



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:47 PM GMT

PDB ID : 4AID
Title : Crystal structure of C. crescentus PNPase bound to RNase E recognition peptide
Authors : Hardwick, S.W.; Gubbey, T.; Hug, I.; Jenal, U.; Luisi, B.F.
Deposited on : 2012-02-09
Resolution : 2.60 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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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

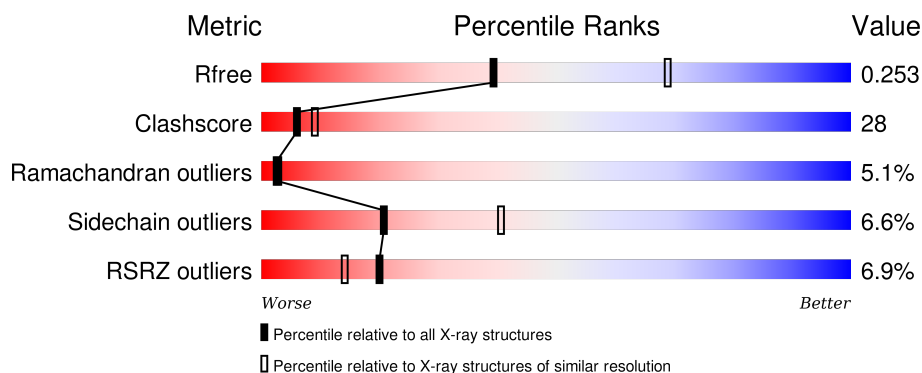
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	726	<div> <div>3%</div> <div> <div></div> <div>48%</div> <div>23%</div> <div>6%</div> <div>•</div> <div>21%</div> </div> </div>
1	B	726	<div> <div>2%</div> <div> <div></div> <div>47%</div> <div>23%</div> <div>6%</div> <div>•</div> <div>23%</div> </div> </div>
1	C	726	<div> <div>11%</div> <div> <div></div> <div>45%</div> <div>26%</div> <div>•</div> <div>26%</div> </div> </div>
2	F	14	<div> <div>7%</div> <div> <div></div> <div>14%</div> <div>21%</div> <div>7%</div> <div>7%</div> <div>50%</div> </div> </div>
2	G	14	<div> <div>7%</div> <div> <div></div> <div>29%</div> <div>21%</div> <div>7%</div> <div>43%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
2	H	14	 <div>29% 7% 64%</div>

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
3	PO4	C	1556	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12655 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 POLYRIBONUCLEOTIDE NUCLEOTIDYLTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	573	Total	C	N	O	S	0	1	0
			4248	2686	720	819	23			
1	B	558	Total	C	N	O	S	0	0	0
			4170	2639	706	802	23			
1	C	539	Total	C	N	O	S	0	0	0
			3836	2425	654	735	22			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-13	MET	-	EXPRESSION TAG	UNP Q9AC32
A	-12	GLY	-	EXPRESSION TAG	UNP Q9AC32
A	-11	SER	-	EXPRESSION TAG	UNP Q9AC32
A	-10	SER	-	EXPRESSION TAG	UNP Q9AC32
A	-9	HIS	-	EXPRESSION TAG	UNP Q9AC32
A	-8	HIS	-	EXPRESSION TAG	UNP Q9AC32
A	-7	HIS	-	EXPRESSION TAG	UNP Q9AC32
A	-6	HIS	-	EXPRESSION TAG	UNP Q9AC32
A	-5	HIS	-	EXPRESSION TAG	UNP Q9AC32
A	-4	HIS	-	EXPRESSION TAG	UNP Q9AC32
A	-3	SER	-	EXPRESSION TAG	UNP Q9AC32
A	-2	GLN	-	EXPRESSION TAG	UNP Q9AC32
A	-1	ASP	-	EXPRESSION TAG	UNP Q9AC32
A	0	PRO	-	EXPRESSION TAG	UNP Q9AC32
B	-13	MET	-	EXPRESSION TAG	UNP Q9AC32
B	-12	GLY	-	EXPRESSION TAG	UNP Q9AC32
B	-11	SER	-	EXPRESSION TAG	UNP Q9AC32
B	-10	SER	-	EXPRESSION TAG	UNP Q9AC32
B	-9	HIS	-	EXPRESSION TAG	UNP Q9AC32
B	-8	HIS	-	EXPRESSION TAG	UNP Q9AC32
B	-7	HIS	-	EXPRESSION TAG	UNP Q9AC32
B	-6	HIS	-	EXPRESSION TAG	UNP Q9AC32

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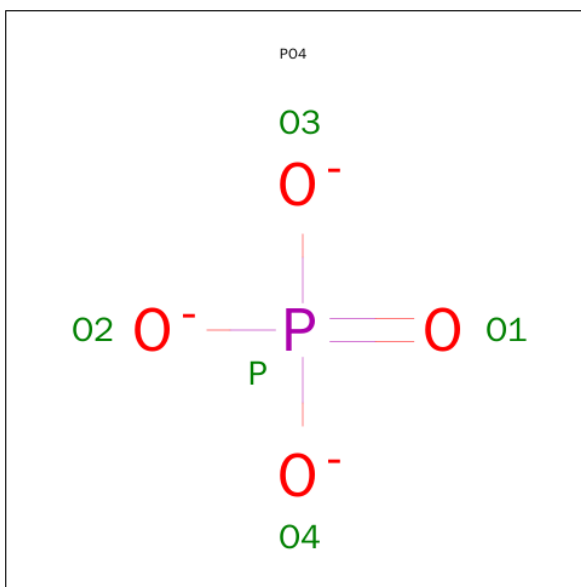
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Chain	Residue	Modelled	Actual	Comment	Reference
B	-5	HIS	-	EXPRESSION TAG	UNP Q9AC32
B	-4	HIS	-	EXPRESSION TAG	UNP Q9AC32
B	-3	SER	-	EXPRESSION TAG	UNP Q9AC32
B	-2	GLN	-	EXPRESSION TAG	UNP Q9AC32
B	-1	ASP	-	EXPRESSION TAG	UNP Q9AC32
B	0	PRO	-	EXPRESSION TAG	UNP Q9AC32
C	-13	MET	-	EXPRESSION TAG	UNP Q9AC32
C	-12	GLY	-	EXPRESSION TAG	UNP Q9AC32
C	-11	SER	-	EXPRESSION TAG	UNP Q9AC32
C	-10	SER	-	EXPRESSION TAG	UNP Q9AC32
C	-9	HIS	-	EXPRESSION TAG	UNP Q9AC32
C	-8	HIS	-	EXPRESSION TAG	UNP Q9AC32
C	-7	HIS	-	EXPRESSION TAG	UNP Q9AC32
C	-6	HIS	-	EXPRESSION TAG	UNP Q9AC32
C	-5	HIS	-	EXPRESSION TAG	UNP Q9AC32
C	-4	HIS	-	EXPRESSION TAG	UNP Q9AC32
C	-3	SER	-	EXPRESSION TAG	UNP Q9AC32
C	-2	GLN	-	EXPRESSION TAG	UNP Q9AC32
C	-1	ASP	-	EXPRESSION TAG	UNP Q9AC32
C	0	PRO	-	EXPRESSION TAG	UNP Q9AC32

- Molecule 2 is a protein called RIBONUCLEASE, RNE/RNG FAMILY PROTEIN.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	F	7	Total	C	N	O	0	0	0
			66	44	15	7			
2	G	8	Total	C	N	O	0	0	0
			77	50	19	8			
2	H	5	Total	C	N	O	0	0	0
			42	30	7	5			

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



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

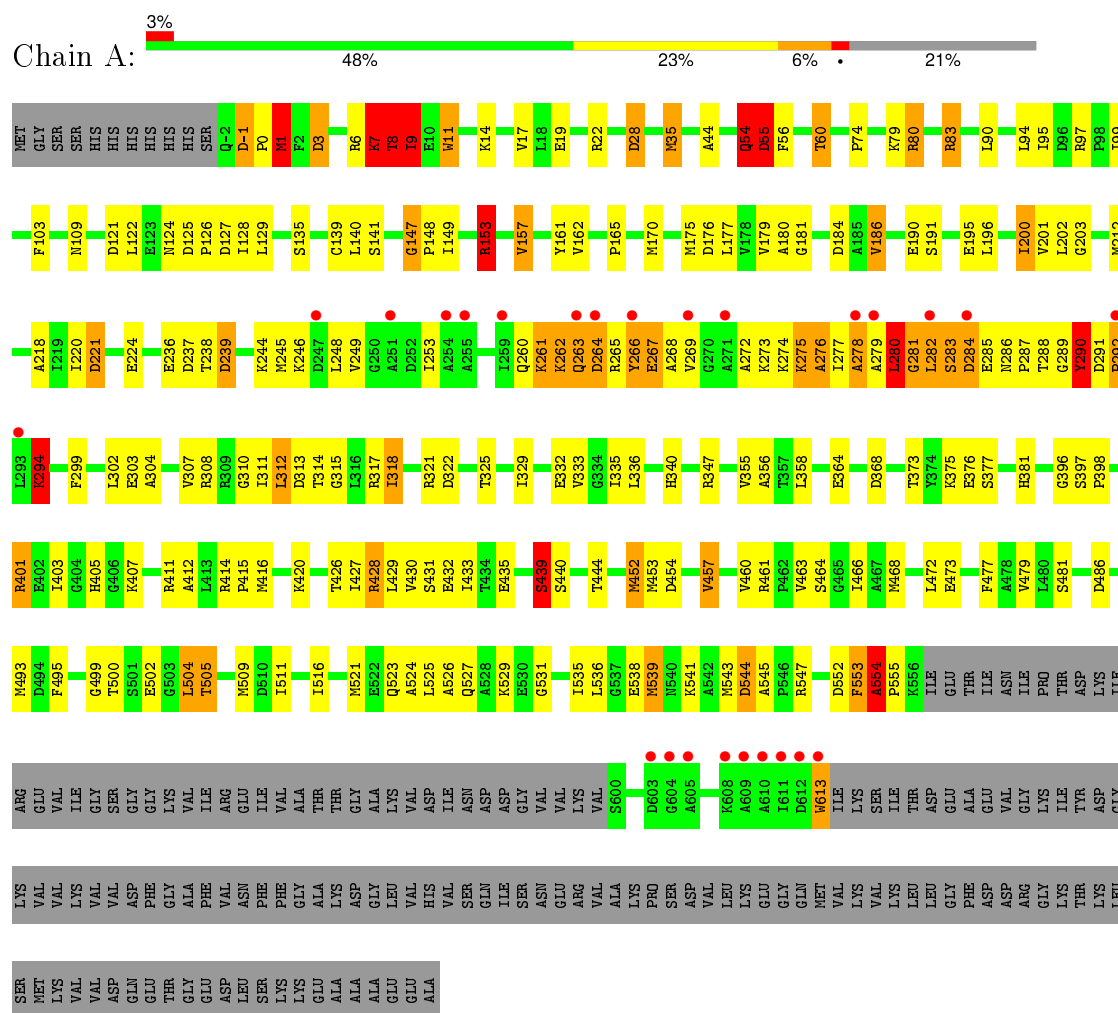
- Molecule 4 is water.

