Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 08:59 AM GMT

PDB ID	:	3GOK
Title	:	Binding site mapping of protein ligands
Authors	:	Scheich, C.
Deposited on	:	2009-03-19
Resolution	:	3.20 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

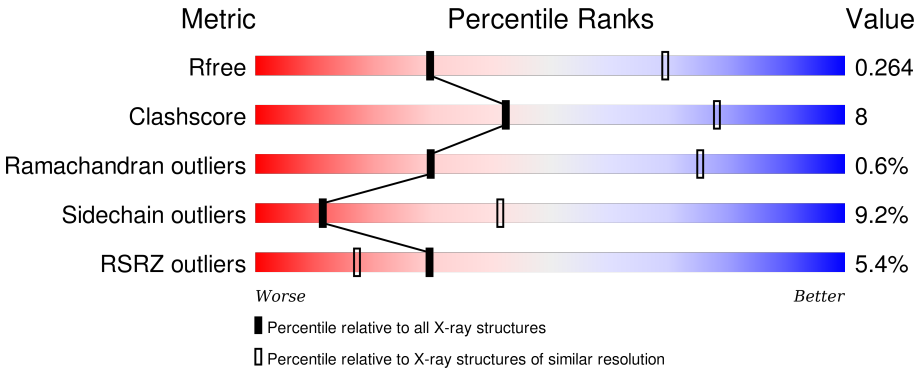
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 3.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1124 (3.24-3.16)
Clashscore	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)
RSRZ outliers	91569	1129 (3.24-3.16)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=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 <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	334	2% 66% 16% • 15%
1	B	334	4% 65% 18% • 13%
1	C	334	4% 67% 16% • 15%
1	D	334	3% 62% 18% 5% 15%
1	E	334	6% 63% 18% • • 13%

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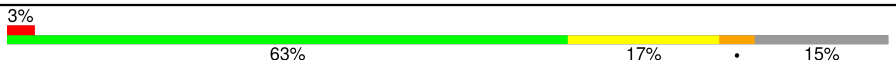
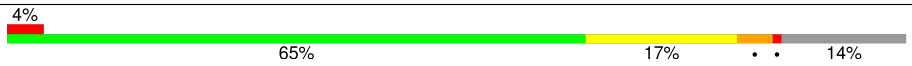
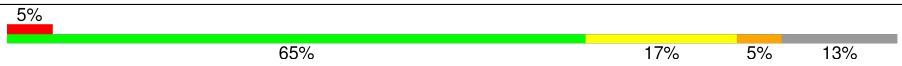
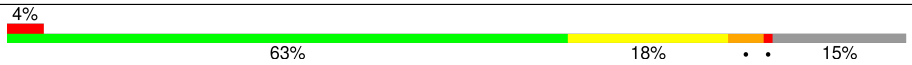
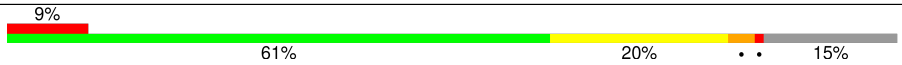
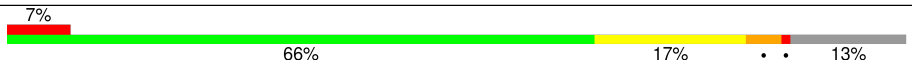
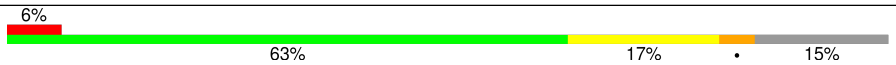
Mol	Chain	Length	Quality of chain
1	F	334	
1	G	334	
1	H	334	
1	I	334	
1	J	334	
1	K	334	
1	L	334	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 28332 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 MAP kinase-activated protein kinase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	285	Total	C	N	O	S	0	0	0
			2317	1481	401	418	17			
1	B	290	Total	C	N	O	S	0	0	0
			2361	1510	407	427	17			
1	C	285	Total	C	N	O	S	0	0	0
			2322	1488	400	417	17			
1	D	283	Total	C	N	O	S	0	0	0
			2298	1467	399	415	17			
1	E	290	Total	C	N	O	S	0	0	0
			2361	1510	407	427	17			
1	F	284	Total	C	N	O	S	0	0	0
			2316	1485	399	415	17			
1	G	286	Total	C	N	O	S	0	0	0
			2329	1490	402	420	17			
1	H	290	Total	C	N	O	S	0	0	0
			2361	1510	407	427	17			
1	I	284	Total	C	N	O	S	0	0	0
			2316	1485	399	415	17			
1	J	283	Total	C	N	O	S	0	0	0
			2298	1467	399	415	17			
1	K	290	Total	C	N	O	S	0	0	0
			2361	1510	407	427	17			
1	L	284	Total	C	N	O	S	0	0	0
			2316	1485	399	415	17			

There are 120 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	31	GLY	-	EXPRESSION TAG	UNP P49137
A	32	ALA	-	EXPRESSION TAG	UNP P49137
A	33	MET	-	EXPRESSION TAG	UNP P49137
A	34	GLY	-	EXPRESSION TAG	UNP P49137
A	35	SER	-	EXPRESSION TAG	UNP P49137

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Chain	Residue	Modelled	Actual	Comment	Reference
A	36	GLY	-	EXPRESSION TAG	UNP P49137
A	37	ALA	-	EXPRESSION TAG	UNP P49137
A	38	MET	-	EXPRESSION TAG	UNP P49137
A	39	GLY	-	EXPRESSION TAG	UNP P49137
A	40	SER	-	EXPRESSION TAG	UNP P49137
B	31	GLY	-	EXPRESSION TAG	UNP P49137
B	32	ALA	-	EXPRESSION TAG	UNP P49137
B	33	MET	-	EXPRESSION TAG	UNP P49137
B	34	GLY	-	EXPRESSION TAG	UNP P49137
B	35	SER	-	EXPRESSION TAG	UNP P49137
B	36	GLY	-	EXPRESSION TAG	UNP P49137
B	37	ALA	-	EXPRESSION TAG	UNP P49137
B	38	MET	-	EXPRESSION TAG	UNP P49137
B	39	GLY	-	EXPRESSION TAG	UNP P49137
B	40	SER	-	EXPRESSION TAG	UNP P49137
C	31	GLY	-	EXPRESSION TAG	UNP P49137
C	32	ALA	-	EXPRESSION TAG	UNP P49137
C	33	MET	-	EXPRESSION TAG	UNP P49137
C	34	GLY	-	EXPRESSION TAG	UNP P49137
C	35	SER	-	EXPRESSION TAG	UNP P49137
C	36	GLY	-	EXPRESSION TAG	UNP P49137
C	37	ALA	-	EXPRESSION TAG	UNP P49137
C	38	MET	-	EXPRESSION TAG	UNP P49137
C	39	GLY	-	EXPRESSION TAG	UNP P49137
C	40	SER	-	EXPRESSION TAG	UNP P49137
D	31	GLY	-	EXPRESSION TAG	UNP P49137
D	32	ALA	-	EXPRESSION TAG	UNP P49137
D	33	MET	-	EXPRESSION TAG	UNP P49137
D	34	GLY	-	EXPRESSION TAG	UNP P49137
D	35	SER	-	EXPRESSION TAG	UNP P49137
D	36	GLY	-	EXPRESSION TAG	UNP P49137
D	37	ALA	-	EXPRESSION TAG	UNP P49137
D	38	MET	-	EXPRESSION TAG	UNP P49137
D	39	GLY	-	EXPRESSION TAG	UNP P49137
D	40	SER	-	EXPRESSION TAG	UNP P49137
E	31	GLY	-	EXPRESSION TAG	UNP P49137
E	32	ALA	-	EXPRESSION TAG	UNP P49137
E	33	MET	-	EXPRESSION TAG	UNP P49137
E	34	GLY	-	EXPRESSION TAG	UNP P49137
E	35	SER	-	EXPRESSION TAG	UNP P49137
E	36	GLY	-	EXPRESSION TAG	UNP P49137
E	37	ALA	-	EXPRESSION TAG	UNP P49137

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Chain	Residue	Modelled	Actual	Comment	Reference
E	38	MET	-	EXPRESSION TAG	UNP P49137
E	39	GLY	-	EXPRESSION TAG	UNP P49137
E	40	SER	-	EXPRESSION TAG	UNP P49137
F	31	GLY	-	EXPRESSION TAG	UNP P49137
F	32	ALA	-	EXPRESSION TAG	UNP P49137
F	33	MET	-	EXPRESSION TAG	UNP P49137
F	34	GLY	-	EXPRESSION TAG	UNP P49137
F	35	SER	-	EXPRESSION TAG	UNP P49137
F	36	GLY	-	EXPRESSION TAG	UNP P49137
F	37	ALA	-	EXPRESSION TAG	UNP P49137
F	38	MET	-	EXPRESSION TAG	UNP P49137
F	39	GLY	-	EXPRESSION TAG	UNP P49137
F	40	SER	-	EXPRESSION TAG	UNP P49137
G	31	GLY	-	EXPRESSION TAG	UNP P49137
G	32	ALA	-	EXPRESSION TAG	UNP P49137
G	33	MET	-	EXPRESSION TAG	UNP P49137
G	34	GLY	-	EXPRESSION TAG	UNP P49137
G	35	SER	-	EXPRESSION TAG	UNP P49137
G	36	GLY	-	EXPRESSION TAG	UNP P49137
G	37	ALA	-	EXPRESSION TAG	UNP P49137
G	38	MET	-	EXPRESSION TAG	UNP P49137
G	39	GLY	-	EXPRESSION TAG	UNP P49137
G	40	SER	-	EXPRESSION TAG	UNP P49137
H	31	GLY	-	EXPRESSION TAG	UNP P49137
H	32	ALA	-	EXPRESSION TAG	UNP P49137
H	33	MET	-	EXPRESSION TAG	UNP P49137
H	34	GLY	-	EXPRESSION TAG	UNP P49137
H	35	SER	-	EXPRESSION TAG	UNP P49137
H	36	GLY	-	EXPRESSION TAG	UNP P49137
H	37	ALA	-	EXPRESSION TAG	UNP P49137
H	38	MET	-	EXPRESSION TAG	UNP P49137
H	39	GLY	-	EXPRESSION TAG	UNP P49137
H	40	SER	-	EXPRESSION TAG	UNP P49137
I	31	GLY	-	EXPRESSION TAG	UNP P49137
I	32	ALA	-	EXPRESSION TAG	UNP P49137
I	33	MET	-	EXPRESSION TAG	UNP P49137
I	34	GLY	-	EXPRESSION TAG	UNP P49137
I	35	SER	-	EXPRESSION TAG	UNP P49137
I	36	GLY	-	EXPRESSION TAG	UNP P49137
I	37	ALA	-	EXPRESSION TAG	UNP P49137
I	38	MET	-	EXPRESSION TAG	UNP P49137
I	39	GLY	-	EXPRESSION TAG	UNP P49137

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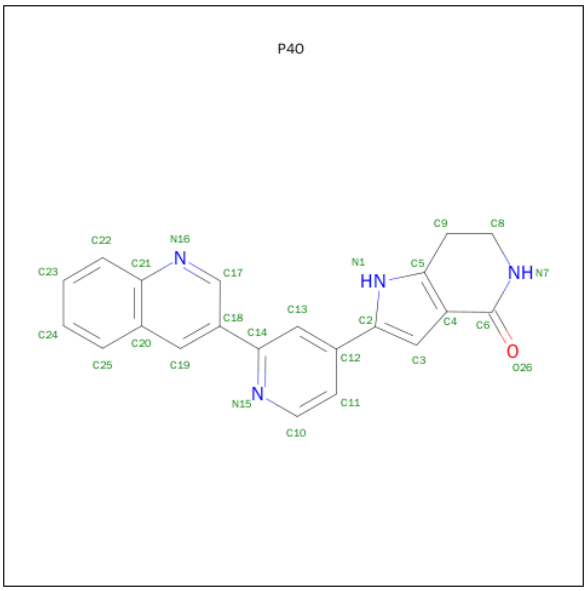
Chain	Residue	Modelled	Actual	Comment	Reference
I	40	SER	-	EXPRESSION TAG	UNP P49137
J	31	GLY	-	EXPRESSION TAG	UNP P49137
J	32	ALA	-	EXPRESSION TAG	UNP P49137
J	33	MET	-	EXPRESSION TAG	UNP P49137
J	34	GLY	-	EXPRESSION TAG	UNP P49137
J	35	SER	-	EXPRESSION TAG	UNP P49137
J	36	GLY	-	EXPRESSION TAG	UNP P49137
J	37	ALA	-	EXPRESSION TAG	UNP P49137
J	38	MET	-	EXPRESSION TAG	UNP P49137
J	39	GLY	-	EXPRESSION TAG	UNP P49137
J	40	SER	-	EXPRESSION TAG	UNP P49137
K	31	GLY	-	EXPRESSION TAG	UNP P49137
K	32	ALA	-	EXPRESSION TAG	UNP P49137
K	33	MET	-	EXPRESSION TAG	UNP P49137
K	34	GLY	-	EXPRESSION TAG	UNP P49137
K	35	SER	-	EXPRESSION TAG	UNP P49137
K	36	GLY	-	EXPRESSION TAG	UNP P49137
K	37	ALA	-	EXPRESSION TAG	UNP P49137
K	38	MET	-	EXPRESSION TAG	UNP P49137
K	39	GLY	-	EXPRESSION TAG	UNP P49137
K	40	SER	-	EXPRESSION TAG	UNP P49137
L	31	GLY	-	EXPRESSION TAG	UNP P49137
L	32	ALA	-	EXPRESSION TAG	UNP P49137
L	33	MET	-	EXPRESSION TAG	UNP P49137
L	34	GLY	-	EXPRESSION TAG	UNP P49137
L	35	SER	-	EXPRESSION TAG	UNP P49137
L	36	GLY	-	EXPRESSION TAG	UNP P49137
L	37	ALA	-	EXPRESSION TAG	UNP P49137
L	38	MET	-	EXPRESSION TAG	UNP P49137
L	39	GLY	-	EXPRESSION TAG	UNP P49137
L	40	SER	-	EXPRESSION TAG	UNP P49137

- Molecule 2 is 2-(2-QUINOLIN-3-YLPYRIDIN-4-YL)-1,5,6,7-TETRAHYDRO-4H-PYRROLO[3,2-C]PYRIDIN-4-ONE (three-letter code: P4O) (formula: $C_{21}H_{16}N_4O$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C N O 26 21 4 1	0	0
2	B	1	Total C N O 26 21 4 1	0	0
2	C	1	Total C N O 26 21 4 1	0	0
2	D	1	Total C N O 26 21 4 1	0	0
2	E	1	Total C N O 26 21 4 1	0	0
2	F	1	Total C N O 26 21 4 1	0	0
2	G	1	Total C N O 26 21 4 1	0	0
2	H	1	Total C N O 26 21 4 1	0	0
2	I	1	Total C N O 26 21 4 1	0	0
2	J	1	Total C N O 26 21 4 1	0	0
2	K	1	Total C N O 26 21 4 1	0	0
2	L	1	Total C N O 26 21 4 1	0	0

- Molecule 3 is water.

