



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 04:02 PM UTC

PDB ID : 1G5X / pdb_00001g5x
Title : The Structure of Beta-Ketoacyl-[Acyl Carrier Protein] Synthase I
Authors : Zhang, Y.M.; Rao, M.S.; Heath, R.J.; Price, A.C.; Olson, A.J.; Rock, C.O.;
White, S.W.
Deposited on : 2000-11-02
Resolution : 2.45 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
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

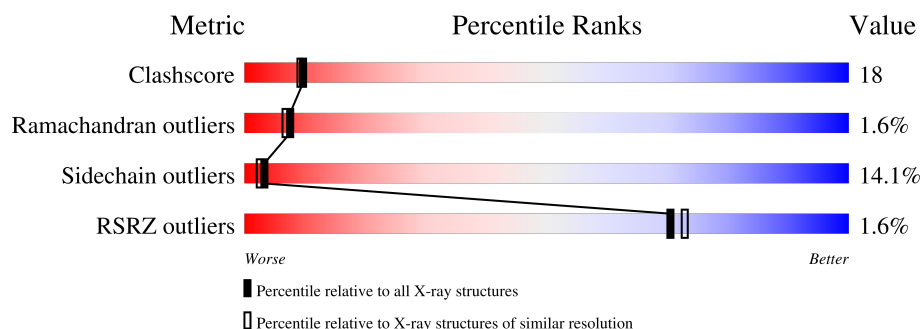
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.45 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	1229 (2.46-2.46)
Ramachandran outliers	187476	1218 (2.46-2.46)
Sidechain outliers	187428	1218 (2.46-2.46)
RSRZ outliers	180081	1190 (2.46-2.46)

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	406	2% 65% 27% 7% ..
1	B	406	2% 66% 25% 8% ..
1	C	406	2% 65% 25% 8% ..
1	D	406	2% 66% 25% 8% ..

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 12220 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 BETA-KETOACYL ACYL CARRIER PROTEIN SYNTHASE I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	403	Total	C	N	O	S	0	0	0
			2955	1838	515	580	22			
1	B	403	Total	C	N	O	S	0	0	0
			2955	1838	515	580	22			
1	C	403	Total	C	N	O	S	0	0	0
			2955	1838	515	580	22			
1	D	403	Total	C	N	O	S	0	0	0
			2955	1838	515	580	22			

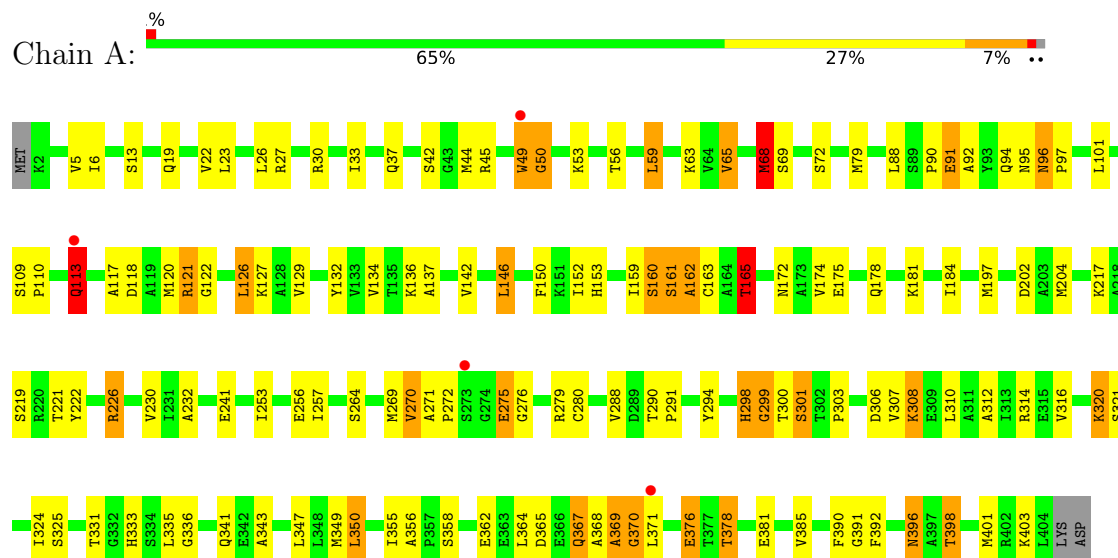
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	95	Total	O	0	0
			95	95		
2	B	104	Total	O	0	0
			104	104		
2	C	89	Total	O	0	0
			89	89		
2	D	112	Total	O	0	0
			112	112		

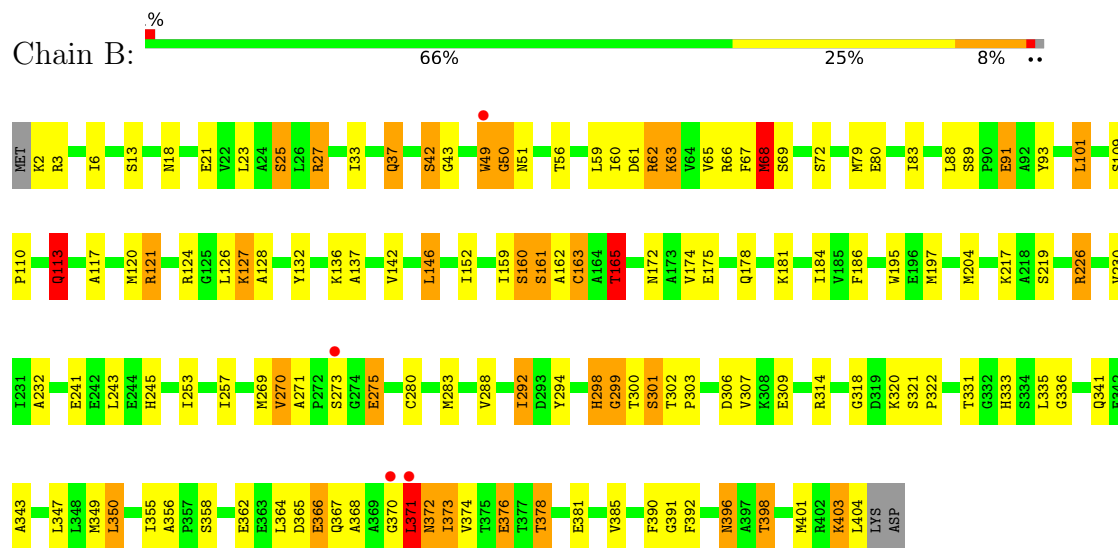
3 Residue-property plots [i](#)