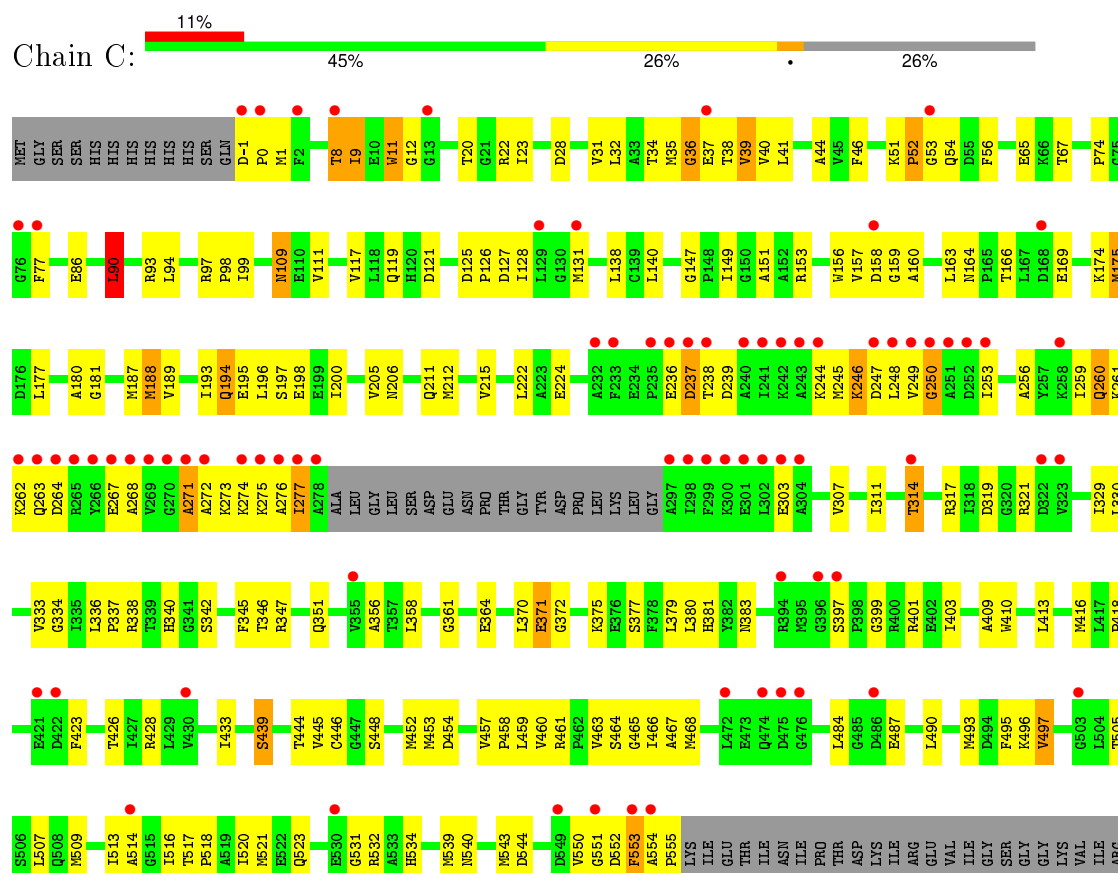
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	96	Total	O	0	0
			96	96		
4	B	80	Total	O	0	0
			80	80		
4	C	24	Total	O	0	0
			24	24		
4	G	1	Total	O	0	0
			1	1		

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: POLYRIBONUCLEOTIDE NUCLEOTIDYLTRANSFERASE

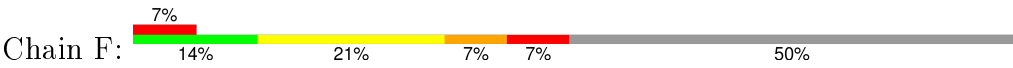




GLU	ILE	ALA	THR	GLY	ALA	LYS	VAL	ASP	ILE	ASN	ASP	ASP	GLY	VAL	LYS	VAL	SER	ALA	SER	ASP	GLY	ALA	ILE	LYS	ALA	ILE	ASP	TRP	ILE	LYS	LYS	ILE	SER	ILE	THR	GLU	ALA	GLU	VAL	GLY	LYS	ILE	TYR	ASP	GLY	LYS	VAL	VAL	VAL	VAL	VAL	ASP	PHE	GLU	THR	GLY	ALA
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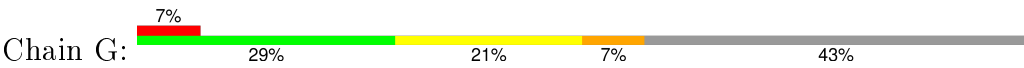
GLU	ASP	LEU	SER	GLU	LYS	GLU	ALA	ALA	GLU	GLU	ALA
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● Molecule 2: RIBONUCLEASE, RNE/RNG FAMILY PROTEIN



THR	ALA	PRO	PRO	GLU	LYS	R891	R892	R893	G894	W895	W896	R897	ARG
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● Molecule 2: RIBONUCLEASE, RNE/RNG FAMILY PROTEIN



THR	ALA	PRO	PRO	GLU	R890	R891	R892	R893	G894	W895	W896	R897	ARG
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● Molecule 2: RIBONUCLEASE, RNE/RNG FAMILY PROTEIN



THR	ALA	PRO	PRO	GLU	LYS	PRO	ARG	R893	W896	R897	ARG
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4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	157.44Å 157.44Å 302.38Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 2.60 29.75 – 2.60	Depositor EDS
% Data completeness (in resolution range)	90.0 (30.00-2.60) 90.0 (29.75-2.60)	Depositor EDS
R_{merge}	0.22	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.92 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.209 , 0.254 0.209 , 0.253	Depositor DCC
R_{free} test set	2587 reflections (3.45%)	DCC
Wilson B-factor (Å ²)	46.7	Xtriage
Anisotropy	0.048	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 52.3	EDS
Estimated twinning fraction	0.357 for h,-h-k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 77316 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	12655	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.87% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 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: PO4

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	1.01	8/4324 (0.2%)	1.15	27/5859 (0.5%)
1	B	1.03	9/4242 (0.2%)	1.21	33/5744 (0.6%)
1	C	0.66	2/3900 (0.1%)	0.87	3/5305 (0.1%)
2	F	1.59	2/70 (2.9%)	1.32	1/94 (1.1%)
2	G	1.30	1/81 (1.2%)	1.14	0/109
2	H	1.49	1/45 (2.2%)	1.03	0/62
All	All	0.94	23/12662 (0.2%)	1.10	64/17173 (0.4%)

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	2
1	B	0	3
1	C	0	1
2	F	0	1
All	All	0	7

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	896	TRP	CD2-CE2	7.50	1.50	1.41
1	B	81	GLU	CD-OE1	6.69	1.33	1.25
2	G	896	TRP	CD2-CE2	6.34	1.49	1.41
1	A	432	GLU	CD-OE1	6.33	1.32	1.25
1	A	332	GLU	CD-OE1	6.26	1.32	1.25
1	A	11	TRP	CD2-CE2	6.05	1.48	1.41
1	B	432	GLU	CD-OE1	5.86	1.32	1.25
1	B	332	GLU	CD-OE1	5.74	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	147	GLY	N-CA	5.73	1.54	1.46
1	A	376	GLU	CD-OE1	5.72	1.31	1.25
2	F	895	TRP	CD2-CE2	5.68	1.48	1.41
1	A	147	GLY	C-O	-5.62	1.14	1.23
1	B	81	GLU	CD-OE2	5.58	1.31	1.25
1	A	435	GLU	CD-OE1	5.57	1.31	1.25
1	B	11	TRP	CD2-CE2	5.49	1.48	1.41
1	B	199	GLU	CG-CD	5.45	1.60	1.51
1	B	190	GLU	CD-OE1	5.44	1.31	1.25
1	A	190	GLU	CD-OE1	5.40	1.31	1.25
1	A	613	TRP	CD2-CE2	5.37	1.47	1.41
1	C	11	TRP	CD2-CE2	5.34	1.47	1.41
1	B	3	ASP	CB-CG	-5.24	1.40	1.51
1	C	410	TRP	CD2-CE2	5.19	1.47	1.41
2	H	896	TRP	CD2-CE2	5.11	1.47	1.41

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	177	LEU	CB-CG-CD1	-10.79	92.66	111.00
1	B	28	ASP	CB-CG-OD2	10.72	127.95	118.30
1	B	3	ASP	CB-CG-OD1	-10.37	108.97	118.30
1	B	153	ARG	NE-CZ-NH1	9.91	125.26	120.30
1	B	486	ASP	CB-CG-OD1	-9.45	109.80	118.30
1	A	9	ILE	N-CA-C	-9.45	85.50	111.00
1	B	28	ASP	CB-CG-OD1	-9.40	109.84	118.30
1	A	80	ARG	NE-CZ-NH1	9.26	124.93	120.30
1	A	80	ARG	NE-CZ-NH2	-8.95	115.83	120.30
1	A	486	ASP	CB-CG-OD1	-8.28	110.85	118.30
1	B	539	MET	CG-SD-CE	-8.26	86.98	100.20
1	A	97	ARG	NE-CZ-NH2	-8.08	116.26	120.30
1	B	55	ASP	CB-CG-OD2	7.99	125.49	118.30
1	A	94	LEU	CB-CG-CD1	-7.84	97.67	111.00
1	B	486	ASP	CB-CG-OD2	7.76	125.28	118.30
1	A	539	MET	CG-SD-CE	-7.54	88.14	100.20
1	B	532	ARG	NE-CZ-NH2	-7.53	116.54	120.30
1	A	452	MET	CG-SD-CE	-7.31	88.50	100.20
1	A	553	PHE	N-CA-C	-6.56	93.29	111.00
1	B	525	LEU	CA-CB-CG	-6.45	100.46	115.30
1	B	291	ASP	C-N-CD	-6.45	106.42	120.60
1	A	439	SER	N-CA-C	6.40	128.28	111.00
1	B	83	ARG	NE-CZ-NH1	6.26	123.43	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	222	LEU	CA-CB-CG	6.24	129.65	115.30
1	B	8	THR	N-CA-C	-6.20	94.26	111.00
1	B	153	ARG	NE-CZ-NH2	-6.17	117.21	120.30
1	B	3	ASP	CB-CG-OD2	6.14	123.83	118.30
1	B	452	MET	CG-SD-CE	-6.05	90.52	100.20
1	A	-1	ASP	C-N-CD	6.05	141.10	128.40
1	A	28	ASP	CB-CG-OD1	-6.04	112.87	118.30
1	B	55	ASP	CB-CG-OD1	-5.99	112.91	118.30
1	B	96	ASP	CB-CG-OD1	5.99	123.69	118.30
1	B	401	ARG	NE-CZ-NH1	-5.96	117.32	120.30
1	B	461	ARG	NE-CZ-NH2	-5.84	117.38	120.30
1	A	153	ARG	NE-CZ-NH2	-5.81	117.39	120.30
1	B	96	ASP	CB-CG-OD2	-5.77	113.10	118.30
1	A	544	ASP	N-CA-CB	-5.67	100.39	110.60
1	A	468	MET	CG-SD-CE	5.63	109.21	100.20
1	B	321	ARG	NE-CZ-NH2	-5.60	117.50	120.30
1	B	7	LYS	N-CA-C	-5.57	95.97	111.00
1	B	510	ASP	CB-CG-OD1	5.53	123.28	118.30
1	B	439	SER	N-CA-C	5.50	125.84	111.00
1	A	294	LYS	N-CA-C	-5.49	96.19	111.00
1	A	411	ARG	NE-CZ-NH2	-5.47	117.56	120.30
1	B	125	ASP	CB-CG-OD1	5.46	123.21	118.30
1	A	428	ARG	NE-CZ-NH2	-5.37	117.61	120.30
1	B	3	ASP	N-CA-CB	-5.35	100.97	110.60
2	F	894	GLY	N-CA-C	5.34	126.45	113.10
1	C	90	LEU	CA-CB-CG	5.31	127.51	115.30
1	A	504	LEU	CB-CG-CD2	-5.30	101.99	111.00
1	A	7	LYS	N-CA-C	-5.29	96.71	111.00
1	B	529	LYS	CD-CE-NZ	-5.27	99.59	111.70
1	A	55	ASP	CB-CA-C	-5.25	99.90	110.40
1	B	1	MET	CB-CG-SD	5.23	128.10	112.40
1	A	317	ARG	NE-CZ-NH1	5.23	122.92	120.30
1	B	194	GLN	CA-CB-CG	5.21	124.87	113.40
1	A	28	ASP	CB-CG-OD2	5.20	122.98	118.30
1	B	192	GLU	N-CA-C	-5.20	96.97	111.00
1	A	19	GLU	OE1-CD-OE2	-5.12	117.15	123.30
1	A	8	THR	N-CA-C	-5.12	97.18	111.00
1	A	184	ASP	CB-CA-C	-5.10	100.19	110.40
1	B	6	ARG	N-CA-C	-5.10	97.23	111.00
1	A	486	ASP	CB-CG-OD2	5.01	122.81	118.30
1	C	463	VAL	CB-CA-C	-5.01	101.88	111.40

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	554	ALA	Peptide
1	A	8	THR	Peptide
1	B	554	ALA	Peptide
1	B	6	ARG	Peptide
1	B	9	ILE	Peptide
1	C	35	MET	Peptide
2	F	892	ARG	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	4248	0	4212	272	1
1	B	4170	0	4161	260	1
1	C	3836	0	3670	172	2
2	F	66	0	58	2	0
2	G	77	0	70	3	0
2	H	42	0	26	1	0
3	A	5	0	0	1	0
3	B	5	0	0	1	0
3	C	5	0	0	1	0
4	A	96	0	0	6	0
4	B	80	0	0	1	0
4	C	24	0	0	3	0
4	G	1	0	0	0	0
All	All	12655	0	12197	699	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 28.

