



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:41 PM UTC

PDB ID : 3HP0 / pdb_00003hp0
Title : Crystal structure of a Putative polyketide biosynthesis enoyl-CoA hydratase (pksH) from *Bacillus subtilis*
Authors : Satyanarayana, L.; Eswaramoorthy, S.; Burley, S.K.; Swaminathan, S.; New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on : 2009-06-03
Resolution : 2.32 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

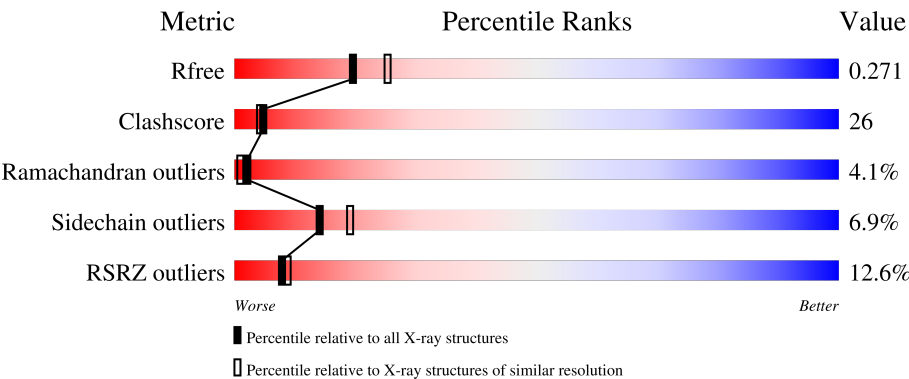
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.32 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}	180053	7754 (2.34-2.30)
Clashscore	190562	8383 (2.34-2.30)
Ramachandran outliers	187476	8303 (2.34-2.30)
Sidechain outliers	187428	8303 (2.34-2.30)
RSRZ outliers	180081	7760 (2.34-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	267	19% 47% 39% 7% 6%
1	B	267	3% 60% 29% • 6%
1	C	267	6% 59% 25% 7% • 6%
1	D	267	10% 46% 39% 9% 6%
1	E	267	11% 47% 39% 6% • 6%

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Mol	Chain	Length	Quality of chain
1	F	267	21% 52% 34% 7% 6%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 11858 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 Putative polyketide biosynthesis enoyl-CoA hydratase homolog pksH.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	250	Total	C	N	O	S	Se	0	0	0
			1836	1161	321	344	4	6			
1	B	251	Total	C	N	O	S	Se	0	0	0
			1995	1269	345	369	5	7			
1	C	251	Total	C	N	O	S	Se	0	0	0
			1995	1269	345	369	5	7			
1	D	251	Total	C	N	O	S	Se	0	0	0
			1995	1269	345	369	5	7			
1	E	251	Total	C	N	O	S	Se	0	0	0
			1995	1269	345	369	5	7			
1	F	251	Total	C	N	O	S	Se	0	0	0
			1833	1158	322	344	4	5			

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	-	expression tag	UNP P40805
A	2	SER	-	expression tag	UNP P40805
A	260	GLU	-	expression tag	UNP P40805
A	261	GLY	-	expression tag	UNP P40805
A	262	HIS	-	expression tag	UNP P40805
A	263	HIS	-	expression tag	UNP P40805
A	264	HIS	-	expression tag	UNP P40805
A	265	HIS	-	expression tag	UNP P40805
A	266	HIS	-	expression tag	UNP P40805
A	267	HIS	-	expression tag	UNP P40805
B	1	MSE	-	expression tag	UNP P40805
B	2	SER	-	expression tag	UNP P40805
B	260	GLU	-	expression tag	UNP P40805
B	261	GLY	-	expression tag	UNP P40805
B	262	HIS	-	expression tag	UNP P40805
B	263	HIS	-	expression tag	UNP P40805

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Chain	Residue	Modelled	Actual	Comment	Reference
B	264	HIS	-	expression tag	UNP P40805
B	265	HIS	-	expression tag	UNP P40805
B	266	HIS	-	expression tag	UNP P40805
B	267	HIS	-	expression tag	UNP P40805
C	1	MSE	-	expression tag	UNP P40805
C	2	SER	-	expression tag	UNP P40805
C	260	GLU	-	expression tag	UNP P40805
C	261	GLY	-	expression tag	UNP P40805
C	262	HIS	-	expression tag	UNP P40805
C	263	HIS	-	expression tag	UNP P40805
C	264	HIS	-	expression tag	UNP P40805
C	265	HIS	-	expression tag	UNP P40805
C	266	HIS	-	expression tag	UNP P40805
C	267	HIS	-	expression tag	UNP P40805
D	1	MSE	-	expression tag	UNP P40805
D	2	SER	-	expression tag	UNP P40805
D	260	GLU	-	expression tag	UNP P40805
D	261	GLY	-	expression tag	UNP P40805
D	262	HIS	-	expression tag	UNP P40805
D	263	HIS	-	expression tag	UNP P40805
D	264	HIS	-	expression tag	UNP P40805
D	265	HIS	-	expression tag	UNP P40805
D	266	HIS	-	expression tag	UNP P40805
D	267	HIS	-	expression tag	UNP P40805
E	1	MSE	-	expression tag	UNP P40805
E	2	SER	-	expression tag	UNP P40805
E	260	GLU	-	expression tag	UNP P40805
E	261	GLY	-	expression tag	UNP P40805
E	262	HIS	-	expression tag	UNP P40805
E	263	HIS	-	expression tag	UNP P40805
E	264	HIS	-	expression tag	UNP P40805
E	265	HIS	-	expression tag	UNP P40805
E	266	HIS	-	expression tag	UNP P40805
E	267	HIS	-	expression tag	UNP P40805
F	1	MSE	-	expression tag	UNP P40805
F	2	SER	-	expression tag	UNP P40805
F	260	GLU	-	expression tag	UNP P40805
F	261	GLY	-	expression tag	UNP P40805
F	262	HIS	-	expression tag	UNP P40805
F	263	HIS	-	expression tag	UNP P40805
F	264	HIS	-	expression tag	UNP P40805
F	265	HIS	-	expression tag	UNP P40805

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Chain	Residue	Modelled	Actual	Comment	Reference
F	266	HIS	-	expression tag	UNP P40805
F	267	HIS	-	expression tag	UNP P40805

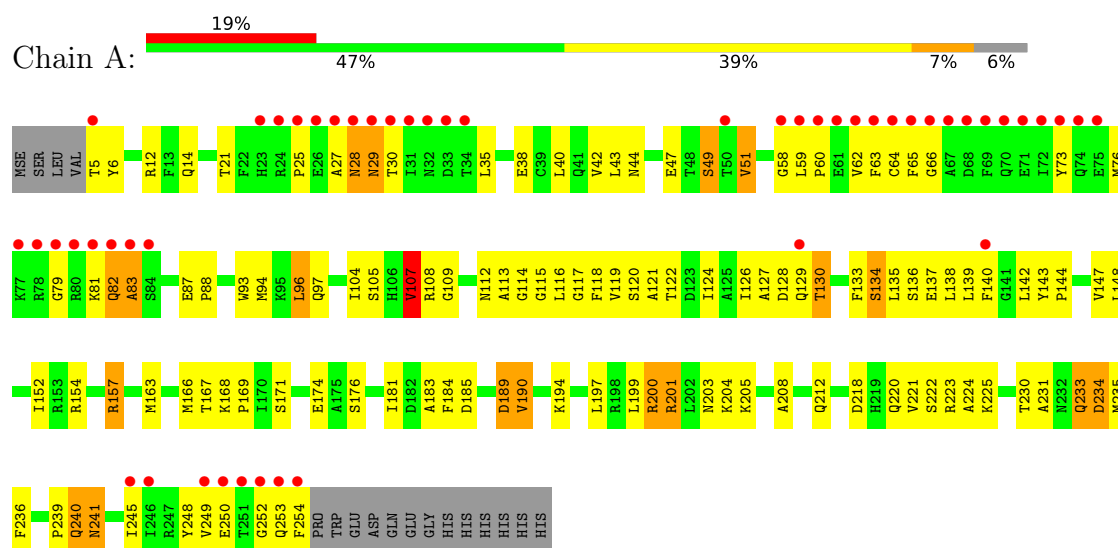
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	33	Total	O	0	0
			33	33		
2	B	44	Total	O	0	0
			44	44		
2	C	49	Total	O	0	0
			49	49		
2	D	23	Total	O	0	0
			23	23		
2	E	31	Total	O	0	0
			31	31		
2	F	29	Total	O	0	0
			29	29		

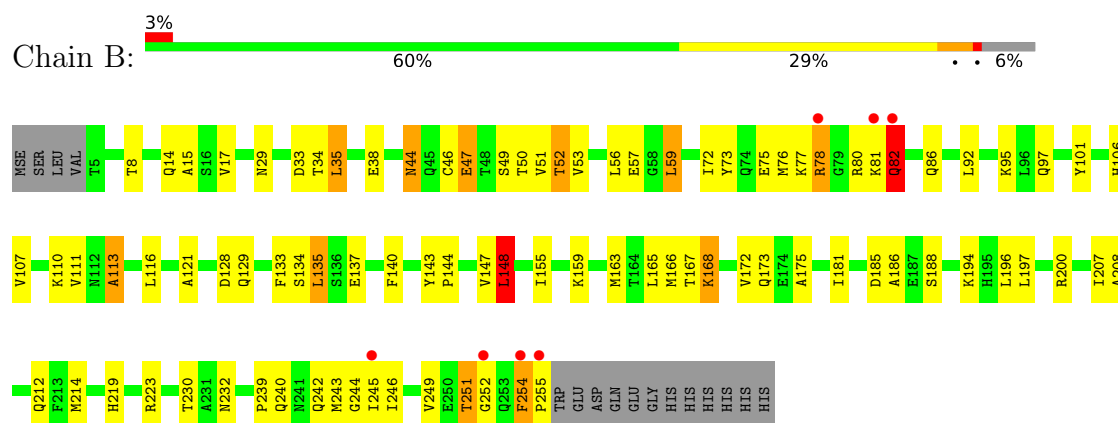
3 Residue-property plots [i](#)