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: BETA-KETOACYL ACYL CARRIER PROTEIN SYNTHASE I

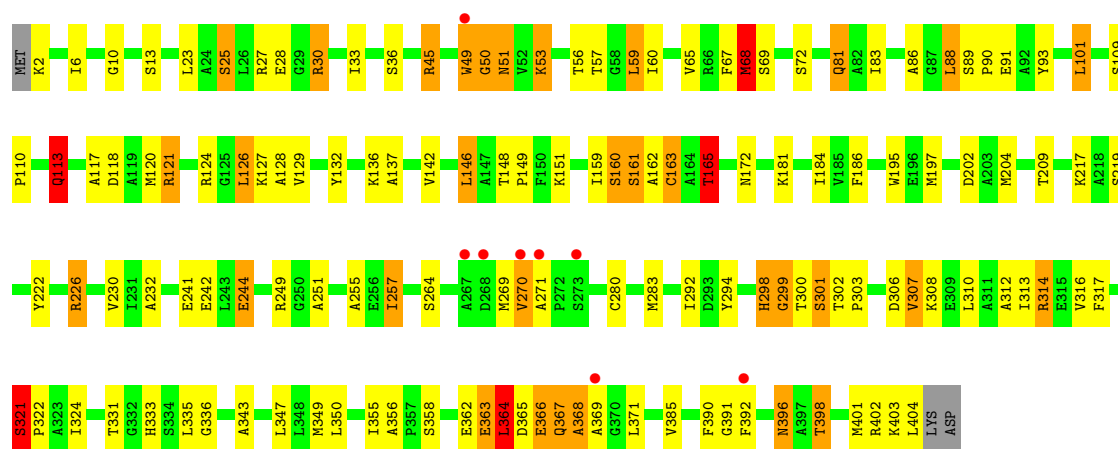


• Molecule 1: BETA-KETOACYL ACYL CARRIER PROTEIN SYNTHASE I

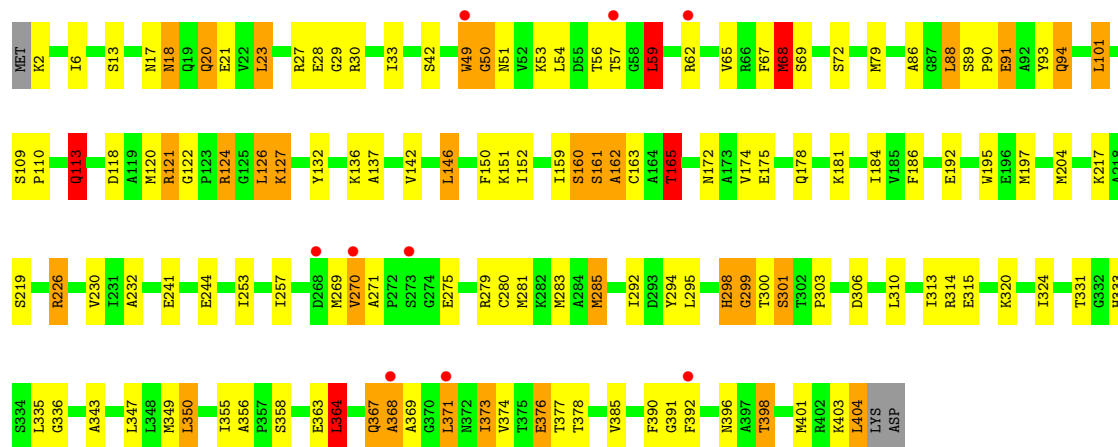


• Molecule 1: BETA-KETOACYL ACYL CARRIER PROTEIN SYNTHASE I





• Molecule 1: BETA-KETOACYL ACYL CARRIER PROTEIN SYNTHASE I



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	59.10Å 139.60Å 212.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.90 – 2.45 19.90 – 2.45	Depositor EDS
% Data completeness (in resolution range)	(Not available) (19.90-2.45) 92.8 (19.90-2.45)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.89 (at 2.47Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.199 , 0.266 0.215 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	21.2	Xtriage
Anisotropy	0.564	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 43.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	12220	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.72% 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	0.48	0/3003	0.99	17/4058 (0.4%)
1	B	0.51	0/3003	0.99	14/4058 (0.3%)
1	C	0.48	0/3003	0.99	14/4058 (0.3%)
1	D	0.50	0/3003	0.99	17/4058 (0.4%)
All	All	0.49	0/12012	0.99	62/16232 (0.4%)

There are no bond length outliers.

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	68	MET	N-CA-C	7.09	121.02	110.52
1	B	68	MET	N-CA-C	6.94	120.79	110.52
1	D	68	MET	N-CA-C	6.75	120.50	110.52
1	B	165	THR	N-CA-C	6.74	119.20	111.11
1	D	69	SER	N-CA-C	-6.71	100.29	109.95
1	A	122	GLY	CA-C-N	6.66	126.29	119.56
1	A	122	GLY	C-N-CA	6.66	126.29	119.56
1	B	69	SER	N-CA-C	-6.58	100.47	110.14
1	D	165	THR	N-CA-C	6.57	119.00	111.11
1	D	113	GLN	N-CA-C	-6.57	103.61	111.69
1	C	69	SER	N-CA-C	-6.46	100.64	110.14
1	A	68	MET	N-CA-C	6.46	120.08	110.52
1	A	165	THR	N-CA-C	6.43	118.82	111.11
1	B	113	GLN	N-CA-C	-6.36	103.87	111.69
1	A	113	GLN	N-CA-C	-6.32	103.91	111.69
1	D	29	GLY	N-CA-C	-6.31	104.03	114.76
1	A	343	ALA	N-CA-C	-6.27	104.53	111.36
1	B	343	ALA	N-CA-C	-6.26	104.53	111.36
1	A	96	ASN	CA-C-N	6.25	125.93	119.56
1	A	96	ASN	C-N-CA	6.25	125.93	119.56
1	C	113	GLN	N-CA-C	-6.09	104.19	111.69
1	A	50	GLY	N-CA-C	-6.03	98.90	113.18
1	C	165	THR	N-CA-C	6.02	118.34	111.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	275	GLU	N-CA-C	-6.00	101.16	110.10
1	B	298	HIS	N-CA-C	-5.99	104.83	111.36
1	B	331	THR	N-CA-C	5.95	120.70	112.90
1	C	343	ALA	N-CA-C	-5.89	104.94	111.36
1	A	69	SER	N-CA-C	-5.88	101.49	110.14
1	C	331	THR	N-CA-C	5.86	120.58	112.90
1	D	343	ALA	N-CA-C	-5.83	105.00	111.36
1	D	50	GLY	N-CA-C	-5.79	99.46	113.18
1	D	93	TYR	N-CA-C	5.79	119.52	112.23
1	C	50	GLY	N-CA-C	-5.77	99.50	113.18
1	D	331	THR	N-CA-C	5.75	120.44	112.90
1	C	129	VAL	N-CA-C	-5.73	104.93	110.72
1	A	298	HIS	N-CA-C	-5.73	105.12	111.36
1	B	50	GLY	N-CA-C	-5.70	99.67	113.18
1	A	331	THR	N-CA-C	5.61	120.25	112.90
1	D	51	ASN	N-CA-C	5.60	118.12	110.55
1	A	162	ALA	CB-CA-C	-5.56	110.14	116.54
1	D	298	HIS	N-CA-C	-5.53	105.33	111.36
1	C	51	ASN	N-CA-C	5.49	118.60	110.48
1	B	37	GLN	N-CA-C	-5.41	105.46	111.36
1	D	122	GLY	CA-C-N	5.38	125.20	119.28
1	D	122	GLY	C-N-CA	5.38	125.20	119.28
1	C	13	SER	N-CA-C	5.36	116.41	108.86
1	A	13	SER	N-CA-C	5.35	116.40	108.86
1	C	298	HIS	N-CA-C	-5.34	105.54	111.36
1	B	43	GLY	N-CA-C	-5.32	107.34	115.00
1	B	373	ILE	N-CA-C	-5.32	99.44	107.73
1	D	59	LEU	N-CA-C	5.29	119.36	113.01
1	A	129	VAL	N-CA-C	-5.27	105.58	110.53
1	A	45	ARG	N-CA-C	-5.26	106.71	113.23
1	B	13	SER	N-CA-C	5.25	116.26	108.86
1	C	321	SER	CA-C-N	-5.23	115.19	120.21
1	C	321	SER	C-N-CA	-5.23	115.19	120.21
1	B	51	ASN	N-CA-C	5.23	118.22	110.48
1	D	162	ALA	CB-CA-C	-5.19	110.57	116.54
1	D	13	SER	N-CA-C	5.14	116.80	109.14
1	D	368	ALA	N-CA-C	-5.13	104.91	110.91
1	A	19	GLN	N-CA-C	5.08	117.56	111.71
1	C	45	ARG	N-CA-C	-5.00	107.03	113.23