All (699) 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:287:PRO:HB2	1:A:288:THR:CG2	1.29	1.60
1:A:287:PRO:CB	1:A:288:THR:CG2	1.84	1.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:282:LEU:HA	1:A:292:PRO:CG	1.44	1.43
1:A:281:GLY:CA	1:A:289:GLY:O	1.68	1.37
1:B:274:LYS:HA	1:B:277:ILE:CG2	1.57	1.34
1:B:291:ASP:O	1:B:293:LEU:N	1.61	1.29
1:A:282:LEU:CA	1:A:292:PRO:HG3	1.66	1.25
1:A:493:MET:HE3	1:A:509:MET:CE	1.70	1.21
1:A:287:PRO:CB	1:A:288:THR:HG22	1.56	1.21
1:B:278:ALA:O	1:B:282:LEU:HD23	1.37	1.18
1:A:493:MET:CE	1:A:509:MET:HE2	1.74	1.18
1:A:274:LYS:O	1:A:277:ILE:HG22	1.43	1.14
1:A:274:LYS:HE2	1:A:274:LYS:HA	1.29	1.13
1:A:277:ILE:O	1:A:282:LEU:HD12	1.46	1.13
1:B:279:ALA:O	1:B:282:LEU:CD2	1.97	1.13
1:A:287:PRO:CB	1:A:288:THR:HG23	1.57	1.13
1:B:274:LYS:CD	1:B:277:ILE:HG21	1.80	1.12
1:B:274:LYS:CD	1:B:277:ILE:HD13	1.80	1.12
1:A:287:PRO:CA	1:A:288:THR:CG2	2.28	1.10
1:A:277:ILE:C	1:A:282:LEU:HD12	1.71	1.09
1:A:543:MET:O	1:A:544:ASP:HB3	1.36	1.09
1:B:279:ALA:O	1:B:282:LEU:HD21	1.53	1.09
1:B:274:LYS:HA	1:B:277:ILE:HG22	1.30	1.09
1:B:274:LYS:HA	1:B:277:ILE:HG21	1.28	1.08
1:A:281:GLY:HA2	1:A:289:GLY:O	0.90	1.08
1:C:338:ARG:HA	1:C:553:PHE:HE1	1.05	1.07
1:A:493:MET:HE3	1:A:509:MET:HE2	1.16	1.07
1:A:416:MET:HE1	1:A:500:THR:HG21	1.30	1.06
1:A:287:PRO:CA	1:A:288:THR:HG22	1.85	1.06
1:B:287:PRO:HB2	1:B:288:THR:HA	1.08	1.05
1:A:453:MET:HB3	1:A:543:MET:CE	1.86	1.05
1:C:249:VAL:CG1	1:C:272:ALA:HB1	1.87	1.04
1:C:338:ARG:HA	1:C:553:PHE:CE1	1.93	1.02
1:B:279:ALA:O	1:B:282:LEU:CG	2.07	1.02
1:C:52:PRO:O	1:C:54:GLN:N	1.92	1.01
1:B:303:GLU:O	1:B:306:VAL:HG12	1.61	1.00
1:A:493:MET:CE	1:A:509:MET:CE	2.36	0.99
1:C:340:HIS:HD2	1:C:358:LEU:H	1.05	0.98
1:A:381:HIS:HD2	1:A:428:ARG:NH1	1.62	0.98
1:B:287:PRO:CB	1:B:288:THR:HA	1.94	0.98
1:B:354:VAL:HG22	1:B:431:SER:HB2	1.42	0.98
1:B:416:MET:CE	1:B:461:ARG:HB2	1.93	0.97
1:C:128:ILE:HD11	1:C:153:ARG:HB2	1.44	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:97:ARG:NH2	1:B:190:GLU:OE1	1.96	0.97
1:A:340:HIS:HD2	1:A:358:LEU:H	1.13	0.97
1:B:83:ARG:HB2	1:B:83:ARG:HH11	1.28	0.97
1:B:275:LYS:O	1:B:277:ILE:N	1.97	0.97
1:A:381:HIS:CD2	1:A:428:ARG:HH11	1.82	0.97
1:A:281:GLY:O	1:A:290:TYR:O	1.82	0.97
1:A:54:GLN:O	1:A:55:ASP:HB2	1.62	0.96
1:C:99:ILE:HG22	1:C:149:ILE:HD12	1.47	0.96
1:B:263:GLN:HG3	1:B:264:ASP:H	1.28	0.96
1:A:364:GLU:HG2	1:A:426:THR:HG21	1.47	0.95
1:A:287:PRO:HB3	1:A:288:THR:HG22	1.49	0.93
1:B:364:GLU:OE1	1:B:375:LYS:HE3	1.68	0.93
1:B:263:GLN:O	1:B:266:TYR:N	2.01	0.93
1:B:93:ARG:HH11	1:B:404:GLY:HA3	1.34	0.93
1:A:8:THR:O	1:A:9:ILE:HG12	1.68	0.93
1:B:279:ALA:O	1:B:282:LEU:HG	1.66	0.93
1:A:493:MET:HG3	1:A:511:ILE:HG13	1.52	0.92
1:B:9:ILE:HG13	1:B:218:ALA:HB2	1.50	0.92
1:B:282:LEU:HB3	1:B:287:PRO:O	1.70	0.92
1:C:39:VAL:HG12	1:C:119:GLN:HB3	1.53	0.91
1:B:283:SER:HB2	1:B:287:PRO:HB3	1.52	0.91
1:B:102:LEU:HD12	1:B:149:ILE:HD11	1.51	0.91
1:A:60:THR:HG23	4:A:2012:HOH:O	1.69	0.91
1:A:543:MET:O	1:A:544:ASP:CB	2.11	0.91
1:C:67:THR:HG21	1:C:74:PRO:HG3	1.52	0.91
1:A:276:ALA:O	1:A:280:LEU:CB	2.19	0.91
1:B:287:PRO:HB2	1:B:288:THR:CA	1.99	0.90
1:B:1:MET:HG2	1:B:22:ARG:HA	1.54	0.90
1:C:94:LEU:HD12	1:C:97:ARG:NH2	1.87	0.90
1:A:281:GLY:O	1:A:292:PRO:HD3	1.73	0.89
1:C:249:VAL:HG13	1:C:272:ALA:HB1	1.54	0.89
1:A:416:MET:CE	1:A:500:THR:HG21	2.03	0.89
1:A:282:LEU:CA	1:A:292:PRO:CG	2.38	0.89
1:B:284:ASP:HA	1:B:285:GLU:HB3	1.51	0.89
1:A:274:LYS:HE2	1:A:277:ILE:HG21	1.52	0.89
1:B:274:LYS:CA	1:B:277:ILE:CG2	2.47	0.88
1:A:287:PRO:HB2	1:A:288:THR:HG23	0.89	0.88
1:A:282:LEU:HA	1:A:292:PRO:HG2	1.56	0.88
1:B:470:LEU:HD12	1:B:478:ALA:O	1.72	0.88
1:C:340:HIS:CD2	1:C:358:LEU:H	1.92	0.88
1:B:275:LYS:HG2	1:B:276:ALA:N	1.87	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:337:PRO:O	1:C:338:ARG:HB2	1.72	0.87
1:A:287:PRO:HB2	1:A:288:THR:HG21	1.53	0.87
1:B:93:ARG:NH1	1:B:404:GLY:HA3	1.88	0.86
1:A:381:HIS:HD2	1:A:428:ARG:HH11	0.91	0.86
1:A:416:MET:CE	1:A:461:ARG:HB2	2.06	0.86
1:A:464:SER:HB2	1:A:539:MET:HE1	1.55	0.85
1:B:274:LYS:CA	1:B:277:ILE:HG22	2.03	0.85
1:B:97:ARG:CZ	1:B:188:MET:HE3	2.06	0.85
1:C:39:VAL:CG1	1:C:119:GLN:HB3	2.05	0.85
1:A:181:GLY:HA3	1:A:212:MET:HE1	1.57	0.85
1:B:275:LYS:HG2	1:B:276:ALA:H	1.39	0.84
1:C:338:ARG:CA	1:C:553:PHE:HE1	1.87	0.84
1:C:409:ALA:O	1:C:413:LEU:HG	1.77	0.83
1:A:249:VAL:CG2	1:A:276:ALA:HB2	2.08	0.82
1:A:502:GLU:OE2	1:B:529:LYS:HE2	1.78	0.82
1:B:-1:ASP:HB3	1:B:0:PRO:HD3	1.61	0.82
1:B:97:ARG:CZ	1:B:188:MET:CE	2.57	0.82
1:A:245:MET:HE3	1:A:299:PHE:HA	1.62	0.82
1:B:263:GLN:HG3	1:B:264:ASP:N	1.95	0.82
1:A:8:THR:HG22	1:A:9:ILE:HD13	1.59	0.82
1:A:277:ILE:C	1:A:282:LEU:CD1	2.49	0.81
1:A:276:ALA:O	1:A:280:LEU:HB3	1.80	0.81
1:A:200:ILE:HD11	1:B:200:ILE:HD11	1.62	0.81
1:C:125:ASP:OD1	1:C:126:PRO:HD2	1.81	0.81
1:C:268:ALA:O	1:C:271:ALA:HB3	1.81	0.81
1:B:283:SER:HB2	1:B:287:PRO:CB	2.11	0.81
1:A:464:SER:HB2	1:A:539:MET:CE	2.10	0.81
1:A:177:LEU:HD12	1:A:191:SER:HB3	1.62	0.81
1:A:364:GLU:OE1	1:A:375:LYS:HE3	1.80	0.80
1:B:309:ARG:HH11	1:B:309:ARG:HG3	1.46	0.80
1:B:277:ILE:O	1:B:278:ALA:C	2.20	0.80
1:A:274:LYS:C	1:A:277:ILE:HG22	2.00	0.80
1:A:274:LYS:CE	1:A:274:LYS:HA	2.10	0.80
1:B:277:ILE:HG23	1:B:278:ALA:H	1.46	0.80
1:B:291:ASP:C	1:B:293:LEU:N	2.32	0.80
1:A:453:MET:HB3	1:A:543:MET:HE3	1.62	0.80
1:C:338:ARG:HG2	1:C:553:PHE:CZ	2.17	0.80
1:B:-1:ASP:HB3	1:B:0:PRO:CD	2.11	0.80
1:B:433:ILE:HD12	1:B:440:SER:HB2	1.63	0.80
1:B:464:SER:HB2	1:B:539:MET:CE	2.12	0.80
1:A:287:PRO:HA	1:A:288:THR:HG22	1.62	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:381:HIS:HD2	1:C:428:ARG:HH11	1.30	0.79
1:A:83:ARG:HG3	1:A:83:ARG:HH11	1.46	0.79
1:A:276:ALA:O	1:A:280:LEU:HB2	1.81	0.79
1:B:338:ARG:HA	1:B:553:PHE:HE1	1.48	0.79
1:A:95:ILE:O	1:A:99:ILE:HG12	1.82	0.79
1:B:249:VAL:O	1:B:253:ILE:HG12	1.82	0.79
1:A:287:PRO:CA	1:A:288:THR:HG23	2.00	0.79
1:A:249:VAL:CG1	1:A:272:ALA:HB1	2.11	0.79
1:A:274:LYS:O	1:A:277:ILE:CG2	2.30	0.78
1:B:278:ALA:O	1:B:282:LEU:CD2	2.28	0.78
1:C:319:ASP:OD2	1:C:321:ARG:NH1	2.16	0.78
1:B:274:LYS:CA	1:B:277:ILE:HG21	2.11	0.77
1:A:277:ILE:HG12	1:A:282:LEU:HD11	1.64	0.77