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

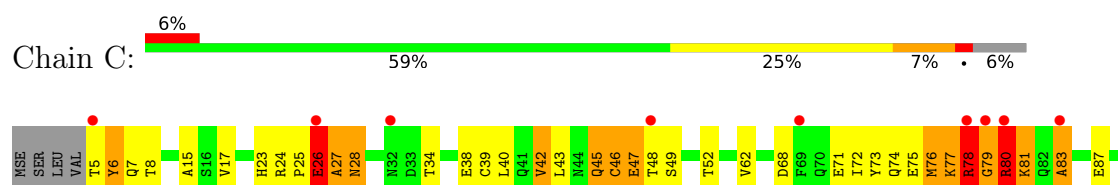
- Molecule 1: Putative polyketide biosynthesis enoyl-CoA hydratase homolog pksH



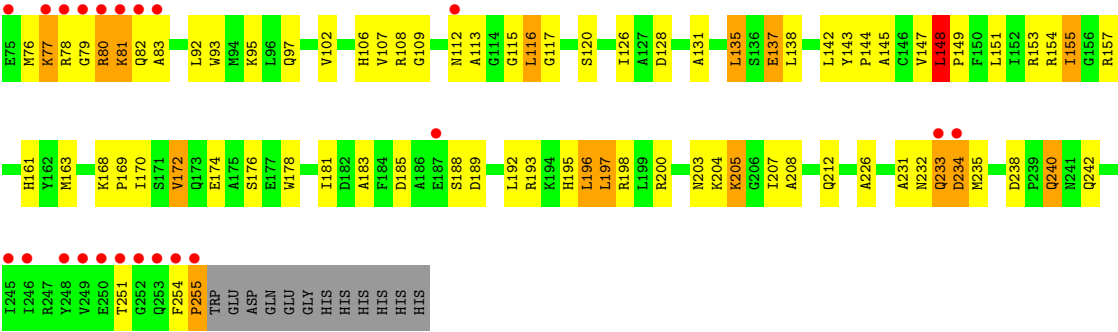
- Molecule 1: Putative polyketide biosynthesis enoyl-CoA hydratase homolog pksH



- Molecule 1: Putative polyketide biosynthesis enoyl-CoA hydratase homolog pksH







4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	80.91Å 80.91Å 218.59Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	43.09 – 2.32 43.09 – 2.32	Depositor EDS
% Data completeness (in resolution range)	96.4 (43.09-2.32) 93.4 (43.09-2.32)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.90 (at 2.32Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.232 , 0.270 0.232 , 0.271	Depositor DCC
R_{free} test set	5004 reflections (3.75%)	wwPDB-VP
Wilson B-factor (Å ²)	33.5	Xtriage
Anisotropy	0.146	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 44.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.010 for -h,-k,l 0.037 for h,-h-k,-l 0.058 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	11858	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.24% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	0.51	0/1859	1.13	17/2514 (0.7%)
1	B	0.50	0/2028	0.96	7/2732 (0.3%)
1	C	0.49	0/2028	1.05	13/2732 (0.5%)
1	D	0.43	0/2028	0.94	8/2732 (0.3%)
1	E	0.44	0/2028	1.02	12/2732 (0.4%)
1	F	0.46	0/1856	1.09	16/2511 (0.6%)
All	All	0.47	0/11827	1.03	73/15953 (0.5%)

There are no bond length outliers.

All (73) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	233	GLN	N-CA-C	-13.89	92.19	110.53
1	F	233	GLN	N-CA-C	-12.04	95.25	110.19
1	F	196	LEU	N-CA-C	-11.41	95.46	110.53
1	A	200	ARG	N-CA-C	-11.32	93.52	110.28
1	C	233	GLN	N-CA-C	-9.26	95.97	109.59
1	C	46	CYS	N-CA-C	-8.90	98.85	110.33
1	D	34	THR	N-CA-C	-8.69	101.29	112.23
1	F	107	VAL	N-CA-C	8.63	120.26	108.17
1	A	241	ASN	N-CA-C	-8.56	102.03	111.36
1	E	245	ILE	N-CA-C	-8.33	102.70	110.53
1	A	115	GLY	N-CA-C	-8.15	102.45	113.37
1	D	50	THR	N-CA-C	-7.79	103.34	112.92
1	C	107	VAL	N-CA-C	7.53	118.99	107.99
1	C	45	GLN	N-CA-C	-7.49	102.80	110.97
1	F	198	ARG	N-CA-C	-7.42	102.88	112.23
1	C	77	LYS	N-CA-C	-7.35	98.00	109.25
1	E	233	GLN	N-CA-C	-7.13	95.62	110.80
1	E	45	GLN	N-CA-C	-7.10	103.88	112.54
1	C	76	MSE	N-CA-C	-6.98	103.61	111.14
1	F	77	LYS	N-CA-C	-6.87	104.87	113.18
1	A	107	VAL	N-CA-C	6.81	118.40	108.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	155	ILE	N-CA-C	6.79	119.42	112.90
1	A	189	ASP	N-CA-C	-6.74	96.45	110.80
1	E	168	LYS	N-CA-C	6.72	118.36	109.83
1	F	60	PRO	N-CA-CB	6.70	110.28	103.25
1	D	107	VAL	N-CA-C	6.59	118.32	108.23
1	F	115	GLY	N-CA-C	-6.59	104.61	113.24
1	F	255	PRO	N-CA-CB	6.57	110.23	103.00
1	F	81	LYS	N-CA-C	-6.57	102.33	110.41
1	E	243	MSE	N-CA-C	-6.55	102.35	110.41
1	B	107	VAL	N-CA-C	6.50	117.95	108.58
1	F	25	PRO	N-CA-CB	6.48	110.06	103.25
1	E	115	GLY	N-CA-C	-6.46	107.57	114.67
1	B	110	LYS	N-CA-C	6.34	119.66	110.28
1	C	78	ARG	N-CA-C	-6.33	97.31	110.80
1	F	69	PHE	N-CA-C	-6.31	104.28	112.23
1	A	83	ALA	N-CA-C	6.25	118.61	110.43
1	E	166	MSE	N-CA-C	-6.23	100.42	110.32
1	D	8	THR	N-CA-C	-6.22	106.92	114.75
1	E	30	THR	N-CA-C	-6.14	102.61	110.53
1	C	238	ASP	CA-C-N	6.04	125.53	119.24
1	C	238	ASP	C-N-CA	6.04	125.53	119.24
1	A	25	PRO	N-CA-C	6.03	121.47	113.57
1	A	60	PRO	N-CA-CB	6.03	110.14	103.26
1	A	130	THR	N-CA-C	5.97	118.75	111.82
1	A	252	GLY	N-CA-C	5.93	122.27	112.66
1	E	50	THR	N-CA-C	-5.90	106.08	113.28
1	C	253	GLN	N-CA-C	5.83	123.21	110.80
1	E	254	PHE	N-CA-C	5.79	122.61	109.81
1	F	76	MSE	N-CA-C	-5.73	106.05	113.16
1	E	227	THR	N-CA-C	-5.70	105.07	111.28
1	D	115	GLY	N-CA-C	-5.68	107.29	114.16
1	C	157	ARG	N-CA-C	5.61	117.48	111.36
1	B	78	ARG	N-CA-C	-5.55	105.23	111.28
1	B	33	ASP	N-CA-C	5.50	118.03	111.71
1	A	190	VAL	N-CA-C	-5.42	105.25	110.72
1	A	143	TYR	CA-C-N	5.41	126.61	119.84
1	A	143	TYR	C-N-CA	5.41	126.61	119.84
1	C	15	ALA	CB-CA-C	-5.39	110.34	116.54
1	F	78	ARG	N-CA-C	-5.35	101.54	109.94
1	B	134	SER	N-CA-C	5.33	117.49	109.23
1	D	129	GLN	N-CA-C	-5.33	101.45	109.60
1	A	225	LYS	N-CA-C	5.27	117.45	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	148	LEU	N-CA-C	5.27	121.45	109.81
1	C	80	ARG	N-CA-C	5.24	121.96	110.80
1	F	32	ASN	N-CA-C	5.20	116.66	107.61
1	A	134	SER	N-CA-C	5.19	117.14	108.99
1	A	25	PRO	N-CA-CB	5.17	109.00	103.52
1	B	148	LEU	N-CA-C	5.16	120.58	113.77
1	E	31	ILE	N-CA-C	5.15	116.00	108.53
1	D	128	ASP	N-CA-C	-5.13	99.88	110.80
1	B	50	THR	N-CA-C	-5.11	106.82	113.16
1	D	155	ILE	N-CA-C	5.06	117.76	112.90

There are no chirality outliers.

There are no planarity outliers.

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	1836	0	1734	98	0
1	B	1995	0	1997	88	0
1	C	1995	0	1997	93	0
1	D	1995	0	1997	134	0
1	E	1995	0	1997	115	0
1	F	1833	0	1720	88	0
2	A	33	0	0	2	0
2	B	44	0	0	3	0
2	C	49	0	0	6	0
2	D	23	0	0	8	0
2	E	31	0	0	7	0
2	F	29	0	0	7	0
All	All	11858	0	11442	592	0

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 26.