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	2955	0	2910	95	0
1	B	2955	0	2910	94	0
1	C	2955	0	2910	121	0
1	D	2955	0	2910	129	0
2	A	95	0	0	4	0
2	B	104	0	0	6	0
2	C	89	0	0	8	0
2	D	112	0	0	6	0
All	All	12220	0	11640	415	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 18.

All (415) 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:B:314:ARG:HH12	1:B:370:GLY:HA3	1.20	1.02
1:D:124:ARG:HH11	1:D:124:ARG:HG2	1.26	0.96
1:D:310:LEU:HD13	1:D:368:ALA:HB2	1.48	0.96
1:D:310:LEU:HD13	1:D:368:ALA:CB	1.98	0.94
1:D:56:THR:HA	1:D:59:LEU:HD22	1.48	0.93
1:D:349:MET:HE3	1:D:356:ALA:H	1.36	0.91
1:B:349:MET:HE3	1:B:356:ALA:H	1.36	0.90
1:D:349:MET:HE3	1:D:355:ILE:HA	1.53	0.90
1:C:349:MET:HE3	1:C:355:ILE:HA	1.55	0.89
1:A:349:MET:HE3	1:A:356:ALA:H	1.38	0.88
1:C:349:MET:HE3	1:C:356:ALA:H	1.38	0.88
1:B:349:MET:HE3	1:B:355:ILE:HA	1.55	0.86
1:A:349:MET:HE3	1:A:355:ILE:HA	1.56	0.86
1:D:314:ARG:NH2	1:D:368:ALA:HA	1.89	0.86
1:C:56:THR:HA	1:C:59:LEU:HD22	1.56	0.84
1:D:6:ILE:HD11	1:D:257:ILE:HD11	1.59	0.83
1:B:314:ARG:HH22	1:B:370:GLY:H	1.27	0.82
1:A:280:CYS:SG	1:A:398:THR:HG23	2.19	0.82
1:C:310:LEU:HD13	1:C:368:ALA:CB	2.10	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:280:CYS:SG	1:C:398:THR:HG23	2.19	0.81
1:B:56:THR:HA	1:B:59:LEU:HD22	1.60	0.81
1:D:314:ARG:HH21	1:D:368:ALA:HA	1.46	0.80
1:A:6:ILE:HD11	1:A:257:ILE:HD11	1.62	0.79
1:A:113:GLN:OE1	1:B:113:GLN:OE1	2.00	0.79
1:D:124:ARG:HG2	1:D:124:ARG:NH1	1.91	0.79
1:D:280:CYS:SG	1:D:398:THR:HG23	2.23	0.78
1:A:110:PRO:HG2	1:A:197:MET:HB2	1.65	0.77
1:D:27:ARG:HD3	2:D:420:HOH:O	1.85	0.77
1:C:110:PRO:HG2	1:C:197:MET:HB2	1.66	0.77
1:B:110:PRO:HG2	1:B:197:MET:HB2	1.68	0.76
1:B:280:CYS:SG	1:B:398:THR:HG23	2.27	0.75
1:A:314:ARG:NH1	1:A:371:LEU:HD11	2.00	0.75
1:D:110:PRO:HG2	1:D:197:MET:HB2	1.68	0.74
1:A:56:THR:HA	1:A:59:LEU:HD22	1.68	0.74
1:B:124:ARG:HB2	1:B:128:ALA:HB2	1.68	0.74
1:C:25:SER:HA	1:C:30:ARG:HD2	1.68	0.73
1:C:113:GLN:OE1	1:D:113:GLN:OE1	2.06	0.73
1:A:42:SER:OG	1:A:44:MET:HG3	1.88	0.73
1:D:349:MET:HE3	1:D:356:ALA:N	2.04	0.72
1:C:310:LEU:HD13	1:C:368:ALA:HB1	1.69	0.72
1:A:272:PRO:O	1:A:308:LYS:HD3	1.88	0.72
1:B:226:ARG:NH2	1:B:365:ASP:OD1	2.23	0.71
1:D:349:MET:CE	1:D:355:ILE:HA	2.19	0.71
1:A:132:TYR:O	1:A:136:LYS:HG3	1.90	0.71
1:A:307:VAL:HG11	1:A:367:GLN:HG3	1.74	0.70
1:B:349:MET:CE	1:B:355:ILE:HA	2.20	0.70
1:C:132:TYR:O	1:C:136:LYS:HG3	1.92	0.70
1:C:118:ASP:OD1	1:D:121:ARG:NH2	2.25	0.70
1:B:6:ILE:HD11	1:B:257:ILE:HD11	1.72	0.70
1:D:62:ARG:HB2	2:D:518:HOH:O	1.91	0.70
1:D:314:ARG:HH21	1:D:368:ALA:CA	2.04	0.69
1:A:349:MET:HE3	1:A:356:ALA:N	2.07	0.69
1:B:132:TYR:O	1:B:136:LYS:HG3	1.92	0.69
1:B:349:MET:HE3	1:B:356:ALA:N	2.05	0.69
1:D:132:TYR:O	1:D:136:LYS:HG3	1.92	0.69
1:C:349:MET:HE3	1:C:356:ALA:N	2.07	0.69
1:C:117:ALA:O	1:C:121:ARG:HD3	1.93	0.69
1:C:349:MET:CE	1:C:355:ILE:HA	2.22	0.69
1:C:118:ASP:CG	1:D:121:ARG:HH22	2.01	0.68
1:C:121:ARG:HD2	1:D:195:TRP:HH2	1.59	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:349:MET:CE	1:A:355:ILE:HA	2.23	0.68
1:D:363:GLU:O	1:D:364:LEU:HB2	1.93	0.67
1:C:184:ILE:HG12	1:C:241:GLU:HG3	1.76	0.67
1:D:371:LEU:HB3	2:D:498:HOH:O	1.94	0.67
1:C:6:ILE:HD11	1:C:257:ILE:HD11	1.76	0.66
1:C:310:LEU:HD13	1:C:368:ALA:HB2	1.78	0.66
1:A:117:ALA:O	1:A:121:ARG:HD2	1.95	0.65
1:D:349:MET:CE	1:D:356:ALA:H	2.09	0.65
1:D:371:LEU:HD22	1:D:373:ILE:HG23	1.77	0.65
1:B:241:GLU:OE1	1:B:245:HIS:HD2	1.78	0.65
1:C:121:ARG:HD2	1:D:195:TRP:CH2	2.32	0.65
1:B:18:ASN:OD1	1:B:21:GLU:HG3	1.97	0.65
1:C:312:ALA:O	1:C:316:VAL:HG23	1.96	0.65
1:C:113:GLN:NE2	2:C:421:HOH:O	2.31	0.64
1:C:160:SER:HA	1:C:165:THR:HB	1.80	0.63
1:B:160:SER:HA	1:B:165:THR:HB	1.78	0.63
1:C:27:ARG:HD3	2:C:463:HOH:O	1.99	0.63