1:A:284:ASP:OD1	1:A:285:GLU:N	2.18	0.77
1:A:282:LEU:HA	1:A:292:PRO:HG3	0.77	0.77
1:C:249:VAL:CG2	1:C:276:ALA:HB2	2.15	0.76
1:B:97:ARG:NH2	1:B:188:MET:HE1	2.00	0.76
1:B:275:LYS:C	1:B:277:ILE:H	1.87	0.76
1:A:464:SER:CB	1:A:539:MET:CE	2.64	0.76
1:A:236:GLU:HB3	1:A:238:THR:HG23	1.66	0.76
1:B:283:SER:CB	1:B:287:PRO:HB3	2.15	0.76
1:A:83:ARG:HH11	1:A:83:ARG:CG	1.98	0.75
1:C:249:VAL:O	1:C:253:ILE:HG12	1.86	0.75
1:C:383:ASN:O	1:C:433:ILE:HG12	1.86	0.75
1:A:287:PRO:C	1:A:288:THR:HG23	2.07	0.75
1:A:401:ARG:NE	1:A:405:HIS:HE1	1.85	0.75
1:C:236:GLU:O	1:C:238:THR:N	2.20	0.74
1:A:308:ARG:O	1:A:312:LEU:HD12	1.87	0.74
1:A:287:PRO:HB3	1:A:288:THR:CG2	2.07	0.74
1:B:286:ASN:N	1:B:287:PRO:O	2.20	0.74
1:C:99:ILE:HG22	1:C:149:ILE:CD1	2.16	0.74
1:A:340:HIS:CD2	1:A:358:LEU:H	2.01	0.74
1:A:7:LYS:O	1:A:8:THR:C	2.26	0.74
1:C:12:GLY:HA3	1:C:163:LEU:HD23	1.67	0.74
1:B:412:ALA:HA	1:B:505:THR:HG23	1.70	0.74
1:A:202:LEU:HD11	1:A:525:LEU:HD12	1.70	0.74
1:A:281:GLY:O	1:A:292:PRO:CD	2.35	0.74
1:B:290:TYR:O	1:B:292:PRO:N	2.21	0.74
1:B:464:SER:HB2	1:B:539:MET:HE1	1.69	0.73
1:A:249:VAL:HG11	1:A:272:ALA:HB1	1.69	0.73
1:C:67:THR:HG21	1:C:74:PRO:CG	2.19	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:454:ASP:OD1	1:A:547:ARG:NH1	2.20	0.73
1:B:97:ARG:HD2	1:B:510:ASP:OD1	1.88	0.73
1:A:303:GLU:O	1:A:307:VAL:HG23	1.88	0.73
1:B:83:ARG:CB	1:B:83:ARG:HH11	1.99	0.73
1:A:464:SER:HB3	1:A:539:MET:HE3	1.69	0.73
1:B:304:ALA:O	1:B:308:ARG:HG3	1.89	0.73
1:A:499:GLY:HA2	1:A:505:THR:HB	1.71	0.73
1:A:8:THR:O	1:A:9:ILE:CG1	2.37	0.72
1:C:128:ILE:HD11	1:C:153:ARG:CB	2.17	0.72
1:B:337:PRO:O	1:B:338:ARG:HB2	1.90	0.72
1:B:416:MET:CE	1:B:461:ARG:CB	2.67	0.72
1:B:454:ASP:OD1	1:B:547:ARG:NH1	2.22	0.72
1:B:253:ILE:CG2	1:B:306:VAL:HG11	2.20	0.71
1:B:260:GLN:O	1:B:261:LYS:CB	2.35	0.71
1:A:181:GLY:CA	1:A:212:MET:HE1	2.21	0.71
1:B:291:ASP:O	1:B:292:PRO:C	2.27	0.71
1:B:176:ASP:O	1:B:191:SER:HA	1.90	0.71
1:B:97:ARG:NH1	1:B:188:MET:HE3	2.06	0.71
1:A:493:MET:CE	1:A:509:MET:HE3	2.21	0.71
1:A:181:GLY:O	1:A:212:MET:HE3	1.91	0.71
1:A:401:ARG:CZ	1:A:405:HIS:HE1	2.05	0.70
1:B:238:THR:O	1:B:241:ILE:HG22	1.91	0.70
1:C:464:SER:HB3	1:C:539:MET:HE1	1.72	0.70
1:B:175:MET:SD	1:B:177:LEU:HD23	2.32	0.70
1:B:439:SER:HA	3:B:1557:PO4:O4	1.91	0.70
1:A:54:GLN:O	1:A:55:ASP:CB	2.36	0.70
1:B:416:MET:HE1	1:B:461:ARG:HB2	1.73	0.69
1:A:377:SER:HB2	1:A:426:THR:HG22	1.74	0.69
1:A:277:ILE:O	1:A:282:LEU:CD1	2.34	0.69
1:C:249:VAL:HG11	1:C:272:ALA:HB1	1.72	0.69
1:C:333:VAL:HG11	1:C:543:MET:HE2	1.73	0.69
1:A:278:ALA:HA	1:A:282:LEU:HD13	1.74	0.69
1:C:452:MET:O	1:C:457:VAL:HG22	1.93	0.69
1:C:157:VAL:O	1:C:159:GLY:N	2.25	0.69
1:A:464:SER:CB	1:A:539:MET:HE3	2.22	0.69
1:B:277:ILE:HG23	1:B:278:ALA:N	2.08	0.69
1:B:277:ILE:O	1:B:279:ALA:N	2.26	0.69
1:C:177:LEU:HD11	1:C:189:VAL:HG13	1.74	0.69
1:B:181:GLY:HA3	1:B:212:MET:HE1	1.75	0.69
1:B:261:LYS:O	1:B:262:LYS:O	2.11	0.69
1:A:464:SER:CB	1:A:539:MET:HE1	2.23	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:39:VAL:O	1:C:40:VAL:HG23	1.91	0.68
1:C:109:ASN:HD22	1:C:109:ASN:N	1.91	0.68
1:C:8:THR:O	1:C:9:ILE:HB	1.93	0.68
1:B:275:LYS:CG	1:B:276:ALA:N	2.55	0.68
1:C:364:GLU:OE2	1:C:375:LYS:HE3	1.93	0.68
1:A:433:ILE:HD12	1:A:440:SER:HB2	1.75	0.68
1:C:94:LEU:HD12	1:C:97:ARG:HH21	1.56	0.68
1:A:181:GLY:CA	1:A:212:MET:CE	2.72	0.68
1:B:291:ASP:OD1	1:B:293:LEU:HB2	1.93	0.68
1:B:364:GLU:OE1	1:B:375:LYS:CE	2.42	0.68
1:A:275:LYS:HG2	1:A:276:ALA:N	2.09	0.67
1:A:181:GLY:C	1:A:212:MET:HE3	2.15	0.67
1:A:453:MET:CB	1:A:543:MET:CE	2.70	0.67
1:A:153:ARG:HD3	1:A:176:ASP:OD1	1.95	0.67
1:B:309:ARG:HG3	1:B:309:ARG:NH1	2.09	0.67
1:C:340:HIS:HB2	1:C:356:ALA:O	1.95	0.67
1:B:274:LYS:C	1:B:277:ILE:HG22	2.15	0.66
1:A:401:ARG:HD2	4:A:2078:HOH:O	1.95	0.66
1:B:263:GLN:O	1:B:267:GLU:N	2.26	0.66
1:A:416:MET:HE1	1:A:500:THR:CG2	2.18	0.66
1:B:83:ARG:NH1	1:B:83:ARG:HB2	2.06	0.66
1:B:9:ILE:HG13	1:B:218:ALA:CB	2.26	0.66
1:C:338:ARG:HG2	1:C:553:PHE:HZ	1.60	0.66
1:A:401:ARG:NE	1:A:405:HIS:CE1	2.63	0.66
1:A:381:HIS:CD2	1:A:428:ARG:NH1	2.54	0.65
1:B:97:ARG:NH1	1:B:188:MET:CE	2.59	0.65
1:B:303:GLU:O	1:B:307:VAL:HG23	1.95	0.65
1:A:249:VAL:HG21	1:A:276:ALA:HB2	1.76	0.65
1:C:249:VAL:HG12	1:C:253:ILE:HG12	1.79	0.65
1:B:9:ILE:HG22	1:B:11:TRP:HB2	1.79	0.65
1:A:265:ARG:HH22	1:A:318:ILE:HA	1.61	0.65
1:C:189:VAL:HG11	1:C:507:LEU:HD12	1.77	0.64
1:A:277:ILE:HG12	1:A:282:LEU:CD1	2.27	0.64
1:B:381:HIS:HD2	1:B:428:ARG:HE	1.45	0.64
1:C:39:VAL:CG1	1:C:119:GLN:CB	2.76	0.64
1:A:266:TYR:O	1:A:267:GLU:C	2.36	0.64
1:B:286:ASN:HB2	1:B:287:PRO:O	1.98	0.63
1:A:502:GLU:O	4:A:2091:HOH:O	2.15	0.63
1:A:427:ILE:HD13	1:A:452:MET:CE	2.27	0.63
1:A:311:ILE:O	1:A:314:THR:O	2.16	0.63
1:A:135:SER:HB2	1:A:149:ILE:HG12	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:249:VAL:HG13	1:B:272:ALA:HB1	1.81	0.63
1:B:535:ILE:HG22	1:B:539:MET:CE	2.27	0.63
1:A:479:VAL:HG23	1:A:527:GLN:CD	2.19	0.62
1:A:281:GLY:C	1:A:289:GLY:O	2.36	0.62
1:B:9:ILE:CG1	1:B:218:ALA:HB2	2.24	0.62
1:B:269:VAL:HG12	1:B:270:GLY:N	2.15	0.62
1:C:40:VAL:HG22	1:C:117:VAL:HA	1.80	0.62
1:C:468:MET:HB2	1:C:495:PHE:CE2	2.34	0.62
1:C:175:MET:HB2	1:C:193:ILE:HG23	1.82	0.62
1:B:468:MET:HB2	1:B:495:PHE:CE1	2.35	0.62
1:B:303:GLU:O	1:B:306:VAL:CG1	2.44	0.62
1:B:337:PRO:O	1:B:338:ARG:CB	2.42	0.62
1:C:340:HIS:HD2	1:C:358:LEU:N	1.87	0.61
1:C:381:HIS:CD2	1:C:428:ARG:HD2	2.35	0.61
1:B:442:MET:HA	1:B:445:VAL:HG13	1.81	0.61
1:A:200:ILE:HD11	1:B:200:ILE:CD1	2.31	0.61
1:A:161:TYR:OH	1:A:203:GLY:HA3	2.00	0.61
1:B:381:HIS:CD2	1:B:428:ARG:HE	2.19	0.61
1:C:423:PHE:CZ	1:C:457:VAL:HG12	2.35	0.61
1:C:256:ALA:O	1:C:259:ILE:CB	2.49	0.60
1:B:181:GLY:O	1:B:212:MET:HE3	2.01	0.60
1:B:253:ILE:HG22	1:B:306:VAL:HG11	1.83	0.60
1:A:495:PHE:HB3	1:A:509:MET:HG2	1.83	0.60
1:C:337:PRO:O	1:C:338:ARG:CB	2.41	0.60
1:A:249:VAL:HG23	1:A:276:ALA:HB2	1.83	0.60
1:B:464:SER:HB2	1:B:539:MET:HE3	1.83	0.60
1:B:259:ILE:O	1:B:265:ARG:NH1	2.34	0.60
1:A:245:MET:CE	1:A:299:PHE:HA	2.31	0.60
1:A:340:HIS:CE1	1:A:554:ALA:HB3	2.36	0.60
1:A:238:THR:HG22	1:A:290:TYR:OH	2.02	0.60
