1:C:566:GLN:HE22	1:C:576:GLN:HA	1.51	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:703:ALA:HA	1:A:807:THR:HG21	1.66	0.75
1:B:550:GLU:HG3	1:B:554:LYS:HA	1.68	0.75
1:D:168:GLN:HG3	1:D:175:GLN:HG3	1.68	0.75
1:D:254:LEU:HA	1:D:259:VAL:HG22	1.69	0.75
1:A:168:GLN:HG3	1:A:175:GLN:HG3	1.69	0.74
1:A:320:ASP:HB2	1:A:324:THR:HA	1.67	0.74
1:B:315:LYS:HA	1:B:318:CYS:SG	2.28	0.74
1:A:336:GLN:HE21	1:A:825:TRP:HE1	1.34	0.73
1:D:550:GLU:HG3	1:D:554:LYS:HA	1.70	0.73
1:C:597:PHE:HE2	1:C:792:LYS:HD2	1.54	0.73
1:B:225:PRO:HB2	1:B:242:ARG:HD2	1.69	0.73
1:B:193:ARG:HB2	1:B:225:PRO:HG2	1.70	0.72
1:C:588:ASN:HD21	1:C:744:GLN:HE22	1.36	0.72
1:D:676:THR:HG21	5:D:1032:HOH:O	1.89	0.71
1:B:588:ASN:HD21	1:B:744:GLN:HE22	1.35	0.71
1:B:378:THR:HG23	5:B:1038:HOH:O	1.89	0.71
1:D:381:PRO:HG2	1:D:382:GLU:HG3	1.72	0.71
1:C:267:LEU:HD23	1:D:266:VAL:HG11	1.73	0.71
1:A:557:ILE:HD11	1:A:643:ILE:HD11	1.71	0.71
1:D:91:MET:SD	5:D:1137:HOH:O	2.49	0.71
1:A:222:LEU:HB2	1:A:247:LYS:HB2	1.71	0.71
1:C:168:GLN:HG3	1:C:175:GLN:HG3	1.74	0.70
1:C:703:ALA:HA	1:C:807:THR:HG21	1.74	0.69
1:B:287:GLU:O	1:B:292:ARG:HD3	1.91	0.69
1:C:336:GLN:NE2	1:C:825:TRP:HE1	1.90	0.69
1:C:322:VAL:HG22	1:C:325:ASN:HD22	1.57	0.68
1:D:322:VAL:CG1	1:D:325:ASN:HB3	2.21	0.68
1:D:173:GLY:CA	1:D:624:THR:HG21	2.22	0.68
1:B:548:TYR:HD1	1:B:551:ARG:HH21	1.41	0.68
1:A:236:ASN:HB2	1:A:834:LEU:O	1.94	0.68
1:C:336:GLN:HE21	1:C:825:TRP:HE1	1.41	0.68
1:B:168:GLN:HG3	1:B:175:GLN:HG3	1.76	0.68
1:A:10:ARG:HG3	1:B:43:ARG:HD3	1.75	0.68
1:C:319:ARG:HE	1:C:321:PRO:HD2	1.56	0.68
1:A:193:ARG:HB3	1:A:196:PHE:HD2	1.57	0.67
1:A:601:ARG:HH22	1:A:784:GLN:NE2	1.92	0.67
1:C:597:PHE:CE2	1:C:792:LYS:HD2	2.29	0.67
1:A:168:GLN:HE21	1:A:647:ASN:H	1.42	0.67
1:B:59:VAL:HG13	1:B:104:LEU:HD23	1.76	0.67
1:C:211:GLN:HG2	1:C:358:ARG:HD2	1.76	0.67
1:C:795:ARG:O	1:C:799:ARG:HG3	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:791:TYR:HA	1:D:797:TRP:CD1	2.30	0.67
1:C:322:VAL:HG22	1:C:325:ASN:ND2	2.10	0.67
1:A:144:LEU:HD12	5:A:1128:HOH:O	1.95	0.66
1:A:463:LEU:HD23	1:A:467:ILE:HD13	1.78	0.66
1:A:173:GLY:HA2	1:A:624:THR:HG21	1.77	0.65
1:C:168:GLN:HE21	1:C:647:ASN:H	1.44	0.65
1:B:836:ALA:HB1	1:B:837:PRO:HA	1.77	0.65
1:C:322:VAL:HG13	1:C:325:ASN:HB2	1.78	0.65
1:D:289:LYS:HG2	1:D:291:LEU:H	1.62	0.65
1:A:343:SER:HB3	1:A:445:CYS:SG	2.36	0.65
1:A:426:ARG:NH1	1:D:755:PRO:HB2	2.11	0.65
1:D:129:ALA:HB1	1:D:131:LEU:HD22	1.77	0.65
1:D:593:GLU:HB3	1:D:596:LYS:HB2	1.77	0.65
1:C:225:PRO:HB2	1:C:242:ARG:HD2	1.79	0.64
1:C:550:GLU:HG3	1:C:554:LYS:HA	1.79	0.64
1:A:142:CYS:SG	1:A:487:THR:HG22	2.37	0.64
1:A:426:ARG:NE	1:D:755:PRO:HD2	2.12	0.64
1:A:91:MET:SD	5:A:1128:HOH:O	2.55	0.64
1:B:193:ARG:HB3	1:B:196:PHE:HD2	1.62	0.64
1:D:322:VAL:HG23	1:D:323:ARG:NH1	2.13	0.64
1:A:168:GLN:NE2	1:A:647:ASN:H	1.96	0.64
1:A:235:ASN:HA	1:A:833:ARG:HG3	1.80	0.64
1:B:615:MET:HE1	1:B:761:ILE:HA	1.79	0.64
1:C:168:GLN:NE2	1:C:647:ASN:H	1.96	0.64
1:D:311:PHE:O	1:D:316:PHE:HB2	1.98	0.64
1:B:676:THR:HG22	3:B:999:PLP:H5A1	1.78	0.63
1:D:545:PHE:O	1:D:549:LEU:HB2	1.98	0.63
1:B:235:ASN:H	1:B:235:ASN:HD22	1.44	0.63
1:A:21:VAL:HG12	1:A:22:GLU:H	1.64	0.62
1:A:336:GLN:NE2	1:A:825:TRP:HE1	1.97	0.62
1:D:144:LEU:HD12	5:D:1137:HOH:O	1.99	0.62
1:D:358:ARG:HD3	1:D:358:ARG:N	2.14	0.62
1:A:480:GLN:HE21	1:A:482:LYS:HZ3	1.47	0.62
1:B:795:ARG:O	1:B:799:ARG:HG3	1.99	0.62
1:C:480:GLN:HE21	1:C:482:LYS:NZ	1.98	0.62
1:D:173:GLY:HA2	1:D:624:THR:HG21	1.81	0.62
1:B:545:PHE:HE2	1:B:604:MET:HE1	1.64	0.62
1:B:34:HIS:HD2	1:B:38:THR:OG1	1.82	0.62
1:B:455:VAL:HG22	1:B:484:ASN:OD1	1.99	0.61
1:A:138:ARG:HB3	5:A:1022:HOH:O	1.99	0.61
1:C:378:THR:O	1:C:459:HIS:HE1	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:467:ILE:H	1:A:467:ILE:HD12	1.66	0.61
1:A:734:ARG:HD2	5:A:1161:HOH:O	1.99	0.61
1:B:263:ILE:HG13	1:C:262:TYR:OH	2.01	0.61
1:C:193:ARG:HB3	1:C:196:PHE:HD2	1.66	0.61
1:D:550:GLU:HA	1:D:553:TYR:O	2.00	0.61
1:D:610:ALA:N	5:D:1158:HOH:O	2.33	0.61
1:D:336:GLN:NE2	1:D:825:TRP:HE1	1.97	0.61
1:B:615:MET:CE	1:B:761:ILE:HG12	2.31	0.61
1:C:721:LEU:HD23	1:C:772:LYS:HD3	1.83	0.61
1:B:161:TYR:HA	1:B:276:SER:O	2.01	0.60
1:B:803:ARG:HB2	1:B:803:ARG:HH11	1.64	0.60
1:C:365:TRP:O	1:C:369:VAL:HG13	2.01	0.60
1:D:601:ARG:HD2	5:D:1172:HOH:O	2.01	0.60
1:A:383:ALA:HA	5:A:1160:HOH:O	1.99	0.60
1:D:173:GLY:HA3	1:D:624:THR:HG21	1.84	0.60
1:B:71:GLN:HG3	5:B:1162:HOH:O	2.00	0.60
1:C:317:GLY:HA2	1:C:324:THR:OG1	2.01	0.60
1:B:144:LEU:HD23	1:B:147:MET:CE	2.32	0.60
1:D:322:VAL:O	1:D:325:ASN:HB2	2.01	0.60
5:A:1108:HOH:O	1:B:33:ARG:HD2	2.02	0.60
1:A:173:GLY:CA	1:A:624:THR:HG21	2.32	0.60
1:C:739:ARG:HH11	1:C:739:ARG:HG3	1.67	0.59
1:A:138:ARG:NH2	1:A:490:ARG:HD3	2.17	0.59
1:D:734:ARG:HD2	5:D:1168:HOH:O	2.03	0.59
1:D:545:PHE:HE2	1:D:604:MET:HE1	1.66	0.59
1:B:320:ASP:HA	1:B:324:THR:HA	1.84	0.59
1:B:588:ASN:HD21	1:B:744:GLN:NE2	2.00	0.59
1:C:588:ASN:HD21	1:C:744:GLN:NE2	1.99	0.59
1:A:198:LEU:HD13	1:A:305:GLN:HB2	1.82	0.59
1:A:550:GLU:HG2	1:A:554:LYS:HA	1.85	0.59
1:C:33:ARG:HD2	5:C:1214:HOH:O	2.01	0.59
1:C:193:ARG:HB2	1:C:225:PRO:HG2	1.85	0.59
1:C:32:ASN:OD1	1:D:13:ILE:HA	2.02	0.59
1:B:47:THR:HG22	1:B:50:ASP:OD2	2.03	0.59
1:B:610:ALA:N	5:B:1155:HOH:O	2.35	0.59
1:A:138:ARG:O	1:A:138:ARG:HD3	2.02	0.59
1:B:173:GLY:CA	1:B:624:THR:HG21	2.32	0.59
1:C:486:ILE:HD11	1:C:676:THR:HG23	1.85	0.59
1:B:381:PRO:HG3	1:B:467:ILE:HG12	1.84	0.58
1:B:741:ILE:HA	1:B:744:GLN:HE21	1.68	0.58
1:C:184:ARG:HD2	1:C:185:TYR:CE2	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:601:ARG:HH22	1:D:784:GLN:NE2	2.01	0.58
1:D:316:PHE:C	1:D:320:ASP:HA	2.24	0.58
1:A:480:GLN:HE21	1:A:482:LYS:NZ	2.01	0.58
1:B:435:ALA:O	1:B:436:VAL:HG12	2.04	0.58
1:A:601:ARG:NH2	1:A:784:GLN:NE2	2.52	0.58
1:C:144:LEU:HD12	5:C:1130:HOH:O	2.03	0.58
1:A:92:GLY:O	1:A:93:ARG:HB2	2.04	0.58
1:B:480:GLN:HE21	1:B:482:LYS:NZ	2.01	0.58
1:B:63:LEU:HD13	1:B:229:PRO:HG2	1.86	0.58
1:A:21:VAL:O	1:A:23:ASN:N	2.37	0.58
1:B:163:PHE:HB2	1:B:278:VAL:HG23	1.85	0.58
1:C:323:ARG:HB3	1:C:325:ASN:HA	1.83	0.58
1:C:555:VAL:HG21	1:C:643:ILE:HG12	1.86	0.58
1:C:610:ALA:N	5:C:1153:HOH:O	2.36	0.57
1:D:171:CYS:SG	1:D:176:MET:HG3	2.44	0.57
1:D:336:GLN:HE21	1:D:825:TRP:HE1	1.52	0.57
1:A:67:TRP:CZ3	1:A:229:PRO:HG3	2.38	0.57
1:A:587:TYR:O	1:A:591:LYS:HG2	2.03	0.57
1:A:714:ARG:HD3	5:A:1185:HOH:O	2.04	0.57
1:D:458:ILE:HG23	5:D:1129:HOH:O	2.05	0.57
1:B:254:LEU:HA	1:B:259:VAL:HG11	1.86	0.57
1:B:455:VAL:H	1:B:459:HIS:HD2	1.53	0.57
1:A:13:ILE:O	1:B:43:ARG:HG2	2.05	0.57
1:A:43:ARG:HE	1:B:11:LYS:HA	1.69	0.57
1:D:522:LEU:O	1:D:525:VAL:HG23	2.05	0.57
1:A:588:ASN:HD21	1:A:744:GLN:NE2	2.03	0.57