All (592) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:76:MSE:HE3	1:D:242:GLN:HG3	1.39	1.02
1:B:82:GLN:HE21	1:E:219:HIS:HB3	1.25	1.01
1:F:205:LYS:H	1:F:205:LYS:HD2	1.19	1.01
1:D:254:PHE:HB2	1:D:255:PRO:CD	1.92	1.00
1:D:113:ALA:HB2	1:D:135:LEU:HA	1.39	1.00
1:E:113:ALA:HB2	1:E:135:LEU:HA	1.45	0.99
1:B:133:PHE:CZ	1:B:181:ILE:HD11	1.96	0.98
1:C:233:GLN:O	1:C:234:ASP:HB2	1.62	0.96
1:C:77:LYS:O	1:C:78:ARG:HB2	1.65	0.93
1:F:163:MSE:HE2	1:F:178:TRP:HZ3	1.34	0.92
1:E:136:SER:HA	1:E:167:THR:HG23	1.49	0.92
1:F:163:MSE:HE2	1:F:178:TRP:CZ3	2.07	0.90
1:A:233:GLN:O	1:A:234:ASP:HB2	1.74	0.86
1:E:81:LYS:O	1:E:82:GLN:HG3	1.75	0.85
1:B:76:MSE:HE1	1:B:242:GLN:HB3	1.60	0.84
1:E:76:MSE:HE1	1:E:242:GLN:HB3	1.59	0.84
1:D:52:THR:HG22	1:D:53:VAL:HG12	1.59	0.84
1:A:94:MSE:HE1	1:A:222:SER:HB3	1.58	0.84
1:F:196:LEU:O	1:F:197:LEU:HB3	1.75	0.84
1:A:12:ARG:HH11	1:A:14:GLN:NE2	1.75	0.83
1:B:81:LYS:C	1:B:82:GLN:HG3	2.04	0.83
1:D:76:MSE:CE	1:D:242:GLN:HG3	2.08	0.82
1:E:6:TYR:O	1:E:7:GLN:HB3	1.78	0.81
1:D:6:TYR:O	1:D:7:GLN:HB3	1.79	0.81
1:F:233:GLN:O	1:F:234:ASP:HB2	1.81	0.81
1:C:136:SER:HA	1:C:167:THR:HG23	1.63	0.79
1:D:46:CYS:HB3	1:D:51:VAL:HG11	1.63	0.79
1:A:66:GLY:HA2	1:A:114:GLY:HA3	1.66	0.78
1:B:144:PRO:HB2	1:B:147:VAL:HB	1.65	0.78
1:E:52:THR:HG21	2:E:271:HOH:O	1.82	0.78
1:C:139:LEU:HD11	1:C:167:THR:HG21	1.66	0.78
1:D:214:MSE:HE1	1:F:148:LEU:HG	1.66	0.78
1:D:32:ASN:ND2	1:D:34:THR:H	1.83	0.77
1:A:12:ARG:HD3	1:A:14:GLN:HE21	1.48	0.77
1:C:83:ALA:HB3	1:C:233:GLN:HG2	1.64	0.77
1:D:254:PHE:CD1	1:D:254:PHE:N	2.46	0.76
1:E:102:VAL:HG23	1:E:207:ILE:HD13	1.66	0.75
1:A:139:LEU:HD11	1:A:167:THR:HG21	1.69	0.75
1:A:168:LYS:HB3	1:E:198:ARG:NH1	2.01	0.75
1:F:197:LEU:HA	1:F:200:ARG:HD3	1.69	0.75
1:B:46:CYS:HB3	1:B:51:VAL:HG11	1.69	0.74
1:D:254:PHE:HB2	1:D:255:PRO:HD3	1.68	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:78:ARG:HG3	1:E:45:GLN:NE2	2.01	0.74
1:F:240:GLN:H	1:F:240:GLN:HE21	1.35	0.74
1:C:74:GLN:O	1:C:78:ARG:HD3	1.88	0.74
1:B:81:LYS:O	1:B:82:GLN:HG3	1.89	0.73
1:A:235:MSE:HE2	1:A:236:PHE:CE1	2.24	0.73
1:F:116:LEU:HD21	1:F:151:LEU:HD13	1.71	0.73
1:B:219:HIS:HB2	1:B:223:ARG:HH11	1.53	0.72
1:C:80:ARG:HG3	1:C:81:LYS:H	1.55	0.72
1:A:239:PRO:O	1:A:240:GLN:CB	2.38	0.72
1:B:49:SER:HB2	1:B:51:VAL:HG12	1.72	0.71
1:B:116:LEU:HD22	1:B:135:LEU:HD13	1.70	0.71
1:A:12:ARG:CD	1:A:14:GLN:HE21	2.03	0.71
1:D:197:LEU:HD12	1:D:200:ARG:HH12	1.56	0.71
1:E:49:SER:HB2	1:E:51:VAL:HG12	1.71	0.71
1:C:68:ASP:HB3	1:C:71:GLU:HB3	1.71	0.71
1:C:108:ARG:HG3	2:C:310:HOH:O	1.91	0.71
1:C:128:ASP:OD1	1:C:130:THR:HG22	1.89	0.70
1:F:144:PRO:HG2	1:F:148:LEU:HD22	1.73	0.70
1:C:6:TYR:HA	1:C:38:GLU:OE2	1.90	0.70
1:D:46:CYS:CB	1:D:51:VAL:HG11	2.21	0.70
1:E:136:SER:HA	1:E:167:THR:CG2	2.21	0.70
1:F:196:LEU:O	1:F:197:LEU:CB	2.40	0.70
1:C:167:THR:O	1:C:167:THR:HG22	1.92	0.70
1:A:116:LEU:HD23	1:A:135:LEU:HD21	1.74	0.69
1:D:214:MSE:CE	1:F:148:LEU:HG	2.23	0.69
1:D:230:THR:O	1:D:233:GLN:HB2	1.91	0.69
1:E:106:HIS:HD2	1:E:192:LEU:HD22	1.58	0.69
1:E:108:ARG:O	1:E:130:THR:HB	1.91	0.69
1:A:248:TYR:C	1:A:250:GLU:H	2.01	0.68
1:B:219:HIS:CB	1:B:223:ARG:HD3	2.22	0.68
1:D:73:TYR:HE1	1:D:246:ILE:HG23	1.57	0.68
1:C:46:CYS:O	1:C:47:GLU:CB	2.41	0.68
1:E:106:HIS:CD2	1:E:192:LEU:HD22	2.28	0.68
1:A:239:PRO:O	1:A:240:GLN:HB3	1.94	0.68
1:B:82:GLN:NE2	1:E:222:SER:HB3	2.09	0.68
1:D:197:LEU:HD12	1:D:200:ARG:NH1	2.08	0.68
1:F:128:ASP:HA	1:F:185:ASP:O	1.94	0.68
1:C:253:GLN:C	1:C:254:PHE:HD2	2.01	0.67
1:B:46:CYS:CB	1:B:51:VAL:HG11	2.23	0.67
1:B:106:HIS:HE1	1:B:188:SER:OG	1.77	0.67
1:B:78:ARG:HG3	1:D:45:GLN:OE1	1.95	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:254:PHE:CD1	1:B:254:PHE:N	2.61	0.67
1:D:34:THR:O	1:D:38:GLU:HG3	1.95	0.67
1:F:226:ALA:HB3	2:F:284:HOH:O	1.94	0.67
1:A:94:MSE:HE3	1:A:221:VAL:HG12	1.77	0.66
1:E:90:TYR:CE2	1:E:225:LYS:HB2	2.30	0.66
1:C:80:ARG:O	1:C:81:LYS:HB2	1.94	0.66
1:D:6:TYR:O	1:D:7:GLN:CB	2.42	0.66
1:D:76:MSE:HE2	1:D:246:ILE:HD11	1.77	0.66
1:A:59:LEU:CB	1:A:63:PHE:HA	2.26	0.66
1:D:128:ASP:HA	1:D:185:ASP:O	1.96	0.66
1:B:254:PHE:N	1:B:254:PHE:HD1	1.93	0.66
1:D:254:PHE:HB2	1:D:255:PRO:HD2	1.74	0.66
1:B:72:ILE:O	1:B:76:MSE:HG3	1.96	0.65
1:A:136:SER:HA	1:A:167:THR:HG23	1.79	0.65
1:B:144:PRO:HG2	1:B:148:LEU:HD22	1.79	0.65
1:B:116:LEU:HD21	1:B:163:MSE:HE1	1.79	0.65
1:E:75:GLU:O	1:E:80:ARG:HB3	1.97	0.65
1:D:38:GLU:O	1:D:42:VAL:HG23	1.97	0.65
1:E:76:MSE:CE	1:E:242:GLN:HB3	2.27	0.65
1:C:128:ASP:O	1:C:129:GLN:NE2	2.29	0.64
1:C:47:GLU:HA	1:C:100:PRO:HG2	1.79	0.64
1:B:17:VAL:HG22	1:B:53:VAL:CG2	2.28	0.64
1:C:34:THR:O	1:C:38:GLU:HG3	1.97	0.64
1:D:116:LEU:HD22	1:D:135:LEU:HD11	1.79	0.64
1:A:200:ARG:O	1:A:201:ARG:HB2	1.95	0.64
1:C:116:LEU:HD21	1:C:180:LEU:HD21	1.80	0.63
1:F:170:ILE:HG23	1:F:174:GLU:HB2	1.81	0.63
1:E:68:ASP:O	1:E:72:ILE:HG13	1.98	0.63
1:A:21:THR:HG23	1:A:58:GLY:HA3	1.80	0.63
1:D:254:PHE:CB	1:D:255:PRO:CD	2.71	0.63
1:B:208:ALA:O	1:B:212:GLN:HG3	1.99	0.63
1:C:5:THR:HG22	2:C:306:HOH:O	1.98	0.62
1:F:254:PHE:O	1:F:255:PRO:C	2.42	0.62
1:F:135:LEU:HG	1:F:144:PRO:HG3	1.82	0.62
1:F:145:ALA:O	1:F:149:PRO:HD3	2.00	0.62
1:E:254:PHE:CD1	1:E:254:PHE:N	2.66	0.62
1:B:44:ASN:O	1:B:47:GLU:HB2	1.99	0.62
1:D:242:GLN:HE21	1:D:242:GLN:HA	1.64	0.62
1:F:137:GLU:CD	1:F:137:GLU:H	2.06	0.62
1:B:17:VAL:HG13	1:B:53:VAL:HG23	1.80	0.62
1:A:200:ARG:O	1:A:201:ARG:CB	2.47	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:233:GLN:O	1:A:234:ASP:CB	2.48	0.62
1:B:76:MSE:HE1	1:B:242:GLN:CB	2.28	0.61
1:D:154:ARG:HH22	1:D:182:ASP:CG	2.08	0.61
1:A:197:LEU:O	1:A:200:ARG:HG2	2.00	0.61
1:F:143:TYR:CE1	1:F:235:MSE:HE2	2.36	0.61
1:D:49:SER:HB2	1:D:51:VAL:HG12	1.83	0.61
1:B:128:ASP:HA	1:B:185:ASP:O	2.01	0.61
1:F:13:PHE:CZ	1:F:45:GLN:NE2	2.69	0.61
1:D:245:ILE:O	1:D:249:VAL:HG23	2.00	0.60
1:A:49:SER:OG	1:A:51:VAL:HG13	2.01	0.60
1:A:144:PRO:O	1:A:148:LEU:HG	2.02	0.60
1:D:46:CYS:CA	1:D:51:VAL:HG11	2.31	0.60
1:D:75:GLU:O	1:D:80:ARG:HB3	2.01	0.60
1:C:80:ARG:CG	1:C:81:LYS:N	2.64	0.60
1:F:8:THR:HB	1:F:35:LEU:HD23	1.83	0.60
1:A:208:ALA:O	1:A:212:GLN:HG3	2.01	0.60
1:B:97:GLN:HG3	1:B:121:ALA:O	2.02	0.60
1:B:133:PHE:HZ	1:B:181:ILE:HD11	1.61	0.60
1:B:144:PRO:O	1:B:148:LEU:HD22	2.02	0.60
1:C:52:THR:HG21	2:C:304:HOH:O	2.01	0.60
1:A:142:LEU:HB3	1:A:235:MSE:HE3	1.82	0.60
1:C:76:MSE:HB3	1:C:81:LYS:HE3	1.84	0.60