1:C:162:ALA:O	1:C:165:THR:CG2	2.47	0.63
1:D:349:MET:HE3	1:D:355:ILE:CA	2.29	0.63
1:D:160:SER:HA	1:D:165:THR:HB	1.80	0.63
1:D:314:ARG:NH2	1:D:368:ALA:CA	2.60	0.62
1:C:314:ARG:HH22	1:C:368:ALA:HA	1.64	0.62
1:A:160:SER:HA	1:A:165:THR:HB	1.81	0.62
1:B:349:MET:CE	1:B:356:ALA:H	2.11	0.62
1:B:292:ILE:HG22	1:B:322:PRO:HB3	1.80	0.62
1:A:90:PRO:HA	1:A:94:GLN:HG3	1.82	0.61
1:B:314:ARG:NH1	1:B:370:GLY:HA3	2.04	0.61
1:D:124:ARG:HH11	1:D:124:ARG:CG	2.05	0.61
1:A:162:ALA:O	1:A:165:THR:CG2	2.49	0.61
1:A:350:LEU:HD22	1:A:403:LYS:HE2	1.83	0.60
1:D:94:GLN:HG2	1:D:151:LYS:HB2	1.83	0.60
1:B:162:ALA:O	1:B:165:THR:CG2	2.50	0.60
1:D:28:GLU:HG3	1:D:30:ARG:HH21	1.67	0.60
1:C:25:SER:HA	1:C:30:ARG:HG3	1.84	0.59
1:C:25:SER:HA	1:C:30:ARG:CD	2.32	0.59
1:A:226:ARG:NH2	1:A:365:ASP:OD1	2.36	0.59
1:A:294:TYR:CZ	1:A:349:MET:HE1	2.38	0.59
1:B:42:SER:OG	1:B:195:TRP:HB2	2.03	0.59
1:B:204:MET:HE1	1:B:270:VAL:HG11	1.84	0.59
1:D:18:ASN:ND2	1:D:21:GLU:H	2.00	0.59
1:D:310:LEU:CD1	1:D:368:ALA:HB2	2.29	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:275:GLU:OE1	1:A:279:ARG:NH2	2.34	0.59
1:B:184:ILE:HG12	1:B:241:GLU:HG3	1.85	0.59
1:A:184:ILE:HG12	1:A:241:GLU:HG3	1.85	0.58
1:A:349:MET:CE	1:A:356:ALA:H	2.13	0.58
1:B:294:TYR:CZ	1:B:349:MET:HE1	2.39	0.58
1:D:94:GLN:CG	1:D:151:LYS:HB2	2.34	0.58
1:D:184:ILE:HG12	1:D:241:GLU:HG3	1.83	0.58
1:D:162:ALA:O	1:D:165:THR:CG2	2.51	0.58
2:A:441:HOH:O	1:B:283:MET:HE2	2.03	0.58
1:C:333:HIS:CE1	1:C:335:LEU:HA	2.38	0.58
1:A:365:ASP:OD2	1:A:367:GLN:HG2	2.03	0.58
1:D:363:GLU:O	1:D:364:LEU:CB	2.52	0.57
1:D:371:LEU:HD22	1:D:373:ILE:CG2	2.34	0.57
1:B:350:LEU:HD22	1:B:403:LYS:HG3	1.85	0.57
1:A:333:HIS:CE1	1:A:335:LEU:HA	2.39	0.57
1:B:61:ASP:O	1:B:65:VAL:HG12	2.05	0.57
1:A:341:GLN:NE2	2:A:476:HOH:O	2.37	0.57
1:B:366:GLU:C	1:B:368:ALA:H	2.13	0.57
1:C:10:GLY:CA	1:C:81:GLN:HB3	2.34	0.57
1:C:349:MET:CE	1:C:356:ALA:H	2.11	0.57
1:D:333:HIS:CE1	1:D:335:LEU:HA	2.40	0.57
1:C:363:GLU:O	1:C:364:LEU:HB2	2.04	0.57
1:D:283:MET:HE2	2:D:504:HOH:O	2.05	0.57
1:C:25:SER:HA	1:C:30:ARG:CG	2.35	0.56
1:C:349:MET:HE3	1:C:355:ILE:CA	2.30	0.56
1:D:374:VAL:HG11	1:D:378:THR:HG22	1.87	0.56
1:A:162:ALA:O	1:A:165:THR:HG23	2.06	0.56
1:B:349:MET:HE3	1:B:355:ILE:CA	2.30	0.56
1:B:333:HIS:CE1	1:B:335:LEU:HA	2.41	0.56
1:C:283:MET:HE2	2:C:431:HOH:O	2.05	0.56
1:B:124:ARG:O	1:B:127:LYS:HD2	2.05	0.56
1:A:349:MET:HE3	1:A:355:ILE:CA	2.32	0.56
1:A:314:ARG:NH2	2:A:466:HOH:O	2.39	0.55
1:D:162:ALA:O	1:D:165:THR:HG23	2.07	0.55
1:B:162:ALA:O	1:B:165:THR:HG23	2.07	0.55
1:C:310:LEU:HD22	1:C:371:LEU:CD1	2.36	0.55
1:C:120:MET:HE1	1:C:126:LEU:HD13	1.89	0.55
1:A:204:MET:HE1	1:A:270:VAL:HG11	1.87	0.55
1:C:204:MET:HE1	1:C:270:VAL:HG11	1.88	0.55
1:A:370:GLY:C	1:A:371:LEU:HD12	2.32	0.55
1:B:307:VAL:HG23	2:B:493:HOH:O	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:89:SER:O	1:C:90:PRO:C	2.48	0.55
1:C:402:ARG:HB3	2:C:479:HOH:O	2.06	0.55
1:D:371:LEU:HD13	1:D:373:ILE:HD12	1.89	0.55
1:D:373:ILE:HD13	1:D:373:ILE:H	1.71	0.55
1:B:117:ALA:O	1:B:121:ARG:HD2	2.07	0.54
1:C:162:ALA:O	1:C:165:THR:HG23	2.08	0.54
1:B:83:ILE:HD13	1:B:93:TYR:CZ	2.42	0.54
1:D:18:ASN:HD21	1:D:20:GLN:HG3	1.71	0.54
1:D:91:GLU:CD	1:D:91:GLU:H	2.14	0.54
1:D:281:MET:O	1:D:285:MET:HG3	2.07	0.54
1:D:324:ILE:O	1:D:373:ILE:HA	2.07	0.54
1:D:253:ILE:HG21	1:D:404:LEU:HD23	1.89	0.54
1:C:363:GLU:O	1:C:364:LEU:CB	2.55	0.54
1:A:376:GLU:O	1:A:378:THR:HG22	2.08	0.54
1:C:294:TYR:CZ	1:C:349:MET:HE1	2.43	0.54
1:D:367:GLN:O	1:D:368:ALA:HB3	2.07	0.54
1:D:124:ARG:O	1:D:127:LYS:HD3	2.08	0.54
2:C:431:HOH:O	1:D:181:LYS:HE2	2.07	0.54
1:D:269:MET:O	1:D:270:VAL:HG22	2.07	0.54
1:D:17:ASN:ND2	1:D:54:LEU:HB2	2.23	0.54
1:C:124:ARG:HB2	1:C:128:ALA:HB2	1.89	0.53