1:A:536:LEU:HA	1:A:539:MET:HE3	1.83	0.60
1:A:364:GLU:HG2	1:A:426:THR:CG2	2.28	0.59
1:C:67:THR:HG21	1:C:74:PRO:CD	2.32	0.59
1:B:3:ASP:O	1:B:4:ILE:HG13	2.01	0.59
1:A:304:ALA:O	1:A:308:ARG:HG3	2.03	0.59
1:B:287:PRO:HD2	1:B:288:THR:HG23	1.82	0.59
1:B:284:ASP:CA	1:B:285:GLU:HB3	2.29	0.59
1:A:401:ARG:CZ	1:A:405:HIS:CE1	2.85	0.59
1:C:264:ASP:O	1:C:267:GLU:N	2.36	0.59
1:A:315:GLY:O	1:A:322:ASP:HA	2.03	0.59
1:A:412:ALA:O	1:A:505:THR:HG21	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:64:GLN:HE21	1:B:116:THR:HG23	1.68	0.59
1:B:99:ILE:HD13	1:B:149:ILE:CD1	2.32	0.58
1:C:550:VAL:HG21	1:C:555:PRO:HB3	1.85	0.58
1:B:274:LYS:CD	1:B:277:ILE:CG2	2.70	0.58
1:C:509:MET:CE	1:C:521:MET:SD	2.91	0.58
1:B:464:SER:CB	1:B:539:MET:HE1	2.34	0.58
1:B:260:GLN:HA	1:B:265:ARG:NH1	2.18	0.58
1:B:470:LEU:HD13	1:B:479:VAL:HG13	1.85	0.58
1:C:67:THR:HG21	1:C:74:PRO:HD3	1.85	0.58
1:C:531:GLY:HA3	4:C:2020:HOH:O	2.03	0.58
1:A:6:ARG:HD3	1:A:221:ASP:HB3	1.85	0.58
1:A:275:LYS:O	1:A:278:ALA:N	2.36	0.58
1:A:412:ALA:HA	1:A:505:THR:CG2	2.34	0.58
1:B:277:ILE:O	1:B:280:LEU:N	2.37	0.58
1:A:83:ARG:HG3	1:A:83:ARG:NH1	2.12	0.58
1:B:253:ILE:HG21	1:B:306:VAL:HG11	1.84	0.58
1:B:303:GLU:HA	1:B:306:VAL:HG12	1.86	0.57
1:A:176:ASP:O	1:A:191:SER:HA	2.04	0.57
1:A:479:VAL:HG23	1:A:527:GLN:NE2	2.19	0.57
1:B:4:ILE:HG22	1:B:222:LEU:HD11	1.87	0.57
2:G:896:TRP:N	2:G:897:ARG:HA	2.19	0.57
1:A:260:GLN:O	1:A:261:LYS:C	2.42	0.57
1:A:262:LYS:O	1:A:263:GLN:C	2.42	0.57
1:C:317:ARG:HG3	1:C:321:ARG:O	2.04	0.57
1:B:499:GLY:HA2	1:B:505:THR:HB	1.87	0.57
1:A:274:LYS:NZ	1:A:277:ILE:HD13	2.20	0.56
1:A:333:VAL:HG11	1:A:543:MET:HG3	1.86	0.56
1:A:200:ILE:CD1	1:B:200:ILE:HD11	2.32	0.56
1:C:93:ARG:HH12	1:C:401:ARG:HA	1.69	0.56
1:A:236:GLU:C	1:A:238:THR:H	2.08	0.56
1:B:303:GLU:C	1:B:306:VAL:HG12	2.23	0.56
1:B:414:ARG:N	1:B:415:PRO:CD	2.67	0.56
1:A:277:ILE:HG23	1:A:278:ALA:N	2.20	0.56
1:A:416:MET:HE3	1:A:461:ARG:HB2	1.83	0.56
1:B:64:GLN:NE2	1:B:116:THR:HG23	2.20	0.56
1:B:282:LEU:CB	1:B:287:PRO:O	2.50	0.56
1:A:535:ILE:HG22	1:A:539:MET:HE2	1.88	0.56
1:B:97:ARG:CZ	1:B:188:MET:HE1	2.35	0.56
1:B:147:GLY:HA2	2:G:896:TRP:O	2.06	0.56
1:A:125:ASP:OD1	1:A:126:PRO:HD2	2.05	0.56
1:A:285:GLU:O	1:A:286:ASN:ND2	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:282:LEU:HA	1:B:284:ASP:O	2.05	0.55
1:B:28:ASP:HB2	1:B:44:ALA:O	2.07	0.55
1:B:315:GLY:O	1:B:322:ASP:HA	2.07	0.55
1:B:291:ASP:O	1:B:293:LEU:CA	2.52	0.55
1:C:333:VAL:HG11	1:C:543:MET:CE	2.37	0.55
1:A:266:TYR:O	1:A:269:VAL:N	2.39	0.55
1:C:246:LYS:O	1:C:247:ASP:C	2.43	0.55
1:A:310:GLY:O	1:A:313:ASP:O	2.24	0.55
1:C:439:SER:HB2	1:C:467:ALA:HB2	1.88	0.55
1:B:181:GLY:CA	1:B:212:MET:HE1	2.37	0.55
1:C:86:GLU:O	1:C:90:LEU:HB2	2.07	0.55
1:B:284:ASP:HA	1:B:285:GLU:CB	2.16	0.55
1:C:493:MET:SD	1:C:516:ILE:HD13	2.47	0.55
1:B:381:HIS:CD2	1:B:428:ARG:HH21	2.25	0.55
1:B:416:MET:HE3	1:B:461:ARG:HB2	1.83	0.55
1:A:261:LYS:O	1:A:262:LYS:C	2.45	0.55
1:B:193:ILE:HD13	1:B:201:VAL:HG21	1.89	0.55
1:A:277:ILE:CG2	1:A:278:ALA:N	2.70	0.54
1:C:490:LEU:O	1:C:490:LEU:HG	2.06	0.54
1:B:263:GLN:O	1:B:265:ARG:N	2.41	0.54
1:B:439:SER:HB2	1:B:467:ALA:HB2	1.90	0.54
1:A:275:LYS:O	1:A:277:ILE:N	2.40	0.54
1:B:464:SER:CB	1:B:539:MET:CE	2.85	0.54
1:B:102:LEU:CD1	1:B:149:ILE:HD11	2.33	0.54
1:A:261:LYS:O	1:A:262:LYS:O	2.25	0.54
1:A:249:VAL:HG21	1:A:276:ALA:CB	2.38	0.54
1:C:98:PRO:HD3	1:C:188:MET:HG2	1.89	0.54
1:C:36:GLY:O	1:C:37:GLU:HB2	2.08	0.54
1:A:368:ASP:N	1:A:368:ASP:OD1	2.37	0.54
1:A:281:GLY:N	1:A:289:GLY:O	2.39	0.54
1:A:431:SER:OG	1:A:444:THR:CG2	2.56	0.54
1:C:377:SER:HA	1:C:426:THR:HG23	1.89	0.54
1:B:100:ARG:HB3	1:B:101:PRO:HD3	1.90	0.54
1:C:20:THR:HG21	1:C:140:LEU:HD21	1.89	0.54
1:C:416:MET:HE3	1:C:460:VAL:HB	1.90	0.54
1:C:509:MET:HE3	1:C:521:MET:SD	2.48	0.54
1:A:127:ASP:OD1	1:A:128:ILE:N	2.41	0.54
1:C:330:LEU:O	1:C:346:THR:HG22	2.09	0.53
1:A:274:LYS:HA	1:A:277:ILE:HG21	1.91	0.53
1:A:464:SER:HB3	1:A:539:MET:CE	2.33	0.53
1:C:22:ARG:HG2	1:C:23:ILE:HG13	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:529:LYS:HE2	1:B:502:GLU:OE2	2.08	0.53
1:C:93:ARG:NH1	1:C:401:ARG:HA	2.24	0.53
1:B:246:LYS:O	1:B:250:GLY:N	2.41	0.53
1:B:181:GLY:CA	1:B:212:MET:CE	2.87	0.53
1:C:32:LEU:HD11	1:C:39:VAL:CG2	2.39	0.53
1:B:145:PHE:HZ	1:B:149:ILE:HD12	1.74	0.53
1:B:470:LEU:HD13	1:B:479:VAL:CG1	2.39	0.53
1:A:287:PRO:HA	1:A:288:THR:CG2	2.25	0.53
1:A:195:GLU:HA	1:A:504:LEU:O	2.09	0.53
1:A:401:ARG:CD	4:A:2078:HOH:O	2.55	0.53
1:A:175:MET:CE	1:A:196:LEU:HD12	2.39	0.53
1:C:259:ILE:O	1:C:260:GLN:O	2.27	0.52
1:A:329:ILE:CG1	1:A:347:ARG:HG3	2.39	0.52
1:B:313:ASP:O	1:B:314:THR:OG1	2.13	0.52
1:C:531:GLY:O	1:C:534:HIS:HB3	2.09	0.52
1:A:157:VAL:HG13	1:A:162:VAL:HG11	1.90	0.52
1:A:274:LYS:CE	1:A:277:ILE:HG21	2.34	0.52
1:B:416:MET:HE2	1:B:461:ARG:CB	2.39	0.52
1:B:193:ILE:HD13	1:B:201:VAL:CG2	2.39	0.52
1:C:163:LEU:HD13	1:C:211:GLN:HG2	1.91	0.52
1:A:253:ILE:HD11	1:A:299:PHE:HE1	1.75	0.52
1:A:493:MET:HE1	1:A:509:MET:CE	2.33	0.52
1:A:440:SER:O	1:A:444:THR:HG23	2.10	0.52
1:A:412:ALA:O	1:A:505:THR:CG2	2.58	0.52
1:B:280:LEU:N	1:B:280:LEU:HD12	2.24	0.51
1:C:249:VAL:CG2	1:C:276:ALA:CB	2.88	0.51
1:B:317:ARG:HD2	1:B:487:GLU:OE2	2.11	0.51
1:B:263:GLN:O	1:B:266:TYR:CA	2.58	0.51
1:A:181:GLY:CA	1:A:212:MET:HE3	2.40	0.51
1:A:479:VAL:CG2	1:A:527:GLN:OE1	2.58	0.51
1:A:427:ILE:HD13	1:A:452:MET:HE3	1.91	0.51
1:A:429:LEU:HD21	1:A:452:MET:HG3	1.92	0.51
1:A:175:MET:HE2	1:A:196:LEU:HD12	1.92	0.51
1:A:157:VAL:CG1	1:A:162:VAL:HG11	2.40	0.51
1:A:35:MET:HB2	1:A:129:LEU:HD13	1.92	0.51
1:A:502:GLU:OE2	1:B:529:LYS:CE	2.55	0.51
1:A:453:MET:CB	1:A:543:MET:HE2	2.41	0.51
1:B:89:THR:HG23	1:B:400:ARG:HG2	1.93	0.51
1:B:298:ILE:N	1:B:298:ILE:HD13	2.25	0.51
1:A:479:VAL:HG23	1:A:527:GLN:OE1	2.11	0.51
1:C:416:MET:HE2	1:C:461:ARG:HB2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:416:MET:CE	1:C:461:ARG:HB2	2.41	0.51
1:A:321:ARG:HB3	1:A:325:THR:HB	1.91	0.51
1:A:260:GLN:O	1:A:261:LYS:O	2.28	0.51
1:A:28:ASP:HB2	1:A:44:ALA:O	2.10	0.51
1:A:453:MET:HB3	1:A:543:MET:HE1	1.88	0.50
1:B:274:LYS:CD	1:B:277:ILE:CD1	2.72	0.50
1:B:293:LEU:C	1:B:295:LEU:H	2.14	0.50