1:B:196:LEU:O	1:B:200:ARG:HG3	2.02	0.60
1:D:249:VAL:O	1:D:250:GLU:HG3	2.01	0.60
1:C:251:THR:HG22	1:C:252:GLY:N	2.17	0.59
1:D:244:GLY:N	2:D:281:HOH:O	2.35	0.59
1:F:106:HIS:HE1	1:F:188:SER:OG	1.84	0.59
1:E:46:CYS:HB3	1:E:51:VAL:HG11	1.84	0.59
1:E:111:VAL:HG12	1:E:116:LEU:HD12	1.83	0.59
1:F:144:PRO:HB2	1:F:147:VAL:HB	1.83	0.59
1:E:163:MSE:O	1:E:166:MSE:O	2.20	0.59
1:F:238:ASP:O	1:F:242:GLN:HG3	2.03	0.59
1:C:251:THR:HG22	1:C:252:GLY:H	1.67	0.59
1:C:254:PHE:N	1:C:254:PHE:CD2	2.69	0.59
1:E:28:ASN:HD22	1:E:62:VAL:HG11	1.68	0.59
1:E:255:PRO:HG2	2:E:269:HOH:O	2.02	0.59
1:F:68:ASP:HA	2:F:282:HOH:O	2.01	0.59
1:A:134:SER:HB3	1:A:169:PRO:HB3	1.85	0.59
1:D:208:ALA:O	1:D:212:GLN:HG3	2.02	0.59
1:D:238:ASP:O	1:D:242:GLN:HB2	2.03	0.59
1:B:17:VAL:HG22	1:B:53:VAL:HG22	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:210:TYR:OH	1:F:161:HIS:HD2	1.85	0.59
1:C:74:GLN:O	1:C:77:LYS:O	2.21	0.59
1:E:81:LYS:O	1:E:82:GLN:O	2.20	0.59
1:C:80:ARG:CG	1:C:81:LYS:H	2.15	0.58
1:E:225:LYS:O	1:E:226:ALA:CB	2.51	0.58
1:B:95:LYS:HE3	2:B:290:HOH:O	2.04	0.58
1:C:97:GLN:HG2	1:C:121:ALA:O	2.04	0.58
1:E:91:ASP:OD1	1:E:225:LYS:NZ	2.35	0.58
1:F:144:PRO:O	1:F:148:LEU:HD22	2.03	0.58
1:D:86:GLN:HE21	1:D:86:GLN:HA	1.68	0.58
1:E:233:GLN:O	1:E:235:MSE:N	2.36	0.58
1:D:47:GLU:HG2	2:D:282:HOH:O	2.03	0.58
1:F:34:THR:O	1:F:38:GLU:HG3	2.04	0.58
1:B:140:PHE:HA	1:B:254:PHE:CZ	2.39	0.58
1:D:111:VAL:HG12	1:D:116:LEU:HD12	1.86	0.58
1:E:6:TYR:O	1:E:7:GLN:CB	2.49	0.58
1:A:66:GLY:HA3	1:A:113:ALA:O	2.04	0.58
1:C:233:GLN:O	1:C:234:ASP:CB	2.45	0.58
1:D:128:ASP:HB3	1:D:188:SER:HB3	1.86	0.57
1:A:241:ASN:O	1:A:245:ILE:HG13	2.03	0.57
1:D:76:MSE:CE	1:D:246:ILE:HD11	2.34	0.57
1:D:243:MSE:HE2	1:D:246:ILE:HD12	1.86	0.57
1:E:116:LEU:HD22	1:E:135:LEU:CD1	2.33	0.57
1:D:60:PRO:HD2	1:D:61:GLU:OE2	2.05	0.57
1:D:254:PHE:N	1:D:254:PHE:HD1	2.02	0.57
1:E:37:GLU:O	1:E:41:GLN:HG3	2.05	0.57
1:A:142:LEU:HB3	1:A:235:MSE:CE	2.35	0.57
1:D:200:ARG:HH11	1:D:200:ARG:HB2	1.68	0.57
1:F:137:GLU:HG3	1:F:144:PRO:HD3	1.87	0.57
1:B:86:GLN:HG3	1:B:232:ASN:ND2	2.20	0.57
1:A:59:LEU:O	1:A:108:ARG:HB2	2.05	0.57
1:C:72:ILE:HG22	1:C:76:MSE:HE2	1.87	0.57
1:F:197:LEU:O	1:F:200:ARG:HG2	2.05	0.56
1:D:218:ASP:HB2	1:F:157:ARG:NE	2.20	0.56
1:B:82:GLN:HG2	1:E:219:HIS:CG	2.40	0.56
1:B:219:HIS:HB3	1:B:223:ARG:HD3	1.86	0.56
1:D:168:LYS:HD2	1:D:168:LYS:O	2.06	0.56
1:F:120:SER:O	1:F:154:ARG:HD2	2.06	0.56
1:A:230:THR:O	1:A:233:GLN:O	2.24	0.56
1:B:86:GLN:HA	1:B:86:GLN:NE2	2.21	0.56
1:A:38:GLU:O	1:A:42:VAL:HG23	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:254:PHE:HD1	1:B:254:PHE:H	1.51	0.56
1:C:109:GLY:H	1:C:130:THR:CG2	2.18	0.56
1:D:77:LYS:O	1:D:78:ARG:HG3	2.05	0.56
1:E:167:THR:HG22	1:E:167:THR:O	2.06	0.56
1:A:65:PHE:O	1:A:112:ASN:HB3	2.06	0.55
1:C:46:CYS:O	1:C:47:GLU:HB2	2.06	0.55
1:C:144:PRO:HB2	1:C:147:VAL:HB	1.88	0.55
1:B:86:GLN:HA	1:B:86:GLN:HE21	1.70	0.55
1:B:155:ILE:HD12	1:B:159:LYS:HB3	1.88	0.55
1:C:129:GLN:HA	1:C:172:VAL:HG11	1.88	0.55
1:D:142:LEU:HD11	1:D:245:ILE:HD11	1.89	0.55
1:C:109:GLY:H	1:C:130:THR:HG23	1.71	0.55
1:F:131:ALA:O	1:F:172:VAL:HG22	2.07	0.55
1:C:253:GLN:C	1:C:254:PHE:CD2	2.85	0.55
1:A:128:ASP:HA	1:A:185:ASP:O	2.07	0.55
1:E:38:GLU:O	1:E:42:VAL:HG12	2.06	0.55
1:E:220:GLN:HA	1:E:223:ARG:HD3	1.89	0.55
1:A:138:LEU:HG	1:E:202:LEU:HD22	1.89	0.55
1:D:32:ASN:ND2	1:D:34:THR:HB	2.22	0.55
1:F:205:LYS:H	1:F:205:LYS:CD	1.99	0.55
1:B:144:PRO:HG2	1:B:148:LEU:CD2	2.37	0.55
1:C:159:LYS:HE2	1:C:178:TRP:NE1	2.22	0.55
1:C:139:LEU:CD1	1:C:167:THR:HG21	2.35	0.54
1:B:34:THR:O	1:B:38:GLU:HG3	2.06	0.54
1:C:83:ALA:CB	1:C:233:GLN:HG2	2.36	0.54
1:D:86:GLN:HA	1:D:86:GLN:NE2	2.22	0.54
1:F:66:GLY:HA3	1:F:113:ALA:O	2.07	0.54
1:B:57:GLU:OE2	1:B:106:HIS:HD2	1.90	0.54
1:A:167:THR:O	1:A:167:THR:HG22	2.08	0.54
1:E:36:ILE:HD13	1:E:89:LEU:HB2	1.90	0.54
1:F:79:GLY:O	1:F:81:LYS:N	2.40	0.54
1:E:220:GLN:HA	1:E:223:ARG:HH11	1.73	0.54
1:C:38:GLU:O	1:C:42:VAL:HG12	2.08	0.53
1:C:73:TYR:HE1	1:C:246:ILE:HG23	1.73	0.53
1:E:144:PRO:HB2	1:E:147:VAL:HB	1.90	0.53
1:F:232:ASN:C	1:F:233:GLN:O	2.40	0.53
1:C:136:SER:CA	1:C:167:THR:HG23	2.35	0.53
1:D:17:VAL:HG13	1:D:53:VAL:HG22	1.89	0.53
1:E:128:ASP:HA	1:E:185:ASP:O	2.08	0.53
1:C:47:GLU:HG2	1:C:100:PRO:CD	2.39	0.53
1:A:73:TYR:O	1:A:76:MSE:N	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:242:GLN:O	1:B:245:ILE:HG12	2.08	0.53
1:F:95:LYS:HE3	2:F:268:HOH:O	2.07	0.53
1:D:131:ALA:HB3	1:D:172:VAL:HG13	1.90	0.53
1:A:66:GLY:N	2:A:296:HOH:O	2.39	0.53
1:B:52:THR:HG22	1:B:53:VAL:HG13	1.90	0.53
1:C:71:GLU:O	1:C:75:GLU:HG3	2.08	0.53
1:D:213:PHE:CD2	1:D:214:MSE:HE2	2.44	0.53
1:E:27:ALA:O	1:E:30:THR:HG23	2.08	0.53
1:E:244:GLY:HA2	2:E:275:HOH:O	2.07	0.53
1:A:109:GLY:H	1:A:130:THR:HG22	1.74	0.53
1:C:79:GLY:O	1:C:80:ARG:O	2.25	0.53
1:D:106:HIS:HE1	1:D:188:SER:OG	1.92	0.53
1:A:107:VAL:HG23	1:A:126:ILE:O	2.09	0.53
1:C:138:LEU:HA	1:C:142:LEU:O	2.09	0.53
1:C:144:PRO:O	1:C:148:LEU:HG	2.09	0.53
1:F:116:LEU:HD13	1:F:135:LEU:HD13	1.90	0.53
1:C:8:THR:HG22	1:C:24:ARG:HD3	1.90	0.52
1:D:106:HIS:HE1	1:D:188:SER:CB	2.21	0.52
1:E:213:PHE:O	1:E:216:SER:HB3	2.08	0.52
1:F:205:LYS:HD2	1:F:205:LYS:N	2.04	0.52
1:A:171:SER:OG	1:A:174:GLU:HG3	2.09	0.52
1:D:32:ASN:HD22	1:D:34:THR:H	1.52	0.52
1:D:76:MSE:HE3	1:D:242:GLN:CG	2.26	0.52
1:A:140:PHE:HB2	1:A:142:LEU:CD2	2.39	0.52
1:C:128:ASP:HA	1:C:185:ASP:O	2.09	0.52
1:D:159:LYS:HD3	1:D:178:TRP:CD2	2.44	0.52
1:F:102:VAL:HG23	1:F:207:ILE:HD13	1.90	0.52
1:E:28:ASN:ND2	1:E:62:VAL:HG11	2.24	0.52
1:C:80:ARG:HB2	1:C:80:ARG:CZ	2.39	0.52
1:B:219:HIS:HB2	1:B:223:ARG:HD3	1.89	0.52
1:C:232:ASN:O	1:C:235:MSE:HG2	2.09	0.52
1:F:9:ILE:HG22	1:F:22:PHE:HD1	1.74	0.52
1:A:104:ILE:HA	1:A:124:ILE:O	2.10	0.52
1:C:214:MSE:SE	2:C:275:HOH:O	2.78	0.52
1:D:12:ARG:O	1:D:12:ARG:HG2	2.08	0.52
1:E:232:ASN:C	1:E:233:GLN:O	2.53	0.52
1:A:137:GLU:H	1:A:137:GLU:CD	2.17	0.52
1:E:57:GLU:HG2	1:E:106:HIS:HB3	1.92	0.52
1:E:81:LYS:C	1:E:82:GLN:HG3	2.35	0.52
1:D:106:HIS:HE1	1:D:188:SER:HB2	1.76	0.51
1:D:225:LYS:O	1:D:229:LEU:HG	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:172:VAL:HG13	1:B:173:GLN:NE2	2.25	0.51
1:D:151:LEU:CD1	1:D:180:LEU:HD13	2.40	0.51
1:F:137:GLU:CG	1:F:144:PRO:HD3	2.40	0.51
1:F:208:ALA:O	1:F:212:GLN:HG3	2.09	0.51
1:A:223:ARG:NH2	1:B:230:THR:HG23	2.25	0.51
1:B:133:PHE:CE1	1:B:181:ILE:HD11	2.42	0.51