1:D:310:LEU:HD13	1:D:368:ALA:HB1	1.87	0.53
1:C:10:GLY:HA3	1:C:81:GLN:HB3	1.89	0.53
1:D:294:TYR:CZ	1:D:349:MET:HE1	2.43	0.53
1:A:33:ILE:HA	1:A:49:TRP:O	2.09	0.53
1:B:292:ILE:HG22	1:B:322:PRO:CB	2.38	0.53
1:D:204:MET:HE1	1:D:270:VAL:HG11	1.90	0.53
1:D:226:ARG:NH1	1:D:303:PRO:HA	2.23	0.53
1:A:300:THR:O	1:A:301:SER:CB	2.57	0.53
1:A:314:ARG:HH12	1:A:371:LEU:HD11	1.72	0.53
1:D:68:MET:HB3	1:D:72:SER:HB2	1.90	0.53
1:C:28:GLU:HB3	1:C:30:ARG:HG2	1.89	0.53
1:B:163:CYS:SG	1:B:391:GLY:HA2	2.49	0.52
1:C:195:TRP:HH2	1:D:121:ARG:HD2	1.73	0.52
1:C:68:MET:HB3	1:C:72:SER:HB2	1.91	0.52
1:A:68:MET:HB3	1:A:72:SER:HB2	1.90	0.52
1:C:163:CYS:SG	1:C:391:GLY:HA2	2.50	0.52
1:A:269:MET:O	1:A:271:ALA:N	2.39	0.52
1:B:314:ARG:HH12	1:B:370:GLY:CA	2.07	0.52
1:A:312:ALA:O	1:A:316:VAL:HG23	2.09	0.52
1:C:36:SER:HB2	1:C:49:TRP:CD2	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:275:GLU:HG3	1:A:276:GLY:N	2.25	0.51
1:D:295:LEU:HD13	1:D:313:ILE:HD13	1.91	0.51
1:B:33:ILE:HA	1:B:49:TRP:O	2.11	0.51
1:B:341:GLN:NE2	2:B:409:HOH:O	2.43	0.51
1:C:142:VAL:O	1:C:146:LEU:HG	2.10	0.51
1:D:269:MET:O	1:D:271:ALA:N	2.39	0.51
1:D:18:ASN:ND2	1:D:20:GLN:HG3	2.25	0.51
1:D:33:ILE:HA	1:D:49:TRP:O	2.10	0.51
1:D:90:PRO:O	1:D:94:GLN:HB2	2.10	0.51
1:D:355:ILE:HB	1:D:378:THR:CG2	2.40	0.51
1:C:159:ILE:HG12	1:D:159:ILE:HG12	1.93	0.51
1:A:307:VAL:CG1	1:A:367:GLN:HG3	2.40	0.51
1:A:369:ALA:C	1:A:371:LEU:HD12	2.36	0.51
1:B:109:SER:HB3	1:B:137:ALA:HA	1.93	0.51
1:B:269:MET:O	1:B:271:ALA:N	2.41	0.51
1:B:371:LEU:HD23	1:B:373:ILE:H	1.76	0.51
1:C:390:PHE:CD1	1:C:396:ASN:HB3	2.45	0.50
1:A:142:VAL:O	1:A:146:LEU:HG	2.10	0.50
1:C:162:ALA:O	1:C:165:THR:HG22	2.10	0.50
1:C:269:MET:O	1:C:270:VAL:HG22	2.11	0.50
1:B:79:MET:O	1:B:83:ILE:HG13	2.12	0.50
1:B:385:VAL:HG23	1:B:401:MET:HE3	1.94	0.50
1:C:385:VAL:HG23	1:C:401:MET:HE3	1.93	0.50
1:D:6:ILE:CD1	1:D:257:ILE:HD11	2.36	0.50
1:B:120:MET:SD	1:B:126:LEU:HD23	2.52	0.50
1:A:390:PHE:CD1	1:A:396:ASN:HB3	2.47	0.49
1:B:226:ARG:NH1	1:B:303:PRO:HA	2.27	0.49
1:D:371:LEU:HD22	1:D:373:ILE:HD12	1.94	0.49
1:C:83:ILE:HD13	1:C:93:TYR:CZ	2.47	0.49
1:D:373:ILE:HG12	1:D:373:ILE:O	2.12	0.49
1:D:385:VAL:HG23	1:D:401:MET:HE3	1.94	0.49
1:B:68:MET:HB3	1:B:72:SER:HB2	1.94	0.49
1:B:142:VAL:O	1:B:146:LEU:HG	2.12	0.49
1:B:300:THR:O	1:B:301:SER:CB	2.61	0.49
1:C:181:LYS:NZ	1:D:175:GLU:OE2	2.46	0.49
1:D:355:ILE:HB	1:D:378:THR:HG22	1.94	0.49
1:A:226:ARG:NH1	1:A:306:ASP:HB2	2.28	0.49
1:D:142:VAL:O	1:D:146:LEU:HG	2.13	0.49
1:A:269:MET:O	1:A:270:VAL:HG22	2.13	0.49
1:C:113:GLN:HG2	1:D:110:PRO:HB3	1.94	0.49
1:D:120:MET:HE1	1:D:126:LEU:HD13	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:385:VAL:HG23	1:A:401:MET:HE3	1.94	0.49
1:C:121:ARG:NH2	1:D:118:ASP:OD1	2.46	0.49
1:D:350:LEU:HD22	1:D:403:LYS:HE2	1.94	0.49
1:A:163:CYS:SG	1:A:391:GLY:HA2	2.53	0.49
1:C:226:ARG:NH1	1:C:306:ASP:HB2	2.26	0.49
1:C:300:THR:O	1:C:301:SER:CB	2.61	0.49
1:D:368:ALA:O	1:D:371:LEU:HG	2.12	0.49
1:B:63:LYS:HZ3	1:B:66:ARG:HH12	1.59	0.48
1:C:110:PRO:HB3	1:D:113:GLN:HG2	1.94	0.48
1:D:368:ALA:HB1	1:D:371:LEU:HD23	1.95	0.48
1:B:269:MET:O	1:B:270:VAL:HG22	2.13	0.48
1:A:226:ARG:NH1	1:A:303:PRO:HA	2.28	0.48
1:C:244:GLU:OE1	1:C:244:GLU:HA	2.13	0.48
1:C:269:MET:C	1:C:271:ALA:H	2.21	0.48
1:A:53:LYS:HD3	1:A:53:LYS:N	2.28	0.48
1:B:390:PHE:CD1	1:B:396:ASN:HB3	2.49	0.48
1:C:165:THR:HG23	1:C:336:GLY:HA2	1.96	0.48
1:C:310:LEU:CD1	1:C:368:ALA:HB2	2.42	0.48
1:C:366:GLU:C	1:C:368:ALA:H	2.22	0.48
1:B:50:GLY:HA3	1:B:232:ALA:HB2	1.96	0.48
1:C:33:ILE:HA	1:C:49:TRP:O	2.12	0.48
1:C:269:MET:HG3	1:D:67:PHE:CD2	2.49	0.48
1:C:298:HIS:O	1:C:299:GLY:C	2.57	0.48
1:A:22:VAL:O	1:A:26:LEU:HG	2.13	0.48
1:A:165:THR:HG23	1:A:336:GLY:HA2	1.96	0.47