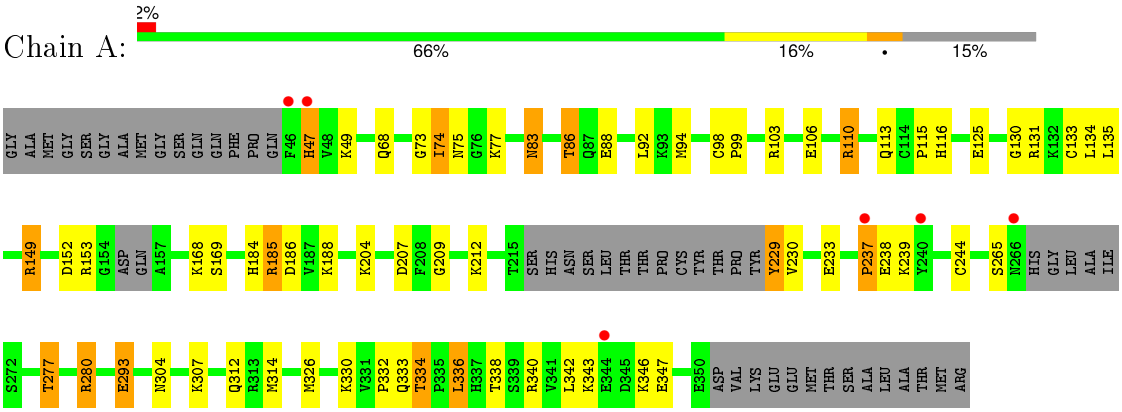
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	3	Total O 3 3	0	0
3	B	8	Total O 8 8	0	0
3	C	6	Total O 6 6	0	0
3	D	8	Total O 8 8	0	0
3	E	5	Total O 5 5	0	0
3	F	2	Total O 2 2	0	0
3	G	6	Total O 6 6	0	0
3	H	7	Total O 7 7	0	0
3	I	2	Total O 2 2	0	0
3	J	6	Total O 6 6	0	0
3	K	4	Total O 4 4	0	0
3	L	7	Total O 7 7	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 errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

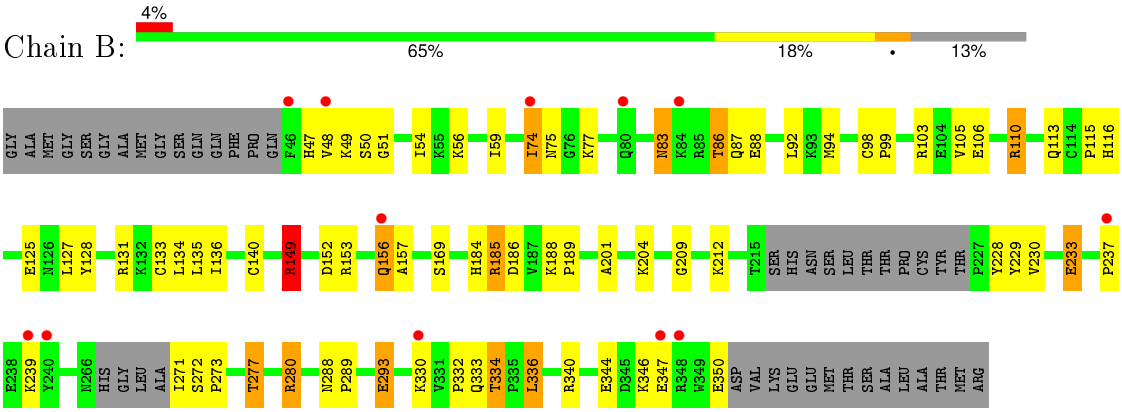
- Molecule 1: MAP kinase-activated protein kinase 2

Chain A:



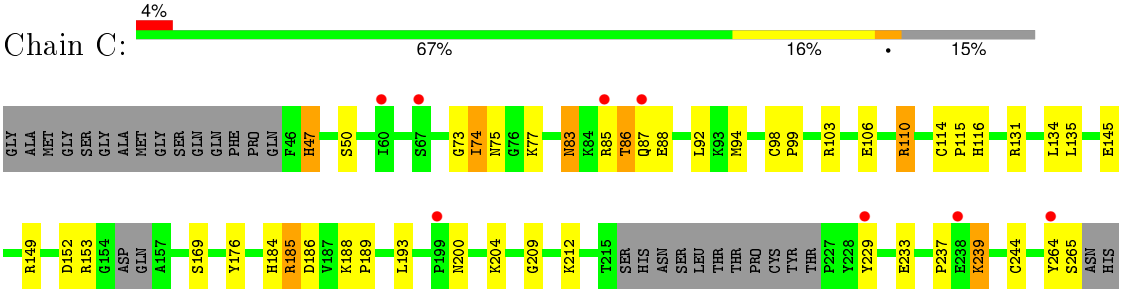
- Molecule 1: MAP kinase-activated protein kinase 2

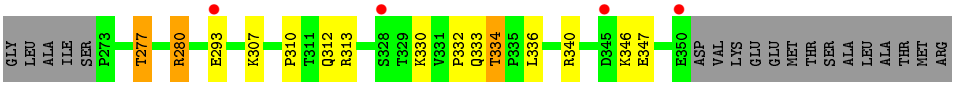
Chain B:



- Molecule 1: MAP kinase-activated protein kinase 2

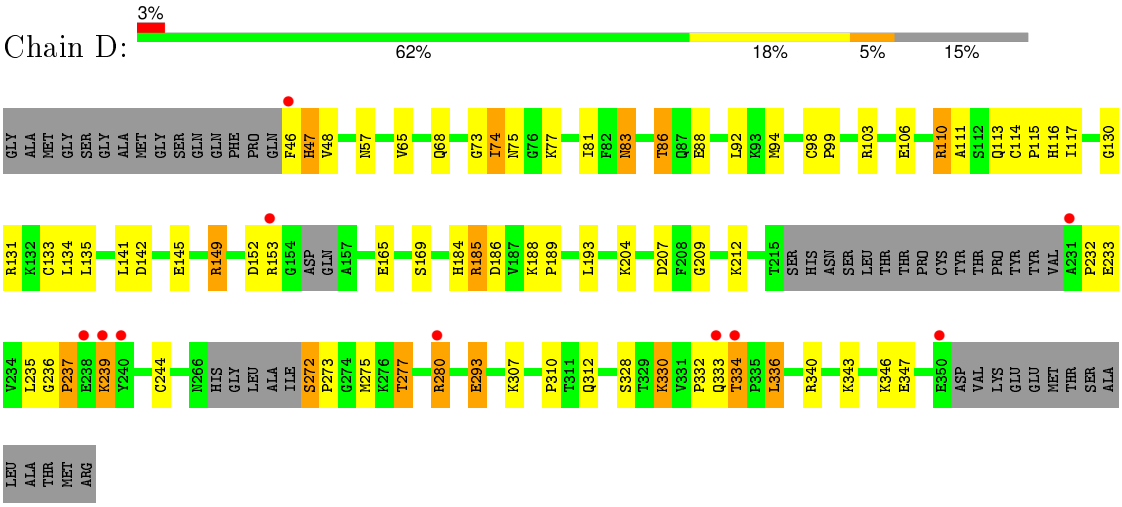
Chain C:





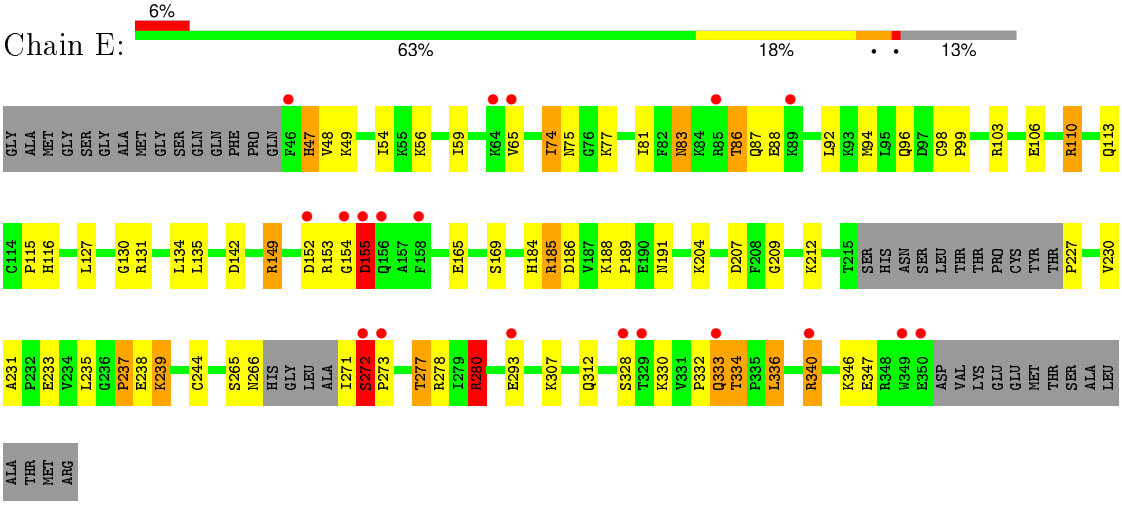
• Molecule 1: MAP kinase-activated protein kinase 2

Chain D:



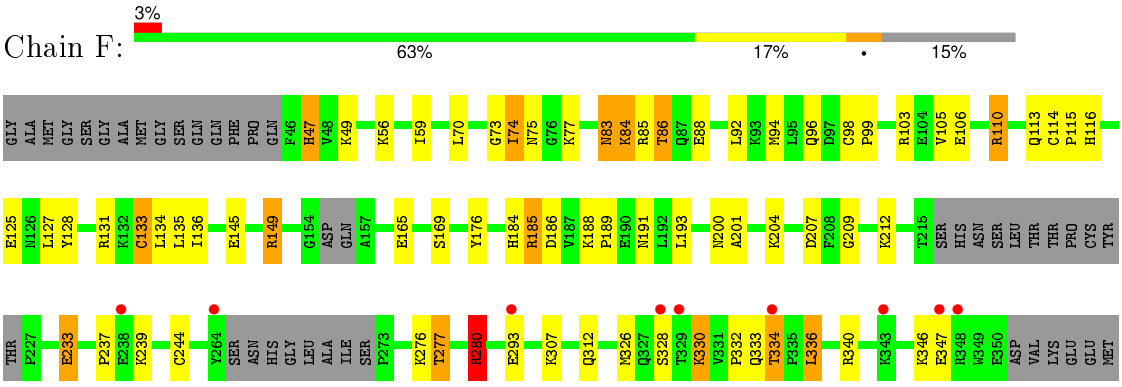
• Molecule 1: MAP kinase-activated protein kinase 2

Chain E:



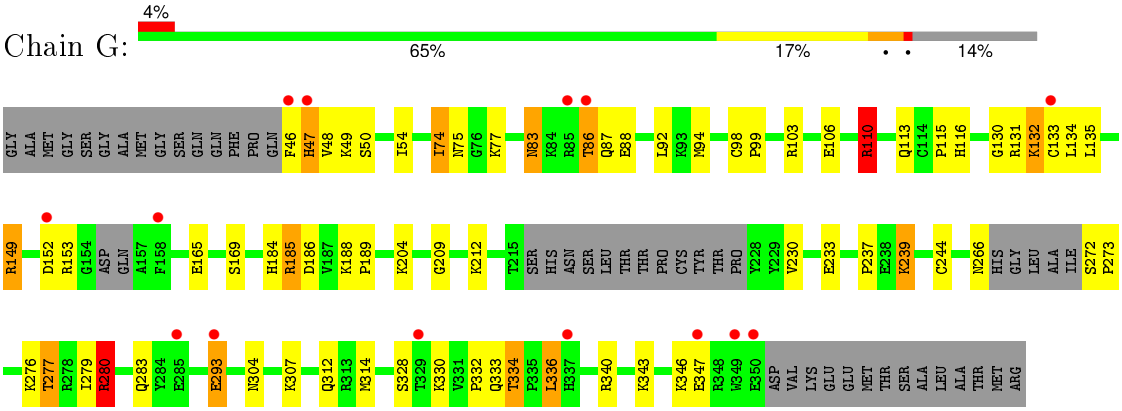
• Molecule 1: MAP kinase-activated protein kinase 2

Chain F:



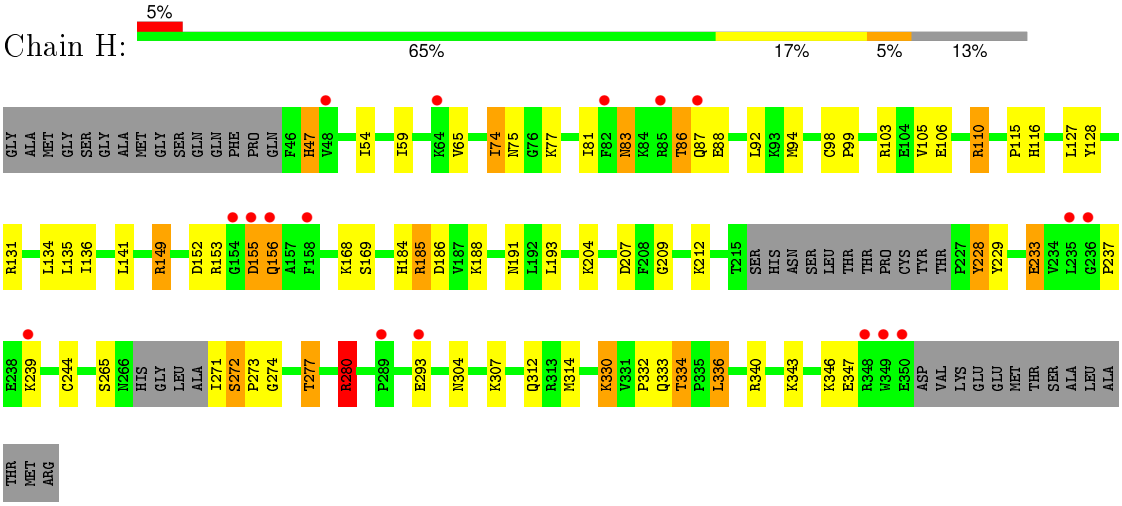
- Molecule 1: MAP kinase-activated protein kinase 2

Chain G:



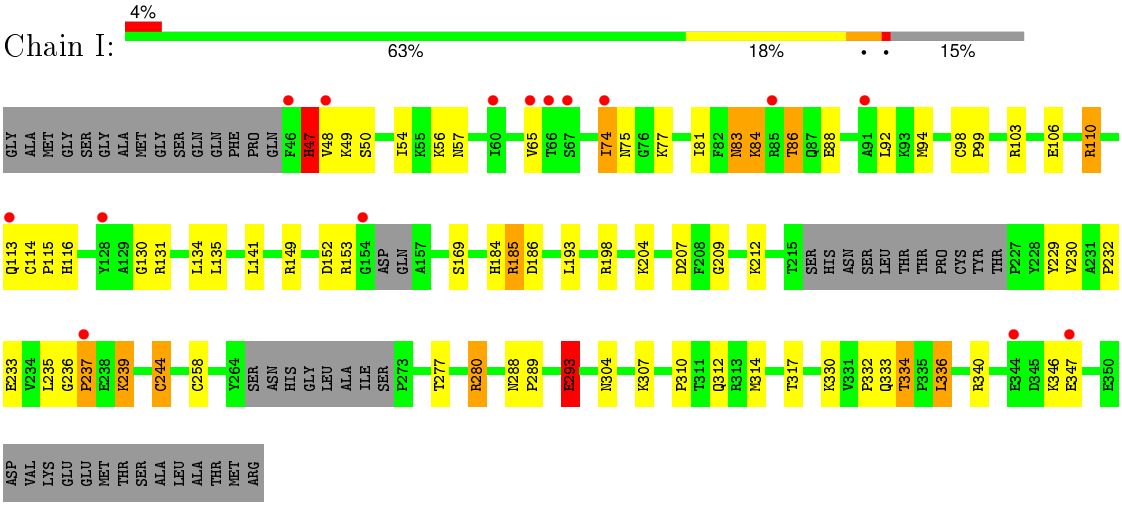
- Molecule 1: MAP kinase-activated protein kinase 2

Chain H:

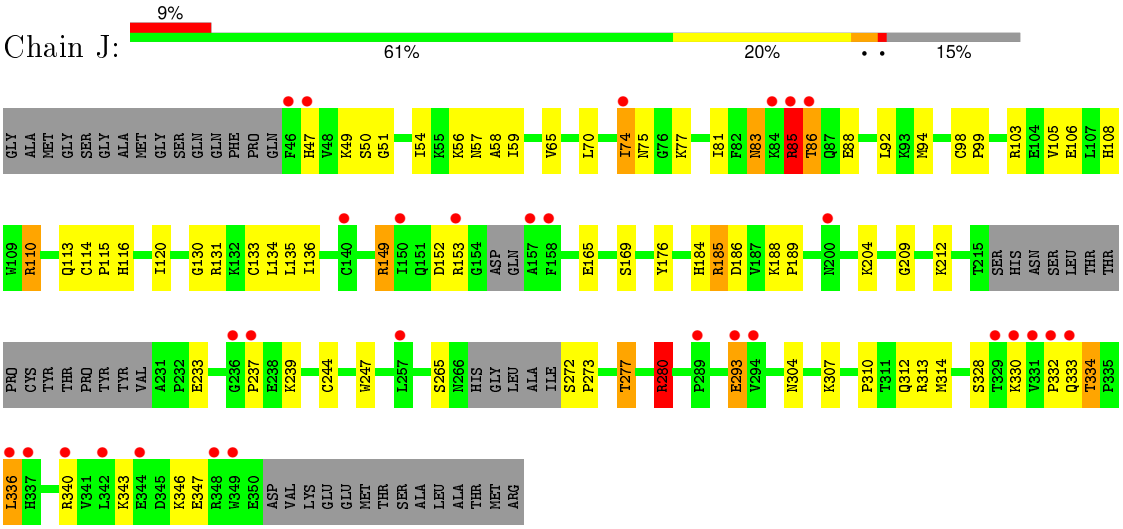


- Molecule 1: MAP kinase-activated protein kinase 2

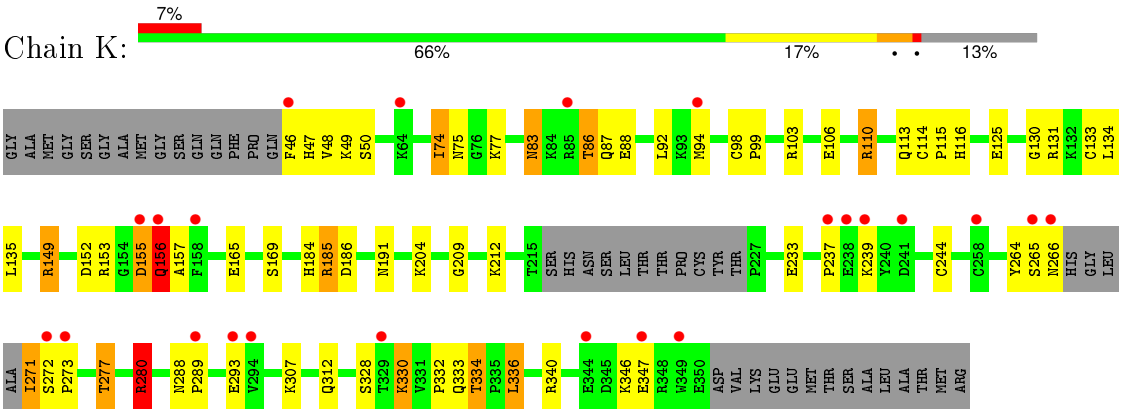
Chain I:



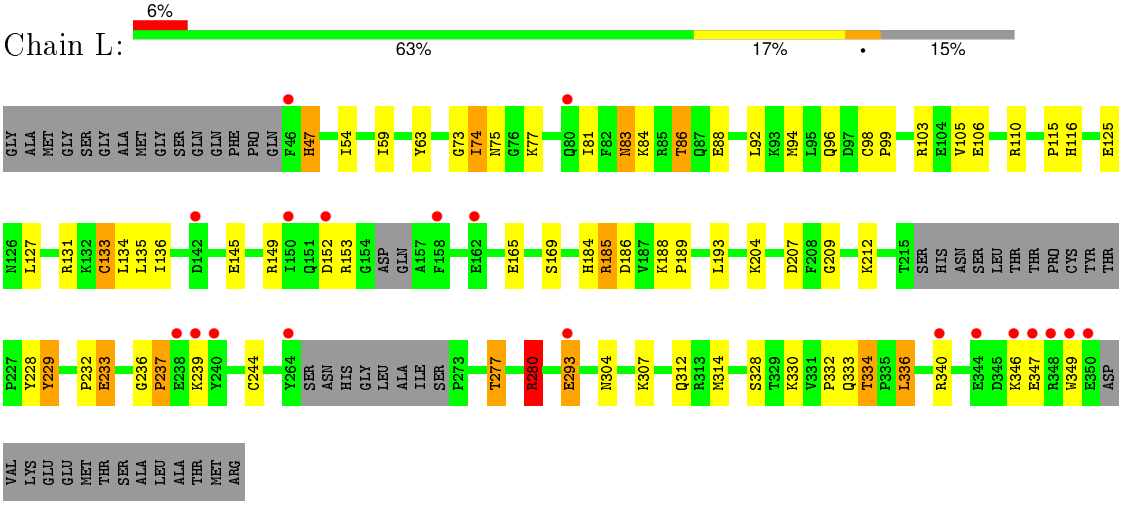
- Molecule 1: MAP kinase-activated protein kinase 2



- Molecule 1: MAP kinase-activated protein kinase 2



- Molecule 1: MAP kinase-activated protein kinase 2



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	140.21Å 183.19Å 217.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.73 – 3.20 46.72 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.8 (46.73-3.20) 99.8 (46.72-3.20)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	0.17	Depositor
$< I/\sigma(I) >$ [1]	2.11 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.238 , 0.258 0.242 , 0.264	Depositor DCC
R_{free} test set	4642 reflections (5.27%)	DCC
Wilson B-factor (Å^2)	91.4	Xtriage
Anisotropy	0.027	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 94.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Outliers	0 of 92694 reflections	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	28332	wwPDB-VP
Average B, all atoms (Å^2)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.88% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: P4O

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	0.80	1/2366 (0.0%)	0.87	15/3188 (0.5%)
1	B	0.72	0/2413	0.91	14/3254 (0.4%)
1	C	0.73	0/2373	1.04	16/3197 (0.5%)
1	D	0.75	1/2346 (0.0%)	0.95	17/3160 (0.5%)
1	E	0.70	1/2413 (0.0%)	0.92	15/3254 (0.5%)
1	F	0.76	1/2367 (0.0%)	1.06	17/3189 (0.5%)
1	G	0.72	1/2379 (0.0%)	0.89	17/3206 (0.5%)
1	H	0.68	0/2413	0.90	12/3254 (0.4%)
1	I	0.74	2/2367 (0.1%)	1.06	19/3189 (0.6%)
1	J	0.68	2/2346 (0.1%)	0.87	15/3160 (0.5%)
1	K	0.65	0/2413	0.92	14/3254 (0.4%)
1	L	0.70	1/2367 (0.0%)	1.07	18/3189 (0.6%)
All	All	0.72	10/28563 (0.0%)	0.96	189/38494 (0.5%)

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	D	0	1
1	E	0	1
All	All	0	2

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	133	CYS	CB-SG	-8.54	1.67	1.82
1	A	244	CYS	CB-SG	-7.02	1.70	1.82
1	D	133	CYS	CB-SG	-7.01	1.70	1.82
1	I	244	CYS	CB-SG	-6.77	1.70	1.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	133	CYS	CB-SG	-6.01	1.72	1.82
1	G	133	CYS	CB-SG	-5.66	1.72	1.81
1	E	340	ARG	CG-CD	5.42	1.65	1.51
1	J	133	CYS	CB-SG	-5.20	1.73	1.81
1	J	85	ARG	CG-CD	5.15	1.64	1.51
1	I	258	CYS	CB-SG	-5.05	1.73	1.81

All (189) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	280	ARG	NE-CZ-NH1	-16.48	112.06	120.30
1	C	280	ARG	NE-CZ-NH1	-16.41	112.09	120.30
1	L	280	ARG	NE-CZ-NH1	-16.27	112.16	120.30
1	I	280	ARG	NE-CZ-NH2	15.77	128.19	120.30
1	L	280	ARG	NE-CZ-NH2	15.77	128.19	120.30
1	I	340	ARG	NE-CZ-NH2	-15.71	112.44	120.30
1	C	280	ARG	NE-CZ-NH2	15.71	128.16	120.30
1	C	340	ARG	NE-CZ-NH2	-15.68	112.46	120.30
1	K	103	ARG	NE-CZ-NH1	-15.52	112.54	120.30
1	F	280	ARG	NE-CZ-NH2	15.46	128.03	120.30
1	B	103	ARG	NE-CZ-NH1	-15.27	112.67	120.30
1	I	280	ARG	NE-CZ-NH1	-15.09	112.76	120.30
1	L	340	ARG	NE-CZ-NH2	-15.09	112.76	120.30
1	L	340	ARG	NE-CZ-NH1	15.08	127.84	120.30
1	H	103	ARG	NE-CZ-NH1	-15.02	112.79	120.30
1	C	340	ARG	NE-CZ-NH1	14.72	127.66	120.30
1	E	103	ARG	NE-CZ-NH1	-14.43	113.09	120.30
1	I	340	ARG	NE-CZ-NH1	14.22	127.41	120.30
1	F	340	ARG	NE-CZ-NH2	-14.13	113.24	120.30
1	F	340	ARG	NE-CZ-NH1	14.05	127.33	120.30
1	K	103	ARG	NE-CZ-NH2	13.98	127.29	120.30
1	E	340	ARG	NE-CZ-NH2	13.47	127.04	120.30
1	B	103	ARG	NE-CZ-NH2	13.34	126.97	120.30
1	H	103	ARG	NE-CZ-NH2	13.33	126.97	120.30
1	D	149	ARG	NE-CZ-NH1	13.19	126.89	120.30
1	L	149	ARG	NE-CZ-NH2	12.96	126.78	120.30
1	L	149	ARG	NE-CZ-NH1	-12.21	114.19	120.30
1	I	149	ARG	NE-CZ-NH2	12.04	126.32	120.30
1	F	131	ARG	NE-CZ-NH1	11.95	126.27	120.30
1	E	103	ARG	NE-CZ-NH2	11.92	126.26	120.30
1	L	131	ARG	NE-CZ-NH1	11.91	126.26	120.30
1	C	131	ARG	NE-CZ-NH1	11.36	125.98	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	I	149	ARG	NE-CZ-NH1	-11.21	114.70	120.30
1	L	131	ARG	NE-CZ-NH2	-11.17	114.71	120.30
1	I	131	ARG	NE-CZ-NH1	11.08	125.84	120.30
1	F	149	ARG	NE-CZ-NH2	10.95	125.77	120.30
1	F	131	ARG	NE-CZ-NH2	-10.77	114.92	120.30
1	I	131	ARG	NE-CZ-NH2	-10.76	114.92	120.30
1	C	131	ARG	NE-CZ-NH2	-10.64	114.98	120.30
1	F	103	ARG	NE-CZ-NH2	-10.36	115.12	120.30
1	D	280	ARG	NE-CZ-NH2	-10.21	115.20	120.30
1	F	149	ARG	NE-CZ-NH1	-10.11	115.25	120.30
1	G	280	ARG	NE-CZ-NH2	-9.82	115.39	120.30
1	C	149	ARG	NE-CZ-NH1	-9.70	115.45	120.30
1	K	280	ARG	NE-CZ-NH1	9.66	125.13	120.30
1	D	149	ARG	NE-CZ-NH2	-9.61	115.50	120.30
1	C	149	ARG	NE-CZ-NH2	9.58	125.09	120.30
1	G	280	ARG	NE-CZ-NH1	9.42	125.01	120.30
1	D	280	ARG	NE-CZ-NH1	9.36	124.98	120.30
1	J	340	ARG	NE-CZ-NH2	9.20	124.90	120.30
1	K	280	ARG	NE-CZ-NH2	-9.18	115.71	120.30
1	B	280	ARG	NE-CZ-NH1	9.05	124.83	120.30
1	A	280	ARG	NE-CZ-NH2	-9.04	115.78	120.30
1	B	280	ARG	NE-CZ-NH2	-9.03	115.78	120.30
1	J	85	ARG	CA-CB-CG	9.02	133.24	113.40
1	J	131	ARG	NE-CZ-NH2	8.96	124.78	120.30
1	D	340	ARG	NE-CZ-NH1	-8.94	115.83	120.30
1	K	149	ARG	NE-CZ-NH1	8.89	124.75	120.30
1	E	280	ARG	NE-CZ-NH1	8.86	124.73	120.30
1	A	280	ARG	NE-CZ-NH1	8.84	124.72	120.30
1	J	280	ARG	NE-CZ-NH1	8.74	124.67	120.30
1	J	280	ARG	NE-CZ-NH2	-8.72	115.94	120.30
1	E	280	ARG	NE-CZ-NH2	-8.60	116.00	120.30
1	H	131	ARG	NE-CZ-NH2	8.49	124.55	120.30
1	H	280	ARG	NE-CZ-NH1	8.46	124.53	120.30
1	C	103	ARG	NE-CZ-NH2	-8.34	116.13	120.30
1	F	103	ARG	NE-CZ-NH1	8.34	124.47	120.30
1	H	280	ARG	NE-CZ-NH2	-8.31	116.15	120.30
1	C	280	ARG	CD-NE-CZ	8.28	135.19	123.60
1	I	280	ARG	CD-NE-CZ	8.27	135.17	123.60
1	I	47	HIS	CB-CA-C	-8.25	93.90	110.40
1	B	340	ARG	NE-CZ-NH1	-8.24	116.18	120.30
1	G	340	ARG	NE-CZ-NH1	-8.20	116.20	120.30
1	B	340	ARG	NE-CZ-NH2	8.09	124.34	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	340	ARG	CD-NE-CZ	8.06	134.88	123.60
1	K	131	ARG	NE-CZ-NH2	8.05	124.32	120.30
1	L	47	HIS	CB-CA-C	-7.95	94.50	110.40
1	L	340	ARG	CD-NE-CZ	7.95	134.72	123.60
1	L	280	ARG	CD-NE-CZ	7.94	134.72	123.60
1	K	340	ARG	NE-CZ-NH2	7.87	124.23	120.30
1	F	280	ARG	CD-NE-CZ	7.86	134.61	123.60
1	D	340	ARG	NE-CZ-NH2	7.84	124.22	120.30
1	L	103	ARG	NE-CZ-NH2	-7.83	116.38	120.30
1	I	340	ARG	CD-NE-CZ	7.82	134.55	123.60
1	G	103	ARG	NE-CZ-NH2	-7.82	116.39	120.30
1	A	340	ARG	NE-CZ-NH1	-7.71	116.44	120.30
1	C	340	ARG	CD-NE-CZ	7.65	134.30	123.60
1	C	47	HIS	CB-CA-C	-7.63	95.13	110.40
1	J	340	ARG	NE-CZ-NH1	-7.57	116.52	120.30
1	K	340	ARG	NE-CZ-NH1	-7.56	116.52	120.30
1	E	131	ARG	NE-CZ-NH2	7.53	124.07	120.30
1	G	47	HIS	CB-CA-C	-7.45	95.50	110.40
1	G	340	ARG	NE-CZ-NH2	7.43	124.02	120.30
1	F	47	HIS	CB-CA-C	-7.24	95.91	110.40
1	H	340	ARG	NE-CZ-NH2	7.19	123.89	120.30
1	D	47	HIS	CB-CA-C	-7.18	96.04	110.40
1	I	103	ARG	NE-CZ-NH1	7.17	123.89	120.30
1	A	340	ARG	NE-CZ-NH2	7.13	123.86	120.30
1	H	47	HIS	CB-CA-C	-7.09	96.21	110.40
1	J	131	ARG	NE-CZ-NH1	-7.09	116.75	120.30
1	J	103	ARG	NE-CZ-NH2	-7.08	116.76	120.30
1	B	47	HIS	CB-CA-C	-7.02	96.36	110.40
1	H	340	ARG	NE-CZ-NH1	-6.99	116.80	120.30
1	K	149	ARG	NE-CZ-NH2	-6.97	116.81	120.30
1	A	149	ARG	NE-CZ-NH1	6.96	123.78	120.30
1	A	103	ARG	NE-CZ-NH2	-6.94	116.83	120.30
1	A	47	HIS	CB-CA-C	-6.94	96.53	110.40
1	E	149	ARG	NE-CZ-NH1	6.92	123.76	120.30
1	E	340	ARG	CD-NE-CZ	6.91	133.27	123.60
1	C	103	ARG	NE-CZ-NH1	6.88	123.74	120.30
1	D	149	ARG	CD-NE-CZ	6.88	133.24	123.60
1	D	131	ARG	NE-CZ-NH2	6.86	123.73	120.30
1	B	131	ARG	NE-CZ-NH2	6.84	123.72	120.30
1	K	103	ARG	CD-NE-CZ	6.83	133.16	123.60
1	A	131	ARG	NE-CZ-NH2	6.82	123.71	120.30
1	H	103	ARG	CD-NE-CZ	6.78	133.09	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	K	47	HIS	CB-CA-C	-6.76	96.87	110.40
1	D	103	ARG	NE-CZ-NH1	6.74	123.67	120.30
1	D	149	ARG	CB-CG-CD	6.69	128.99	111.60
1	I	103	ARG	NE-CZ-NH2	-6.61	117.00	120.30
1	E	103	ARG	CD-NE-CZ	6.59	132.82	123.60
1	B	131	ARG	NE-CZ-NH1	-6.57	117.01	120.30
1	B	103	ARG	CD-NE-CZ	6.53	132.74	123.60
1	E	47	HIS	CB-CA-C	-6.51	97.38	110.40
1	G	132	LYS	CD-CE-NZ	6.50	126.64	111.70
1	G	131	ARG	NE-CZ-NH2	6.49	123.54	120.30
1	B	149	ARG	NE-CZ-NH1	6.46	123.53	120.30
1	H	149	ARG	NE-CZ-NH1	6.45	123.53	120.30
1	K	131	ARG	NE-CZ-NH1	-6.39	117.11	120.30
1	H	131	ARG	NE-CZ-NH1	-6.37	117.11	120.30
1	G	103	ARG	NE-CZ-NH1	6.37	123.48	120.30
1	G	149	ARG	NE-CZ-NH1	6.33	123.46	120.30
1	D	131	ARG	NE-CZ-NH1	-6.27	117.16	120.30
1	B	336	LEU	CA-CB-CG	6.13	129.39	115.30
1	G	336	LEU	CA-CB-CG	6.09	129.30	115.30
1	A	131	ARG	NE-CZ-NH1	-6.05	117.28	120.30
1	D	336	LEU	CA-CB-CG	6.04	129.19	115.30
1	D	346	LYS	CD-CE-NZ	-6.04	97.81	111.70
1	F	336	LEU	CA-CB-CG	6.03	129.18	115.30
1	J	85	ARG	N-CA-CB	6.00	121.40	110.60
1	G	293	GLU	CA-CB-CG	6.00	126.60	113.40
1	G	110	ARG	NE-CZ-NH1	5.98	123.29	120.30
1	J	47	HIS	CB-CA-C	-5.96	98.48	110.40
1	J	293	GLU	CA-CB-CG	5.94	126.47	113.40
1	E	340	ARG	NE-CZ-NH1	-5.92	117.34	120.30
1	I	47	HIS	N-CA-CB	5.88	121.18	110.60
1	J	149	ARG	NE-CZ-NH1	5.87	123.23	120.30
1	E	131	ARG	NE-CZ-NH1	-5.86	117.37	120.30
1	G	131	ARG	NE-CZ-NH1	-5.85	117.38	120.30
1	I	336	LEU	CA-CB-CG	5.84	128.73	115.30
1	D	103	ARG	NE-CZ-NH2	-5.80	117.40	120.30
1	D	110	ARG	NE-CZ-NH1	5.73	123.16	120.30
1	L	103	ARG	NE-CZ-NH1	5.73	123.16	120.30
1	A	103	ARG	NE-CZ-NH1	5.71	123.15	120.30
1	E	149	ARG	NE-CZ-NH2	-5.67	117.46	120.30
1	A	293	GLU	N-CA-CB	-5.66	100.41	110.60
1	L	336	LEU	CA-CB-CG	5.66	128.32	115.30
1	L	293	GLU	CA-CB-CG	5.66	125.84	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	J	336	LEU	CA-CB-CG	5.65	128.29	115.30
1	L	131	ARG	CD-NE-CZ	5.65	131.50	123.60
1	J	103	ARG	NE-CZ-NH1	5.63	123.12	120.30
1	F	149	ARG	CD-NE-CZ	5.63	131.48	123.60
1	G	346	LYS	CD-CE-NZ	-5.62	98.78	111.70
1	L	346	LYS	CD-CE-NZ	-5.61	98.81	111.70
1	A	293	GLU	CA-CB-CG	5.57	125.65	113.40
1	B	149	ARG	NE-CZ-NH2	-5.57	117.52	120.30
1	F	84	LYS	CB-CG-CD	5.55	126.04	111.60
1	I	84	LYS	CB-CG-CD	5.54	125.99	111.60
1	I	149	ARG	CD-NE-CZ	5.53	131.34	123.60
1	A	336	LEU	CA-CB-CG	5.53	128.01	115.30
1	L	149	ARG	CD-NE-CZ	5.43	131.21	123.60
1	G	132	LYS	CG-CD-CE	5.42	128.16	111.90
1	A	149	ARG	NE-CZ-NH2	-5.39	117.60	120.30
1	K	336	LEU	CA-CB-CG	5.37	127.66	115.30
1	I	293	GLU	CB-CA-C	-5.31	99.78	110.40
1	C	131	ARG	CD-NE-CZ	5.29	131.01	123.60
1	E	280	ARG	CD-NE-CZ	5.27	130.98	123.60
1	F	131	ARG	CD-NE-CZ	5.20	130.88	123.60
1	C	47	HIS	N-CA-CB	5.19	119.94	110.60
1	I	131	ARG	CD-NE-CZ	5.17	130.83	123.60
1	E	336	LEU	CA-CB-CG	5.15	127.14	115.30
1	J	149	ARG	NE-CZ-NH2	-5.14	117.73	120.30
1	B	293	GLU	CB-CA-C	-5.12	100.16	110.40
1	H	336	LEU	CA-CB-CG	5.12	127.07	115.30
1	G	280	ARG	CD-NE-CZ	5.06	130.68	123.60
1	C	149	ARG	CD-NE-CZ	5.03	130.64	123.60
1	K	280	ARG	CD-NE-CZ	5.03	130.64	123.60
1	A	280	ARG	CD-NE-CZ	5.02	130.63	123.60
1	D	293	GLU	CB-CA-C	-5.02	100.35	110.40