1:E:254:PHE:N	1:E:254:PHE:HD1	2.07	0.51
1:A:144:PRO:HB2	1:A:147:VAL:HB	1.93	0.51
1:A:6:TYR:HB3	1:A:38:GLU:OE1	2.10	0.51
1:D:254:PHE:CB	1:D:255:PRO:HD2	2.38	0.51
1:E:241:ASN:O	1:E:243:MSE:O	2.29	0.51
1:A:12:ARG:NH1	1:A:14:GLN:NE2	2.54	0.51
1:B:82:GLN:NE2	1:E:219:HIS:HB3	2.08	0.51
1:B:244:GLY:HA3	1:B:254:PHE:CE2	2.46	0.51
1:F:109:GLY:O	1:F:131:ALA:HA	2.11	0.51
1:A:133:PHE:O	1:A:169:PRO:HA	2.10	0.51
1:B:81:LYS:HD2	1:B:81:LYS:N	2.26	0.51
1:C:167:THR:O	1:C:167:THR:CG2	2.59	0.51
1:C:208:ALA:O	1:C:212:GLN:HG3	2.10	0.51
1:E:70:GLN:CD	1:E:70:GLN:H	2.19	0.51
1:F:83:ALA:HB3	1:F:233:GLN:CD	2.37	0.50
1:F:144:PRO:HG2	1:F:148:LEU:CD2	2.41	0.50
1:E:37:GLU:HG3	1:E:41:GLN:HE21	1.76	0.50
1:C:230:THR:O	1:C:234:ASP:HB2	2.11	0.50
1:B:116:LEU:HD22	1:B:135:LEU:CD1	2.37	0.50
1:D:116:LEU:HD22	1:D:135:LEU:CD1	2.40	0.50
1:A:248:TYR:C	1:A:250:GLU:N	2.69	0.50
1:B:82:GLN:HE22	1:E:223:ARG:HG3	1.77	0.50
1:C:254:PHE:HD2	1:C:254:PHE:N	2.09	0.50
1:A:128:ASP:OD1	1:A:130:THR:HB	2.12	0.50
1:A:166:MSE:HE1	1:E:199:LEU:HD21	1.94	0.50
1:B:75:GLU:O	1:B:80:ARG:HB3	2.12	0.50
1:C:116:LEU:HD11	1:C:163:MSE:HE1	1.92	0.50
1:D:57:GLU:HG2	1:D:106:HIS:HB3	1.94	0.50
1:B:82:GLN:NE2	1:E:223:ARG:HG3	2.27	0.50
1:B:140:PHE:CD1	1:B:254:PHE:CE1	2.99	0.50
1:B:140:PHE:CD1	1:B:254:PHE:HE1	2.30	0.50
1:C:129:GLN:O	1:C:129:GLN:HG2	2.09	0.50
1:E:238:ASP:O	1:E:242:GLN:HG2	2.12	0.50
1:C:45:GLN:C	1:C:46:CYS:O	2.52	0.50
1:C:142:LEU:HD11	1:C:245:ILE:HD11	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:193:ARG:HD2	2:F:294:HOH:O	2.12	0.50
1:B:113:ALA:HB1	1:B:137:GLU:HG2	1.93	0.49
1:C:47:GLU:HG3	2:C:282:HOH:O	2.11	0.49
1:C:230:THR:O	1:C:233:GLN:O	2.30	0.49
1:C:232:ASN:HA	1:C:235:MSE:HE3	1.93	0.49
1:F:203:ASN:OD1	1:F:205:LYS:HD2	2.12	0.49
1:D:87:GLU:HG2	1:D:229:LEU:HD13	1.93	0.49
1:D:220:GLN:HG3	1:D:221:VAL:N	2.28	0.49
1:F:176:SER:HA	1:F:181:ILE:HG13	1.94	0.49
1:D:106:HIS:CE1	1:D:188:SER:HB2	2.48	0.49
1:A:109:GLY:HA2	1:A:130:THR:HG22	1.95	0.49
1:B:78:ARG:HG3	1:D:45:GLN:CD	2.38	0.49
1:D:129:GLN:NE2	2:D:277:HOH:O	2.46	0.49
1:E:233:GLN:O	1:E:234:ASP:C	2.55	0.49
1:A:118:PHE:O	1:A:122:THR:HG23	2.13	0.49
1:D:32:ASN:ND2	1:D:34:THR:CB	2.76	0.49
1:E:220:GLN:HA	1:E:223:ARG:NH1	2.28	0.49
1:E:254:PHE:HD1	1:E:254:PHE:H	1.59	0.49
1:E:116:LEU:HD21	1:E:163:MSE:HE1	1.93	0.49
1:A:21:THR:HG23	1:A:58:GLY:CA	2.41	0.49
1:A:97:GLN:HG2	1:A:121:ALA:O	2.13	0.49
1:C:47:GLU:HG2	1:C:100:PRO:HD2	1.95	0.49
1:E:239:PRO:HA	1:E:242:GLN:HG3	1.95	0.49
1:C:129:GLN:HE21	1:C:186:ALA:HA	1.77	0.48
1:D:65:PHE:HE1	1:D:110:LYS:HB3	1.78	0.48
1:D:254:PHE:CG	1:D:255:PRO:HD2	2.48	0.48
1:A:181:ILE:HD12	1:A:181:ILE:O	2.14	0.48
1:D:242:GLN:HA	1:D:242:GLN:NE2	2.28	0.48
1:E:29:ASN:HD21	1:E:59:LEU:HG	1.78	0.48
1:B:168:LYS:HE3	1:B:168:LYS:O	2.13	0.48
1:D:75:GLU:HB3	1:D:80:ARG:CD	2.43	0.48
1:B:251:THR:OG1	1:B:252:GLY:N	2.45	0.48
1:C:109:GLY:O	1:C:131:ALA:HA	2.14	0.48
1:D:133:PHE:O	1:D:169:PRO:HA	2.14	0.48
1:C:93:TRP:O	1:C:96:LEU:HB2	2.13	0.48
1:E:12:ARG:HH11	1:E:12:ARG:HG2	1.79	0.48
1:E:140:PHE:HA	1:E:254:PHE:CZ	2.48	0.48
1:B:76:MSE:HE1	1:B:242:GLN:CG	2.43	0.48
1:D:8:THR:HB	1:D:35:LEU:HD23	1.95	0.48
1:E:76:MSE:HE3	1:E:242:GLN:OE1	2.14	0.48
1:E:232:ASN:O	1:E:233:GLN:O	2.32	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:142:LEU:HD12	1:A:235:MSE:HE3	1.95	0.48
1:B:129:GLN:HG3	1:B:186:ALA:HA	1.95	0.48
1:E:40:LEU:HD22	2:E:284:HOH:O	2.13	0.48
1:F:153:ARG:NH2	2:F:276:HOH:O	2.46	0.47
1:C:128:ASP:O	1:C:128:ASP:CG	2.56	0.47
1:B:214:MSE:HG3	2:B:288:HOH:O	2.13	0.47
1:D:232:ASN:HA	1:D:235:MSE:HE3	1.97	0.47
1:A:152:ILE:HD11	1:E:214:MSE:CE	2.45	0.47
1:A:218:ASP:OD1	1:A:220:GLN:HB2	2.14	0.47
1:E:35:LEU:HD13	1:E:35:LEU:C	2.40	0.47
1:F:163:MSE:HE2	1:F:178:TRP:CE3	2.48	0.47
1:C:251:THR:CG2	1:C:252:GLY:H	2.25	0.47
1:E:112:ASN:O	1:E:113:ALA:C	2.56	0.47
1:A:83:ALA:HB3	1:A:233:GLN:NE2	2.28	0.47
1:B:254:PHE:N	1:B:255:PRO:HD2	2.30	0.47
1:E:24:ARG:HG2	1:E:27:ALA:HB3	1.95	0.47
1:D:46:CYS:HA	1:D:51:VAL:HG11	1.97	0.47
1:E:71:GLU:O	1:E:75:GLU:HG3	2.14	0.47
1:E:133:PHE:O	1:E:169:PRO:HA	2.14	0.47
1:E:46:CYS:CB	1:E:51:VAL:HG11	2.45	0.47
1:D:190:VAL:O	1:D:194:LYS:HG3	2.15	0.47
1:A:40:LEU:HD11	2:A:274:HOH:O	2.14	0.46
1:A:116:LEU:HA	1:A:116:LEU:HD12	1.76	0.46
1:F:10:LYS:HB2	1:F:21:THR:HB	1.97	0.46
1:F:126:ILE:HD11	1:F:192:LEU:HB2	1.97	0.46
1:A:51:VAL:O	1:A:204:LYS:NZ	2.47	0.46
1:B:29:ASN:CG	1:B:59:LEU:HD22	2.41	0.46
1:B:76:MSE:HE1	1:B:242:GLN:CD	2.40	0.46
1:D:246:ILE:HB	2:D:281:HOH:O	2.14	0.46
1:F:200:ARG:HG2	1:F:200:ARG:HH11	1.80	0.46
1:F:231:ALA:O	1:F:235:MSE:HB2	2.16	0.46
1:A:203:ASN:OD1	1:A:205:LYS:HB3	2.15	0.46
1:B:244:GLY:HA3	1:B:254:PHE:CZ	2.50	0.46
1:D:14:GLN:O	1:D:15:ALA:HB3	2.15	0.46
1:A:109:GLY:N	1:A:130:THR:HG22	2.31	0.46
1:E:139:LEU:HD11	1:E:167:THR:HG21	1.98	0.46
1:F:83:ALA:C	1:F:233:GLN:HE22	2.24	0.46
1:C:218:ASP:OD1	1:C:220:GLN:HG2	2.15	0.46
1:C:238:ASP:O	1:C:242:GLN:HG3	2.16	0.46
1:D:23:HIS:O	1:D:24:ARG:HG2	2.16	0.46
1:F:231:ALA:O	1:F:233:GLN:O	2.33	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:87:GLU:HB2	1:D:88:PRO:HD3	1.98	0.46
1:E:44:ASN:HA	1:E:47:GLU:HB2	1.98	0.46
1:A:224:ALA:HB1	1:E:217:LEU:HD22	1.97	0.46
1:D:200:ARG:HH11	1:D:200:ARG:CB	2.29	0.46
1:B:52:THR:HG23	1:B:207:ILE:CD1	2.47	0.45
1:D:129:GLN:C	1:D:131:ALA:H	2.24	0.45
1:D:159:LYS:HD3	1:D:178:TRP:CG	2.51	0.45
1:A:113:ALA:HB2	1:A:135:LEU:CD2	2.46	0.45
1:C:116:LEU:HD23	1:C:116:LEU:HA	1.83	0.45
1:D:51:VAL:O	1:D:51:VAL:HG13	2.17	0.45
1:D:144:PRO:HG2	1:D:148:LEU:HD22	1.99	0.45
1:E:138:LEU:HD13	1:E:138:LEU:O	2.16	0.45
1:A:59:LEU:CB	1:A:63:PHE:CA	2.95	0.45
1:D:248:TYR:HD1	1:D:253:GLN:N	2.14	0.45
1:E:116:LEU:HD22	1:E:135:LEU:HD13	1.98	0.45
1:D:32:ASN:HB3	1:D:35:LEU:HB2	1.98	0.45
1:E:95:LYS:NZ	2:E:281:HOH:O	2.48	0.45
1:A:142:LEU:CB	1:A:235:MSE:HE3	2.47	0.45
1:B:197:LEU:O	1:B:200:ARG:HB2	2.16	0.45
1:D:129:GLN:O	1:D:130:THR:OG1	2.32	0.45
1:E:106:HIS:HE1	1:E:188:SER:OG	1.99	0.45
1:F:59:LEU:CB	1:F:108:ARG:HB2	2.47	0.45
1:F:83:ALA:HB3	1:F:233:GLN:OE1	2.16	0.45
1:B:242:GLN:O	1:B:246:ILE:HG12	2.16	0.45
1:E:113:ALA:N	1:E:134:SER:O	2.44	0.45
1:A:44:ASN:O	1:A:47:GLU:HB3	2.17	0.45
1:D:138:LEU:HA	1:D:142:LEU:O	2.17	0.45
1:A:27:ALA:O	1:A:28:ASN:C	2.59	0.45
1:D:197:LEU:HA	1:D:200:ARG:NH1	2.31	0.45
1:E:189:ASP:O	1:E:193:ARG:HG3	2.17	0.45
1:F:73:TYR:O	1:F:77:LYS:CB	2.64	0.45