1:C:358:LEU:HD21	1:C:457:VAL:HG11	1.94	0.50
1:B:256:ALA:O	1:B:259:ILE:HB	2.11	0.50
1:A:265:ARG:O	1:A:266:TYR:O	2.29	0.50
1:C:39:VAL:HG13	1:C:119:GLN:HB3	1.90	0.50
1:A:236:GLU:CB	1:A:238:THR:HG23	2.38	0.50
1:C:249:VAL:HG22	1:C:276:ALA:HB2	1.91	0.50
1:B:311:ILE:O	1:B:314:THR:O	2.29	0.50
1:B:416:MET:CE	1:B:500:THR:HG21	2.41	0.50
1:C:329:ILE:CG1	1:C:347:ARG:HG3	2.41	0.50
1:B:154:VAL:CG2	1:B:208:ALA:HB2	2.42	0.50
1:C:340:HIS:HE1	1:C:554:ALA:H	1.59	0.50
1:B:99:ILE:HD13	1:B:149:ILE:HD12	1.94	0.50
1:B:381:HIS:HD2	1:B:428:ARG:HH21	1.59	0.50
1:C:439:SER:HA	3:C:1556:PO4:P	2.51	0.50
1:A:523:GLN:O	1:A:526:ALA:N	2.44	0.50
1:A:535:ILE:HG22	1:A:539:MET:CE	2.42	0.50
1:A:401:ARG:HE	1:A:405:HIS:HE1	1.59	0.50
1:C:131:MET:HE1	1:C:151:ALA:HB1	1.93	0.50
1:B:97:ARG:NH2	1:B:188:MET:CE	2.68	0.50
1:C:416:MET:CE	1:C:460:VAL:HB	2.42	0.49
1:C:181:GLY:O	1:C:212:MET:HE3	2.12	0.49
1:C:38:THR:OG1	1:C:121:ASP:N	2.34	0.49
1:C:39:VAL:HG13	1:C:119:GLN:CB	2.42	0.49
1:B:308:ARG:HB3	1:B:471:ILE:HG21	1.93	0.49
1:C:370:LEU:C	1:C:372:GLY:H	2.15	0.49
1:B:286:ASN:H	1:B:287:PRO:C	2.14	0.49
1:B:275:LYS:C	1:B:277:ILE:N	2.53	0.49
1:A:493:MET:HE1	1:A:509:MET:HE3	1.92	0.49
1:C:-1:ASP:O	1:C:0:PRO:C	2.49	0.49
1:B:264:ASP:HA	1:B:267:GLU:CB	2.42	0.49
1:B:9:ILE:HG21	1:B:16:LEU:HD23	1.93	0.49
1:A:274:LYS:HA	1:A:277:ILE:CG2	2.43	0.49
1:A:278:ALA:CA	1:A:282:LEU:HD13	2.42	0.49
1:C:509:MET:HE1	1:C:521:MET:SD	2.51	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:403:ILE:HA	4:A:2080:HOH:O	2.12	0.49
1:A:340:HIS:HB2	1:A:356:ALA:O	2.13	0.48
1:A:263:GLN:O	1:A:264:ASP:C	2.52	0.48
1:A:460:VAL:O	1:A:461:ARG:HG3	2.13	0.48
1:A:99:ILE:CG2	1:A:103:PHE:HE1	2.26	0.48
1:B:181:GLY:C	1:B:212:MET:HE3	2.34	0.48
1:C:330:LEU:O	1:C:346:THR:CG2	2.61	0.48
1:B:237:ASP:OD1	1:B:239:ASP:HB2	2.12	0.48
1:C:193:ILE:CG2	1:C:196:LEU:HB2	2.43	0.48
1:B:281:GLY:O	1:B:289:GLY:O	2.32	0.48
1:B:427:ILE:HG21	1:B:452:MET:HE2	1.95	0.48
1:C:531:GLY:CA	4:C:2020:HOH:O	2.58	0.48
1:B:551:GLY:O	1:B:552:ASP:C	2.51	0.48
1:B:8:THR:O	1:B:9:ILE:C	2.48	0.48
1:A:452:MET:HE1	1:A:457:VAL:HG21	1.95	0.48
1:A:335:ILE:HG13	1:A:336:LEU:N	2.28	0.48
1:A:377:SER:CB	1:A:426:THR:HG22	2.41	0.48
1:B:535:ILE:HG22	1:B:539:MET:HE2	1.93	0.48
1:C:333:VAL:HG12	1:C:334:GLY:N	2.28	0.48
1:A:165:PRO:HG2	1:A:170:MET:SD	2.53	0.48
1:C:468:MET:HB2	1:C:495:PHE:CZ	2.48	0.48
1:C:370:LEU:O	1:C:372:GLY:N	2.47	0.48
1:A:414:ARG:N	1:A:415:PRO:HD2	2.28	0.48
1:C:195:GLU:OE2	1:C:461:ARG:NH1	2.47	0.48
1:A:282:LEU:N	1:A:292:PRO:HG3	2.25	0.47
1:A:181:GLY:C	1:A:212:MET:CE	2.82	0.47
1:B:468:MET:HB2	1:B:495:PHE:CZ	2.48	0.47
1:A:263:GLN:O	1:A:265:ARG:N	2.47	0.47
1:B:4:ILE:HG22	1:B:222:LEU:CD1	2.43	0.47
1:A:220:ILE:HG12	2:F:896:TRP:CD1	2.50	0.47
1:A:273:LYS:HB2	1:A:299:PHE:CE2	2.50	0.47
1:B:303:GLU:CA	1:B:306:VAL:HG12	2.43	0.47
1:C:109:ASN:ND2	1:C:109:ASN:N	2.61	0.47
1:C:336:LEU:HB2	1:C:342:SER:HB3	1.97	0.47
1:C:516:ILE:HG22	1:C:521:MET:HG3	1.96	0.47
1:A:401:ARG:NH2	1:A:405:HIS:HE1	2.12	0.47
1:B:414:ARG:N	1:B:415:PRO:HD2	2.29	0.47
1:C:346:THR:HB	1:C:351:GLN:HG3	1.96	0.47
1:C:513:ILE:HD12	1:C:514:ALA:O	2.13	0.47
1:A:277:ILE:HG23	1:A:282:LEU:HD11	1.96	0.47
1:B:295:LEU:HA	1:B:298:ILE:HG12	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:54:GLN:NE2	1:C:56:PHE:CE1	2.82	0.47
1:B:543:MET:O	1:B:545:ALA:N	2.45	0.47
1:C:197:SER:H	1:C:200:ILE:HD12	1.79	0.47
1:B:125:ASP:OD1	1:B:126:PRO:HD2	2.14	0.47
1:C:338:ARG:HG2	1:C:553:PHE:CE1	2.50	0.47
1:C:8:THR:O	1:C:9:ILE:CB	2.63	0.47
1:C:65:GLU:HB3	1:C:370:LEU:HD11	1.95	0.47
1:A:8:THR:C	1:A:9:ILE:HD13	2.35	0.47
1:B:8:THR:HG23	1:B:9:ILE:H	1.80	0.47
1:B:279:ALA:C	1:B:282:LEU:HD21	2.26	0.46
1:C:446:CYS:SG	4:C:2015:HOH:O	2.50	0.46
1:A:0:PRO:O	1:A:1:MET:HB2	2.15	0.46
1:B:274:LYS:CB	1:B:277:ILE:HG21	2.44	0.46
1:C:381:HIS:CD2	1:C:428:ARG:HH11	2.22	0.46
1:C:466:ILE:HG12	1:C:467:ALA:N	2.31	0.46
1:C:418:PRO:HG3	1:C:458:PRO:HD2	1.96	0.46
1:B:261:LYS:C	1:B:262:LYS:O	2.52	0.46
1:A:9:ILE:HG22	1:A:11:TRP:HB2	1.98	0.46
1:B:89:THR:CG2	1:B:400:ARG:HG2	2.46	0.46
1:A:139:CYS:HA	4:A:2030:HOH:O	2.15	0.46
1:B:207:PHE:O	1:B:211:GLN:HG2	2.15	0.46
1:B:280:LEU:N	1:B:280:LEU:CD1	2.79	0.46
1:B:266:TYR:C	1:B:266:TYR:CD1	2.89	0.46
1:C:131:MET:HE2	1:C:151:ALA:HB2	1.97	0.46
1:C:237:ASP:C	1:C:239:ASP:H	2.19	0.46
1:A:299:PHE:O	1:A:302:LEU:N	2.48	0.46
1:A:265:ARG:O	1:A:266:TYR:C	2.52	0.46
1:A:109:ASN:N	1:A:109:ASN:HD22	2.14	0.46
1:C:551:GLY:O	1:C:552:ASP:C	2.52	0.46
1:C:127:ASP:OD1	1:C:128:ILE:N	2.47	0.46
1:A:373:THR:CG2	1:A:373:THR:O	2.63	0.46
1:A:90:LEU:HD13	1:A:407:LYS:HG2	1.97	0.46
1:C:31:VAL:O	1:C:41:LEU:HD12	2.16	0.46
1:C:330:LEU:HB3	1:C:346:THR:HG23	1.98	0.46
1:B:55:ASP:N	1:B:55:ASP:OD1	2.48	0.46
1:C:311:ILE:O	1:C:314:THR:O	2.33	0.46
1:B:286:ASN:N	1:B:287:PRO:CA	2.79	0.45
1:B:83:ARG:CG	1:B:83:ARG:HH11	2.28	0.45
1:B:127:ASP:O	1:B:131:MET:HG3	2.16	0.45
1:C:181:GLY:CA	1:C:212:MET:HE1	2.46	0.45
1:A:74:PRO:O	1:A:79:LYS:HD3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:224:GLU:O	2:F:892:ARG:HD3	2.16	0.45
1:B:295:LEU:O	1:B:295:LEU:HG	2.16	0.45
1:A:9:ILE:HG13	1:A:218:ALA:HB2	1.98	0.45
1:C:174:LYS:O	1:C:194:GLN:HG3	2.16	0.45
1:B:462:PRO:HB2	1:B:536:LEU:HD11	1.99	0.45
1:B:61:VAL:HG22	1:B:113:VAL:CG1	2.47	0.45
1:B:3:ASP:HB2	4:B:2002:HOH:O	2.17	0.45
1:A:466:ILE:HD12	1:A:531:GLY:HA3	1.99	0.45
1:B:279:ALA:C	1:B:280:LEU:HD12	2.37	0.45
1:B:260:GLN:HA	1:B:265:ARG:HH12	1.82	0.45
1:A:543:MET:HB3	1:A:543:MET:HE3	1.92	0.45
1:A:416:MET:HE1	1:A:461:ARG:HB2	1.92	0.45
1:A:14:LYS:HD3	1:A:124:ASN:OD1	2.17	0.45
1:C:484:LEU:HB2	1:C:487:GLU:HG3	1.98	0.45
1:A:275:LYS:C	1:A:277:ILE:N	2.70	0.45
1:B:273:LYS:O	1:B:275:LYS:N	2.50	0.45
1:C:189:VAL:HB	1:C:509:MET:HB2	1.99	0.45
1:B:147:GLY:HA2	2:G:896:TRP:CA	2.47	0.45
1:A:175:MET:HE3	1:A:196:LEU:CD1	2.47	0.45
1:C:147:GLY:H	2:H:896:TRP:HA	1.82	0.45
1:A:179:VAL:HG12	1:A:180:ALA:N	2.32	0.45
1:B:198:GLU:O	1:B:202:LEU:HB2	2.17	0.45
1:A:202:LEU:HA	1:A:202:LEU:HD23	1.82	0.45
1:A:414:ARG:N	1:A:415:PRO:CD	2.80	0.45
1:A:236:GLU:O	1:A:238:THR:N	2.49	0.44
1:B:286:ASN:N	1:B:287:PRO:HA	2.31	0.44