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	272	SER	Peptide
1	E	154	GLY	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	2317	0	2344	34	2
1	B	2361	0	2385	52	2
1	C	2322	0	2351	39	1
1	D	2298	0	2326	47	1
1	E	2361	0	2385	54	8
1	F	2316	0	2346	49	1
1	G	2329	0	2353	42	0
1	H	2361	0	2385	42	2
1	I	2316	0	2346	43	3
1	J	2298	0	2326	50	8
1	K	2361	0	2385	39	0
1	L	2316	0	2346	42	2
2	A	26	0	16	1	0
2	B	26	0	16	1	0
2	C	26	0	16	1	0
2	D	26	0	16	3	0
2	E	26	0	16	2	0
2	F	26	0	16	3	0
2	G	26	0	16	0	0
2	H	26	0	16	1	0
2	I	26	0	16	0	0
2	J	26	0	16	2	0
2	K	26	0	16	1	0
2	L	26	0	16	1	0
3	A	3	0	0	1	0
3	B	8	0	0	2	0
3	C	6	0	0	0	0
3	D	8	0	0	3	0
3	E	5	0	0	1	0
3	F	2	0	0	0	0
3	G	6	0	0	1	0
3	H	7	0	0	0	0
3	I	2	0	0	0	0
3	J	6	0	0	1	0
3	K	4	0	0	1	0
3	L	7	0	0	1	0
All	All	28332	0	28470	473	15