1:A:166:MSE:HE3	1:E:124:ILE:CD1	2.47	0.44
1:A:176:SER:HB2	1:A:181:ILE:HD11	1.99	0.44
1:A:223:ARG:HH21	1:B:230:THR:HG23	1.81	0.44
1:C:23:HIS:C	1:C:25:PRO:HD3	2.42	0.44
1:E:79:GLY:O	1:E:80:ARG:C	2.58	0.44
1:E:87:GLU:N	1:E:88:PRO:CD	2.80	0.44
1:A:35:LEU:C	1:A:35:LEU:HD23	2.43	0.44
1:D:112:ASN:O	1:D:113:ALA:C	2.61	0.44
1:D:143:TYR:O	1:D:235:MSE:HE1	2.16	0.44
1:D:255:PRO:HA	2:D:269:HOH:O	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:118:PHE:O	1:E:122:THR:HG23	2.17	0.44
1:F:32:ASN:O	1:F:34:THR:N	2.51	0.44
1:F:79:GLY:O	1:F:80:ARG:C	2.59	0.44
1:A:166:MSE:CE	1:E:199:LEU:HD21	2.48	0.44
1:F:65:PHE:O	1:F:112:ASN:HB3	2.18	0.44
1:A:28:ASN:O	1:A:30:THR:N	2.51	0.44
1:B:240:GLN:HE21	1:B:243:MSE:HE1	1.82	0.44
1:D:81:LYS:HB2	1:D:82:GLN:H	1.37	0.44
1:D:166:MSE:HA	1:D:166:MSE:HE2	1.99	0.44
1:F:126:ILE:HA	1:F:183:ALA:O	2.17	0.44
1:C:25:PRO:C	1:C:27:ALA:H	2.24	0.44
1:A:190:VAL:O	1:A:194:LYS:HG3	2.18	0.44
1:F:112:ASN:O	1:F:113:ALA:C	2.60	0.44
1:F:93:TRP:CH2	1:F:117:GLY:HA3	2.53	0.44
1:D:113:ALA:N	1:D:134:SER:O	2.46	0.43
1:E:36:ILE:CD1	1:E:89:LEU:HB2	2.48	0.43
1:E:255:PRO:HD3	2:E:290:HOH:O	2.18	0.43
1:A:120:SER:HA	1:A:154:ARG:HD2	2.00	0.43
1:C:46:CYS:O	1:C:47:GLU:HB3	2.18	0.43
1:B:166:MSE:HB2	1:B:168:LYS:HE2	2.00	0.43
1:B:240:GLN:HE21	1:B:243:MSE:CE	2.31	0.43
1:C:78:ARG:O	1:C:79:GLY:O	2.37	0.43
1:C:244:GLY:HA3	2:C:293:HOH:O	2.18	0.43
1:C:62:VAL:O	1:C:62:VAL:HG13	2.19	0.43
1:A:49:SER:OG	1:A:51:VAL:CG1	2.66	0.43
1:C:107:VAL:O	1:C:127:ALA:HA	2.19	0.43
1:D:10:LYS:HE2	1:D:23:HIS:CG	2.54	0.43
1:D:68:ASP:O	1:D:72:ILE:HG13	2.18	0.43
1:D:85:SER:C	1:D:87:GLU:H	2.25	0.43
1:D:32:ASN:HD22	1:D:34:THR:N	2.17	0.43
1:D:79:GLY:O	1:D:80:ARG:C	2.61	0.43
1:E:77:LYS:C	1:E:79:GLY:N	2.75	0.43
1:E:197:LEU:HD12	1:E:197:LEU:O	2.19	0.43
1:F:66:GLY:CA	1:F:113:ALA:O	2.65	0.43
1:F:155:ILE:CD1	1:F:163:MSE:HE1	2.49	0.43
1:B:95:LYS:CE	2:B:290:HOH:O	2.64	0.43
1:B:113:ALA:CB	1:B:137:GLU:HG2	2.49	0.43
1:D:61:GLU:CD	1:D:61:GLU:H	2.25	0.43
1:E:60:PRO:HB2	1:E:61:GLU:OE2	2.18	0.43
1:A:81:LYS:O	1:A:82:GLN:CB	2.66	0.43
1:C:159:LYS:HE2	1:C:178:TRP:CE2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:35:LEU:C	1:D:35:LEU:HD13	2.44	0.43
1:F:8:THR:OG1	1:F:38:GLU:OE1	2.37	0.43
1:F:233:GLN:O	1:F:235:MSE:N	2.47	0.43
1:A:127:ALA:O	1:A:184:PHE:HA	2.19	0.43
1:D:27:ALA:O	1:D:30:THR:HG23	2.19	0.43
1:F:128:ASP:C	1:F:128:ASP:OD1	2.62	0.43
1:C:39:CYS:O	1:C:42:VAL:HG13	2.19	0.42
1:D:75:GLU:HB3	1:D:80:ARG:HD3	2.01	0.42
1:D:87:GLU:CB	1:D:88:PRO:HD3	2.49	0.42
1:E:97:GLN:HG2	1:E:121:ALA:O	2.19	0.42
1:E:225:LYS:O	1:E:226:ALA:HB2	2.19	0.42
1:E:254:PHE:HB3	2:E:275:HOH:O	2.18	0.42
1:F:203:ASN:OD1	1:F:205:LYS:CD	2.67	0.42
1:C:113:ALA:O	1:C:116:LEU:HB2	2.20	0.42
1:D:144:PRO:HB2	1:D:147:VAL:HB	2.02	0.42
1:E:140:PHE:HA	1:E:254:PHE:HZ	1.85	0.42
1:A:231:ALA:C	1:A:233:GLN:O	2.62	0.42
1:B:14:GLN:O	1:B:15:ALA:HB3	2.18	0.42
1:C:43:LEU:HD23	1:C:43:LEU:HA	1.90	0.42
1:E:197:LEU:HA	1:E:200:ARG:HD3	2.01	0.42
1:D:9:ILE:HA	1:D:21:THR:O	2.19	0.42
1:D:57:GLU:OE2	1:D:106:HIS:HD2	2.02	0.42
1:F:57:GLU:OE2	1:F:106:HIS:HD2	2.02	0.42
1:F:58:GLY:HA3	2:F:270:HOH:O	2.19	0.42
1:A:87:GLU:HB3	1:A:88:PRO:HD3	2.01	0.42
1:C:49:SER:O	1:C:204:LYS:HE3	2.20	0.42
1:C:52:THR:HG23	1:C:207:ILE:HD12	2.00	0.42
1:D:80:ARG:NH1	1:D:80:ARG:HG3	2.34	0.42
1:E:138:LEU:HA	1:E:142:LEU:O	2.19	0.42
1:B:239:PRO:HG2	1:B:240:GLN:OE1	2.20	0.42
1:F:143:TYR:CD1	1:F:235:MSE:HE2	2.55	0.42
1:A:253:GLN:O	1:A:254:PHE:CB	2.68	0.42
1:D:186:ALA:HA	2:D:276:HOH:O	2.20	0.42
1:C:80:ARG:O	1:C:81:LYS:CB	2.67	0.42
1:F:176:SER:HB2	1:F:181:ILE:HD11	2.00	0.42
1:A:135:LEU:HD13	1:A:144:PRO:HG3	2.01	0.42
1:B:8:THR:OG1	1:B:35:LEU:HA	2.20	0.42
1:D:128:ASP:HB3	1:D:188:SER:CB	2.50	0.42
1:D:144:PRO:HG2	1:D:148:LEU:CD2	2.50	0.42
1:F:65:PHE:O	1:F:113:ALA:O	2.37	0.42
1:D:24:ARG:CZ	1:D:32:ASN:HB2	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:143:TYR:O	1:D:145:ALA:N	2.51	0.41
1:E:251:THR:OG1	1:E:252:GLY:N	2.52	0.41
1:A:167:THR:O	1:A:167:THR:CG2	2.68	0.41
1:A:157:ARG:NE	1:E:218:ASP:HB2	2.36	0.41
1:A:199:LEU:HD23	1:A:199:LEU:HA	1.81	0.41
1:E:127:ALA:HB1	1:E:131:ALA:HB2	2.02	0.41
1:E:185:ASP:OD1	1:E:186:ALA:N	2.53	0.41
1:A:224:ALA:CB	1:E:217:LEU:HD22	2.50	0.41
1:D:134:SER:HB3	1:D:169:PRO:HA	2.02	0.41
1:E:142:LEU:HD11	1:E:245:ILE:HD11	2.02	0.41
1:A:28:ASN:O	1:A:29:ASN:C	2.63	0.41
1:C:52:THR:O	1:C:52:THR:HG22	2.20	0.41
1:D:226:ALA:HB3	2:D:288:HOH:O	2.20	0.41
1:E:77:LYS:C	1:E:79:GLY:H	2.27	0.41
1:F:13:PHE:HZ	1:F:45:GLN:HE22	1.63	0.41
1:F:30:THR:HA	1:F:66:GLY:O	2.20	0.41
1:F:97:GLN:NE2	2:F:293:HOH:O	2.53	0.41
1:D:32:ASN:HD22	1:D:35:LEU:H	1.69	0.41
1:A:43:LEU:HD11	1:A:96:LEU:CD1	2.51	0.41
1:D:247:ARG:N	2:D:281:HOH:O	2.33	0.41
1:E:243:MSE:HE2	1:E:246:ILE:HD12	2.03	0.41
1:B:51:VAL:O	1:B:51:VAL:HG13	2.21	0.41
1:C:24:ARG:N	1:C:25:PRO:HD3	2.35	0.41
1:C:26:GLU:O	1:C:27:ALA:HB2	2.20	0.41
1:C:108:ARG:HD2	1:C:128:ASP:OD2	2.21	0.41
1:D:73:TYR:CZ	1:D:77:LYS:HE2	2.55	0.41
1:D:82:GLN:H	1:D:82:GLN:HG3	1.53	0.41
1:E:42:VAL:O	1:E:45:GLN:HB3	2.20	0.41
1:B:57:GLU:HG2	1:B:106:HIS:HB3	2.03	0.41
1:B:73:TYR:OH	1:B:77:LYS:HE3	2.20	0.41
1:B:111:VAL:HG12	1:B:116:LEU:HD12	2.03	0.41
1:D:129:GLN:C	1:D:130:THR:HG23	2.45	0.41
1:D:200:ARG:NH1	1:D:200:ARG:CB	2.84	0.41
1:E:107:VAL:HB	1:E:127:ALA:HB2	2.02	0.41
1:E:248:TYR:HD1	1:E:253:GLN:N	2.19	0.41
1:F:52:THR:HG22	1:F:204:LYS:HB2	2.03	0.41
1:D:241:ASN:O	1:D:243:MSE:O	2.39	0.41
1:F:138:LEU:HA	1:F:142:LEU:O	2.20	0.41
1:A:190:VAL:HG12	1:A:194:LYS:HE3	2.03	0.40
1:D:9:ILE:HG23	1:D:35:LEU:HD22	2.03	0.40
1:D:71:GLU:O	1:D:75:GLU:HG3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:35:LEU:HD13	1:F:35:LEU:C	2.46	0.40
1:F:143:TYR:CZ	1:F:235:MSE:HE2	2.56	0.40
1:F:195:HIS:C	1:F:196:LEU:O	2.58	0.40
1:A:105:SER:OG	1:A:119:VAL:HA	2.20	0.40
1:A:128:ASP:OD1	1:A:128:ASP:C	2.64	0.40
1:A:129:GLN:H	1:A:129:GLN:HG2	1.66	0.40
1:B:245:ILE:O	1:B:249:VAL:HG23	2.22	0.40
1:E:245:ILE:O	1:E:249:VAL:HG23	2.22	0.40
1:A:93:TRP:CZ2	1:A:117:GLY:HA3	2.57	0.40
1:B:175:ALA:HB3	1:B:181:ILE:HD12	2.02	0.40
1:C:28:ASN:HD22	1:C:28:ASN:HA	1.65	0.40
1:B:73:TYR:CZ	1:B:77:LYS:HE3	2.56	0.40
1:D:136:SER:HA	1:D:167:THR:HB	2.04	0.40
1:D:198:ARG:O	1:D:201:ARG:HG3	2.21	0.40
1:E:168:LYS:HA	1:E:169:PRO:HD3	1.92	0.40
1:E:220:GLN:HG3	1:E:221:VAL:N	2.36	0.40
1:F:168:LYS:HA	1:F:169:PRO:HD3	1.97	0.40