1:A:7:LYS:C	1:A:8:THR:O	2.50	0.44
1:A:452:MET:CE	1:A:457:VAL:HG21	2.46	0.44
1:C:44:ALA:HB1	1:C:138:LEU:HD23	1.99	0.44
1:B:68:PHE:C	1:B:68:PHE:CD1	2.90	0.44
1:B:274:LYS:CG	1:B:277:ILE:HG21	2.46	0.44
1:C:206:ASN:OD1	1:C:518:PRO:HG3	2.18	0.44
1:A:284:ASP:C	1:A:286:ASN:H	2.20	0.44
1:C:166:THR:HG23	1:C:169:GLU:OE2	2.18	0.44
1:A:420:LYS:HA	1:A:420:LYS:HD3	1.77	0.44
1:A:266:TYR:O	1:A:268:ALA:N	2.51	0.44
1:B:368:ASP:N	1:B:368:ASP:OD1	2.50	0.44
1:A:3:ASP:N	1:A:3:ASP:OD1	2.50	0.44
1:B:63:TYR:HD2	1:B:115:VAL:HG22	1.82	0.44
1:B:401:ARG:HH21	1:B:405:HIS:HE1	1.65	0.44
1:B:401:ARG:NH2	1:B:405:HIS:HE1	2.14	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:94:LEU:HA	1:B:94:LEU:HD12	1.75	0.44
1:B:509:MET:HE2	1:B:511:ILE:HD11	1.99	0.44
1:B:303:GLU:HA	1:B:306:VAL:CG1	2.48	0.44
1:B:535:ILE:HG22	1:B:539:MET:HE3	1.96	0.44
1:B:347:ARG:NH2	1:B:439:SER:O	2.51	0.44
1:B:283:SER:N	1:B:284:ASP:C	2.71	0.44
1:B:427:ILE:HD13	1:B:452:MET:CE	2.48	0.44
1:A:7:LYS:O	1:A:9:ILE:N	2.50	0.44
1:A:1:MET:HG2	1:A:22:ARG:HA	1.99	0.44
1:B:307:VAL:O	1:B:311:ILE:HG13	2.18	0.43
1:B:246:LYS:HA	1:B:302:LEU:HD21	2.00	0.43
1:A:472:LEU:HD12	1:A:477:PHE:HB3	1.99	0.43
1:C:553:PHE:O	1:C:553:PHE:CD1	2.71	0.43
1:A:55:ASP:HB3	1:A:56:PHE:HD1	1.83	0.43
1:A:177:LEU:CD1	1:A:191:SER:HB3	2.40	0.43
1:B:248:LEU:HG	1:B:249:VAL:HG23	1.99	0.43
1:C:246:LYS:O	1:C:250:GLY:N	2.50	0.43
1:B:35:MET:HE3	1:B:129:LEU:HB2	2.00	0.43
1:C:198:GLU:OE2	1:C:532:ARG:NH2	2.47	0.43
1:A:516:ILE:HG22	1:A:521:MET:HG2	2.01	0.43
1:A:275:LYS:CG	1:A:276:ALA:N	2.76	0.43
1:B:263:GLN:CG	1:B:264:ASP:H	2.04	0.43
1:C:256:ALA:O	1:C:259:ILE:N	2.50	0.43
1:C:345:PHE:O	1:C:351:GLN:HA	2.19	0.43
1:C:329:ILE:HG13	1:C:347:ARG:HG3	2.00	0.43
1:C:131:MET:CE	1:C:151:ALA:CB	2.97	0.43
1:B:551:GLY:O	1:B:552:ASP:O	2.37	0.43
1:B:283:SER:N	1:B:285:GLU:N	2.67	0.43
1:B:338:ARG:HA	1:B:553:PHE:CE1	2.38	0.43
1:C:180:ALA:O	1:C:187:MET:N	2.42	0.43
1:C:303:GLU:O	1:C:307:VAL:HG12	2.18	0.43
1:B:107:PHE:CZ	1:B:109:ASN:HB2	2.54	0.43
1:A:7:LYS:HG2	1:A:17:VAL:HG13	2.01	0.42
1:B:65:GLU:HG3	1:B:88:GLU:HG2	2.01	0.42
1:A:543:MET:O	1:A:545:ALA:N	2.44	0.42
1:C:329:ILE:HG12	1:C:347:ARG:HG3	2.01	0.42
1:C:466:ILE:CG1	1:C:467:ALA:N	2.83	0.42
1:A:249:VAL:HG12	1:A:253:ILE:HG13	2.00	0.42
1:B:145:PHE:CZ	1:B:149:ILE:HD12	2.54	0.42
1:B:381:HIS:HD2	1:B:428:ARG:NE	2.12	0.42
1:C:94:LEU:HD12	1:C:97:ARG:HH22	1.80	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:490:LEU:O	1:B:490:LEU:HG	2.20	0.42
1:B:109:ASN:HD22	1:B:109:ASN:N	2.17	0.42
1:B:195:GLU:HA	1:B:504:LEU:O	2.19	0.42
1:B:273:LYS:C	1:B:275:LYS:H	2.23	0.42
1:A:201:VAL:HG21	1:A:504:LEU:HD12	2.02	0.42
1:B:286:ASN:CA	1:B:287:PRO:O	2.68	0.42
1:C:177:LEU:HD21	1:C:205:VAL:HG23	2.01	0.42
1:C:361:GLY:O	1:C:364:GLU:HG2	2.20	0.42
1:C:465:GLY:HA2	1:C:497:VAL:O	2.20	0.42
1:A:274:LYS:CA	1:A:274:LYS:CE	2.92	0.42
1:C:128:ILE:CD1	1:C:153:ARG:CB	2.95	0.42
1:B:99:ILE:O	1:B:100:ARG:C	2.58	0.42
1:A:265:ARG:HH22	1:A:318:ILE:CA	2.32	0.42
1:C:189:VAL:HB	1:C:509:MET:CB	2.50	0.41
1:B:468:MET:CB	1:B:495:PHE:CZ	3.03	0.41
1:A:121:ASP:O	1:A:122:LEU:HB2	2.20	0.41
1:A:274:LYS:HZ3	1:A:277:ILE:HD13	1.84	0.41
1:C:28:ASP:HB2	1:C:44:ALA:O	2.20	0.41
1:C:11:TRP:CZ3	1:C:215:VAL:HG21	2.56	0.41
1:C:453:MET:HG3	1:C:459:LEU:HD12	2.02	0.41
1:B:279:ALA:C	1:B:282:LEU:CD2	2.79	0.41
1:C:317:ARG:NH2	1:C:321:ARG:NH2	2.67	0.41
1:A:525:LEU:HA	1:A:525:LEU:HD23	1.81	0.41
1:C:156:TRP:HA	1:C:160:ALA:O	2.19	0.41
1:B:286:ASN:H	1:B:287:PRO:HA	1.85	0.41
1:A:8:THR:C	1:A:9:ILE:CG1	2.89	0.41
1:C:163:LEU:HD22	1:C:211:GLN:HG2	2.02	0.41
1:C:193:ILE:O	1:C:505:THR:HG22	2.20	0.41
1:C:380:LEU:HD21	1:C:444:THR:HG21	2.01	0.41
1:C:399:GLY:O	1:C:403:ILE:HG13	2.20	0.41
1:B:287:PRO:CB	1:B:288:THR:CA	2.77	0.41
1:C:553:PHE:HD1	1:C:553:PHE:O	2.03	0.41
1:B:553:PHE:HA	1:B:554:ALA:HA	1.72	0.41
1:C:163:LEU:O	1:C:164:ASN:C	2.59	0.41
1:A:135:SER:HB2	1:A:149:ILE:CG1	2.48	0.41
1:B:427:ILE:HG21	1:B:452:MET:CE	2.51	0.41
1:B:35:MET:HB2	1:B:129:LEU:HD13	2.01	0.41
1:B:544:ASP:C	1:B:544:ASP:OD1	2.59	0.41
1:C:334:GLY:HA2	1:C:342:SER:OG	2.20	0.41
1:A:277:ILE:CG2	1:A:278:ALA:H	2.34	0.41
1:A:401:ARG:NH2	1:A:405:HIS:CE1	2.87	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:127:ASP:OD1	1:A:128:ILE:HG12	2.21	0.41
1:A:281:GLY:O	1:A:292:PRO:CG	2.69	0.41
1:A:253:ILE:HD11	1:A:299:PHE:CE1	2.53	0.41
1:B:336:LEU:C	1:B:337:PRO:O	2.59	0.41
1:A:397[A]:SER:HA	1:A:398:PRO:HD2	1.93	0.41
1:B:450:LEU:HA	1:B:450:LEU:HD23	1.94	0.41
1:A:281:GLY:O	1:A:292:PRO:HG3	2.21	0.41
1:B:273:LYS:HD2	1:B:299:PHE:CD2	2.55	0.41
1:A:186:VAL:O	1:A:511:ILE:HD13	2.20	0.41
1:A:181:GLY:N	1:A:212:MET:CE	2.84	0.41
1:C:493:MET:CE	1:C:495:PHE:CD1	3.04	0.41
1:B:512:LYS:C	1:B:513:ILE:HG23	2.41	0.41
1:A:245:MET:CE	1:A:299:PHE:CA	2.98	0.41
1:B:286:ASN:H	1:B:287:PRO:CA	2.34	0.41
1:C:381:HIS:HD2	1:C:428:ARG:HD2	1.80	0.41
1:C:177:LEU:HD21	1:C:205:VAL:CG2	2.51	0.41
1:A:28:ASP:HB3	1:A:141:SER:HB2	2.03	0.41
1:C:46:PHE:CB	1:C:111:VAL:HG22	2.51	0.41
1:A:147:GLY:HA3	1:A:148:PRO:HA	1.86	0.41
1:A:538:GLU:HA	1:A:541:LYS:HD2	2.03	0.41
1:A:495:PHE:CZ	1:A:524:ALA:HB1	2.56	0.40
1:B:263:GLN:CG	1:B:264:ASP:N	2.70	0.40
1:C:256:ALA:HB1	1:C:268:ALA:HB3	2.02	0.40
1:A:308:ARG:NH2	1:A:473:GLU:OE2	2.55	0.40
1:B:308:ARG:CZ	1:B:471:ILE:HG23	2.51	0.40
1:B:191:SER:OG	1:B:507:LEU:O	2.40	0.40
1:B:269:VAL:CG1	1:B:270:GLY:N	2.83	0.40
1:B:99:ILE:HA	1:B:99:ILE:HD13	1.91	0.40
1:C:256:ALA:HB2	1:C:268:ALA:HB1	2.03	0.40
1:A:279:ALA:O	1:A:280:LEU:HD22	2.21	0.40
1:B:238:THR:HG22	1:B:290:TYR:OH	2.22	0.40
1:C:256:ALA:CB	1:C:268:ALA:HB1	2.51	0.40
1:B:15:THR:O	1:B:35:MET:HA	2.21	0.40
1:C:274:LYS:O	1:C:277:ILE:CB	2.70	0.40
1:A:439:SER:HA	3:A:1614:PO4:O1	2.22	0.40
1:B:446:CYS:SG	1:B:539:MET:HE1	2.62	0.40
1:C:333:VAL:HG13	1:C:454:ASP:HB2	2.03	0.40
1:B:349:GLU:OE1	1:B:437:ASN:ND2	2.54	0.40
1:C:517:THR:OG1	1:C:520:ILE:HG12	2.21	0.40
1:A:291:ASP:O	1:A:294:LYS:HB3	2.21	0.40
1:B:335:ILE:HG13	1:B:342:SER:OG	2.21	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)
1:A:8:THR:OG1	1:C:540:ASN:O[2_555]	1.87	0.33
1:B:6:ARG:NH2	1:C:224:GLU:OE2[3_565]	2.10	0.10