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (473) 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:47:HIS:HA	3:A:366:HOH:O	1.52	1.08
1:H:265:SER:O	1:H:272:SER:HA	1.71	0.88
1:H:271:ILE:HG12	1:H:274:GLY:HA3	1.53	0.88
1:F:332:PRO:HB2	1:F:334:THR:HG22	1.55	0.88
1:I:332:PRO:HB2	1:I:334:THR:HG22	1.53	0.87
1:B:48:VAL:HG21	1:J:59:ILE:HG22	1.57	0.87
1:B:59:ILE:HG22	1:I:48:VAL:HG21	1.59	0.84
1:G:332:PRO:HB2	1:G:334:THR:HG22	1.57	0.84
1:C:332:PRO:HB2	1:C:334:THR:HG22	1.60	0.83
1:A:83:ASN:HB3	1:A:86:THR:HG22	1.60	0.83
1:D:83:ASN:HB3	1:D:86:THR:HG22	1.60	0.82
1:A:110:ARG:NH1	1:G:130:GLY:O	2.13	0.82
1:J:83:ASN:HB3	1:J:86:THR:HG22	1.59	0.82
1:J:332:PRO:HB2	1:J:334:THR:HG22	1.60	0.82
1:L:332:PRO:HB2	1:L:334:THR:HG22	1.60	0.82
1:B:332:PRO:HB2	1:B:334:THR:HG22	1.60	0.81
1:K:266:ASN:HB2	1:K:271:ILE:HA	1.62	0.81
1:B:127:LEU:HD13	1:I:113:GLN:HE21	1.46	0.80
1:E:332:PRO:HB2	1:E:334:THR:HG22	1.61	0.80
1:D:332:PRO:HB2	1:D:334:THR:HG22	1.61	0.79
1:I:116:HIS:CE1	1:I:169:SER:HB2	2.17	0.79
1:A:332:PRO:HB2	1:A:334:THR:HG22	1.62	0.79
1:L:83:ASN:HB3	1:L:86:THR:HG22	1.63	0.79
1:K:332:PRO:HB2	1:K:334:THR:HG22	1.62	0.79
1:H:83:ASN:HB3	1:H:86:THR:HG22	1.61	0.79
1:B:83:ASN:HB3	1:B:86:THR:HG22	1.65	0.79
1:E:83:ASN:HB3	1:E:86:THR:HG22	1.63	0.77
1:F:83:ASN:HB3	1:F:86:THR:HG22	1.65	0.77
1:B:110:ARG:NH1	1:J:130:GLY:O	2.17	0.77
1:C:83:ASN:HB3	1:C:86:THR:HG22	1.65	0.77
1:K:83:ASN:HB3	1:K:86:THR:HG22	1.65	0.77
1:I:83:ASN:HB3	1:I:86:THR:HG22	1.66	0.76
1:H:332:PRO:HB2	1:H:334:THR:HG22	1.67	0.76
1:A:83:ASN:CB	1:A:86:THR:HG22	2.16	0.76
1:D:83:ASN:CB	1:D:86:THR:HG22	2.16	0.75
1:D:48:VAL:HG21	1:L:59:ILE:HG22	1.68	0.74
1:B:50:SER:HB2	1:J:57:ASN:HA	1.70	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:83:ASN:HB3	1:G:86:THR:HG22	1.70	0.73
1:F:330:LYS:O	1:F:330:LYS:HG3	1.85	0.73
1:B:184:HIS:HD2	1:B:186:ASP:H	1.37	0.73
1:B:116:HIS:CE1	1:B:169:SER:HB2	2.25	0.72
1:E:83:ASN:CB	1:E:86:THR:HG22	2.20	0.72
1:B:233:GLU:HG2	1:C:310:PRO:HG3	1.72	0.72
1:D:235:LEU:O	1:E:280:ARG:NH2	2.23	0.72
1:J:83:ASN:CB	1:J:86:THR:HG22	2.19	0.71
1:K:116:HIS:CE1	1:K:169:SER:HB2	2.25	0.71
1:G:266:ASN:HB2	1:G:272:SER:N	2.05	0.71
1:E:116:HIS:CE1	1:E:169:SER:HB2	2.26	0.71
1:D:272:SER:HB2	1:D:273:PRO:HD2	1.73	0.70
1:K:155:ASP:O	1:K:156:GLN:HB2	1.88	0.70
1:H:83:ASN:CB	1:H:86:THR:HG22	2.21	0.70
1:D:46:PHE:N	3:D:372:HOH:O	2.24	0.69
1:C:83:ASN:CB	1:C:86:THR:HG22	2.23	0.69
1:C:330:LYS:O	1:C:330:LYS:HG2	1.91	0.69
1:D:116:HIS:CE1	1:D:169:SER:HB2	2.26	0.69
1:D:310:PRO:HG3	1:F:233:GLU:HG2	1.75	0.69
1:E:265:SER:O	1:E:272:SER:HA	1.92	0.68
1:K:98:CYS:HB2	1:K:99:PRO:HD2	1.75	0.68
1:L:184:HIS:HD2	1:L:186:ASP:H	1.41	0.68
1:K:330:LYS:O	1:K:330:LYS:HG3	1.94	0.67
1:E:227:PRO:HB2	1:E:230:VAL:HB	1.77	0.67
1:D:330:LYS:O	1:D:330:LYS:HG3	1.95	0.66
1:B:56:LYS:O	1:I:50:SER:HB2	1.95	0.66
1:A:184:HIS:HD2	1:A:186:ASP:H	1.42	0.66
1:K:152:ASP:O	1:K:153:ARG:HG3	1.95	0.66
1:G:152:ASP:O	1:G:153:ARG:HG3	1.96	0.66
1:B:83:ASN:CB	1:B:86:THR:HG22	2.24	0.66
1:J:116:HIS:CE1	1:J:169:SER:HB2	2.31	0.66
1:F:128:TYR:HD1	1:G:47:HIS:O	1.78	0.66
1:K:83:ASN:CB	1:K:86:THR:HG22	2.25	0.66
1:H:330:LYS:HG3	1:H:330:LYS:O	1.93	0.66
1:H:184:HIS:HD2	1:H:186:ASP:H	1.44	0.66
1:J:185:ARG:HH21	1:J:212:LYS:HD2	1.61	0.66
1:F:83:ASN:CB	1:F:86:THR:HG22	2.25	0.65
1:L:116:HIS:CE1	1:L:169:SER:HB2	2.31	0.65
1:G:188:LYS:HE2	1:I:229:TYR:OH	1.96	0.64
1:L:98:CYS:HB2	1:L:99:PRO:HD2	1.79	0.64
1:I:83:ASN:CB	1:I:86:THR:HG22	2.27	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:184:HIS:HD2	1:E:186:ASP:H	1.46	0.64
1:L:83:ASN:CB	1:L:86:THR:HG22	2.28	0.64
1:E:59:ILE:HG22	1:K:48:VAL:HG21	1.81	0.63
1:A:115:PRO:O	1:A:204:LYS:HE2	1.98	0.63
1:F:127:LEU:N	1:G:49:LYS:O	2.27	0.63
1:G:46:PHE:N	3:G:368:HOH:O	2.31	0.62
1:E:48:VAL:HG21	1:H:59:ILE:HG22	1.80	0.62
1:H:98:CYS:HB2	1:H:99:PRO:HD2	1.81	0.62
1:E:152:ASP:O	1:E:153:ARG:HG3	2.00	0.62
1:H:185:ARG:HH21	1:H:212:LYS:HD2	1.62	0.62
1:G:83:ASN:CB	1:G:86:THR:HG22	2.30	0.62
1:E:113:GLN:HE21	1:H:127:LEU:HD13	1.63	0.62
1:L:74:ILE:HG12	1:L:209:GLY:HA3	1.81	0.62
1:A:98:CYS:HB2	1:A:99:PRO:HD2	1.80	0.62
1:A:185:ARG:HH21	1:A:212:LYS:HD2	1.64	0.62
1:F:116:HIS:CE1	1:F:169:SER:HB2	2.35	0.61
1:D:184:HIS:HD2	1:D:186:ASP:H	1.48	0.61
1:A:116:HIS:CE1	1:A:169:SER:HB2	2.36	0.61
1:J:92:LEU:HD11	1:J:135:LEU:HB3	1.83	0.61
1:F:184:HIS:HD2	1:F:186:ASP:H	1.49	0.61
1:D:92:LEU:HD11	1:D:135:LEU:HB3	1.83	0.61
1:D:152:ASP:O	1:D:153:ARG:HG3	2.01	0.60
1:G:94:MET:HG2	1:G:135:LEU:HD22	1.84	0.60
1:G:98:CYS:HB2	1:G:99:PRO:HD2	1.82	0.60
1:J:152:ASP:O	1:J:153:ARG:HG3	2.02	0.60
1:H:272:SER:HB3	1:H:273:PRO:HD2	1.83	0.60
1:I:57:ASN:HA	1:J:50:SER:HB2	1.84	0.60
1:J:313:ARG:NH1	1:L:233:GLU:OE1	2.33	0.60
1:J:110:ARG:HG2	1:J:110:ARG:HH11	1.67	0.60
1:K:185:ARG:HH21	1:K:212:LYS:HD2	1.65	0.59
1:H:92:LEU:HD11	1:H:135:LEU:HB3	1.84	0.59
1:K:271:ILE:HG23	1:K:273:PRO:HD2	1.83	0.59
1:K:184:HIS:HD2	1:K:186:ASP:H	1.48	0.59
1:F:98:CYS:HB2	1:F:99:PRO:HD2	1.83	0.59
1:D:232:PRO:HB3	1:E:280:ARG:HA	1.84	0.59
1:I:184:HIS:HD2	1:I:186:ASP:H	1.47	0.59
1:E:330:LYS:HG2	1:E:330:LYS:O	2.03	0.59
1:G:184:HIS:HD2	1:G:186:ASP:H	1.51	0.59
1:B:98:CYS:HB2	1:B:99:PRO:HD2	1.83	0.59
1:E:333:GLN:HG3	3:E:366:HOH:O	2.02	0.58
1:F:185:ARG:HH21	1:F:212:LYS:HD2	1.67	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:330:LYS:HG2	1:I:330:LYS:O	2.03	0.58
1:F:127:LEU:HD13	1:G:113:GLN:HE21	1.69	0.58
1:D:98:CYS:HB2	1:D:99:PRO:HD2	1.85	0.58
1:B:185:ARG:HH21	1:B:212:LYS:HD2	1.68	0.58
1:D:272:SER:HB2	1:D:273:PRO:CD	2.33	0.58
1:G:185:ARG:HH21	1:G:212:LYS:HD2	1.68	0.58
1:B:127:LEU:HB2	1:I:49:LYS:HB2	1.85	0.58
1:K:46:PHE:N	3:K:366:HOH:O	2.36	0.58
1:G:330:LYS:HG2	1:G:330:LYS:O	2.03	0.58
1:I:92:LEU:HD11	1:I:135:LEU:HB3	1.86	0.58
1:E:98:CYS:HB2	1:E:99:PRO:HD2	1.85	0.57
1:L:330:LYS:O	1:L:330:LYS:HG2	2.04	0.57
1:H:228:TYR:HD1	1:H:228:TYR:O	1.87	0.57
1:H:116:HIS:CE1	1:H:169:SER:HB2	2.39	0.57
1:J:98:CYS:HB2	1:J:99:PRO:HD2	1.87	0.57
1:C:184:HIS:HD2	1:C:186:ASP:H	1.52	0.57
1:C:73:GLY:HA2	2:C:1:P4O:H8C1	1.86	0.57
1:C:185:ARG:HH21	1:C:212:LYS:HD2	1.69	0.57
1:A:92:LEU:HD11	1:A:135:LEU:HB3	1.86	0.57
1:C:116:HIS:CE1	1:C:169:SER:HB2	2.40	0.57
1:I:98:CYS:HB2	1:I:99:PRO:HD2	1.86	0.57
1:I:130:GLY:O	1:J:110:ARG:NH1	2.38	0.57
1:F:128:TYR:CD1	1:G:47:HIS:O	2.58	0.57
1:L:92:LEU:HD11	1:L:135:LEU:HB3	1.87	0.56
1:A:229:TYR:CD1	1:A:229:TYR:N	2.70	0.56
1:G:92:LEU:HD11	1:G:135:LEU:HB3	1.88	0.56
1:K:94:MET:HG2	1:K:135:LEU:HD22	1.88	0.56
1:H:110:ARG:NH1	1:K:130:GLY:O	2.39	0.56
1:B:152:ASP:O	1:B:153:ARG:HG3	2.05	0.56
1:C:98:CYS:HB2	1:C:99:PRO:HD2	1.88	0.56
1:B:50:SER:HB3	1:J:58:ALA:N	2.21	0.56
1:G:116:HIS:CE1	1:G:169:SER:HB2	2.41	0.56
1:H:74:ILE:HG12	1:H:209:GLY:HA3	1.87	0.56
1:B:127:LEU:HD13	1:I:113:GLN:NE2	2.19	0.55
1:D:185:ARG:HH21	1:D:212:LYS:HD2	1.71	0.55
1:E:185:ARG:HH21	1:E:212:LYS:HD2	1.71	0.55
1:J:184:HIS:HD2	1:J:186:ASP:H	1.53	0.55
1:B:92:LEU:HD11	1:B:135:LEU:HB3	1.87	0.55
1:G:272:SER:N	1:G:273:PRO:HD2	2.22	0.55
1:E:266:ASN:HB3	1:E:271:ILE:HG23	1.88	0.55
1:B:50:SER:CB	1:J:57:ASN:HA	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:330:LYS:O	1:A:330:LYS:HG2	2.06	0.55
1:J:330:LYS:O	1:J:330:LYS:HG2	2.06	0.55
1:B:350:GLU:O	3:B:369:HOH:O	2.18	0.54
1:L:115:PRO:O	1:L:204:LYS:HE2	2.07	0.54
1:D:310:PRO:CG	1:F:233:GLU:HG2	2.38	0.54
1:A:152:ASP:O	1:A:153:ARG:HG3	2.08	0.54
1:G:86:THR:HG23	1:G:88:GLU:HB2	1.89	0.54
1:D:115:PRO:O	1:D:204:LYS:HE2	2.08	0.54
1:H:152:ASP:O	1:H:153:ARG:HG3	2.08	0.54
1:L:152:ASP:O	1:L:153:ARG:HG3	2.09	0.53
1:L:185:ARG:HH21	1:L:212:LYS:HD2	1.74	0.53
1:B:50:SER:HB3	1:J:58:ALA:H	1.73	0.53
1:I:152:ASP:O	1:I:153:ARG:HG3	2.09	0.53
1:F:92:LEU:HD11	1:F:135:LEU:HB3	1.91	0.53
1:E:47:HIS:O	1:H:128:TYR:HD1	1.92	0.53
1:G:272:SER:N	1:G:273:PRO:CD	2.72	0.53
1:L:94:MET:HG2	1:L:135:LEU:HD22	1.91	0.53
1:K:307:LYS:HD3	1:K:312:GLN:HB3	1.91	0.53
1:C:92:LEU:HD11	1:C:135:LEU:HB3	1.90	0.52
1:F:74:ILE:HG12	1:F:209:GLY:HA3	1.91	0.52
1:H:272:SER:HB3	1:H:273:PRO:CD	2.39	0.52
1:I:94:MET:HG2	1:I:135:LEU:HD22	1.91	0.52
1:B:94:MET:HG2	1:B:135:LEU:HD22	1.91	0.52
1:F:73:GLY:HA2	2:F:1:P4O:C8	2.39	0.52
1:J:188:LYS:HD3	1:L:229:TYR:CZ	2.43	0.52
1:C:94:MET:HG2	1:C:135:LEU:HD22	1.91	0.52
1:E:74:ILE:HG12	1:E:209:GLY:HA3	1.90	0.52
1:B:230:VAL:HB	3:B:370:HOH:O	2.09	0.52
1:J:74:ILE:HG12	1:J:209:GLY:HA3	1.91	0.52
1:I:185:ARG:HH21	1:I:212:LYS:HD2	1.74	0.52
1:L:86:THR:HG23	1:L:88:GLU:H	1.75	0.52
1:B:233:GLU:HG2	1:C:310:PRO:CG	2.38	0.52
1:B:105:VAL:HG22	1:B:136:ILE:HD11	1.92	0.52
1:B:115:PRO:O	1:B:204:LYS:HE2	2.10	0.52
1:B:74:ILE:HG12	1:B:209:GLY:HA3	1.91	0.52
1:D:73:GLY:HA2	2:D:1:P4O:C8	2.40	0.52
1:F:74:ILE:HG23	1:F:207:ASP:OD2	2.10	0.51
1:F:83:ASN:ND2	1:F:86:THR:H	2.08	0.51
1:E:191:ASN:ND2	2:E:1:P4O:H8C2	2.25	0.51
1:K:115:PRO:O	1:K:204:LYS:HE2	2.10	0.51
1:G:115:PRO:O	1:G:204:LYS:HE2	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:73:GLY:HA2	2:D:1:P4O:H8C1	1.92	0.51
1:F:110:ARG:HH11	1:F:110:ARG:HG2	1.75	0.51
1:K:92:LEU:HD11	1:K:135:LEU:HB3	1.93	0.51
1:G:283:GLN:HG3	1:I:317:THR:HG21	1.93	0.51
1:J:115:PRO:O	1:J:204:LYS:HE2	2.10	0.51
1:G:277:THR:HA	1:G:280:ARG:HG2	1.93	0.51
1:J:272:SER:N	3:J:367:HOH:O	2.44	0.51
1:C:115:PRO:O	1:C:204:LYS:HE2	2.11	0.51
1:E:92:LEU:HD11	1:E:135:LEU:HB3	1.93	0.51
1:G:307:LYS:HD3	1:G:312:GLN:HB3	1.93	0.51
1:L:74:ILE:HG23	1:L:207:ASP:OD2	2.12	0.50
1:H:105:VAL:HG22	1:H:136:ILE:HD11	1.93	0.50
1:I:74:ILE:HG12	1:I:209:GLY:HA3	1.91	0.50
1:K:191:ASN:ND2	2:K:1:P4O:H8C2	2.27	0.50
1:J:70:LEU:HD13	2:J:1:P4O:C17	2.42	0.50
1:A:304:ASN:HD22	1:A:314:MET:HB2	1.76	0.50
1:E:127:LEU:HD13	1:K:113:GLN:HE21	1.76	0.50
1:C:83:ASN:C	1:C:83:ASN:HD22	2.15	0.50
1:D:86:THR:HG23	1:D:88:GLU:HB2	1.94	0.50
1:E:307:LYS:HD3	1:E:312:GLN:HB3	1.93	0.50
1:A:83:ASN:CG	1:A:86:THR:HG22	2.32	0.50
1:F:105:VAL:HG22	1:F:136:ILE:HD11	1.93	0.50
1:B:128:TYR:HD1	1:I:47:HIS:O	1.95	0.50
1:E:188:LYS:HB2	1:E:189:PRO:HD2	1.94	0.50
1:C:110:ARG:NH1	1:D:130:GLY:O	2.45	0.49
1:E:110:ARG:HH11	1:E:110:ARG:HG2	1.76	0.49
1:I:332:PRO:HB2	1:I:334:THR:CG2	2.34	0.49
1:G:86:THR:O	1:G:87:GLN:HB2	2.13	0.49
1:E:94:MET:HG2	1:E:135:LEU:HD22	1.94	0.49
1:K:165:GLU:HG3	1:K:328:SER:HB3	1.95	0.49
1:G:266:ASN:CB	1:G:272:SER:N	2.73	0.49
1:E:56:LYS:O	1:K:50:SER:HB2	2.12	0.49
1:L:83:ASN:ND2	1:L:86:THR:H	2.11	0.49
1:F:332:PRO:HB2	1:F:334:THR:CG2	2.35	0.49
1:E:235:LEU:HD13	1:F:276:LYS:HG3	1.95	0.49
1:E:266:ASN:CB	1:E:271:ILE:HG23	2.43	0.49
1:K:266:ASN:HB2	1:K:271:ILE:CA	2.40	0.49
1:C:330:LYS:O	1:C:330:LYS:CG	2.60	0.49
1:E:265:SER:O	1:E:271:ILE:O	2.31	0.49
1:A:307:LYS:HD3	1:A:312:GLN:HB3	1.94	0.49
1:H:233:GLU:HG2	1:I:310:PRO:HG3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:247:TRP:CD2	1:L:232:PRO:HD3	2.48	0.49
1:G:304:ASN:HD22	1:G:314:MET:HB2	1.78	0.49
1:L:86:THR:HG23	1:L:88:GLU:HB2	1.95	0.48
1:H:74:ILE:HG23	1:H:207:ASP:OD2	2.13	0.48
1:G:74:ILE:HG12	1:G:209:GLY:HA3	1.95	0.48
1:H:228:TYR:CD1	1:H:228:TYR:O	2.66	0.48
1:E:277:THR:HA	1:E:280:ARG:HG2	1.95	0.48
1:C:307:LYS:HD3	1:C:312:GLN:HB3	1.96	0.48
1:F:115:PRO:O	1:F:204:LYS:HE2	2.13	0.48
1:J:310:PRO:HB3	1:L:233:GLU:HG2	1.95	0.48
1:D:141:LEU:HD13	1:D:193:LEU:HB2	1.96	0.48
1:C:86:THR:HG23	1:C:88:GLU:HB2	1.95	0.48
1:J:94:MET:HG2	1:J:135:LEU:HD22	1.96	0.48
1:J:307:LYS:HD3	1:J:312:GLN:HB3	1.95	0.48
1:D:153:ARG:HB3	3:D:371:HOH:O	2.13	0.48
1:E:165:GLU:HG3	1:E:328:SER:HB3	1.96	0.48
1:E:115:PRO:O	1:E:204:LYS:HE2	2.14	0.47
1:C:50:SER:HB2	1:D:57:ASN:HA	1.96	0.47
1:J:310:PRO:HG3	1:L:233:GLU:HG2	1.96	0.47
1:B:272:SER:N	1:B:273:PRO:HD2	2.29	0.47
1:I:307:LYS:HD3	1:I:312:GLN:HB3	1.96	0.47
1:D:74:ILE:HG12	1:D:209:GLY:HA3	1.95	0.47
1:D:65:VAL:HA	1:D:81:ILE:HG22	1.96	0.47
1:L:73:GLY:HA2	2:L:1:P4O:H8C1	1.96	0.47
1:I:115:PRO:O	1:I:204:LYS:HE2	2.14	0.47
1:B:86:THR:HG23	1:B:88:GLU:HB2	1.96	0.47
1:E:86:THR:HG23	1:E:88:GLU:H	1.80	0.47
1:I:83:ASN:HD22	1:I:83:ASN:C	2.18	0.47
1:B:330:LYS:HG2	1:B:330:LYS:O	2.14	0.47
1:I:65:VAL:HA	1:I:81:ILE:HG22	1.95	0.47
1:D:272:SER:N	1:D:275:MET:H	2.12	0.47
1:J:70:LEU:HD22	2:J:1:P4O:N16	2.30	0.47
1:F:165:GLU:HG3	1:F:328:SER:HB3	1.97	0.47
1:I:86:THR:HG23	1:I:88:GLU:H	1.80	0.47
1:H:155:ASP:O	1:H:156:GLN:HB2	2.15	0.47
1:K:74:ILE:HG12	1:K:209:GLY:HA3	1.96	0.47
1:G:86:THR:HG23	1:G:88:GLU:CB	2.45	0.46
1:I:74:ILE:HG23	1:I:207:ASP:OD2	2.15	0.46
1:I:288:ASN:HB3	1:I:289:PRO:HA	1.97	0.46
1:G:332:PRO:HB2	1:G:334:THR:CG2	2.37	0.46
1:J:110:ARG:HG2	1:J:110:ARG:NH1	2.29	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:277:THR:HA	1:J:280:ARG:HG2	1.98	0.46
1:H:94:MET:HG2	1:H:135:LEU:HD22	1.98	0.46
1:F:145:GLU:HA	1:F:193:LEU:HD23	1.97	0.46
1:F:307:LYS:HD3	1:F:312:GLN:HB3	1.96	0.46
1:A:186:ASP:OD1	1:A:188:LYS:HE3	2.15	0.46
1:H:86:THR:HG23	1:H:88:GLU:H	1.81	0.46
1:D:307:LYS:HD3	1:D:312:GLN:HB3	1.96	0.46
1:L:83:ASN:C	1:L:83:ASN:HD22	2.19	0.46
1:C:110:ARG:HH11	1:C:110:ARG:HG2	1.81	0.46
1:H:86:THR:O	1:H:87:GLN:HB2	2.16	0.46
1:B:184:HIS:CD2	1:B:186:ASP:H	2.26	0.46
1:D:86:THR:HG23	1:D:88:GLU:H	1.80	0.46
1:J:86:THR:HG23	1:J:88:GLU:HB2	1.98	0.46
1:H:86:THR:HG23	1:H:88:GLU:HB2	1.97	0.46
1:C:152:ASP:O	1:C:153:ARG:HG3	2.16	0.46
1:K:125:GLU:HA	1:K:133:CYS:O	2.16	0.46
1:H:191:ASN:ND2	2:H:1:P4O:H8C2	2.31	0.46
1:B:288:ASN:HB3	1:B:289:PRO:HA	1.97	0.46
1:A:74:ILE:HG12	1:A:209:GLY:HA3	1.97	0.46
1:C:86:THR:HG23	1:C:88:GLU:H	1.80	0.45
1:A:229:TYR:HD1	1:A:229:TYR:N	2.14	0.45
1:G:279:ILE:HG22	1:I:232:PRO:HG3	1.99	0.45
1:K:110:ARG:HG2	1:K:110:ARG:HH11	1.81	0.45
1:G:276:LYS:HG3	1:I:235:LEU:HD13	1.97	0.45
1:C:188:LYS:HB2	1:C:189:PRO:HD2	1.98	0.45
1:F:200:ASN:H	1:F:200:ASN:ND2	2.14	0.45
1:H:307:LYS:HD3	1:H:312:GLN:HB3	1.97	0.45
1:K:277:THR:HA	1:K:280:ARG:HG2	1.97	0.45
1:C:86:THR:HG23	1:C:88:GLU:CB	2.47	0.45
1:H:184:HIS:CD2	1:H:186:ASP:H	2.28	0.45
1:E:153:ARG:HB3	1:E:155:ASP:O	2.17	0.45
1:C:264:TYR:HB3	1:C:265:SER:H	1.50	0.45
1:E:83:ASN:CG	1:E:86:THR:HG22	2.36	0.45
1:F:83:ASN:HD22	1:F:83:ASN:C	2.19	0.45
1:L:188:LYS:HB2	1:L:189:PRO:HD2	1.99	0.45
1:H:277:THR:HA	1:H:280:ARG:HG2	1.98	0.45
1:L:307:LYS:HD3	1:L:312:GLN:HB3	1.96	0.45
1:C:332:PRO:HB2	1:C:334:THR:CG2	2.41	0.45
1:L:165:GLU:HG3	1:L:328:SER:HB3	1.97	0.45
1:J:332:PRO:HB2	1:J:334:THR:CG2	2.41	0.45
1:A:184:HIS:HD2	1:A:186:ASP:N	2.13	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:65:VAL:HA	1:H:81:ILE:HG22	1.97	0.45
1:B:149:ARG:NH2	1:B:201:ALA:HB3	2.32	0.45
1:G:239:LYS:NZ	1:G:239:LYS:HB3	2.31	0.45
1:B:110:ARG:HG2	1:B:110:ARG:HH11	1.80	0.45
1:E:74:ILE:HG23	1:E:207:ASP:OD2	2.17	0.45
1:L:105:VAL:HG22	1:L:136:ILE:HD11	1.99	0.45
1:F:127:LEU:HB2	1:G:49:LYS:HB2	1.98	0.45
1:A:110:ARG:HH11	1:A:110:ARG:HG2	1.81	0.44
1:I:141:LEU:HD13	1:I:193:LEU:HB2	1.97	0.44
1:J:272:SER:HB3	1:J:273:PRO:HD3	1.98	0.44
1:J:304:ASN:HD22	1:J:314:MET:HB2	1.83	0.44
1:I:239:LYS:NZ	1:I:239:LYS:HB3	2.33	0.44
1:I:110:ARG:HG2	1:I:110:ARG:HH11	1.81	0.44
1:E:272:SER:H	1:E:273:PRO:HD2	1.83	0.44
1:F:277:THR:HA	1:F:280:ARG:HG2	2.00	0.44
1:H:115:PRO:O	1:H:204:LYS:HE2	2.17	0.44
1:G:110:ARG:HH11	1:G:110:ARG:HG2	1.83	0.44
1:I:86:THR:HG23	1:I:88:GLU:HB2	2.00	0.44
1:H:110:ARG:HG2	1:H:110:ARG:HH11	1.82	0.44
1:B:83:ASN:ND2	1:B:86:THR:H	2.15	0.44
1:F:73:GLY:HA2	2:F:1:P4O:H8C1	1.98	0.44
1:E:127:LEU:N	1:K:49:LYS:O	2.34	0.44
1:B:140:CYS:SG	2:B:1:P4O:H17	2.58	0.44
1:E:239:LYS:NZ	1:E:239:LYS:HB3	2.33	0.44
1:E:271:ILE:HG12	1:E:278:ARG:HH12	1.82	0.44
1:E:49:LYS:O	1:H:127:LEU:N	2.43	0.44
1:A:74:ILE:HG23	1:A:207:ASP:OD2	2.17	0.44
1:E:65:VAL:HA	1:E:81:ILE:HG22	2.00	0.44
1:C:86:THR:O	1:C:87:GLN:HB2	2.18	0.43
1:J:272:SER:HB3	1:J:273:PRO:CD	2.48	0.43
1:F:114:CYS:HB2	1:F:176:TYR:CD2	2.53	0.43
1:B:51:GLY:N	1:J:56:LYS:O	2.48	0.43
1:B:272:SER:H	1:B:273:PRO:HD2	1.83	0.43
1:L:125:GLU:HA	1:L:133:CYS:O	2.18	0.43
1:D:239:LYS:HB3	1:D:239:LYS:NZ	2.33	0.43
1:D:94:MET:HG2	1:D:135:LEU:HD22	2.00	0.43
1:C:145:GLU:HA	1:C:193:LEU:HD23	2.00	0.43
1:G:86:THR:HG23	1:G:88:GLU:H	1.83	0.43
1:J:114:CYS:HB2	1:J:176:TYR:CD2	2.53	0.43
1:J:108:HIS:CG	1:J:120:ILE:HD11	2.54	0.43
1:A:86:THR:HG23	1:A:88:GLU:H	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:83:ASN:CG	1:C:86:THR:HG22	2.39	0.43
1:B:184:HIS:HD2	1:B:186:ASP:N	2.11	0.43
1:F:59:ILE:HG22	1:G:48:VAL:HG21	2.00	0.43
1:D:142:ASP:HA	2:D:1:P4O:N16	2.33	0.43
1:C:114:CYS:HA	1:C:115:PRO:HD3	1.90	0.43
1:L:277:THR:HA	1:L:280:ARG:HG2	2.00	0.43
1:L:304:ASN:HD22	1:L:314:MET:HB2	1.83	0.43
1:E:237:PRO:HB2	1:E:238:GLU:H	1.73	0.43
1:C:200:ASN:H	1:C:200:ASN:ND2	2.15	0.43
1:C:239:LYS:NZ	1:C:239:LYS:HB3	2.33	0.43
1:K:264:TYR:HB3	1:K:265:SER:H	1.56	0.43
1:F:114:CYS:HA	1:F:115:PRO:HD3	1.90	0.43
1:J:165:GLU:HG3	1:J:328:SER:HB3	1.99	0.43
1:D:332:PRO:HB2	1:D:334:THR:CG2	2.42	0.43
1:F:94:MET:HG2	1:F:135:LEU:HD22	2.00	0.43
1:E:110:ARG:NH1	1:E:110:ARG:HG2	2.34	0.43
1:A:277:THR:HA	1:A:280:ARG:HG2	2.01	0.43
1:B:277:THR:HA	1:B:280:ARG:HG2	2.01	0.43
1:L:228:TYR:CD2	1:L:228:TYR:N	2.87	0.43
1:A:125:GLU:HA	1:A:133:CYS:O	2.19	0.43
1:E:86:THR:O	1:E:87:GLN:HB2	2.18	0.42
1:K:86:THR:HG23	1:K:88:GLU:HB2	2.00	0.42
1:G:165:GLU:HG3	1:G:328:SER:HB3	2.01	0.42
1:J:105:VAL:HG22	1:J:136:ILE:HD11	2.01	0.42
1:E:142:ASP:HA	2:E:1:P4O:N16	2.34	0.42
1:E:130:GLY:O	1:K:110:ARG:HG2	2.19	0.42
1:L:86:THR:HG23	1:L:88:GLU:CB	2.49	0.42
1:H:83:ASN:ND2	1:H:86:THR:H	2.17	0.42
1:B:86:THR:HG23	1:B:88:GLU:H	1.85	0.42
1:H:186:ASP:OD1	1:H:188:LYS:HE3	2.20	0.42
1:L:74:ILE:CG1	1:L:209:GLY:HA3	2.49	0.42
1:I:184:HIS:CD2	1:I:186:ASP:H	2.33	0.42
1:D:188:LYS:HB2	1:D:189:PRO:HD2	2.01	0.42
1:C:277:THR:HA	1:C:280:ARG:HG2	2.01	0.42
1:F:49:LYS:HG3	1:F:113:GLN:OE1	2.19	0.42
1:D:83:ASN:CG	1:D:86:THR:HG22	2.39	0.42
1:K:266:ASN:CB	1:K:271:ILE:HA	2.42	0.42
1:I:236:GLY:HA2	1:I:237:PRO:HD3	1.94	0.42
1:H:304:ASN:HD22	1:H:314:MET:HB2	1.85	0.42
1:I:304:ASN:HD22	1:I:314:MET:HB2	1.85	0.42
1:D:86:THR:HG23	1:D:88:GLU:CB	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:332:PRO:HB2	1:L:334:THR:CG2	2.41	0.42
1:B:233:GLU:OE1	1:C:313:ARG:NH1	2.49	0.42
1:B:271:ILE:HG23	1:B:273:PRO:HG2	2.02	0.42
1:K:288:ASN:HB3	1:K:289:PRO:HA	2.02	0.42
1:F:125:GLU:HA	1:F:133:CYS:O	2.19	0.42
1:C:74:ILE:HG12	1:C:209:GLY:HA3	2.00	0.42
1:A:83:ASN:ND2	1:A:86:THR:H	2.18	0.41
1:B:86:THR:O	1:B:87:GLN:HB2	2.20	0.41
1:K:86:THR:O	1:K:87:GLN:HB2	2.19	0.41
1:I:86:THR:HG23	1:I:88:GLU:CB	2.49	0.41
1:B:186:ASP:OD1	1:B:188:LYS:HE3	2.20	0.41
1:B:188:LYS:HB2	1:B:189:PRO:HD2	2.01	0.41
1:A:130:GLY:O	1:F:110:ARG:NH1	2.53	0.41
1:J:65:VAL:HA	1:J:81:ILE:HG22	2.02	0.41
1:G:188:LYS:HB2	1:G:189:PRO:HD2	2.02	0.41
1:F:149:ARG:HH22	1:F:201:ALA:HB3	1.85	0.41
1:D:165:GLU:HG3	1:D:328:SER:HB3	2.02	0.41
1:D:47:HIS:HA	3:D:370:HOH:O	2.19	0.41
1:B:86:THR:HG23	1:B:88:GLU:CB	2.50	0.41
1:F:86:THR:HG23	1:F:88:GLU:HB2	2.01	0.41
1:I:114:CYS:HA	1:I:115:PRO:HD3	1.96	0.41
1:B:83:ASN:HD22	1:B:83:ASN:C	2.23	0.41
1:E:86:THR:HG23	1:E:88:GLU:HB2	2.02	0.41
1:K:86:THR:HG23	1:K:88:GLU:CB	2.51	0.41
1:F:70:LEU:HD13	2:F:1:P4O:C17	2.51	0.41
1:J:114:CYS:HA	1:J:115:PRO:HD3	1.90	0.41
1:A:49:LYS:HG3	1:A:113:GLN:OE1	2.20	0.41
1:F:191:ASN:HA	1:F:191:ASN:HD22	1.72	0.41
1:A:73:GLY:HA2	2:A:1:P4O:C8	2.50	0.41
1:A:94:MET:HG2	1:A:135:LEU:HD22	2.02	0.41
1:C:114:CYS:HB2	1:C:176:TYR:CD2	2.55	0.41
1:D:277:THR:HA	1:D:280:ARG:HG2	2.02	0.41
1:J:83:ASN:CG	1:J:86:THR:HG22	2.41	0.41
1:H:83:ASN:CG	1:H:86:THR:HG22	2.40	0.41
1:B:49:LYS:HG3	1:B:113:GLN:OE1	2.21	0.41
1:L:184:HIS:CD2	1:L:186:ASP:H	2.29	0.41
1:A:188:LYS:HD3	1:C:229:TYR:CZ	2.56	0.41
1:E:235:LEU:HD13	1:F:276:LYS:CG	2.50	0.41
1:D:145:GLU:HA	1:D:193:LEU:HD23	2.01	0.41
1:F:188:LYS:HB2	1:F:189:PRO:HD2	2.01	0.41
1:L:349:TRP:HE3	3:L:370:HOH:O	2.04	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:237:PRO:O	1:A:238:GLU:HB3	2.20	0.41
1:B:125:GLU:HA	1:B:133:CYS:O	2.20	0.41
1:I:56:LYS:O	1:J:51:GLY:N	2.49	0.41
1:E:86:THR:HG23	1:E:88:GLU:CB	2.51	0.41
1:E:230:VAL:HG22	1:E:231:ALA:H	1.86	0.41
1:E:235:LEU:HD22	1:F:276:LYS:HE3	2.02	0.41
1:H:141:LEU:HD13	1:H:193:LEU:HB2	2.02	0.41
1:J:49:LYS:HG3	1:J:113:GLN:OE1	2.21	0.41
1:F:56:LYS:O	1:G:50:SER:HB2	2.21	0.41
1:D:236:GLY:HA2	1:D:237:PRO:HD3	1.94	0.41
1:F:86:THR:HG23	1:F:88:GLU:H	1.85	0.40
1:K:114:CYS:HA	1:K:115:PRO:HD3	1.94	0.40
1:D:111:ALA:HB1	1:D:117:ILE:HD13	2.03	0.40
1:K:272:SER:N	1:K:273:PRO:HD2	2.35	0.40
1:L:145:GLU:HA	1:L:193:LEU:HD23	2.02	0.40
1:J:188:LYS:HB2	1:J:189:PRO:HD2	2.02	0.40
1:L:236:GLY:HA2	1:L:237:PRO:HD3	1.93	0.40
1:F:83:ASN:CG	1:F:86:THR:HG22	2.42	0.40
1:K:83:ASN:ND2	1:K:86:THR:H	2.19	0.40
1:A:338:THR:O	1:A:342:LEU:HB2	2.22	0.40
1:D:113:GLN:HE21	1:L:127:LEU:HD13	1.86	0.40
1:L:63:TYR:CD1	1:L:81:ILE:HD12	2.56	0.40
1:J:86:THR:HG23	1:J:88:GLU:CB	2.51	0.40
1:C:83:ASN:ND2	1:C:86:THR:H	2.19	0.40
1:D:74:ILE:HG23	1:D:207:ASP:OD2	2.21	0.40
1:D:114:CYS:HB3	1:D:117:ILE:HD12	2.03	0.40