1:B:763:ASN:O	1:B:767:HIS:HB2	2.05	0.57
1:B:601:ARG:HH22	1:B:784:GLN:NE2	2.03	0.57
1:C:287:GLU:O	1:C:292:ARG:HD3	2.05	0.57
1:C:455:VAL:H	1:C:459:HIS:HD2	1.52	0.57
1:B:18:LEU:HD12	5:B:1008:HOH:O	2.04	0.57
1:D:545:PHE:CE2	1:D:604:MET:HE1	2.40	0.57
1:A:430:LEU:HD22	1:A:443:HIS:HB3	1.87	0.56
1:C:528:GLU:O	1:C:532:ARG:HG2	2.05	0.56
1:A:566:GLN:HE22	1:A:576:GLN:HA	1.68	0.56
1:D:143:PHE:O	1:D:147:MET:HG3	2.04	0.56
1:D:235:ASN:H	1:D:235:ASN:HD22	1.53	0.56
1:B:605:ILE:HG21	1:B:623:ILE:HD13	1.86	0.56
1:B:129:ALA:HB1	1:B:131:LEU:HD22	1.87	0.56
1:D:455:VAL:H	1:D:459:HIS:HD2	1.51	0.56
1:B:703:ALA:CA	1:B:807:THR:HG21	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:82:ILE:HB	5:A:1142:HOH:O	2.06	0.56
1:B:734:ARG:HD2	5:B:1166:HOH:O	2.05	0.56
1:C:224:MET:HB2	1:C:247:LYS:NZ	2.22	0.55
1:C:573:TYR:CZ	1:C:574:LYS:HE2	2.41	0.55
1:A:615:MET:HE3	1:A:761:ILE:HG12	1.88	0.55
1:B:615:MET:HE3	1:B:761:ILE:HG12	1.89	0.55
1:B:525:VAL:O	1:B:531:ILE:HD11	2.07	0.55
1:B:601:ARG:HD2	5:B:1170:HOH:O	2.07	0.55
1:B:727:ASN:O	1:B:730:GLU:HG2	2.06	0.55
1:D:184:ARG:HD2	1:D:185:TYR:CE2	2.42	0.55
1:A:795:ARG:O	1:A:799:ARG:HG3	2.06	0.55
1:D:157:TYR:CE1	1:D:242:ARG:HG2	2.42	0.55
1:B:423:ASP:O	1:B:426:ARG:HD3	2.07	0.55
1:D:193:ARG:HB2	1:D:225:PRO:HG2	1.89	0.55
1:C:550:GLU:HA	1:C:554:LYS:HA	1.89	0.54
1:B:600:PRO:HB3	1:B:639:ARG:HA	1.89	0.54
1:D:355:ASP:OD2	1:D:398:ARG:HD3	2.07	0.54
1:A:227:ASP:OD1	1:A:242:ARG:HD3	2.08	0.54
1:A:53:PHE:CE1	1:A:188:PRO:HD3	2.42	0.54
1:C:548:TYR:HD1	1:C:551:ARG:NH2	2.04	0.54
1:C:791:TYR:HA	1:C:797:TRP:CD1	2.42	0.54
1:A:311:PHE:O	1:A:316:PHE:CD1	2.61	0.54
1:B:14:SER:OG	1:B:16:ARG:HG3	2.08	0.54
1:D:227:ASP:OD1	1:D:242:ARG:HD3	2.08	0.54
1:C:11:LYS:HA	1:D:43:ARG:HE	1.72	0.54
1:A:610:ALA:N	5:A:1149:HOH:O	2.37	0.54
1:C:391:LEU:O	1:C:395:LEU:HD23	2.08	0.54
1:B:395:LEU:HD23	1:B:395:LEU:H	1.72	0.54
1:C:727:ASN:O	1:C:730:GLU:HG2	2.08	0.54
1:B:336:GLN:NE2	1:B:825:TRP:HE1	2.06	0.53
1:D:692:MET:SD	1:D:710:ILE:HD12	2.48	0.53
1:D:250:ASN:HD22	1:D:269:ARG:HH22	1.56	0.53
1:D:568:LYS:HZ1	1:D:665:GLN:NE2	2.06	0.53
1:B:336:GLN:HE21	1:B:825:TRP:HE1	1.55	0.53
1:D:21:VAL:HG22	1:D:62:HIS:HD2	1.73	0.53
1:A:717:ASP:HA	1:A:720:ARG:HG2	1.91	0.53
1:B:164:GLY:O	1:B:279:LEU:HB2	2.09	0.53
1:D:289:LYS:HD3	1:D:291:LEU:HB2	1.90	0.53
1:A:719:ASP:O	1:A:722:ASP:HB2	2.09	0.53
1:B:168:GLN:NE2	1:B:647:ASN:H	2.02	0.53
1:D:641:ARG:HG3	5:D:1128:HOH:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:458:ILE:O	1:A:462:ILE:HG23	2.08	0.53
1:A:756:ASP:HB2	1:A:759:LYS:HG3	1.91	0.53
1:A:778:GLU:O	1:A:782:LYS:HG2	2.09	0.53
1:B:480:GLN:HE21	1:B:482:LYS:HZ3	1.56	0.53
1:D:583:VAL:HG22	1:D:603:VAL:HG11	1.91	0.53
1:D:562:LEU:HD21	1:D:662:LEU:HB2	1.91	0.53
1:B:173:GLY:HA2	1:B:624:THR:HG21	1.90	0.52
1:C:322:VAL:HG13	1:C:325:ASN:CB	2.38	0.52
1:C:82:ILE:HB	5:C:1145:HOH:O	2.08	0.52
1:D:133:ASN:OD1	1:D:165:ILE:HG21	2.08	0.52
1:A:69:ARG:HE	1:A:837:PRO:HB2	1.75	0.52
1:D:280:TYR:HB3	1:D:292:ARG:HD2	1.90	0.52
1:D:597:PHE:CE2	1:D:792:LYS:HD2	2.43	0.52
1:C:157:TYR:CE1	1:C:242:ARG:HG2	2.45	0.52
1:D:316:PHE:HB3	1:D:320:ASP:O	2.09	0.52
1:A:792:LYS:O	1:A:794:PRO:HD3	2.10	0.52
1:C:110:GLU:O	1:C:113:TYR:HB3	2.10	0.52
1:A:528:GLU:OE2	1:A:795:ARG:HD2	2.10	0.52
1:C:322:VAL:O	1:C:325:ASN:HB2	2.09	0.52
1:C:525:VAL:O	1:C:799:ARG:HD2	2.09	0.52
1:D:480:GLN:HE21	1:D:482:LYS:NZ	2.08	0.52
1:D:568:LYS:NZ	1:D:665:GLN:HE22	2.08	0.52
1:A:615:MET:CE	1:A:761:ILE:HG12	2.40	0.52
1:B:804:ASN:O	1:B:807:THR:HG22	2.09	0.52
1:D:144:LEU:HD23	1:D:147:MET:CE	2.38	0.52
1:D:803:ARG:HH11	1:D:803:ARG:HB2	1.74	0.52
1:B:184:ARG:HD2	1:B:185:TYR:CE2	2.45	0.52
1:C:480:GLN:HE21	1:C:482:LYS:HZ3	1.57	0.52
1:C:584:ILE:HG21	1:C:741:ILE:HG23	1.91	0.52
1:D:386:ARG:HB3	1:D:438:ARG:HD3	1.91	0.51
1:D:727:ASN:O	1:D:730:GLU:HG2	2.10	0.51
1:B:171:CYS:SG	1:B:176:MET:HG3	2.50	0.51
1:C:423:ASP:OD1	1:C:426:ARG:HD2	2.09	0.51
1:A:129:ALA:HB1	1:A:131:LEU:HD22	1.92	0.51
1:A:396:LEU:HB3	1:A:399:HIS:HB2	1.91	0.51
1:A:435:ALA:HB2	1:D:174:TRP:CE3	2.46	0.51
1:A:588:ASN:HD21	1:A:744:GLN:HE22	1.59	0.51
1:C:463:LEU:HD23	1:C:467:ILE:HD12	1.91	0.51
1:C:568:LYS:NZ	1:C:665:GLN:HE22	2.09	0.51
1:A:594:PRO:HB3	1:A:635:VAL:HG13	1.93	0.51
1:C:268:ASP:HB2	5:C:1104:HOH:O	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:319:ARG:HH21	1:C:320:ASP:HA	1.76	0.51
1:D:293:LEU:HD23	1:D:395:LEU:HD21	1.92	0.51
1:C:261:GLY:O	1:C:262:TYR:HB2	2.11	0.51
1:D:168:GLN:NE2	1:D:647:ASN:H	2.08	0.51
1:C:93:ARG:HG2	1:C:126:GLU:HG2	1.93	0.51
1:B:300:VAL:HG13	1:B:345:ALA:HA	1.92	0.51
1:A:713:MET:HE1	1:A:721:LEU:HD22	1.93	0.51
1:B:568:LYS:HZ1	1:B:665:GLN:HE22	1.57	0.51
1:D:316:PHE:HA	1:D:319:ARG:O	2.11	0.51
1:B:626:ILE:O	1:B:630:VAL:HG13	2.11	0.50
1:A:322:VAL:HG22	1:A:325:ASN:ND2	2.26	0.50
1:B:566:GLN:HE22	1:B:576:GLN:HA	1.75	0.50
1:C:235:ASN:ND2	1:C:235:ASN:H	2.09	0.50
1:B:426:ARG:CZ	1:C:755:PRO:HD2	2.42	0.50
1:C:421:ASP:OD2	1:C:424:ARG:HD2	2.11	0.50
1:B:173:GLY:HA3	1:B:624:THR:HG21	1.93	0.50
1:A:522:LEU:O	1:A:525:VAL:HG23	2.11	0.50
1:D:130:GLY:O	1:D:164:GLY:HA2	2.10	0.50
1:D:446:ILE:O	1:D:478:LYS:HE3	2.12	0.50
1:A:166:PHE:CD1	1:A:177:GLU:HB3	2.47	0.50
1:A:193:ARG:HB3	1:A:196:PHE:CD2	2.44	0.50
1:C:571:HIS:ND1	1:C:573:TYR:HD1	2.09	0.50
1:B:716:GLU:OE2	1:B:720:ARG:HD3	2.12	0.49
1:C:235:ASN:N	1:C:235:ASN:HD22	2.10	0.49
1:A:426:ARG:CZ	1:D:755:PRO:HD2	2.41	0.49
1:B:235:ASN:ND2	1:B:235:ASN:H	2.10	0.49
1:D:170:ILE:HG12	1:D:646:GLU:HG3	1.94	0.49
1:A:426:ARG:CD	1:D:755:PRO:HD2	2.42	0.49
1:B:548:TYR:HD1	1:B:551:ARG:NH2	2.08	0.49
1:C:232:GLY:HA3	1:C:235:ASN:HD21	1.76	0.49
1:A:34:HIS:HD2	1:A:38:THR:OG1	1.94	0.49
1:B:386:ARG:HB3	1:B:438:ARG:HD3	1.94	0.49
1:C:254:LEU:HD11	1:C:257:PHE:CZ	2.47	0.49
1:D:752:PRO:O	1:D:755:PRO:HD3	2.13	0.49
1:C:266:VAL:HG11	1:D:267:LEU:HD23	1.94	0.49
1:C:57:HIS:HE1	5:C:1129:HOH:O	1.95	0.49
1:B:717:ASP:HA	1:B:720:ARG:HG2	1.95	0.49
1:C:13:ILE:HA	1:D:32:ASN:OD1	2.13	0.49
1:A:435:ALA:HB2	1:D:174:TRP:CZ3	2.48	0.49
1:D:70:THR:O	1:D:73:HIS:HB3	2.13	0.49
1:A:235:ASN:H	1:A:235:ASN:HD22	1.60	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:150:LEU:HB3	1:A:829:PRO:HB3	1.95	0.49
1:D:241:MET:HG2	1:D:243:LEU:HD13	1.94	0.49
1:D:252:PHE:CE2	1:D:269:ARG:HG3	2.47	0.49
1:D:338:ASN:O	1:D:339:ASP:HB2	2.13	0.49
1:B:311:PHE:O	1:B:316:PHE:HB2	2.13	0.49
1:B:73:HIS:O	1:B:77:LYS:HB2	2.13	0.49
1:C:138:ARG:HD3	1:C:138:ARG:O	2.13	0.49
1:A:423:ASP:O	1:A:426:ARG:HD3	2.13	0.48
1:B:280:TYR:HB3	1:B:292:ARG:HD2	1.95	0.48
1:C:250:ASN:ND2	1:C:269:ARG:HG2	2.28	0.48
1:C:355:ASP:OD2	1:C:398:ARG:HD3	2.12	0.48
1:D:618:MET:O	1:D:621:LYS:HB3	2.12	0.48
1:A:171:CYS:SG	1:A:176:MET:HG3	2.53	0.48