1:C:45:ARG:NH1	1:C:209:THR:HG21	2.29	0.47
1:C:314:ARG:NH2	1:C:368:ALA:HA	2.28	0.47
1:D:161:SER:OG	1:D:165:THR:HA	2.14	0.47
1:B:226:ARG:NH1	1:B:306:ASP:HB2	2.30	0.47
1:C:86:ALA:O	1:C:88:LEU:HD22	2.13	0.47
1:A:5:VAL:HG12	1:A:256:GLU:HB2	1.96	0.47
1:A:79:MET:HE2	1:A:150:PHE:CG	2.49	0.47
1:A:109:SER:HB3	1:A:137:ALA:HA	1.96	0.47
1:A:270:VAL:HG12	1:A:392:PHE:CD2	2.50	0.47
1:A:368:ALA:C	1:A:371:LEU:HD13	2.39	0.47
1:B:27:ARG:HD3	2:B:438:HOH:O	2.15	0.47
1:D:390:PHE:CD1	1:D:396:ASN:HB3	2.49	0.47
1:C:28:GLU:CB	1:C:30:ARG:HG2	2.44	0.47
1:D:20:GLN:HG3	1:D:21:GLU:N	2.29	0.47
1:A:113:GLN:HG2	1:B:110:PRO:HB3	1.97	0.47
1:A:300:THR:O	1:A:301:SER:HB3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:79:MET:HE2	1:D:150:PHE:CG	2.50	0.47
1:A:159:ILE:HG12	1:B:159:ILE:HG12	1.96	0.46
1:B:161:SER:OG	1:B:165:THR:HA	2.15	0.46
1:C:226:ARG:NH2	1:C:365:ASP:CG	2.73	0.46
1:A:161:SER:OG	1:A:165:THR:HA	2.16	0.46
1:D:300:THR:O	1:D:301:SER:CB	2.62	0.46
1:B:62:ARG:CZ	1:B:62:ARG:HB3	2.45	0.46
1:C:50:GLY:HA3	1:C:232:ALA:HB2	1.96	0.46
1:D:269:MET:C	1:D:271:ALA:H	2.23	0.46
1:C:10:GLY:HA2	1:C:81:GLN:HB3	1.98	0.46
1:D:18:ASN:C	1:D:18:ASN:HD22	2.22	0.46
1:D:109:SER:HB3	1:D:137:ALA:HA	1.97	0.46
1:C:33:ILE:HG13	2:C:485:HOH:O	2.15	0.46
1:C:67:PHE:O	1:C:136:LYS:HG2	2.15	0.46
1:D:86:ALA:HB3	1:D:88:LEU:HD22	1.97	0.46
1:D:163:CYS:SG	1:D:391:GLY:HA2	2.55	0.46
1:A:174:VAL:O	1:A:178:GLN:HG3	2.15	0.46
1:B:300:THR:O	1:B:301:SER:HB3	2.16	0.46
1:C:33:ILE:HD12	1:C:230:VAL:HG11	1.97	0.46
1:A:110:PRO:HB3	1:B:113:GLN:HG2	1.98	0.46
1:B:67:PHE:O	1:B:136:LYS:HG2	2.16	0.46
1:C:161:SER:OG	1:C:165:THR:HA	2.16	0.46
1:C:109:SER:HB3	1:C:137:ALA:HA	1.96	0.46
1:A:162:ALA:O	1:A:165:THR:HG22	2.16	0.46
1:C:242:GLU:OE1	1:C:244:GLU:HB2	2.16	0.46
1:B:309:GLU:HB3	2:B:508:HOH:O	2.14	0.46
1:C:270:VAL:HG12	1:C:392:PHE:CD2	2.50	0.46
1:D:89:SER:OG	1:D:91:GLU:HG2	2.15	0.46
1:B:270:VAL:HG12	1:B:392:PHE:CD2	2.51	0.45
1:A:65:VAL:HA	1:A:68:MET:HG3	1.97	0.45
1:C:255:ALA:HB1	1:C:402:ARG:O	2.17	0.45
1:C:269:MET:O	1:C:271:ALA:N	2.38	0.45
1:D:244:GLU:OE1	1:D:244:GLU:HA	2.16	0.45
1:D:298:HIS:O	1:D:299:GLY:C	2.59	0.45
1:A:269:MET:C	1:A:271:ALA:H	2.22	0.45
1:B:298:HIS:O	1:B:299:GLY:C	2.60	0.45
1:C:51:ASN:O	1:C:53:LYS:NZ	2.45	0.45
1:D:86:ALA:CB	1:D:88:LEU:HD22	2.47	0.45
1:D:269:MET:O	1:D:270:VAL:CG2	2.65	0.45
1:D:373:ILE:H	1:D:373:ILE:CD1	2.30	0.45
1:D:376:GLU:O	1:D:377:THR:C	2.59	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:368:ALA:C	2:C:417:HOH:O	2.59	0.45
1:D:300:THR:O	1:D:301:SER:HB3	2.17	0.45
1:B:269:MET:C	1:B:271:ALA:H	2.25	0.45
1:D:165:THR:HG23	1:D:336:GLY:HA2	1.99	0.45
1:D:270:VAL:HG12	1:D:392:PHE:CD2	2.51	0.45
1:C:404:LEU:HD23	1:C:404:LEU:HA	1.84	0.45
1:C:366:GLU:O	1:C:368:ALA:N	2.39	0.44
1:B:376:GLU:O	1:B:378:THR:CG2	2.65	0.44
1:B:101:LEU:HD23	1:B:186:PHE:HB2	1.99	0.44
1:C:121:ARG:HH22	1:D:118:ASP:CG	2.25	0.44
1:C:390:PHE:HD1	1:C:396:ASN:HB3	1.82	0.44
1:A:90:PRO:CA	1:A:94:GLN:HG3	2.47	0.44
1:A:118:ASP:OD1	1:B:121:ARG:NH2	2.36	0.44
1:B:309:GLU:HG3	1:B:390:PHE:HE2	1.83	0.44
1:A:181:LYS:NZ	1:B:175:GLU:OE2	2.47	0.44
1:B:33:ILE:HD12	1:B:230:VAL:HG11	1.99	0.44
1:D:174:VAL:O	1:D:178:GLN:HG3	2.18	0.44
1:C:222:TYR:CD2	1:C:310:LEU:HD11	2.53	0.44
1:C:244:GLU:OE1	1:C:244:GLU:CA	2.66	0.44
1:C:300:THR:O	1:C:301:SER:HB3	2.18	0.44
1:D:28:GLU:HG3	1:D:30:ARG:NH2	2.33	0.44
1:D:281:MET:O	1:D:285:MET:CG	2.66	0.44
1:B:6:ILE:CD1	1:B:257:ILE:HD11	2.43	0.43
1:B:89:SER:OG	1:B:91:GLU:HG2	2.17	0.43
1:D:295:LEU:C	1:D:295:LEU:HD23	2.43	0.43
1:A:367:GLN:HG2	1:A:367:GLN:H	1.64	0.43
1:B:165:THR:HG23	1:B:336:GLY:HA2	1.99	0.43
1:A:264:SER:HB3	1:B:152:ILE:O	2.18	0.43
1:B:161:SER:H	1:B:165:THR:HG22	1.83	0.43
1:C:59:LEU:C	1:C:60:ILE:HG13	2.43	0.43