All (15) 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:I:198:ARG:NH2	1:L:84:LYS:O[2_555]	1.26	0.94
1:E:340:ARG:NE	1:J:85:ARG:NE[2_554]	1.50	0.70
1:E:340:ARG:NH1	1:J:85:ARG:CZ[2_554]	1.57	0.63
1:E:340:ARG:CB	1:J:85:ARG:CD[2_554]	1.66	0.54
1:E:340:ARG:NH1	1:J:85:ARG:NH2[2_554]	1.70	0.50
1:A:68:GLN:OE1	1:C:85:ARG:NH1[4_455]	1.75	0.45
1:E:340:ARG:CZ	1:J:85:ARG:NE[2_554]	1.83	0.37
1:E:340:ARG:CB	1:J:85:ARG:CG[2_554]	1.87	0.33
1:D:68:GLN:OE1	1:F:85:ARG:NH1[4_555]	1.92	0.28

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:168:LYS:NZ	1:I:293:GLU:OE1[3_555]	2.01	0.19
1:E:340:ARG:CZ	1:J:85:ARG:CZ[2_554]	2.08	0.12
1:I:198:ARG:CZ	1:L:84:LYS:O[2_555]	2.09	0.11
1:B:293:GLU:OE1	1:H:168:LYS:NZ[3_555]	2.10	0.10
1:E:340:ARG:CD	1:J:85:ARG:CG[2_554]	2.11	0.09
1:B:344:GLU:O	1:H:47:HIS:CE1[3_555]	2.13	0.07