1:A:280:TYR:HB3	1:A:292:ARG:HD2	1.95	0.48
1:A:676:THR:HB	5:A:1043:HOH:O	2.13	0.48
1:C:713:MET:CE	1:C:775:ALA:HB1	2.43	0.48
1:B:601:ARG:NH2	1:B:784:GLN:NE2	2.60	0.48
1:D:82:ILE:HG12	1:D:83:TYR:N	2.28	0.48
1:D:492:LEU:HD22	1:D:500:ALA:HB2	1.95	0.48
1:A:528:GLU:O	1:A:532:ARG:HG2	2.13	0.48
1:B:57:HIS:HE1	5:B:1134:HOH:O	1.96	0.48
1:B:69:ARG:HG2	1:B:69:ARG:HH11	1.79	0.48
1:A:548:TYR:HD2	1:A:551:ARG:HH21	1.62	0.48
1:C:224:MET:HB2	1:C:247:LYS:HZ3	1.77	0.48
1:C:252:PHE:CD2	1:C:265:ALA:HB1	2.48	0.48
1:D:322:VAL:HG23	1:D:323:ARG:HH11	1.76	0.48
1:D:568:LYS:NZ	1:D:665:GLN:NE2	2.62	0.48
1:D:797:TRP:HZ3	5:D:1114:HOH:O	1.94	0.48
1:B:53:PHE:CE2	1:B:188:PRO:HD3	2.49	0.48
1:B:550:GLU:HA	1:B:554:LYS:HA	1.96	0.48
1:B:600:PRO:HA	1:B:639:ARG:O	2.14	0.48
1:C:152:LEU:HD22	1:C:827:VAL:HG21	1.95	0.48
1:D:235:ASN:OD1	1:D:237:VAL:HG13	2.14	0.48
1:D:60:ARG:O	1:D:64:VAL:HG22	2.13	0.48
1:A:49:ARG:HA	1:A:125:ILE:HG21	1.96	0.48
1:B:56:ALA:O	1:B:60:ARG:HB2	2.14	0.48
1:C:18:LEU:HG	1:D:33:ARG:NH1	2.28	0.48
1:C:584:ILE:CG2	1:C:741:ILE:HD12	2.44	0.48
1:D:251:ASP:HB3	1:D:255:LYS:HD3	1.96	0.48
1:A:21:VAL:HG21	1:A:66:ARG:HH22	1.79	0.47
1:A:11:LYS:HA	1:B:43:ARG:HH21	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:761:ILE:HG22	1:B:765:LEU:HD22	1.95	0.47
1:C:235:ASN:HD22	1:C:235:ASN:H	1.61	0.47
1:D:168:GLN:HE21	1:D:647:ASN:H	1.62	0.47
1:D:160:ARG:HB2	1:D:243:LEU:HB3	1.95	0.47
1:A:322:VAL:HG13	1:A:325:ASN:CG	2.35	0.47
1:A:316:PHE:O	1:A:324:THR:HG23	2.14	0.47
1:A:32:ASN:HB3	1:B:18:LEU:HD11	1.95	0.47
1:C:777:TYR:O	1:C:781:VAL:HG13	2.14	0.47
1:A:235:ASN:H	1:A:235:ASN:ND2	2.13	0.47
1:B:211:GLN:HG2	1:B:358:ARG:HD2	1.97	0.47
1:C:583:VAL:HG21	1:C:603:VAL:HG21	1.96	0.47
1:A:703:ALA:CA	1:A:807:THR:HG21	2.41	0.47
1:C:442:ALA:O	1:C:446:ILE:HG13	2.14	0.47
1:A:636:VAL:O	1:A:639:ARG:HD3	2.14	0.47
1:B:127:GLU:HG3	1:B:182:TRP:HA	1.97	0.47
1:D:316:PHE:O	1:D:320:ASP:HA	2.15	0.47
1:A:446:ILE:O	1:A:478:LYS:HE3	2.15	0.47
1:C:822:ARG:HD3	1:C:828:GLU:OE2	2.15	0.47
1:D:557:ILE:HD12	1:D:557:ILE:N	2.30	0.47
1:D:604:MET:HA	1:D:643:ILE:O	2.14	0.47
1:C:170:ILE:HA	1:C:174:TRP:O	2.15	0.47
1:D:486:ILE:HD11	1:D:680:LYS:HE3	1.96	0.47
1:A:235:ASN:ND2	1:A:237:VAL:H	2.13	0.47
1:B:615:MET:HE1	1:B:761:ILE:HG12	1.96	0.47
1:A:266:VAL:HG12	1:B:266:VAL:HG12	1.96	0.47
1:B:568:LYS:NZ	1:B:665:GLN:HE22	2.13	0.47
1:C:105:GLU:HB3	5:C:1090:HOH:O	2.14	0.47
1:C:545:PHE:HE2	1:C:604:MET:HE1	1.81	0.46
1:D:803:ARG:HG3	5:D:1147:HOH:O	2.14	0.46
1:B:233:TYR:CZ	1:B:234:ARG:HD3	2.51	0.46
1:C:20:GLY:O	1:C:23:ASN:HB3	2.15	0.46
1:D:803:ARG:NE	5:D:1117:HOH:O	2.47	0.46
1:B:292:ARG:O	1:B:296:GLU:HG3	2.15	0.46
1:B:480:GLN:NE2	1:B:482:LYS:NZ	2.64	0.46
1:C:316:PHE:HE1	1:C:332:LYS:NZ	2.13	0.46
1:D:322:VAL:HG13	1:D:325:ASN:CB	2.31	0.46
1:A:119:MET:O	1:A:123:GLU:HG3	2.16	0.46
1:C:173:GLY:CA	1:C:624:THR:HG21	2.38	0.46
1:C:601:ARG:HH22	1:C:784:GLN:NE2	2.14	0.46
1:D:253:ASN:O	1:D:259:VAL:HG21	2.15	0.46
1:D:193:ARG:HB3	1:D:196:PHE:HD2	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:566:GLN:NE2	1:C:576:GLN:HA	2.25	0.46
1:A:800:MET:HA	1:A:803:ARG:NH1	2.31	0.46
1:B:221:VAL:HG13	1:B:272:ALA:HB1	1.97	0.46
1:C:582:HIS:HB2	1:C:780:TYR:CE2	2.51	0.46
1:C:803:ARG:HG3	5:C:1141:HOH:O	2.14	0.46
1:D:557:ILE:HA	5:D:1128:HOH:O	2.16	0.46
1:A:380:ILE:O	1:A:382:GLU:N	2.49	0.46
1:C:584:ILE:HG22	1:C:741:ILE:HD12	1.97	0.46
1:C:717:ASP:HA	1:C:720:ARG:HG2	1.98	0.46
1:B:82:ILE:HB	5:B:1148:HOH:O	2.15	0.45
1:A:221:VAL:HG13	1:A:272:ALA:HB1	1.98	0.45
1:D:47:THR:HG22	1:D:50:ASP:OD2	2.17	0.45
1:A:138:ARG:C	1:A:138:ARG:HD3	2.37	0.45
1:C:43:ARG:HE	1:D:11:LYS:HG3	1.81	0.45
1:A:506:ARG:HB3	1:A:524:TYR:CZ	2.52	0.45
1:B:18:LEU:HA	5:B:1008:HOH:O	2.16	0.45
1:C:336:GLN:HE22	1:C:373:ALA:HB3	1.80	0.45
1:C:525:VAL:O	1:C:531:ILE:HD11	2.16	0.45
1:C:726:TYR:OH	1:C:774:PHE:HB2	2.17	0.45
1:A:480:GLN:NE2	1:A:482:LYS:NZ	2.63	0.45
1:C:262:TYR:HB3	1:C:264:GLN:OE1	2.17	0.45
1:D:343:SER:HB3	1:D:445:CYS:SG	2.56	0.45
1:B:456:ALA:C	1:B:481:ASN:HD21	2.19	0.45
1:C:475:GLU:CD	1:C:478:LYS:HE2	2.36	0.45
1:C:479:PHE:N	1:C:479:PHE:CD1	2.83	0.45
1:C:522:LEU:O	1:C:525:VAL:HG23	2.16	0.45
1:C:548:TYR:HD1	1:C:551:ARG:HH21	1.63	0.45
1:C:67:TRP:CZ3	1:C:229:PRO:HG3	2.50	0.45
1:A:174:TRP:CH2	1:D:435:ALA:HB2	2.51	0.45
1:A:80:LYS:HE2	1:A:825:TRP:O	2.17	0.45
1:B:479:PHE:N	1:B:479:PHE:CD1	2.85	0.45
1:B:724:ARG:O	1:C:729:GLN:HG2	2.17	0.45
1:C:568:LYS:HZ3	1:C:665:GLN:HE22	1.65	0.45
1:C:604:MET:HE1	1:C:645:LEU:HD21	1.98	0.45
1:C:69:ARG:HD2	1:C:836:ALA:HA	1.99	0.45
1:C:67:TRP:O	1:C:71:GLN:HG2	2.17	0.45
1:C:817:ILE:HA	1:C:817:ILE:HD13	1.74	0.45
1:D:795:ARG:O	1:D:799:ARG:HG3	2.16	0.45
1:A:319:ARG:HE	1:A:320:ASP:HA	1.80	0.45
1:A:784:GLN:HA	1:A:784:GLN:HE21	1.82	0.45
1:D:736:PRO:HG3	1:D:739:ARG:NH2	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:361:TRP:CH2	1:A:409:ARG:HD2	2.51	0.45
1:A:355:ASP:OD2	1:A:398:ARG:HD3	2.16	0.45
1:A:53:PHE:HE1	1:A:188:PRO:HD3	1.80	0.45
1:A:740:GLN:O	1:A:744:GLN:HG3	2.16	0.45
1:B:516:ASP:O	1:B:519:ARG:HB2	2.17	0.45
1:C:592:LYS:HG2	1:C:593:GLU:HG3	1.98	0.45
1:C:797:TRP:HZ3	5:C:1105:HOH:O	1.98	0.45
1:D:423:ASP:OD1	1:D:426:ARG:HD2	2.16	0.45
1:A:426:ARG:HD2	1:D:755:PRO:HD2	1.98	0.45
1:D:379:VAL:HG11	1:D:671:THR:HA	1.98	0.45
1:A:475:GLU:OE1	1:A:478:LYS:HE2	2.18	0.44
1:B:252:PHE:HE1	1:B:269:ARG:HG2	1.82	0.44
1:B:269:ARG:O	1:B:273:GLU:HG3	2.17	0.44
1:B:365:TRP:O	1:B:369:VAL:HG13	2.18	0.44
1:C:475:GLU:OE1	1:C:478:LYS:HE2	2.17	0.44
1:A:713:MET:HE1	1:A:775:ALA:HB1	2.00	0.44
1:C:815:ARG:O	1:C:819:GLN:HG3	2.17	0.44
1:D:34:HIS:HD2	1:D:38:THR:OG1	1.99	0.44
1:D:568:LYS:HZ3	1:D:665:GLN:HE22	1.65	0.44
1:A:472:TYR:O	1:A:476:PRO:HG3	2.17	0.44
1:B:322:VAL:HG23	1:B:323:ARG:NH2	2.32	0.44
1:C:338:ASN:O	1:C:339:ASP:HB2	2.18	0.44
1:C:91:MET:HE1	5:C:1130:HOH:O	2.16	0.44
1:B:518:LEU:O	1:B:521:LEU:HB2	2.17	0.44
1:B:91:MET:SD	5:B:1135:HOH:O	2.60	0.44
1:C:480:GLN:NE2	1:C:482:LYS:NZ	2.65	0.44
1:C:549:LEU:O	1:C:550:GLU:HG3	2.17	0.44
1:C:70:THR:O	1:C:73:HIS:HB3	2.17	0.44
1:A:626:ILE:O	1:A:630:VAL:HG13	2.18	0.44
1:A:566:GLN:O	1:A:605:ILE:HA	2.17	0.44
1:C:166:PHE:CG	1:C:177:GLU:HB2	2.52	0.44
1:A:399:HIS:HD2	5:A:1129:HOH:O	2.00	0.44
1:C:615:MET:HE1	1:C:761:ILE:HA	1.99	0.44
1:D:34:HIS:HE1	1:D:61:ASP:OD2	1.99	0.44
1:A:548:TYR:HD2	1:A:551:ARG:NH2	2.16	0.44
1:C:325:ASN:C	1:C:327:ASP:N	2.70	0.44
1:D:332:LYS:HD3	1:D:332:LYS:HA	1.69	0.44
1:A:662:LEU:HD22	1:A:689:ILE:HG22	1.99	0.44
1:B:144:LEU:HD23	1:B:147:MET:HE2	2.00	0.44
1:B:335:ILE:HG22	1:B:337:LEU:HD13	1.99	0.44
1:D:504:ALA:HA	1:D:508:GLY:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:319:ARG:HH21	1:A:320:ASP:HA	1.83	0.43