There are no symmetry-related clashes.

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	248/267 (93%)	219 (88%)	16 (6%)	13 (5%)	1	0
1	B	249/267 (93%)	231 (93%)	14 (6%)	4 (2%)	7	7
1	C	249/267 (93%)	223 (90%)	13 (5%)	13 (5%)	1	0
1	D	249/267 (93%)	215 (86%)	24 (10%)	10 (4%)	2	1
1	E	249/267 (93%)	221 (89%)	18 (7%)	10 (4%)	2	1
1	F	249/267 (93%)	223 (90%)	15 (6%)	11 (4%)	2	1
All	All	1493/1602 (93%)	1332 (89%)	100 (7%)	61 (4%)	2	1

All (61) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	234	ASP
1	A	240	GLN
1	B	82	GLN
1	B	167	THR
1	C	27	ALA
1	C	78	ARG
1	C	80	ARG
1	C	81	LYS
1	C	234	ASP
1	C	253	GLN
1	D	7	GLN
1	D	33	ASP
1	D	254	PHE
1	E	7	GLN
1	E	82	GLN
1	E	226	ALA
1	E	233	GLN
1	E	234	ASP
1	E	253	GLN
1	F	7	GLN
1	F	33	ASP
1	F	59	LEU
1	F	60	PRO
1	F	80	ARG
1	A	28	ASN
1	A	29	ASN
1	A	62	VAL
1	A	183	ALA
1	A	189	ASP
1	A	201	ARG
1	A	249	VAL
1	B	113	ALA
1	C	47	GLU
1	C	79	GLY
1	D	80	ARG
1	D	113	ALA
1	D	233	GLN
1	D	250	GLU
1	E	80	ARG
1	F	49	SER
1	F	197	LEU
1	A	79	GLY