1:C:310:LEU:CD1	1:C:368:ALA:CB	2.91	0.43
1:C:314:ARG:HH12	1:C:369:ALA:H	1.64	0.43
1:B:162:ALA:O	1:B:165:THR:HG22	2.17	0.43
1:C:226:ARG:NH1	1:C:303:PRO:HA	2.33	0.43
1:C:310:LEU:HD22	1:C:371:LEU:HD13	1.99	0.43
1:D:65:VAL:HA	1:D:68:MET:HG3	2.00	0.43
1:A:134:VAL:HB	2:A:497:HOH:O	2.17	0.43
1:C:195:TRP:CH2	1:D:121:ARG:HD2	2.53	0.43
1:D:50:GLY:HA3	1:D:232:ALA:HB2	2.00	0.43
1:D:285:MET:HE1	1:D:292:ILE:HG12	2.00	0.43
1:B:273:SER:O	2:B:475:HOH:O	2.21	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:120:MET:HE1	1:A:126:LEU:HD13	2.01	0.42
1:A:298:HIS:O	1:A:299:GLY:C	2.63	0.42
1:C:307:VAL:HG11	1:C:365:ASP:OD1	2.19	0.42
1:D:314:ARG:HH21	1:D:368:ALA:N	2.16	0.42
1:A:50:GLY:HA3	1:A:232:ALA:HB2	2.01	0.42
1:B:376:GLU:O	1:B:378:THR:HG22	2.18	0.42
1:A:68:MET:HB3	1:A:72:SER:CB	2.49	0.42
1:B:136:LYS:HA	2:B:446:HOH:O	2.18	0.42
1:A:90:PRO:C	1:A:92:ALA:H	2.28	0.42
1:A:90:PRO:O	1:A:92:ALA:N	2.53	0.42
1:A:324:ILE:HG22	1:A:325:SER:N	2.33	0.42
1:C:101:LEU:HD23	1:C:186:PHE:HB2	2.01	0.42
1:D:269:MET:C	1:D:270:VAL:HG22	2.44	0.42
1:A:5:VAL:HB	1:A:253:ILE:HG23	2.01	0.42
1:A:175:GLU:OE2	1:B:181:LYS:NZ	2.49	0.42
1:A:269:MET:C	1:A:270:VAL:HG22	2.45	0.42
1:B:300:THR:OG1	1:B:302:THR:HG23	2.19	0.42
1:D:162:ALA:O	1:D:165:THR:HG22	2.19	0.42
1:A:290:THR:HA	1:A:291:PRO:HD3	1.90	0.42
1:C:292:ILE:O	1:C:322:PRO:HB3	2.20	0.42
1:C:300:THR:OG1	1:C:302:THR:HG23	2.20	0.42
1:D:373:ILE:O	1:D:373:ILE:CG1	2.68	0.42
1:B:3:ARG:HD3	1:B:243:LEU:HD23	2.01	0.42
1:C:65:VAL:HA	1:C:68:MET:HG3	2.01	0.42
1:C:65:VAL:HG22	1:C:65:VAL:O	2.19	0.42
1:C:118:ASP:CG	1:D:121:ARG:NH2	2.69	0.42
1:D:226:ARG:NH1	1:D:306:ASP:HB2	2.35	0.42
1:B:294:TYR:CE1	1:B:349:MET:HE1	2.55	0.41
1:C:313:ILE:HG21	1:C:324:ILE:HD11	2.01	0.41
1:B:60:ILE:O	1:B:61:ASP:C	2.63	0.41
1:C:45:ARG:NH2	1:C:202:ASP:O	2.53	0.41
1:D:279:ARG:HD2	2:D:445:HOH:O	2.20	0.41
1:A:294:TYR:CE1	1:A:349:MET:HE1	2.55	0.41
1:C:269:MET:C	1:C:270:VAL:HG22	2.46	0.41
1:C:321:SER:HB3	2:C:494:HOH:O	2.19	0.41
1:C:401:MET:HE3	1:C:401:MET:HB2	1.97	0.41
1:D:161:SER:H	1:D:165:THR:HG22	1.84	0.41
1:D:253:ILE:HG21	1:D:404:LEU:CD2	2.51	0.41
1:C:148:THR:N	1:C:149:PRO:HD2	2.36	0.41
1:D:94:GLN:HG2	1:D:151:LYS:CB	2.51	0.41
1:A:33:ILE:HD12	1:A:230:VAL:HG11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:264:SER:HB3	1:D:152:ILE:O	2.20	0.41
1:B:65:VAL:HG22	1:B:65:VAL:O	2.21	0.41
1:B:371:LEU:HB3	1:B:372:ASN:H	1.42	0.41
1:A:95:ASN:HA	1:A:153:HIS:CE1	2.56	0.41
1:C:269:MET:O	1:C:270:VAL:CG2	2.69	0.41
1:A:96:ASN:HA	1:A:97:PRO:HD3	1.88	0.41
1:A:269:MET:O	1:A:270:VAL:CG2	2.69	0.41
1:B:366:GLU:C	1:B:368:ALA:N	2.74	0.41
1:C:120:MET:SD	1:C:126:LEU:HD13	2.61	0.41
1:D:23:LEU:HD22	1:D:27:ARG:HE	1.86	0.41
1:D:369:ALA:C	1:D:371:LEU:H	2.29	0.41
1:A:204:MET:HE1	1:A:270:VAL:CG1	2.51	0.40
1:A:221:THR:O	1:A:222:TYR:HB2	2.21	0.40
1:B:21:GLU:O	1:B:25:SER:HB2	2.21	0.40
1:D:192:GLU:HG2	2:D:449:HOH:O	2.21	0.40
1:A:320:LYS:HB2	1:A:320:LYS:HE2	1.71	0.40
1:C:249:ARG:CZ	1:C:251:ALA:HB2	2.51	0.40
1:B:366:GLU:O	1:B:368:ALA:N	2.54	0.40
1:C:317:PHE:CD2	1:C:322:PRO:HD3	2.56	0.40
1:A:44:MET:HE3	1:A:202:ASP:HB2	2.03	0.40
1:A:90:PRO:C	1:A:92:ALA:N	2.79	0.40
1:B:174:VAL:O	1:B:178:GLN:HG3	2.21	0.40
1:D:33:ILE:HD12	1:D:230:VAL:HG11	2.03	0.40
1:A:42:SER:HG	1:A:44:MET:HG3	1.82	0.40
1:A:390:PHE:HD1	1:A:396:ASN:HB3	1.86	0.40
1:C:280:CYS:SG	1:C:398:THR:CG2	3.02	0.40
1:D:101:LEU:HD23	1:D:186:PHE:HB2	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	401/406 (99%)	374 (93%)	21 (5%)	6 (2%)	8	7
1	B	401/406 (99%)	376 (94%)	18 (4%)	7 (2%)	7	6
1	C	401/406 (99%)	374 (93%)	20 (5%)	7 (2%)	7	6
1	D	401/406 (99%)	373 (93%)	23 (6%)	5 (1%)	10	11
All	All	1604/1624 (99%)	1497 (93%)	82 (5%)	25 (2%)	7	7