1:B:382:GLU:HA	1:B:386:ARG:HH12	1.83	0.43
1:C:380:ILE:HD12	1:C:380:ILE:HA	1.73	0.43
1:C:739:ARG:HH11	1:C:739:ARG:CG	2.31	0.43
1:C:741:ILE:O	1:C:744:GLN:HB2	2.18	0.43
1:C:741:ILE:HA	1:C:744:GLN:HE21	1.82	0.43
1:C:82:ILE:HD12	1:C:147:MET:SD	2.58	0.43
1:B:16:ARG:NH2	1:B:18:LEU:HD13	2.34	0.43
1:B:343:SER:HB3	1:B:445:CYS:SG	2.57	0.43
1:C:49:ARG:O	1:C:53:PHE:HD1	2.00	0.43
1:C:499:LEU:O	1:C:503:ILE:HG13	2.18	0.43
1:A:341:HIS:HB2	1:A:342:PRO:HD3	2.01	0.43
1:B:399:HIS:HD2	5:B:1136:HOH:O	2.00	0.43
1:D:269:ARG:O	1:D:273:GLU:HG3	2.18	0.43
1:A:89:PHE:O	1:A:131:LEU:HB3	2.19	0.43
1:B:395:LEU:HD23	1:B:395:LEU:N	2.33	0.43
1:C:676:THR:HB	5:C:1044:HOH:O	2.18	0.43
1:D:196:PHE:HB3	5:D:1183:HOH:O	2.17	0.43
1:D:790:LEU:HG	1:D:797:TRP:CD1	2.53	0.43
1:D:268:ASP:HB2	5:D:1113:HOH:O	2.18	0.43
1:A:386:ARG:HH21	1:A:440:ASN:ND2	2.17	0.43
1:A:732:TYR:O	1:A:739:ARG:NH1	2.52	0.43
1:C:399:HIS:HD2	5:C:1131:HOH:O	2.02	0.43
1:C:648:TYR:CE2	3:C:999:PLP:H2A2	2.54	0.43
1:D:469:LYS:HB2	1:D:469:LYS:HE2	1.86	0.43
1:D:736:PRO:O	1:D:739:ARG:HB3	2.19	0.43
1:D:703:ALA:CA	1:D:807:THR:HG21	2.43	0.43
1:A:596:LYS:HD3	1:A:597:PHE:H	1.84	0.43
1:B:489:ARG:HB3	5:B:1154:HOH:O	2.19	0.43
1:B:562:LEU:HD21	1:B:662:LEU:HB2	2.00	0.43
1:B:604:MET:HA	1:B:643:ILE:O	2.18	0.43
1:D:21:VAL:HG22	1:D:62:HIS:CD2	2.53	0.43
1:B:174:TRP:HH2	1:B:757:LEU:HD11	1.84	0.43
1:C:233:TYR:CE1	1:C:234:ARG:HD3	2.54	0.43
1:C:269:ARG:O	1:C:273:GLU:HG3	2.18	0.43
1:C:536:LYS:HD2	1:C:536:LYS:HA	1.86	0.43
1:D:225:PRO:CB	1:D:242:ARG:HD2	2.39	0.43
1:D:34:HIS:CD2	1:D:38:THR:OG1	2.72	0.43
1:A:421:ASP:O	1:A:424:ARG:HB3	2.19	0.43
1:C:713:MET:HB3	5:C:1148:HOH:O	2.18	0.43
1:A:442:ALA:O	1:A:446:ILE:HG13	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:557:ILE:N	1:B:557:ILE:HD12	2.34	0.42
1:B:174:TRP:CH2	1:B:757:LEU:HD11	2.54	0.42
1:C:129:ALA:HB1	1:C:131:LEU:HD22	2.01	0.42
1:C:168:GLN:HE21	1:C:647:ASN:N	2.14	0.42
1:C:43:ARG:HG3	1:C:43:ARG:HH11	1.83	0.42
1:C:651:SER:HB3	5:C:1026:HOH:O	2.18	0.42
1:C:703:ALA:CA	1:C:807:THR:HG21	2.47	0.42
1:D:565:VAL:HG22	1:D:681:PHE:CZ	2.53	0.42
1:A:815:ARG:O	1:A:819:GLN:HG3	2.18	0.42
1:B:190:GLU:HA	1:B:227:ASP:O	2.19	0.42
1:C:135:GLY:HA3	2:C:997:PO4:O3	2.19	0.42
1:D:322:VAL:CB	1:D:325:ASN:HB3	2.48	0.42
1:D:698:GLU:O	1:D:702:GLU:HG2	2.18	0.42
1:A:601:ARG:HD2	5:A:1166:HOH:O	2.19	0.42
1:D:289:LYS:HG2	1:D:291:LEU:N	2.31	0.42
1:D:432:GLU:O	1:D:437:LYS:HA	2.19	0.42
1:B:329:PHE:HB3	1:B:330:PRO:HD3	2.01	0.42
1:C:450:HIS:HE1	1:C:824:ILE:O	2.03	0.42
1:D:761:ILE:HG22	1:D:765:LEU:HD22	2.01	0.42
1:B:166:PHE:HB2	1:B:178:GLU:O	2.19	0.42
1:D:519:ARG:O	1:D:522:LEU:HB2	2.19	0.42
1:D:754:GLN:O	1:D:756:ASP:N	2.52	0.42
1:B:181:ASP:O	1:B:184:ARG:HB2	2.20	0.42
1:C:320:ASP:CB	1:C:324:THR:H	2.33	0.42
1:D:459:HIS:HB2	1:D:673:ALA:O	2.19	0.42
1:D:569:ARG:O	1:D:574:LYS:HD2	2.20	0.42
1:D:676:THR:HB	5:D:1053:HOH:O	2.20	0.42
1:B:233:TYR:CE1	1:B:234:ARG:HD3	2.55	0.42
1:B:785:GLU:HG3	5:B:1130:HOH:O	2.19	0.42
1:C:319:ARG:O	1:C:324:THR:HA	2.20	0.42
1:C:756:ASP:O	1:C:759:LYS:HB2	2.19	0.42
1:D:682:MET:HB2	1:D:699:MET:HE3	2.02	0.42
1:A:168:GLN:HE21	1:A:647:ASN:N	2.14	0.42
1:A:42:ASP:H	1:A:45:VAL:HG12	1.85	0.42
1:A:713:MET:HG2	1:A:717:ASP:HB2	2.01	0.42
1:B:30:ASN:HB3	5:B:1003:HOH:O	2.19	0.42
1:D:102:LEU:HD23	1:D:104:LEU:HD22	2.02	0.42
1:D:585:THR:O	1:D:589:ARG:HD3	2.20	0.42
1:B:251:ASP:HB2	1:B:255:LYS:HG3	2.02	0.42
1:C:432:GLU:O	1:C:437:LYS:HA	2.19	0.42
1:C:446:ILE:O	1:C:478:LYS:HE3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:161:TYR:HA	1:D:276:SER:O	2.20	0.42
1:D:758:PHE:O	1:D:762:VAL:HG23	2.19	0.42
1:B:196:PHE:HB3	5:B:1182:HOH:O	2.20	0.41
1:A:739:ARG:HH11	1:A:739:ARG:HG3	1.85	0.41
1:B:413:ARG:O	1:B:416:ALA:HB3	2.20	0.41
1:B:418:PHE:CG	1:B:424:ARG:HD3	2.55	0.41
1:B:612:GLY:H	1:B:617:LYS:HE3	1.85	0.41
1:C:316:PHE:HE1	1:C:332:LYS:HZ2	1.68	0.41
1:C:784:GLN:O	1:C:787:VAL:HB	2.20	0.41
1:A:138:ARG:NH1	1:A:142:CYS:SG	2.81	0.41
1:B:525:VAL:O	1:B:799:ARG:HD2	2.21	0.41
1:C:228:THR:HA	1:C:229:PRO:HD3	1.85	0.41
1:C:758:PHE:CD1	1:C:761:ILE:HD12	2.55	0.41
1:D:793:ASN:HD21	1:D:796:GLU:HG2	1.85	0.41
1:A:738:LEU:HA	1:A:738:LEU:HD12	1.81	0.41
1:B:386:ARG:HA	1:B:439:ILE:O	2.19	0.41
1:C:550:GLU:CG	1:C:554:LYS:HA	2.50	0.41
1:B:105:GLU:O	1:B:109:ASP:HB2	2.21	0.41
1:B:162:GLU:HG2	1:B:183:LEU:HD12	2.02	0.41
1:C:380:ILE:HG13	1:C:382:GLU:OE1	2.21	0.41
1:C:709:PHE:HB3	1:C:783:CYS:SG	2.60	0.41
1:D:386:ARG:HA	1:D:439:ILE:O	2.20	0.41
1:A:433:GLU:HB2	1:D:754:GLN:HG2	2.02	0.41
1:D:790:LEU:HG	1:D:797:TRP:HD1	1.84	0.41
1:A:225:PRO:HB3	1:A:244:TRP:CZ3	2.56	0.41
1:B:15:VAL:O	1:B:18:LEU:HD22	2.20	0.41
1:B:288:GLY:HA2	1:B:387:TRP:CH2	2.56	0.41
1:B:522:LEU:O	1:B:525:VAL:HG23	2.20	0.41
1:C:734:ARG:HD2	5:C:1165:HOH:O	2.20	0.41
1:C:761:ILE:O	1:C:765:LEU:HB2	2.21	0.41
1:B:570:ILE:HB	1:B:609:PRO:HA	2.03	0.41
1:C:594:PRO:HB3	1:C:635:VAL:CG1	2.51	0.41
1:C:818:ALA:O	1:C:822:ARG:HG3	2.21	0.41
1:D:480:GLN:HE21	1:D:482:LYS:HZ3	1.67	0.41
1:A:72:GLN:O	1:A:75:TYR:HB3	2.21	0.41
1:B:458:ILE:O	1:B:462:ILE:HG23	2.21	0.41
1:C:37:PHE:CZ	1:D:18:LEU:HB3	2.56	0.41
1:C:636:VAL:O	1:C:639:ARG:HD3	2.21	0.41
1:D:738:LEU:O	1:D:742:ILE:HG12	2.21	0.41
1:B:568:LYS:NZ	1:B:665:GLN:NE2	2.69	0.41
1:A:206:VAL:CG1	1:A:213:ALA:HB1	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:157:TYR:CE1	1:A:242:ARG:HG2	2.56	0.41
1:A:596:LYS:HD3	1:A:597:PHE:N	2.36	0.41
1:B:554:LYS:O	1:B:555:VAL:HG23	2.21	0.41
1:B:522:LEU:HD13	1:B:806:ALA:HB3	2.03	0.41
1:C:235:ASN:ND2	1:C:235:ASN:N	2.69	0.41
1:C:85:LEU:HD23	1:C:157:TYR:HB2	2.03	0.41
1:D:287:GLU:H	1:D:292:ARG:CD	2.34	0.41
1:D:49:ARG:O	1:D:53:PHE:HD1	2.03	0.41
1:B:467:ILE:H	1:B:467:ILE:HG13	1.57	0.41
1:B:803:ARG:HG3	5:B:1145:HOH:O	2.20	0.41
1:C:63:LEU:HG	1:C:98:THR:HG23	2.03	0.41
1:A:322:VAL:HG13	1:A:325:ASN:CB	2.51	0.40
1:A:713:MET:CE	1:A:721:LEU:HD22	2.51	0.40
1:C:481:ASN:O	1:C:482:LYS:HG2	2.21	0.40
1:A:399:HIS:CD2	5:A:1129:HOH:O	2.73	0.40
1:A:803:ARG:O	1:A:807:THR:HB	2.20	0.40
1:B:312:LYS:O	1:B:317:GLY:N	2.55	0.40
1:B:548:TYR:CD1	1:B:551:ARG:NH2	2.88	0.40
1:B:815:ARG:O	1:B:819:GLN:HG3	2.21	0.40
1:C:36:HIS:O	1:C:40:VAL:HA	2.21	0.40
1:A:249:PRO:O	1:A:252:PHE:CE2	2.74	0.40
1:B:139:LEU:HD11	1:B:143:PHE:CE1	2.57	0.40
1:C:319:ARG:NH2	1:C:322:VAL:O	2.54	0.40
1:C:316:PHE:C	1:C:324:THR:HG23	2.41	0.40
1:D:49:ARG:HA	1:D:125:ILE:HG21	2.02	0.40
1:B:446:ILE:O	1:B:478:LYS:HE3	2.21	0.40
1:C:623:ILE:H	1:C:623:ILE:HG13	1.76	0.40
1:D:287:GLU:H	1:D:292:ARG:HD3	1.87	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:1030:HOH:O	5:D:1049:HOH:O[2_646]	1.46	0.74
1:B:550:GLU:OE2	5:C:1030:HOH:O[2_746]	2.04	0.16