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	277/334 (83%)	257 (93%)	18 (6%)	2 (1%)	26	72
1	B	284/334 (85%)	260 (92%)	21 (7%)	3 (1%)	17	62
1	C	277/334 (83%)	259 (94%)	17 (6%)	1 (0%)	39	80
1	D	275/334 (82%)	258 (94%)	16 (6%)	1 (0%)	39	80
1	E	284/334 (85%)	260 (92%)	21 (7%)	3 (1%)	17	62
1	F	276/334 (83%)	257 (93%)	18 (6%)	1 (0%)	39	80
1	G	278/334 (83%)	260 (94%)	17 (6%)	1 (0%)	39	80
1	H	284/334 (85%)	258 (91%)	23 (8%)	3 (1%)	17	62
1	I	276/334 (83%)	260 (94%)	15 (5%)	1 (0%)	39	80
1	J	275/334 (82%)	258 (94%)	16 (6%)	1 (0%)	39	80
1	K	284/334 (85%)	260 (92%)	21 (7%)	3 (1%)	17	62
1	L	276/334 (83%)	258 (94%)	17 (6%)	1 (0%)	39	80
All	All	3346/4008 (84%)	3105 (93%)	220 (7%)	21 (1%)	30	75

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	230	VAL

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Mol	Chain	Res	Type
1	A	237	PRO
1	B	157	ALA
1	B	237	PRO
1	C	237	PRO
1	D	237	PRO
1	E	237	PRO
1	F	237	PRO
1	G	237	PRO
1	H	156	GLN
1	H	237	PRO
1	I	237	PRO
1	J	237	PRO
1	K	156	GLN
1	K	157	ALA
1	K	237	PRO
1	L	237	PRO
1	B	156	GLN
1	E	155	ASP
1	E	272	SER
1	H	272	SER

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	257/297 (86%)	234 (91%)	23 (9%)	12 44
1	B	262/297 (88%)	240 (92%)	22 (8%)	14 48
1	C	257/297 (86%)	237 (92%)	20 (8%)	16 53
1	D	255/297 (86%)	234 (92%)	21 (8%)	14 50
1	E	262/297 (88%)	237 (90%)	25 (10%)	11 40
1	F	256/297 (86%)	231 (90%)	25 (10%)	10 38
1	G	258/297 (87%)	234 (91%)	24 (9%)	11 41
1	H	262/297 (88%)	235 (90%)	27 (10%)	9 36

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	I	256/297 (86%)	232 (91%)	24 (9%)	11 41
1	J	255/297 (86%)	230 (90%)	25 (10%)	10 38
1	K	262/297 (88%)	237 (90%)	25 (10%)	11 40
1	L	256/297 (86%)	233 (91%)	23 (9%)	12 43
All	All	3098/3564 (87%)	2814 (91%)	284 (9%)	11 41

All (284) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	74	ILE
1	A	75	ASN
1	A	77	LYS
1	A	83	ASN
1	A	86	THR
1	A	106	GLU
1	A	110	ARG
1	A	134	LEU
1	A	149	ARG
1	A	185	ARG
1	A	229	TYR
1	A	233	GLU
1	A	239	LYS
1	A	265	SER
1	A	277	THR
1	A	293	GLU
1	A	326	MET
1	A	333	GLN
1	A	334	THR
1	A	336	LEU
1	A	343	LYS
1	A	346	LYS
1	A	347	GLU
1	B	54	ILE
1	B	74	ILE
1	B	75	ASN
1	B	77	LYS
1	B	83	ASN
1	B	86	THR
1	B	106	GLU
1	B	110	ARG
1	B	134	LEU

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Mol	Chain	Res	Type
1	B	149	ARG
1	B	156	GLN
1	B	185	ARG
1	B	228	TYR
1	B	229	TYR
1	B	233	GLU
1	B	239	LYS
1	B	277	THR
1	B	333	GLN
1	B	334	THR
1	B	336	LEU
1	B	346	LYS
1	B	347	GLU
1	C	47	HIS
1	C	74	ILE
1	C	75	ASN
1	C	77	LYS
1	C	83	ASN
1	C	86	THR
1	C	106	GLU
1	C	110	ARG
1	C	134	LEU
1	C	185	ARG
1	C	233	GLU
1	C	239	LYS
1	C	244	CYS
1	C	277	THR
1	C	293	GLU
1	C	333	GLN
1	C	334	THR
1	C	336	LEU
1	C	346	LYS
1	C	347	GLU
1	D	74	ILE
1	D	75	ASN
1	D	77	LYS
1	D	83	ASN
1	D	86	THR
1	D	106	GLU
1	D	110	ARG
1	D	134	LEU
1	D	149	ARG

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Mol	Chain	Res	Type
1	D	185	ARG
1	D	233	GLU
1	D	239	LYS
1	D	244	CYS
1	D	277	THR
1	D	293	GLU
1	D	330	LYS
1	D	333	GLN
1	D	334	THR
1	D	336	LEU
1	D	343	LYS
1	D	347	GLU
1	E	54	ILE
1	E	74	ILE
1	E	75	ASN
1	E	77	LYS
1	E	83	ASN
1	E	86	THR
1	E	96	GLN
1	E	106	GLU
1	E	110	ARG
1	E	134	LEU
1	E	149	ARG
1	E	155	ASP
1	E	185	ARG
1	E	233	GLU
1	E	239	LYS
1	E	244	CYS
1	E	272	SER
1	E	277	THR
1	E	280	ARG
1	E	293	GLU
1	E	333	GLN
1	E	334	THR
1	E	336	LEU
1	E	346	LYS
1	E	347	GLU
1	F	47	HIS
1	F	74	ILE
1	F	75	ASN
1	F	77	LYS
1	F	83	ASN

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Mol	Chain	Res	Type
1	F	84	LYS
1	F	86	THR
1	F	96	GLN
1	F	106	GLU
1	F	110	ARG
1	F	134	LEU
1	F	185	ARG
1	F	233	GLU
1	F	239	LYS
1	F	244	CYS
1	F	277	THR
1	F	280	ARG
1	F	293	GLU
1	F	326	MET
1	F	330	LYS
1	F	333	GLN
1	F	334	THR
1	F	336	LEU
1	F	346	LYS
1	F	347	GLU
1	G	54	ILE
1	G	74	ILE
1	G	75	ASN
1	G	77	LYS
1	G	83	ASN
1	G	86	THR
1	G	106	GLU
1	G	110	ARG
1	G	132	LYS
1	G	134	LEU
1	G	149	ARG
1	G	185	ARG
1	G	230	VAL
1	G	233	GLU
1	G	239	LYS
1	G	244	CYS
1	G	277	THR
1	G	280	ARG
1	G	293	GLU
1	G	333	GLN
1	G	334	THR
1	G	336	LEU

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Mol	Chain	Res	Type
1	G	343	LYS
1	G	347	GLU
1	H	54	ILE
1	H	74	ILE
1	H	75	ASN
1	H	77	LYS
1	H	83	ASN
1	H	86	THR
1	H	106	GLU
1	H	110	ARG
1	H	134	LEU
1	H	149	ARG
1	H	155	ASP
1	H	185	ARG
1	H	228	TYR
1	H	229	TYR
1	H	233	GLU
1	H	239	LYS
1	H	244	CYS
1	H	277	THR
1	H	280	ARG
1	H	293	GLU
1	H	330	LYS
1	H	333	GLN
1	H	334	THR
1	H	336	LEU
1	H	343	LYS
1	H	346	LYS
1	H	347	GLU
1	I	47	HIS
1	I	54	ILE
1	I	74	ILE
1	I	75	ASN
1	I	77	LYS
1	I	83	ASN
1	I	84	LYS
1	I	86	THR
1	I	106	GLU
1	I	110	ARG
1	I	134	LEU
1	I	185	ARG
1	I	230	VAL

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Mol	Chain	Res	Type
1	I	233	GLU
1	I	239	LYS
1	I	244	CYS
1	I	277	THR
1	I	280	ARG
1	I	293	GLU
1	I	333	GLN
1	I	334	THR
1	I	336	LEU
1	I	346	LYS
1	I	347	GLU
1	J	54	ILE
1	J	74	ILE
1	J	75	ASN
1	J	77	LYS
1	J	83	ASN
1	J	85	ARG
1	J	86	THR
1	J	106	GLU
1	J	110	ARG
1	J	134	LEU
1	J	149	ARG
1	J	185	ARG
1	J	233	GLU
1	J	239	LYS
1	J	244	CYS
1	J	265	SER
1	J	277	THR
1	J	280	ARG
1	J	293	GLU
1	J	333	GLN
1	J	334	THR
1	J	336	LEU
1	J	343	LYS
1	J	346	LYS
1	J	347	GLU
1	K	74	ILE
1	K	75	ASN
1	K	77	LYS
1	K	83	ASN
1	K	86	THR
1	K	106	GLU

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Mol	Chain	Res	Type
1	K	110	ARG
1	K	134	LEU
1	K	149	ARG
1	K	155	ASP
1	K	156	GLN
1	K	185	ARG
1	K	233	GLU
1	K	239	LYS
1	K	244	CYS
1	K	271	ILE
1	K	277	THR
1	K	280	ARG
1	K	293	GLU
1	K	330	LYS
1	K	333	GLN
1	K	334	THR
1	K	336	LEU
1	K	346	LYS
1	K	347	GLU
1	L	47	HIS
1	L	54	ILE
1	L	74	ILE
1	L	75	ASN
1	L	77	LYS
1	L	83	ASN
1	L	86	THR
1	L	96	GLN
1	L	106	GLU
1	L	110	ARG
1	L	134	LEU
1	L	185	ARG
1	L	229	TYR
1	L	233	GLU
1	L	239	LYS
1	L	244	CYS
1	L	277	THR
1	L	280	ARG
1	L	293	GLU
1	L	333	GLN
1	L	334	THR
1	L	336	LEU
1	L	347	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (82) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	75	ASN
1	A	83	ASN
1	A	184	HIS
1	A	191	ASN
1	A	304	ASN
1	A	333	GLN
1	B	83	ASN
1	B	116	HIS
1	B	184	HIS
1	B	191	ASN
1	B	266	ASN
1	B	304	ASN
1	B	333	GLN
1	C	75	ASN
1	C	83	ASN
1	C	184	HIS
1	C	191	ASN
1	C	200	ASN
1	C	304	ASN
1	C	333	GLN
1	D	75	ASN
1	D	83	ASN
1	D	184	HIS
1	D	191	ASN
1	D	304	ASN
1	D	333	GLN
1	E	83	ASN
1	E	113	GLN
1	E	184	HIS
1	E	191	ASN
1	E	200	ASN
1	E	304	ASN
1	E	333	GLN
1	F	75	ASN
1	F	83	ASN
1	F	184	HIS
1	F	191	ASN
1	F	200	ASN
1	F	304	ASN
1	F	333	GLN
1	G	75	ASN

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Mol	Chain	Res	Type
1	G	83	ASN
1	G	113	GLN
1	G	184	HIS
1	G	191	ASN
1	G	200	ASN
1	G	283	GLN
1	G	304	ASN
1	G	333	GLN
1	H	75	ASN
1	H	83	ASN
1	H	184	HIS
1	H	191	ASN
1	H	266	ASN
1	H	304	ASN
1	H	333	GLN
1	I	75	ASN
1	I	83	ASN
1	I	113	GLN
1	I	184	HIS
1	I	191	ASN
1	I	304	ASN
1	I	333	GLN
1	J	75	ASN
1	J	83	ASN
1	J	184	HIS
1	J	191	ASN
1	J	304	ASN
1	J	333	GLN
1	K	75	ASN
1	K	83	ASN
1	K	113	GLN
1	K	184	HIS
1	K	191	ASN
1	K	304	ASN
1	K	333	GLN
1	L	75	ASN
1	L	83	ASN
1	L	184	HIS
1	L	191	ASN
1	L	304	ASN
1	L	333	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	P4O	A	1	-	28,30,30	1.33	2 (7%)	35,43,43	1.78	9 (25%)
2	P4O	B	1	-	28,30,30	1.37	1 (3%)	35,43,43	1.92	8 (22%)
2	P4O	C	1	-	28,30,30	1.41	3 (10%)	35,43,43	2.02	10 (28%)
2	P4O	D	1	-	28,30,30	1.61	3 (10%)	35,43,43	1.60	5 (14%)
2	P4O	E	1	-	28,30,30	1.33	2 (7%)	35,43,43	1.62	7 (20%)
2	P4O	F	1	-	28,30,30	1.44	1 (3%)	35,43,43	1.98	10 (28%)
2	P4O	G	1	-	28,30,30	1.41	2 (7%)	35,43,43	1.85	11 (31%)
2	P4O	H	1	-	28,30,30	1.39	1 (3%)	35,43,43	1.70	9 (25%)
2	P4O	I	1	-	28,30,30	1.42	2 (7%)	35,43,43	2.04	14 (40%)
2	P4O	J	1	-	28,30,30	1.54	3 (10%)	35,43,43	2.10	11 (31%)
2	P4O	K	1	-	28,30,30	1.47	2 (7%)	35,43,43	1.48	2 (5%)
2	P4O	L	1	-	28,30,30	1.40	3 (10%)	35,43,43	2.11	10 (28%)

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	P4O	A	1	-	-	0/8/18/18	0/5/5/5
2	P4O	B	1	-	-	0/8/18/18	0/5/5/5
2	P4O	C	1	-	-	0/8/18/18	0/5/5/5
2	P4O	D	1	-	-	0/8/18/18	0/5/5/5
2	P4O	E	1	-	-	0/8/18/18	0/5/5/5
2	P4O	F	1	-	-	0/8/18/18	0/5/5/5
2	P4O	G	1	-	-	0/8/18/18	0/5/5/5
2	P4O	H	1	-	-	0/8/18/18	0/5/5/5
2	P4O	I	1	-	-	0/8/18/18	0/5/5/5
2	P4O	J	1	-	-	0/8/18/18	0/5/5/5
2	P4O	K	1	-	-	0/8/18/18	0/5/5/5
2	P4O	L	1	-	-	0/8/18/18	0/5/5/5

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1	P4O	C6-N7	-2.54	1.32	1.34
2	J	1	P4O	C6-N7	-2.11	1.32	1.34
2	C	1	P4O	C23-C22	2.01	1.41	1.36
2	E	1	P4O	C17-N16	2.04	1.35	1.31
2	L	1	P4O	C23-C22	2.05	1.41	1.36
2	J	1	P4O	C17-N16	2.08	1.35	1.31
2	C	1	P4O	C17-N16	2.10	1.35	1.31
2	I	1	P4O	C17-N16	2.14	1.35	1.31
2	K	1	P4O	C17-N16	2.25	1.35	1.31
2	A	1	P4O	C17-N16	2.34	1.35	1.31
2	L	1	P4O	C17-N16	2.38	1.35	1.31
2	G	1	P4O	C17-N16	2.60	1.36	1.31
2	D	1	P4O	C17-N16	2.65	1.36	1.31
2	E	1	P4O	C20-C21	4.77	1.48	1.42
2	G	1	P4O	C20-C21	5.09	1.49	1.42
2	B	1	P4O	C20-C21	5.15	1.49	1.42
2	A	1	P4O	C20-C21	5.23	1.49	1.42
2	I	1	P4O	C20-C21	5.39	1.49	1.42
2	K	1	P4O	C20-C21	5.41	1.49	1.42
2	L	1	P4O	C20-C21	5.42	1.49	1.42
2	C	1	P4O	C20-C21	5.49	1.49	1.42
2	H	1	P4O	C20-C21	5.50	1.49	1.42
2	F	1	P4O	C20-C21	5.54	1.50	1.42
2	D	1	P4O	C20-C21	6.19	1.50	1.42
2	J	1	P4O	C20-C21	6.35	1.51	1.42