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Mol	Chain	Res	Type
1	A	82	GLN
1	C	254	PHE
1	D	234	ASP
1	E	49	SER
1	E	113	ALA
1	F	62	VAL
1	F	67	ALA
1	F	251	THR
1	A	64	CYS
1	B	251	THR
1	C	83	ALA
1	C	251	THR
1	F	82	GLN
1	C	6	TYR
1	C	26	GLU
1	D	32	ASN
1	A	49	SER
1	D	144	PRO
1	E	254	PHE

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	178/225 (79%)	172 (97%)	6 (3%)	32	47
1	B	218/225 (97%)	202 (93%)	16 (7%)	13	17
1	C	218/225 (97%)	200 (92%)	18 (8%)	10	13
1	D	218/225 (97%)	197 (90%)	21 (10%)	8	10
1	E	218/225 (97%)	207 (95%)	11 (5%)	22	32
1	F	176/225 (78%)	163 (93%)	13 (7%)	13	16
All	All	1226/1350 (91%)	1141 (93%)	85 (7%)	14	19

All (85) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	THR
1	A	51	VAL
1	A	96	LEU
1	A	107	VAL
1	A	157	ARG
1	A	163	MSE
1	B	35	LEU
1	B	44	ASN
1	B	47	GLU
1	B	52	THR
1	B	56	LEU
1	B	59	LEU
1	B	82	GLN
1	B	92	LEU
1	B	101	TYR
1	B	135	LEU
1	B	143	TYR
1	B	148	LEU
1	B	165	LEU
1	B	168	LYS
1	B	194	LYS
1	B	254	PHE
1	C	7	GLN
1	C	17	VAL
1	C	26	GLU
1	C	28	ASN
1	C	40	LEU
1	C	42	VAL
1	C	48	THR
1	C	78	ARG
1	C	87	GLU
1	C	96	LEU
1	C	108	ARG
1	C	129	GLN
1	C	130	THR
1	C	203	ASN
1	C	217	LEU
1	C	233	GLN
1	C	253	GLN
1	C	254	PHE
1	D	12	ARG
1	D	48	THR
1	D	52	THR

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Mol	Chain	Res	Type
1	D	53	VAL
1	D	61	GLU
1	D	65	PHE
1	D	81	LYS
1	D	87	GLU
1	D	95	LYS
1	D	116	LEU
1	D	148	LEU
1	D	157	ARG
1	D	163	MSE
1	D	165	LEU
1	D	172	VAL
1	D	181	ILE
1	D	200	ARG
1	D	205	LYS
1	D	242	GLN
1	D	253	GLN
1	D	254	PHE
1	E	31	ILE
1	E	52	THR
1	E	53	VAL
1	E	80	ARG
1	E	81	LYS
1	E	105	SER
1	E	135	LEU
1	E	138	LEU
1	E	168	LYS
1	E	253	GLN
1	E	254	PHE
1	F	42	VAL
1	F	47	GLU
1	F	56	LEU
1	F	92	LEU
1	F	116	LEU
1	F	135	LEU
1	F	137	GLU
1	F	148	LEU
1	F	172	VAL
1	F	189	ASP
1	F	205	LYS
1	F	234	ASP
1	F	240	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	14	GLN
1	A	41	GLN
1	A	106	HIS
1	A	129	GLN
1	A	209	HIS
1	A	219	HIS
1	A	232	ASN
1	A	233	GLN
1	A	242	GLN
1	B	28	ASN
1	B	82	GLN
1	B	86	GLN
1	B	97	GLN
1	B	106	HIS
1	B	173	GLN
1	B	212	GLN
1	B	233	GLN
1	B	240	GLN
1	C	14	GLN
1	C	28	ASN
1	C	45	GLN
1	C	129	GLN
1	C	158	GLN
1	C	203	ASN
1	C	240	GLN
1	D	7	GLN
1	D	28	ASN
1	D	32	ASN
1	D	86	GLN
1	D	97	GLN
1	D	106	HIS
1	D	129	GLN
1	D	219	HIS
1	D	242	GLN
1	E	28	ASN
1	E	41	GLN
1	E	45	GLN
1	E	86	GLN
1	E	106	HIS
1	E	129	GLN
1	F	86	GLN

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Mol	Chain	Res	Type
1	F	106	HIS
1	F	161	HIS
1	F	212	GLN
1	F	232	ASN
1	F	233	GLN
1	F	240	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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	243/267 (91%)	0.98	50 (20%) 2 3	16, 40, 79, 85	0
1	B	244/267 (91%)	0.23	7 (2%) 53 56	14, 30, 58, 73	0
1	C	244/267 (91%)	0.26	15 (6%) 27 30	13, 32, 58, 74	0
1	D	244/267 (91%)	0.88	27 (11%) 10 11	19, 45, 72, 77	0
1	E	244/267 (91%)	0.85	29 (11%) 9 10	17, 46, 68, 77	0
1	F	244/267 (91%)	1.10	56 (22%) 2 2	16, 42, 82, 87	0
All	All	1463/1602 (91%)	0.72	184 (12%) 8 9	13, 39, 74, 87	0

All (184) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	252	GLY	6.4
1	A	254	PHE	6.1
1	A	77	LYS	6.1
1	F	64	CYS	5.6
1	F	70	GLN	5.5
1	A	58	GLY	5.5
1	F	31	ILE	5.4
1	E	255	PRO	5.4
1	F	69	PHE	5.1
1	E	254	PHE	5.1
1	F	28	ASN	5.0
1	A	69	PHE	4.9
1	E	113	ALA	4.9
1	F	75	GLU	4.9
1	B	254	PHE	4.8
1	A	73	TYR	4.7
1	F	83	ALA	4.7
1	A	28	ASN	4.7
1	A	59	LEU	4.7

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Mol	Chain	Res	Type	RSRZ
1	F	79	GLY	4.7
1	A	26	GLU	4.7
1	F	29	ASN	4.6
1	B	255	PRO	4.6
1	A	31	ILE	4.6
1	F	25	PRO	4.6
1	F	255	PRO	4.6
1	F	254	PHE	4.5
1	A	60	PRO	4.5
1	F	72	ILE	4.5
1	F	63	PHE	4.5
1	A	64	CYS	4.5
1	A	29	ASN	4.4
1	D	254	PHE	4.3
1	A	74	GLN	4.3
1	A	72	ILE	4.2
1	A	63	PHE	4.0
1	F	245	ILE	4.0
1	F	73	TYR	3.9
1	A	84	SER	3.9
1	D	113	ALA	3.9
1	F	23	HIS	3.9
1	A	65	PHE	3.8
1	A	66	GLY	3.8
1	F	27	ALA	3.8
1	F	60	PRO	3.8
1	E	244	GLY	3.8
1	D	69	PHE	3.7
1	A	25	PRO	3.7
1	F	74	GLN	3.7
1	A	68	ASP	3.7
1	A	75	GLU	3.7
1	F	61	GLU	3.6
1	A	82	GLN	3.6
1	F	30	THR	3.6
1	A	27	ALA	3.6
1	A	251	THR	3.6
1	D	255	PRO	3.6
1	C	252	GLY	3.5
1	F	246	ILE	3.5
1	F	253	GLN	3.5
1	F	59	LEU	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	70	GLN	3.5
1	F	249	VAL	3.5
1	A	32	ASN	3.5
1	A	250	GLU	3.5
1	E	137	GLU	3.5
1	A	67	ALA	3.4
1	D	252	GLY	3.4
1	F	66	GLY	3.4
1	A	78	ARG	3.4
1	B	82	GLN	3.3
1	F	81	LYS	3.3
1	A	62	VAL	3.3
1	E	252	GLY	3.2
1	C	255	PRO	3.2
1	F	26	GLU	3.2
1	A	79	GLY	3.1
1	A	129	GLN	3.1
1	D	249	VAL	3.1
1	A	246	ILE	3.1
1	F	82	GLN	3.1
1	A	249	VAL	3.1
1	F	71	GLU	3.1
1	A	24	ARG	3.1
1	A	30	THR	3.0
1	A	23	HIS	3.0
1	A	253	GLN	3.0
1	F	78	ARG	3.0
1	D	245	ILE	3.0
1	F	248	TYR	3.0
1	D	59	LEU	3.0
1	F	251	THR	3.0
1	A	252	GLY	3.0
1	E	42	VAL	2.9
1	F	32	ASN	2.9
1	E	82	GLN	2.9
1	C	80	ARG	2.9
1	C	48	THR	2.9
1	E	251	THR	2.9
1	D	70	GLN	2.8
1	F	48	THR	2.8
1	F	62	VAL	2.8
1	F	77	LYS	2.8

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Mol	Chain	Res	Type	RSRZ
1	E	5	THR	2.8
1	F	45	GLN	2.8
1	F	233	GLN	2.7
1	A	245	ILE	2.7
1	C	78	ARG	2.7
1	A	83	ALA	2.7
1	D	248	TYR	2.7
1	F	67	ALA	2.7
1	E	22	PHE	2.7
1	F	65	PHE	2.7
1	D	81	LYS	2.7
1	F	250	GLU	2.7
1	F	80	ARG	2.7
1	E	61	GLU	2.7
1	D	236	PHE	2.6
1	F	234	ASP	2.6
1	A	50	THR	2.6
1	D	251	THR	2.6
1	B	81	LYS	2.6
1	C	251	THR	2.6
1	F	5	THR	2.6
1	D	246	ILE	2.6
1	E	78	ARG	2.5
1	F	33	ASP	2.5
1	F	58	GLY	2.5
1	C	254	PHE	2.5
1	E	237	SER	2.5
1	D	67	ALA	2.5
1	E	253	GLN	2.5
1	D	242	GLN	2.4
1	A	5	THR	2.4
1	D	66	GLY	2.4
1	E	79	GLY	2.4
1	A	80	ARG	2.4
1	D	82	GLN	2.4
1	F	6	TYR	2.4
1	D	31	ILE	2.4
1	B	78	ARG	2.3
1	A	61	GLU	2.3
1	A	71	GLU	2.3
1	D	241	ASN	2.3
1	A	33	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	E	239	PRO	2.3
1	D	79	GLY	2.3
1	E	50	THR	2.3
1	D	32	ASN	2.3
1	E	70	GLN	2.3
1	E	233	GLN	2.3
1	E	246	ILE	2.3
1	B	252	GLY	2.2
1	E	167	THR	2.2
1	F	187	GLU	2.2
1	D	237	SER	2.2
1	D	73	TYR	2.2
1	F	112	ASN	2.2
1	C	5	THR	2.2
1	C	217	LEU	2.2
1	F	24	ARG	2.2
1	E	81	LYS	2.2
1	E	80	ARG	2.1
1	B	245	ILE	2.1
1	C	26	GLU	2.1
1	D	65	PHE	2.1
1	A	81	LYS	2.1
1	F	68	ASP	2.1
1	C	79	GLY	2.1
1	A	34	THR	2.1
1	E	249	VAL	2.1
1	E	46	CYS	2.1
1	C	83	ALA	2.1
1	C	32	ASN	2.1
1	C	253	GLN	2.1
1	A	140	PHE	2.1
1	C	69	PHE	2.1
1	E	85	SER	2.0
1	D	60	PRO	2.0
1	F	49	SER	2.0
1	E	219	HIS	2.0
1	F	35	LEU	2.0
1	D	239	PRO	2.0
1	E	31	ILE	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.