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	822/842 (98%)	741 (90%)	52 (6%)	29 (4%)	3	4
1	B	822/842 (98%)	743 (90%)	59 (7%)	20 (2%)	6	9
1	C	822/842 (98%)	751 (91%)	46 (6%)	25 (3%)	4	6
1	D	822/842 (98%)	746 (91%)	51 (6%)	25 (3%)	4	6
All	All	3288/3368 (98%)	2981 (91%)	208 (6%)	99 (3%)	4	6

All (99) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	16	ARG
1	A	19	ALA
1	A	22	GLU
1	A	166	PHE
1	A	253	ASN
1	A	281	PRO
1	A	321	PRO
1	A	323	ARG
1	A	381	PRO
1	A	555	VAL
1	A	610	ALA
1	A	837	PRO
1	B	16	ARG
1	B	166	PHE
1	B	256	ASP
1	B	257	PHE
1	B	261	GLY
1	B	281	PRO
1	B	321	PRO
1	B	380	ILE
1	B	555	VAL
1	B	556	HIS

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Mol	Chain	Res	Type
1	B	609	PRO
1	B	610	ALA
1	C	16	ARG
1	C	166	PHE
1	C	234	ARG
1	C	254	LEU
1	C	262	TYR
1	C	264	GLN
1	C	281	PRO
1	C	315	LYS
1	C	323	ARG
1	C	555	VAL
1	C	556	HIS
1	C	609	PRO
1	C	610	ALA
1	D	16	ARG
1	D	166	PHE
1	D	256	ASP
1	D	257	PHE
1	D	321	PRO
1	D	324	THR
1	D	555	VAL
1	D	556	HIS
1	D	609	PRO
1	D	610	ALA
1	A	21	VAL
1	A	287	GLU
1	A	436	VAL
1	A	556	HIS
1	A	609	PRO
1	B	92	GLY
1	B	258	ASN
1	B	436	VAL
1	C	17	GLY
1	C	22	GLU
1	C	250	ASN
1	C	256	ASP
1	D	264	GLN
1	D	755	PRO
1	D	836	ALA
1	A	17	GLY
1	A	165	ILE