All (106) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	1	P4O	C4-C6-N7	-6.09	112.13	115.81
2	F	1	P4O	C3-C2-C12	-4.30	123.42	129.40
2	B	1	P4O	C11-C10-N15	-4.21	119.09	123.90
2	F	1	P4O	C4-C6-N7	-4.03	113.38	115.81
2	L	1	P4O	C9-C8-N7	-3.94	105.02	109.69
2	J	1	P4O	C3-C2-C12	-3.84	124.05	129.40
2	L	1	P4O	C3-C2-C12	-3.64	124.33	129.40
2	C	1	P4O	C18-C17-N16	-3.63	120.87	125.46
2	E	1	P4O	C11-C10-N15	-3.56	119.84	123.90
2	G	1	P4O	C3-C2-C12	-3.49	124.55	129.40
2	D	1	P4O	C11-C10-N15	-3.45	119.96	123.90
2	J	1	P4O	C11-C10-N15	-3.41	120.01	123.90
2	I	1	P4O	C11-C10-N15	-3.40	120.02	123.90
2	I	1	P4O	C3-C2-C12	-3.39	124.68	129.40
2	L	1	P4O	C11-C10-N15	-3.37	120.05	123.90
2	J	1	P4O	C18-C17-N16	-3.33	121.25	125.46
2	F	1	P4O	C11-C10-N15	-3.30	120.13	123.90
2	B	1	P4O	C3-C2-C12	-3.29	124.82	129.40
2	L	1	P4O	C18-C17-N16	-3.26	121.34	125.46
2	H	1	P4O	C11-C10-N15	-3.19	120.26	123.90
2	J	1	P4O	C4-C6-N7	-3.17	113.90	115.81
2	A	1	P4O	C18-C17-N16	-3.05	121.60	125.46
2	A	1	P4O	C9-C8-N7	-3.05	106.08	109.69
2	C	1	P4O	C3-C2-C12	-2.94	125.31	129.40
2	G	1	P4O	C11-C10-N15	-2.92	120.56	123.90
2	F	1	P4O	C18-C17-N16	-2.82	121.90	125.46
2	I	1	P4O	C18-C17-N16	-2.69	122.06	125.46
2	C	1	P4O	C11-C10-N15	-2.69	120.83	123.90
2	I	1	P4O	C4-C3-C2	-2.62	104.20	105.98
2	E	1	P4O	C18-C17-N16	-2.55	122.23	125.46
2	F	1	P4O	C18-C19-C20	-2.53	116.89	121.44
2	A	1	P4O	C4-C3-C2	-2.52	104.27	105.98
2	G	1	P4O	C18-C17-N16	-2.48	122.33	125.46
2	H	1	P4O	C18-C17-N16	-2.40	122.43	125.46
2	H	1	P4O	C4-C3-C2	-2.40	104.35	105.98
2	G	1	P4O	C4-C3-C2	-2.35	104.38	105.98
2	G	1	P4O	C22-C21-C20	-2.26	116.78	119.05
2	I	1	P4O	C8-C9-C5	-2.26	109.24	113.15
2	A	1	P4O	C11-C10-N15	-2.24	121.34	123.90
2	J	1	P4O	C8-C9-C5	-2.19	109.36	113.15
2	J	1	P4O	C4-C3-C2	-2.18	104.50	105.98
2	L	1	P4O	O26-C6-C4	-2.08	119.91	123.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	1	P4O	C12-C13-C14	-2.05	117.94	119.89
2	B	1	P4O	C20-C21-N16	-2.05	119.15	122.08
2	E	1	P4O	C20-C21-N16	-2.00	119.22	122.08
2	B	1	P4O	O26-C6-C4	-2.00	120.05	123.33
2	K	1	P4O	C10-N15-C14	2.00	119.96	117.20
2	I	1	P4O	C24-C23-C22	2.03	123.40	120.45
2	I	1	P4O	C25-C20-C21	2.03	121.60	118.44
2	D	1	P4O	C19-C18-C17	2.04	120.16	116.00
2	G	1	P4O	C9-C8-N7	2.16	112.25	109.69
2	C	1	P4O	C22-C21-N16	2.18	122.13	118.52
2	I	1	P4O	C19-C18-C17	2.21	120.50	116.00
2	A	1	P4O	C22-C21-N16	2.26	122.27	118.52
2	I	1	P4O	C22-C21-N16	2.27	122.28	118.52
2	E	1	P4O	C12-C2-N1	2.28	123.74	120.62
2	G	1	P4O	C19-C18-C17	2.29	120.67	116.00
2	I	1	P4O	C11-C12-C13	2.32	121.24	118.17
2	H	1	P4O	C17-N16-C21	2.33	119.61	116.95
2	F	1	P4O	C9-C8-N7	2.34	112.46	109.69
2	D	1	P4O	C12-C2-N1	2.38	123.87	120.62
2	L	1	P4O	C22-C21-N16	2.40	122.51	118.52
2	G	1	P4O	C22-C21-N16	2.41	122.53	118.52
2	A	1	P4O	C17-N16-C21	2.42	119.71	116.95
2	I	1	P4O	C17-N16-C21	2.47	119.76	116.95
2	H	1	P4O	C19-C18-C17	2.49	121.07	116.00
2	H	1	P4O	C11-C12-C13	2.49	121.47	118.17
2	C	1	P4O	C10-N15-C14	2.58	120.76	117.20
2	F	1	P4O	C10-N15-C14	2.61	120.79	117.20
2	C	1	P4O	C19-C18-C17	2.61	121.32	116.00
2	A	1	P4O	C19-C18-C17	2.67	121.43	116.00
2	J	1	P4O	C17-N16-C21	2.79	120.13	116.95
2	I	1	P4O	C12-C2-N1	2.82	124.47	120.62
2	A	1	P4O	C10-N15-C14	2.83	121.10	117.20
2	B	1	P4O	C17-N16-C21	2.84	120.18	116.95
2	G	1	P4O	C12-C2-N1	3.00	124.72	120.62
2	J	1	P4O	C19-C18-C17	3.05	122.20	116.00
2	J	1	P4O	C10-N15-C14	3.21	121.62	117.20
2	C	1	P4O	C12-C2-N1	3.21	125.01	120.62
2	L	1	P4O	C10-N15-C14	3.24	121.67	117.20
2	G	1	P4O	C10-N15-C14	3.33	121.79	117.20
2	F	1	P4O	C19-C18-C17	3.35	122.82	116.00
2	D	1	P4O	C3-C4-C5	3.37	108.57	104.10
2	H	1	P4O	C10-N15-C14	3.39	121.87	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	1	P4O	C17-N16-C21	3.41	120.84	116.95
2	D	1	P4O	C10-N15-C14	3.49	122.01	117.20
2	C	1	P4O	C3-C4-C5	3.55	108.82	104.10
2	J	1	P4O	C12-C2-N1	3.59	125.52	120.62
2	G	1	P4O	C3-C4-C5	3.62	108.91	104.10
2	F	1	P4O	C3-C4-C5	3.62	108.91	104.10
2	E	1	P4O	C3-C4-C5	3.64	108.93	104.10
2	C	1	P4O	C17-N16-C21	3.68	121.14	116.95
2	L	1	P4O	C17-N16-C21	3.73	121.19	116.95
2	I	1	P4O	C10-N15-C14	3.74	122.35	117.20
2	E	1	P4O	C10-N15-C14	3.76	122.38	117.20
2	F	1	P4O	C12-C2-N1	4.05	126.16	120.62
2	B	1	P4O	C12-C2-N1	4.06	126.17	120.62
2	L	1	P4O	C3-C4-C5	4.10	109.55	104.10
2	B	1	P4O	C10-N15-C14	4.11	122.86	117.20
2	H	1	P4O	C3-C4-C5	4.13	109.58	104.10
2	B	1	P4O	C3-C4-C5	4.19	109.66	104.10
2	J	1	P4O	C3-C4-C5	4.43	109.98	104.10
2	K	1	P4O	C3-C4-C5	4.43	109.99	104.10
2	I	1	P4O	C3-C4-C5	4.52	110.10	104.10
2	A	1	P4O	C3-C4-C5	4.54	110.13	104.10
2	L	1	P4O	C12-C2-N1	4.94	127.37	120.62

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

10 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1	P4O	1	0
2	B	1	P4O	1	0
2	C	1	P4O	1	0
2	D	1	P4O	3	0
2	E	1	P4O	2	0
2	F	1	P4O	3	0
2	H	1	P4O	1	0
2	J	1	P4O	2	0
2	K	1	P4O	1	0
2	L	1	P4O	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	285/334 (85%)	0.31	6 (2%) 67 52	42, 63, 95, 119	0
1	B	290/334 (86%)	0.35	12 (4%) 41 27	42, 64, 94, 118	0
1	C	285/334 (85%)	0.40	12 (4%) 40 26	42, 63, 93, 119	0
1	D	283/334 (84%)	0.36	10 (3%) 48 32	42, 63, 93, 118	0
1	E	290/334 (86%)	0.47	19 (6%) 22 12	42, 64, 95, 119	0
1	F	284/334 (85%)	0.45	9 (3%) 51 36	42, 63, 93, 118	0
1	G	286/334 (85%)	0.44	14 (4%) 33 20	42, 63, 93, 118	0
1	H	290/334 (86%)	0.46	17 (5%) 26 14	42, 64, 94, 119	0
1	I	284/334 (85%)	0.43	15 (5%) 30 17	42, 63, 93, 118	0
1	J	283/334 (84%)	0.52	30 (10%) 8 4	42, 63, 93, 119	0
1	K	290/334 (86%)	0.55	23 (7%) 15 9	42, 64, 95, 119	0
1	L	284/334 (85%)	0.47	19 (6%) 21 12	42, 63, 93, 118	0
All	All	3434/4008 (85%)	0.44	186 (5%) 29 17	42, 63, 95, 119	0

All (186) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	350	GLU	6.7
1	H	155	ASP	5.5
1	I	237	PRO	4.7
1	L	239	LYS	4.7
1	E	329	THR	4.6
1	J	157	ALA	4.6
1	I	46	PHE	4.4
1	A	237	PRO	4.3
1	K	85	ARG	4.3
1	H	156	GLN	4.1
1	J	289	PRO	4.1

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Mol	Chain	Res	Type	RSRZ
1	K	155	ASP	4.0
1	L	293	GLU	4.0
1	K	349	TRP	4.0
1	J	158	PHE	4.0
1	K	273	PRO	3.9
1	E	155	ASP	3.9
1	E	156	GLN	3.9
1	K	237	PRO	3.9
1	J	329	THR	3.8
1	L	348	ARG	3.7
1	J	294	VAL	3.7
1	D	350	GLU	3.7
1	L	158	PHE	3.7
1	L	347	GLU	3.7
1	G	47	HIS	3.7
1	D	238	GLU	3.6
1	J	140	CYS	3.5
1	H	348	ARG	3.5
1	B	46	PHE	3.5
1	H	349	TRP	3.4
1	J	333	GLN	3.4
1	G	86	THR	3.4
1	H	64	LYS	3.4
1	K	272	SER	3.4
1	G	46	PHE	3.3
1	A	46	PHE	3.3
1	L	152	ASP	3.3
1	I	66	THR	3.3
1	D	239	LYS	3.3
1	G	347	GLU	3.3
1	H	293	GLU	3.3
1	J	349	TRP	3.2
1	C	293	GLU	3.2
1	I	154	GLY	3.2
1	H	236	GLY	3.2
1	F	347	GLU	3.2
1	F	238	GLU	3.2
1	I	74	ILE	3.1
1	J	46	PHE	3.1
1	H	85	ARG	3.1
1	L	340	ARG	3.1
1	J	150	ILE	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	67	SER	3.0
1	K	239	LYS	3.0
1	J	348	ARG	2.9
1	J	340	ARG	2.9
1	K	156	GLN	2.9
1	L	350	GLU	2.9
1	G	329	THR	2.9
1	L	238	GLU	2.9
1	B	237	PRO	2.8
1	G	337	HIS	2.8
1	K	347	GLU	2.8
1	E	46	PHE	2.8
1	J	330	LYS	2.8
1	K	258	CYS	2.8
1	C	199	PRO	2.8
1	F	293	GLU	2.7
1	K	289	PRO	2.7
1	I	347	GLU	2.7
1	J	337	HIS	2.7
1	K	158	PHE	2.7
1	C	350	GLU	2.7
1	L	264	TYR	2.7
1	C	264	TYR	2.6
1	K	329	THR	2.6
1	K	294	VAL	2.6
1	L	46	PHE	2.6
1	I	48	VAL	2.6
1	J	332	PRO	2.6
1	A	344	GLU	2.6
1	G	85	ARG	2.6
1	E	89	LYS	2.6
1	J	47	HIS	2.6
1	B	347	GLU	2.6
1	E	333	GLN	2.5
1	J	293	GLU	2.5
1	B	239	LYS	2.5
1	J	342	LEU	2.5
1	F	329	THR	2.5
1	B	48	VAL	2.5
1	D	46	PHE	2.5
1	J	85	ARG	2.5
1	L	346	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
1	L	80	GLN	2.5
1	G	152	ASP	2.5
1	D	280	ARG	2.5
1	L	240	TYR	2.5
1	J	200	ASN	2.5
1	D	153	ARG	2.4
1	K	241	ASP	2.4
1	F	348	ARG	2.4
1	D	334	THR	2.4
1	F	343	LYS	2.4
1	I	113	GLN	2.4
1	L	142	ASP	2.4
1	I	85	ARG	2.4
1	G	293	GLU	2.4
1	D	333	GLN	2.4
1	H	235	LEU	2.4
1	L	349	TRP	2.4
1	J	237	PRO	2.4
1	I	91	ALA	2.4
1	A	266	ASN	2.3
1	B	84	LYS	2.3
1	B	330	LYS	2.3
1	K	94	MET	2.3
1	K	293	GLU	2.3
1	E	349	TRP	2.3
1	E	340	ARG	2.3
1	L	162	GLU	2.3
1	E	64	LYS	2.3
1	K	46	PHE	2.3
1	C	328	SER	2.3
1	I	67	SER	2.3
1	H	239	LYS	2.3
1	K	238	GLU	2.3
1	G	158	PHE	2.3
1	C	60	ILE	2.3
1	B	80	GLN	2.3
1	L	344	GLU	2.2
1	D	240	TYR	2.2
1	I	60	ILE	2.2
1	K	265	SER	2.2
1	E	152	ASP	2.2
1	E	154	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	J	336	LEU	2.2
1	K	64	LYS	2.2
1	K	344	GLU	2.2
1	H	87	GLN	2.2
1	G	133	CYS	2.2
1	J	344	GLU	2.2
1	B	240	TYR	2.2
1	F	264	TYR	2.2
1	E	85	ARG	2.2
1	E	350	GLU	2.1
1	H	350	GLU	2.1
1	H	158	PHE	2.1
1	G	349	TRP	2.1
1	B	156	GLN	2.1
1	C	87	GLN	2.1
1	E	272	SER	2.1
1	L	150	ILE	2.1
1	H	82	PHE	2.1
1	I	344	GLU	2.1
1	H	289	PRO	2.1
1	C	345	ASP	2.1
1	K	266	ASN	2.1
1	C	238	GLU	2.1
1	I	65	VAL	2.1
1	F	328	SER	2.1
1	E	65	VAL	2.1
1	G	285	GLU	2.1
1	B	348	ARG	2.1
1	C	85	ARG	2.1
1	D	231	ALA	2.1
1	J	331	VAL	2.1
1	F	334	THR	2.1
1	A	240	TYR	2.1
1	H	154	GLY	2.1
1	B	74	ILE	2.1
1	J	236	GLY	2.1
1	A	47	HIS	2.0
1	J	153	ARG	2.0
1	E	158	PHE	2.0
1	H	48	VAL	2.0
1	J	84	LYS	2.0
1	J	257	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	E	293	GLU	2.0
1	E	328	SER	2.0
1	C	229	TYR	2.0
1	I	128	TYR	2.0
1	E	273	PRO	2.0
1	J	74	ILE	2.0
1	J	86	THR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	P4O	C	1	26/26	0.94	0.34	1.57	70,79,93,95	0
2	P4O	F	1	26/26	0.93	0.34	0.98	70,74,86,88	0
2	P4O	J	1	26/26	0.88	0.38	0.87	97,110,120,120	0
2	P4O	B	1	26/26	0.95	0.38	0.87	70,77,95,96	0
2	P4O	L	1	26/26	0.90	0.34	0.84	93,97,105,106	0
2	P4O	E	1	26/26	0.94	0.29	0.64	87,91,98,100	0
2	P4O	H	1	26/26	0.95	0.29	0.64	78,82,92,93	0
2	P4O	D	1	26/26	0.97	0.28	0.45	62,71,80,81	0
2	P4O	I	1	26/26	0.95	0.35	0.42	83,86,93,95	0
2	P4O	A	1	26/26	0.96	0.29	0.40	62,68,78,78	0
2	P4O	K	1	26/26	0.91	0.30	0.26	95,97,106,107	0
2	P4O	G	1	26/26	0.95	0.24	0.19	71,77,88,88	0

6.5 Other polymers (i)

There are no such residues in this entry.