5.3 Torsion angles

5.3.1 Protein backbone

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

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	570/726 (78%)	502 (88%)	37 (6%)	31 (5%)	2	2
1	B	556/726 (77%)	490 (88%)	41 (7%)	25 (4%)	3	4
1	C	535/726 (74%)	476 (89%)	32 (6%)	27 (5%)	3	3
2	F	5/14 (36%)	4 (80%)	0	1 (20%)	0	0
2	G	6/14 (43%)	5 (83%)	0	1 (17%)	0	0
2	H	3/14 (21%)	2 (67%)	1 (33%)	0	100	100
All	All	1675/2220 (76%)	1479 (88%)	111 (7%)	85 (5%)	2	3

All (85) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	9	ILE
1	A	55	ASP
1	A	239	ASP
1	A	248	LEU
1	A	262	LYS
1	A	263	GLN
1	A	266	TYR
1	A	275	LYS
1	A	294	LYS
1	A	554	ALA
1	B	248	LEU

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Mol	Chain	Res	Type
1	B	264	ASP
1	B	276	ALA
1	B	278	ALA
1	B	287	PRO
1	B	290	TYR
1	B	291	ASP
1	B	292	PRO
1	B	552	ASP
1	B	554	ALA
1	C	8	THR
1	C	53	GLY
1	C	158	ASP
1	C	237	ASP
1	C	244	LYS
1	C	248	LEU
1	C	262	LYS
1	C	271	ALA
1	C	275	LYS
1	C	277	ILE
1	C	397	SER
1	C	544	ASP
1	A	54	GLN
1	A	246	LYS
1	A	261	LYS
1	A	264	ASP
1	A	267	GLU
1	A	276	ALA
1	A	278	ALA
1	A	284	ASP
1	A	318	ILE
1	A	396	GLY
1	B	261	LYS
1	B	262	LYS
1	B	269	VAL
1	B	273	LYS
1	B	274	LYS
1	B	277	ILE
1	B	396	GLY
1	B	439	SER
1	C	1	MET
1	C	9	ILE
1	C	36	GLY

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Mol	Chain	Res	Type
1	C	52	PRO
1	C	260	GLN
1	C	261	LYS
1	C	263	GLN
1	C	371	GLU
1	C	439	SER
1	A	244	LYS
1	A	280	LEU
1	A	283	SER
1	A	290	TYR
1	B	279	ALA
1	B	285	GLU
1	B	371	GLU
1	C	246	LYS
1	B	294	LYS
1	C	245	MET
1	C	273	LYS
1	C	314	THR
2	G	894	GLY
1	A	237	ASP
1	A	292	PRO
1	A	439	SER
1	A	552	ASP
1	B	267	GLU
1	B	397	SER
2	F	892	ARG
1	A	1	MET
1	A	281	GLY
1	B	52	PRO
1	C	51	LYS
1	C	250	GLY
1	A	555	PRO

5.3.2 Protein sidechains ⓘ

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

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	432/578 (75%)	401 (93%)	31 (7%)	18	35
1	B	428/578 (74%)	397 (93%)	31 (7%)	18	35
1	C	364/578 (63%)	348 (96%)	16 (4%)	35	63
2	F	5/12 (42%)	3 (60%)	2 (40%)	0	0
2	G	6/12 (50%)	5 (83%)	1 (17%)	3	4
2	H	2/12 (17%)	2 (100%)	0	100	100
All	All	1237/1770 (70%)	1156 (94%)	81 (6%)	21	42

All (81) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-1	ASP
1	A	1	MET
1	A	3	ASP
1	A	7	LYS
1	A	35	MET
1	A	54	GLN
1	A	55	ASP
1	A	60	THR
1	A	80	ARG
1	A	83	ARG
1	A	140	LEU
1	A	153	ARG
1	A	157	VAL
1	A	186	VAL
1	A	200	ILE
1	A	221	ASP
1	A	239	ASP
1	A	280	LEU
1	A	282	LEU
1	A	283	SER
1	A	290	TYR
1	A	312	LEU
1	A	355	VAL
1	A	401	ARG
1	A	430	VAL
1	A	457	VAL
1	A	463	VAL
1	A	481	SER
1	A	505	THR
1	A	553	PHE

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Mol	Chain	Res	Type
1	A	613	TRP
1	B	-1	ASP
1	B	1	MET
1	B	8	THR
1	B	10	GLU
1	B	31	VAL
1	B	64	GLN
1	B	83	ARG
1	B	120	HIS
1	B	177	LEU
1	B	178	VAL
1	B	188	MET
1	B	194	GLN
1	B	200	ILE
1	B	202	LEU
1	B	242	LYS
1	B	290	TYR
1	B	293	LEU
1	B	308	ARG
1	B	309	ARG
1	B	333	VAL
1	B	335	ILE
1	B	336	LEU
1	B	368	ASP
1	B	431	SER
1	B	445	VAL
1	B	449	SER
1	B	457	VAL
1	B	489	HIS
1	B	505	THR
1	B	518	PRO
1	B	553	PHE
1	C	34	THR
1	C	39	VAL
1	C	77	PHE
1	C	90	LEU
1	C	109	ASN
1	C	175	MET
1	C	188	MET
1	C	194	GLN
1	C	371	GLU
1	C	379	LEU

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Mol	Chain	Res	Type
1	C	445	VAL
1	C	448	SER
1	C	496	LYS
1	C	497	VAL
1	C	523	GLN
1	C	553	PHE
2	F	892	ARG
2	F	897	ARG
2	G	892	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	62	ASN
1	A	109	ASN
1	A	112	GLN
1	A	119	GLN
1	A	209	HIS
1	A	225	HIS
1	A	286	ASN
1	A	340	HIS
1	A	381	HIS
1	A	405	HIS
1	A	508	GLN
1	B	26	GLN
1	B	62	ASN
1	B	64	GLN
1	B	109	ASN
1	B	112	GLN
1	B	119	GLN
1	B	206	ASN
1	B	209	HIS
1	B	381	HIS
1	B	405	HIS
1	B	489	HIS
1	C	62	ASN
1	C	109	ASN
1	C	112	GLN
1	C	119	GLN
1	C	225	HIS
1	C	340	HIS
1	C	381	HIS

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 ⓘ

3 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	$\# Z > 2$
3	PO4	A	1614	-	4,4,4	0.25	0	6,6,6	0.33	0
3	PO4	B	1557	-	4,4,4	0.15	0	6,6,6	0.28	0
3	PO4	C	1556	-	4,4,4	0.31	0	6,6,6	0.29	0

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
3	PO4	A	1614	-	-	0/0/0/0	0/0/0/0
3	PO4	B	1557	-	-	0/0/0/0	0/0/0/0
3	PO4	C	1556	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1614	PO4	1	0
3	B	1557	PO4	1	0
3	C	1556	PO4	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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	573/726 (78%)	-0.09	25 (4%) 38 30	24, 34, 123, 161	0
1	B	558/726 (76%)	-0.23	12 (2%) 65 59	24, 33, 109, 147	0
1	C	539/726 (74%)	0.59	78 (14%) 3 2	53, 87, 184, 253	0
2	F	7/14 (50%)	0.56	1 (14%) 4 2	40, 67, 84, 94	0
2	G	8/14 (57%)	0.35	1 (12%) 5 3	37, 68, 86, 93	0
2	H	5/14 (35%)	0.33	0 100 100	82, 97, 103, 107	0
All	All	1690/2220 (76%)	0.09	117 (6%) 20 14	24, 49, 135, 253	0

All (117) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	276	ALA	6.3
1	C	270	GLY	6.2
1	C	269	VAL	5.7
1	C	297	ALA	5.5
1	C	271	ALA	5.4
1	C	268	ALA	5.4
1	A	605	ALA	5.2
1	C	0	PRO	5.2
1	A	613	TRP	5.2
1	A	611	ILE	5.2
1	C	278	ALA	4.9
1	C	233	PHE	4.7
1	A	247	ASP	4.7
1	C	253	ILE	4.6
1	C	553	PHE	4.5
1	C	240	ALA	4.5
1	A	278	ALA	4.5
1	C	265	ARG	4.5
1	C	251	ALA	4.4

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Mol	Chain	Res	Type	RSRZ
1	C	249	VAL	4.3
1	C	238	THR	4.2
1	C	237	ASP	4.2
1	A	251	ALA	4.2
1	C	421	GLU	4.1
1	A	259	ILE	4.0
1	C	277	ILE	4.0
1	C	158	ASP	4.0
1	C	299	PHE	4.0
1	C	301	GLU	3.9
1	C	275	LYS	3.9
1	C	298	ILE	3.9
1	C	472	LEU	3.8
1	C	304	ALA	3.8
1	A	612	ASP	3.8
1	C	263	GLN	3.7
1	C	262	LYS	3.7
1	A	279	ALA	3.7
1	C	266	TYR	3.7
1	C	8	THR	3.6
1	C	235	PRO	3.6
1	A	604	GLY	3.6
1	A	264	ASP	3.5
1	A	610	ALA	3.5
1	A	284	ASP	3.5
1	A	255	ALA	3.5
1	C	250	GLY	3.5
1	A	254	ALA	3.5
1	B	284	ASP	3.4
1	B	260	GLN	3.4
1	C	551	GLY	3.4
1	C	243	ALA	3.4
1	C	13	GLY	3.4
1	C	2	PHE	3.4
1	B	264	ASP	3.3
1	C	131	MET	3.3
2	F	893	ARG	3.2
1	C	232	ALA	3.1
1	C	475	ASP	3.1
1	B	288	THR	3.0
1	C	554	ALA	2.9
1	C	394	ARG	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	474	GLN	2.9
1	C	77	PHE	2.9
1	C	241	ILE	2.9
1	C	530	GLU	2.9
1	C	-1	ASP	2.9
1	A	609	ALA	2.9
1	C	397	SER	2.8
1	C	549	ASP	2.8
1	C	314	THR	2.8
1	C	236	GLU	2.8
1	C	272	ALA	2.7
1	A	603	ASP	2.7
1	A	263	GLN	2.7
1	A	292	PRO	2.7
1	C	248	LEU	2.6
1	B	263	GLN	2.6
1	C	264	ASP	2.5
1	C	302	LEU	2.5
1	A	271	ALA	2.5
1	B	259	ILE	2.5
1	C	300	LYS	2.5
1	C	129	LEU	2.4
1	C	486	ASP	2.4
1	A	282	LEU	2.4
1	A	608	LYS	2.4
1	B	279	ALA	2.4
1	C	396	GLY	2.4
1	C	476	GLY	2.4
1	C	323	VAL	2.4
1	A	269	VAL	2.4
1	C	430	VAL	2.3
1	B	299	PHE	2.3
1	C	252	ASP	2.3
1	C	322	ASP	2.3
1	B	268	ALA	2.3
1	C	422	ASP	2.3
1	C	244	LYS	2.3
1	B	286	ASN	2.3
1	C	76	GLY	2.3
1	C	274	LYS	2.3
1	B	548	ALA	2.2
1	A	293	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	242	LYS	2.2
1	C	168	ASP	2.2
1	C	267	GLU	2.2
1	C	53	GLY	2.2
1	C	303	GLU	2.1
1	A	266	TYR	2.1
1	C	258	LYS	2.1
1	C	355	VAL	2.1
1	C	247	ASP	2.1
1	B	282	LEU	2.1
2	G	893	ARG	2.1
1	C	37	GLU	2.1
1	C	503	GLY	2.0
1	C	514	ALA	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	PO4	C	1556	5/5	0.81	0.29	5.60	86,89,109,117	0
3	PO4	B	1557	5/5	0.97	0.11	-1.34	76,82,92,104	0
3	PO4	A	1614	5/5	0.96	0.12	-1.54	58,60,69,75	0

6.5 Other polymers [i](#)

There are no such residues in this entry.