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Mol	Chain	Res	Type
1	A	256	ASP
1	A	264	GLN
1	A	835	PRO
1	B	22	GLU
1	B	253	ASN
1	B	314	SER
1	C	317	GLY
1	C	436	VAL
1	D	21	VAL
1	D	92	GLY
1	D	93	ARG
1	D	254	LEU
1	D	436	VAL
1	D	549	LEU
1	A	78	ASP
1	A	251	ASP
1	A	320	ASP
1	A	324	THR
1	A	836	ALA
1	B	209	THR
1	C	21	VAL
1	C	263	ILE
1	D	255	LYS
1	D	262	TYR
1	A	676	THR
1	D	281	PRO
1	D	315	LYS
1	B	381	PRO
1	C	339	ASP
1	D	249	PRO
1	D	837	PRO
1	C	594	PRO
1	A	92	GLY
1	C	92	GLY
1	C	836	ALA

5.3.2 Protein sidechains (i)

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	712/732 (97%)	592 (83%)	120 (17%)	2	3
1	B	712/732 (97%)	615 (86%)	97 (14%)	3	7
1	C	712/732 (97%)	617 (87%)	95 (13%)	4	7
1	D	712/732 (97%)	605 (85%)	107 (15%)	3	5
All	All	2848/2928 (97%)	2429 (85%)	419 (15%)	3	5

All (419) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	ARG
1	A	14	SER
1	A	15	VAL
1	A	43	ARG
1	A	45	VAL
1	A	47	THR
1	A	48	PRO
1	A	63	LEU
1	A	76	GLU
1	A	77	LYS
1	A	78	ASP
1	A	79	PRO
1	A	82	ILE
1	A	85	LEU
1	A	90	TYR
1	A	95	LEU
1	A	100	VAL
1	A	104	LEU
1	A	121	GLU
1	A	128	ASP
1	A	131	LEU
1	A	136	LEU
1	A	138	ARG
1	A	165	ILE
1	A	169	LYS
1	A	177	GLU
1	A	191	LYS
1	A	214	LYS
1	A	230	VAL
1	A	231	PRO
1	A	234	ARG

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Mol	Chain	Res	Type
1	A	235	ASN
1	A	242	ARG
1	A	243	LEU
1	A	245	SER
1	A	251	ASP
1	A	255	LYS
1	A	257	PHE
1	A	258	ASN
1	A	274	ASN
1	A	278	VAL
1	A	279	LEU
1	A	281	PRO
1	A	287	GLU
1	A	289	LYS
1	A	291	LEU
1	A	306	ASP
1	A	319	ARG
1	A	321	PRO
1	A	322	VAL
1	A	325	ASN
1	A	327	ASP
1	A	337	LEU
1	A	356	LEU
1	A	358	ARG
1	A	360	ASP
1	A	369	VAL
1	A	378	THR
1	A	379	VAL
1	A	381	PRO
1	A	382	GLU
1	A	391	LEU
1	A	392	LEU
1	A	394	THR
1	A	395	LEU
1	A	396	LEU
1	A	400	LEU
1	A	405	GLU
1	A	426	ARG
1	A	436	VAL
1	A	444	LEU
1	A	455	VAL
1	A	467	ILE

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Mol	Chain	Res	Type
1	A	474	LEU
1	A	486	ILE
1	A	490	ARG
1	A	492	LEU
1	A	494	LEU
1	A	506	ARG
1	A	513	SER
1	A	522	LEU
1	A	543	LEU
1	A	553	TYR
1	A	554	LYS
1	A	565	VAL
1	A	568	LYS
1	A	576	GLN
1	A	579	ASN
1	A	586	LEU
1	A	589	ARG
1	A	598	VAL
1	A	603	VAL
1	A	613	TYR
1	A	622	LEU
1	A	630	VAL
1	A	640	LEU
1	A	649	ARG
1	A	652	LEU
1	A	662	LEU
1	A	676	THR
1	A	683	LEU
1	A	708	PHE
1	A	714	ARG
1	A	727	ASN
1	A	753	LYS
1	A	755	PRO
1	A	756	ASP
1	A	759	LYS
1	A	765	LEU
1	A	770	ARG
1	A	779	GLU
1	A	784	GLN
1	A	792	LYS
1	A	795	ARG
1	A	803	ARG

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Mol	Chain	Res	Type
1	A	807	THR
1	A	833	ARG
1	A	834	LEU
1	A	835	PRO
1	A	837	PRO
1	B	11	LYS
1	B	16	ARG
1	B	18	LEU
1	B	43	ARG
1	B	63	LEU
1	B	77	LYS
1	B	79	PRO
1	B	82	ILE
1	B	87	LEU
1	B	90	TYR
1	B	95	LEU
1	B	100	VAL
1	B	104	LEU
1	B	121	GLU
1	B	131	LEU
1	B	136	LEU
1	B	138	ARG
1	B	165	ILE
1	B	169	LYS
1	B	191	LYS
1	B	214	LYS
1	B	225	PRO
1	B	235	ASN
1	B	242	ARG
1	B	243	LEU
1	B	253	ASN
1	B	254	LEU
1	B	257	PHE
1	B	264	GLN
1	B	274	ASN
1	B	279	LEU
1	B	281	PRO
1	B	287	GLU
1	B	291	LEU
1	B	318	CYS
1	B	319	ARG
1	B	320	ASP

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Mol	Chain	Res	Type
1	B	321	PRO
1	B	323	ARG
1	B	325	ASN
1	B	337	LEU
1	B	342	PRO
1	B	358	ARG
1	B	360	ASP
1	B	363	LYS
1	B	369	VAL
1	B	396	LEU
1	B	419	PRO
1	B	426	ARG
1	B	444	LEU
1	B	455	VAL
1	B	474	LEU
1	B	486	ILE
1	B	490	ARG
1	B	492	LEU
1	B	494	LEU
1	B	506	ARG
1	B	519	ARG
1	B	521	LEU
1	B	522	LEU
1	B	543	LEU
1	B	550	GLU
1	B	552	GLU
1	B	553	TYR
1	B	554	LYS
1	B	573	TYR
1	B	576	GLN
1	B	579	ASN
1	B	589	ARG
1	B	596	LYS
1	B	603	VAL
1	B	613	TYR
1	B	622	LEU
1	B	640	LEU
1	B	649	ARG
1	B	652	LEU
1	B	655	LYS
1	B	662	LEU
1	B	676	THR

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Mol	Chain	Res	Type
1	B	683	LEU
1	B	705	GLU
1	B	708	PHE
1	B	714	ARG
1	B	721	LEU
1	B	753	LYS
1	B	765	LEU
1	B	770	ARG
1	B	781	VAL
1	B	782	LYS
1	B	784	GLN
1	B	792	LYS
1	B	794	PRO
1	B	803	ARG
1	B	807	THR
1	B	830	SER
1	B	831	ARG
1	B	833	ARG
1	C	12	GLN
1	C	22	GLU
1	C	43	ARG
1	C	47	THR
1	C	48	PRO
1	C	63	LEU
1	C	82	ILE
1	C	90	TYR
1	C	95	LEU
1	C	100	VAL
1	C	104	LEU
1	C	121	GLU
1	C	131	LEU
1	C	136	LEU
1	C	138	ARG
1	C	169	LYS
1	C	191	LYS
1	C	214	LYS
1	C	225	PRO
1	C	231	PRO
1	C	235	ASN
1	C	242	ARG
1	C	243	LEU
1	C	252	PHE

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Mol	Chain	Res	Type
1	C	255	LYS
1	C	256	ASP
1	C	257	PHE
1	C	262	TYR
1	C	264	GLN
1	C	274	ASN
1	C	278	VAL
1	C	279	LEU
1	C	281	PRO
1	C	287	GLU
1	C	289	LYS
1	C	291	LEU
1	C	316	PHE
1	C	319	ARG
1	C	321	PRO
1	C	323	ARG
1	C	337	LEU
1	C	358	ARG
1	C	361	TRP
1	C	369	VAL
1	C	379	VAL
1	C	380	ILE
1	C	391	LEU
1	C	392	LEU
1	C	395	LEU
1	C	396	LEU
1	C	400	LEU
1	C	426	ARG
1	C	436	VAL
1	C	444	LEU
1	C	455	VAL
1	C	462	ILE
1	C	474	LEU
1	C	486	ILE
1	C	490	ARG
1	C	492	LEU
1	C	506	ARG
1	C	513	SER
1	C	521	LEU
1	C	525	VAL
1	C	543	LEU
1	C	550	GLU

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Mol	Chain	Res	Type
1	C	552	GLU
1	C	553	TYR
1	C	554	LYS
1	C	565	VAL
1	C	579	ASN
1	C	586	LEU
1	C	613	TYR
1	C	622	LEU
1	C	630	VAL
1	C	640	LEU
1	C	649	ARG
1	C	652	LEU
1	C	662	LEU
1	C	676	THR
1	C	708	PHE
1	C	714	ARG
1	C	716	GLU
1	C	753	LYS
1	C	755	PRO
1	C	756	ASP
1	C	759	LYS
1	C	766	MET
1	C	779	GLU
1	C	782	LYS
1	C	792	LYS
1	C	797	TRP
1	C	803	ARG
1	C	807	THR
1	C	833	ARG
1	D	11	LYS
1	D	12	GLN
1	D	15	VAL
1	D	22	GLU
1	D	23	ASN
1	D	43	ARG
1	D	45	VAL
1	D	48	PRO
1	D	76	GLU
1	D	77	LYS
1	D	82	ILE
1	D	87	LEU
1	D	90	TYR

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Mol	Chain	Res	Type
1	D	95	LEU
1	D	104	LEU
1	D	121	GLU
1	D	128	ASP
1	D	131	LEU
1	D	136	LEU
1	D	138	ARG
1	D	165	ILE
1	D	169	LYS
1	D	177	GLU
1	D	195	GLU
1	D	199	PRO
1	D	230	VAL
1	D	235	ASN
1	D	242	ARG
1	D	243	LEU
1	D	257	PHE
1	D	262	TYR
1	D	263	ILE
1	D	274	ASN
1	D	278	VAL
1	D	279	LEU
1	D	281	PRO
1	D	287	GLU
1	D	289	LYS
1	D	309	ARG
1	D	315	LYS
1	D	319	ARG
1	D	322	VAL
1	D	323	ARG
1	D	337	LEU
1	D	342	PRO
1	D	358	ARG
1	D	360	ASP
1	D	369	VAL
1	D	378	THR
1	D	379	VAL
1	D	380	ILE
1	D	382	GLU
1	D	392	LEU
1	D	395	LEU
1	D	396	LEU

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Mol	Chain	Res	Type
1	D	400	LEU
1	D	422	VAL
1	D	424	ARG
1	D	426	ARG
1	D	436	VAL
1	D	437	LYS
1	D	444	LEU
1	D	455	VAL
1	D	462	ILE
1	D	474	LEU
1	D	475	GLU
1	D	490	ARG
1	D	492	LEU
1	D	506	ARG
1	D	521	LEU
1	D	522	LEU
1	D	543	LEU
1	D	550	GLU
1	D	553	TYR
1	D	554	LYS
1	D	568	LYS
1	D	573	TYR
1	D	579	ASN
1	D	586	LEU
1	D	589	ARG
1	D	613	TYR
1	D	622	LEU
1	D	630	VAL
1	D	640	LEU
1	D	649	ARG
1	D	652	LEU
1	D	662	LEU
1	D	676	THR
1	D	683	LEU
1	D	705	GLU
1	D	708	PHE
1	D	714	ARG
1	D	715	VAL
1	D	716	GLU
1	D	753	LYS
1	D	755	PRO
1	D	756	ASP

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Mol	Chain	Res	Type
1	D	765	LEU
1	D	766	MET
1	D	770	ARG
1	D	782	LYS
1	D	784	GLN
1	D	797	TRP
1	D	803	ARG
1	D	807	THR
1	D	832	GLN
1	D	837	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (77) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	GLN
1	A	34	HIS
1	A	168	GLN
1	A	235	ASN
1	A	264	GLN
1	A	336	GLN
1	A	390	HIS
1	A	399	HIS
1	A	412	ASN
1	A	459	HIS
1	A	477	HIS
1	A	480	GLN
1	A	481	ASN
1	A	566	GLN
1	A	576	GLN
1	A	579	ASN
1	A	665	GLN
1	A	727	ASN
1	A	744	GLN
1	A	784	GLN
1	B	34	HIS
1	B	167	ASN
1	B	168	GLN
1	B	235	ASN
1	B	336	GLN
1	B	399	HIS
1	B	480	GLN
1	B	481	ASN

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Mol	Chain	Res	Type
1	B	566	GLN
1	B	576	GLN
1	B	579	ASN
1	B	665	GLN
1	B	727	ASN
1	B	744	GLN
1	B	784	GLN
1	C	34	HIS
1	C	57	HIS
1	C	167	ASN
1	C	168	GLN
1	C	235	ASN
1	C	274	ASN
1	C	336	GLN
1	C	399	HIS
1	C	412	ASN
1	C	459	HIS
1	C	480	GLN
1	C	481	ASN
1	C	541	ASN
1	C	566	GLN
1	C	576	GLN
1	C	579	ASN
1	C	665	GLN
1	C	727	ASN
1	C	744	GLN
1	C	763	ASN
1	C	767	HIS
1	C	784	GLN
1	D	12	GLN
1	D	34	HIS
1	D	62	HIS
1	D	168	GLN
1	D	235	ASN
1	D	250	ASN
1	D	336	GLN
1	D	390	HIS
1	D	399	HIS
1	D	412	ASN
1	D	459	HIS
1	D	480	GLN
1	D	481	ASN

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Mol	Chain	Res	Type
1	D	566	GLN
1	D	576	GLN
1	D	579	ASN
1	D	665	GLN
1	D	727	ASN
1	D	744	GLN
1	D	784	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

12 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	PO4	D	997	-	4,4,4	3.49	3 (75%)	6,6,6	2.30	4 (66%)
4	NTZ	C	998	-	13,15,15	2.04	4 (30%)	12,22,22	1.70	1 (8%)
3	PLP	D	999	1	15,15,16	1.54	1 (6%)	20,22,23	1.13	2 (10%)
2	PO4	B	997	-	4,4,4	3.66	4 (100%)	6,6,6	2.15	2 (33%)
2	PO4	A	997	-	4,4,4	3.44	4 (100%)	6,6,6	2.68	4 (66%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	PO4	C	997	-	4,4,4	3.78	4 (100%)	6,6,6	2.46	4 (66%)
3	PLP	B	999	1	15,15,16	1.43	2 (13%)	20,22,23	1.11	1 (5%)
3	PLP	C	999	1	15,15,16	1.70	3 (20%)	20,22,23	1.18	2 (10%)
3	PLP	A	999	1	15,15,16	1.04	1 (6%)	20,22,23	1.28	2 (10%)
4	NTZ	D	998	-	13,15,15	1.83	4 (30%)	12,22,22	3.31	3 (25%)
4	NTZ	B	998	-	13,15,15	1.80	5 (38%)	12,22,22	1.69	3 (25%)
4	NTZ	A	998	-	13,15,15	1.20	2 (15%)	12,22,22	1.84	1 (8%)

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
4	NTZ	C	998	-	-	1/2/22/22	0/1/2/2
3	PLP	D	999	1	-	1/6/6/8	0/1/1/1
3	PLP	B	999	1	-	1/6/6/8	0/1/1/1
3	PLP	C	999	1	-	1/6/6/8	0/1/1/1
3	PLP	A	999	1	-	1/6/6/8	0/1/1/1
4	NTZ	D	998	-	-	0/2/22/22	0/1/2/2
4	NTZ	B	998	-	-	0/2/22/22	0/1/2/2
4	NTZ	A	998	-	-	1/2/22/22	0/1/2/2

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	997	PO4	P-O2	-4.78	1.40	1.54
3	D	999	PLP	C3-C2	-4.54	1.36	1.40
2	D	997	PO4	P-O2	-4.44	1.41	1.54
2	B	997	PO4	P-O2	-4.27	1.41	1.54
4	C	998	NTZ	N21-N18	4.22	1.41	1.34
2	B	997	PO4	P-O3	-4.20	1.42	1.54
4	C	998	NTZ	N17-N18	4.12	1.40	1.30
2	C	997	PO4	P-O4	-3.93	1.42	1.54
2	A	997	PO4	P-O2	-3.91	1.42	1.54
2	A	997	PO4	P-O3	-3.84	1.43	1.54
2	D	997	PO4	P-O3	-3.84	1.43	1.54
4	D	998	NTZ	N17-N18	3.79	1.39	1.30
3	C	999	PLP	C3-C2	-3.76	1.37	1.40
2	D	997	PO4	P-O4	-3.71	1.43	1.54
4	B	998	NTZ	N17-N18	3.68	1.39	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	997	PO4	P-O4	-3.66	1.43	1.54
2	C	997	PO4	P-O3	-3.58	1.43	1.54
2	A	997	PO4	P-O4	-3.48	1.44	1.54
4	B	998	NTZ	N21-N18	3.13	1.39	1.34
4	D	998	NTZ	N17-N1	3.12	1.40	1.34
4	C	998	NTZ	N17-N1	3.11	1.40	1.34
3	C	999	PLP	C4A-C4	2.86	1.57	1.51
4	A	998	NTZ	C1-C2	2.75	1.56	1.51
3	B	999	PLP	C3-C2	-2.69	1.38	1.40
2	C	997	PO4	P-O1	2.47	1.56	1.50
3	A	999	PLP	C3-C2	-2.46	1.38	1.40
4	D	998	NTZ	N21-N18	2.44	1.38	1.34
4	B	998	NTZ	N17-N1	2.36	1.39	1.34
3	B	999	PLP	C5-C4	-2.31	1.37	1.40
3	C	999	PLP	C5-C4	-2.30	1.38	1.40
2	A	997	PO4	P-O1	2.27	1.56	1.50
4	B	998	NTZ	C1-C2	-2.26	1.47	1.51
4	A	998	NTZ	N17-N18	2.25	1.35	1.30
4	B	998	NTZ	C4-C5	-2.18	1.49	1.53
4	C	998	NTZ	C1-N21	2.11	1.40	1.34
2	B	997	PO4	P-O1	2.10	1.55	1.50
4	D	998	NTZ	C1-N21	2.01	1.40	1.34

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	998	NTZ	N18-N17-N1	9.19	113.51	106.02
4	A	998	NTZ	N18-N17-N1	5.74	110.69	106.02
4	D	998	NTZ	N21-N18-N17	-5.37	104.04	110.09
4	C	998	NTZ	N18-N17-N1	5.31	110.34	106.02
4	B	998	NTZ	N18-N17-N1	4.11	109.37	106.02
2	A	997	PO4	O3-P-O1	-3.84	96.86	110.89
2	A	997	PO4	O4-P-O2	3.83	120.25	107.97
4	D	998	NTZ	C1-N21-N18	3.55	108.54	105.28
2	B	997	PO4	O4-P-O2	3.48	119.14	107.97
2	D	997	PO4	O4-P-O2	3.44	119.02	107.97
2	C	997	PO4	O4-P-O1	-3.36	98.61	110.89
3	A	999	PLP	O2P-P-O4P	-3.21	98.19	106.73
2	C	997	PO4	O4-P-O2	3.17	118.14	107.97
2	B	997	PO4	O3-P-O1	-2.98	99.97	110.89
3	A	999	PLP	O3P-P-O4P	2.92	114.49	106.73
3	C	999	PLP	O4P-C5A-C5	-2.75	104.11	109.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	997	PO4	O3-P-O1	-2.73	100.92	110.89
3	B	999	PLP	O3P-P-O1P	2.68	121.18	110.68
2	A	997	PO4	O4-P-O1	-2.67	101.14	110.89
4	B	998	NTZ	C6-C5-C4	2.60	117.14	112.45
3	D	999	PLP	O3P-P-O4P	2.55	113.53	106.73
2	D	997	PO4	O3-P-O1	-2.41	102.08	110.89
2	A	997	PO4	O4-P-O3	2.29	115.31	107.97
3	C	999	PLP	O3P-P-O1P	2.25	119.50	110.68
2	C	997	PO4	O4-P-O3	2.18	114.97	107.97
4	B	998	NTZ	O2-C2-C3	2.11	112.98	108.55
2	D	997	PO4	O4-P-O1	-2.09	103.26	110.89
2	D	997	PO4	O2-P-O1	-2.08	103.28	110.89
3	D	999	PLP	O3P-P-O1P	2.01	118.56	110.68

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	998	NTZ	C4-C5-C6-O6
3	D	999	PLP	C4-C5-C5A-O4P
3	C	999	PLP	C4-C5-C5A-O4P
4	A	998	NTZ	C4-C5-C6-O6
3	B	999	PLP	C6-C5-C5A-O4P
3	A	999	PLP	C6-C5-C5A-O4P

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	997	PO4	1	0
3	B	999	PLP	1	0
3	C	999	PLP	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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.