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	270	VAL
1	A	299	GLY
1	A	369	ALA
1	B	270	VAL
1	B	299	GLY
1	C	57	THR
1	C	270	VAL
1	C	299	GLY
1	C	364	LEU
1	D	270	VAL
1	D	299	GLY
1	B	367	GLN
1	B	371	LEU
1	D	57	THR
1	D	364	LEU
1	C	367	GLN
1	A	91	GLU
1	A	301	SER
1	B	301	SER
1	B	372	ASN
1	C	368	ALA
1	C	301	SER
1	D	301	SER
1	A	370	GLY
1	B	318	GLY

5.3.2 Protein sidechains ⓘ

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

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

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	306/309 (99%)	264 (86%)	42 (14%)	3	3
1	B	306/309 (99%)	259 (85%)	47 (15%)	2	2
1	C	306/309 (99%)	263 (86%)	43 (14%)	3	2
1	D	306/309 (99%)	266 (87%)	40 (13%)	4	3
All	All	1224/1236 (99%)	1052 (86%)	172 (14%)	3	2

All (172) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	LEU
1	A	27	ARG
1	A	30	ARG
1	A	37	GLN
1	A	49	TRP
1	A	59	LEU
1	A	63	LYS
1	A	65	VAL
1	A	68	MET
1	A	88	LEU
1	A	91	GLU
1	A	101	LEU
1	A	113	GLN
1	A	121	ARG
1	A	126	LEU
1	A	127	LYS
1	A	146	LEU
1	A	152	ILE
1	A	160	SER
1	A	161	SER
1	A	165	THR
1	A	172	ASN
1	A	217	LYS
1	A	219	SER
1	A	226	ARG
1	A	275	GLU
1	A	288	VAL
1	A	308	LYS
1	A	310	LEU
1	A	320	LYS
1	A	321	SER

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Mol	Chain	Res	Type
1	A	347	LEU
1	A	350	LEU
1	A	358	SER
1	A	362	GLU
1	A	364	LEU
1	A	367	GLN
1	A	376	GLU
1	A	378	THR
1	A	381	GLU
1	A	396	ASN
1	A	398	THR
1	B	2	LYS
1	B	23	LEU
1	B	25	SER
1	B	27	ARG
1	B	37	GLN
1	B	42	SER
1	B	49	TRP
1	B	62	ARG
1	B	63	LYS
1	B	68	MET
1	B	80	GLU
1	B	88	LEU
1	B	91	GLU
1	B	101	LEU
1	B	113	GLN
1	B	121	ARG
1	B	127	LYS
1	B	146	LEU
1	B	160	SER
1	B	161	SER
1	B	163	CYS
1	B	165	THR
1	B	172	ASN
1	B	217	LYS
1	B	219	SER
1	B	226	ARG
1	B	253	ILE
1	B	275	GLU
1	B	288	VAL
1	B	292	ILE
1	B	320	LYS

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Mol	Chain	Res	Type
1	B	321	SER
1	B	347	LEU
1	B	350	LEU
1	B	358	SER
1	B	362	GLU
1	B	364	LEU
1	B	366	GLU
1	B	371	LEU
1	B	374	VAL
1	B	376	GLU
1	B	378	THR
1	B	381	GLU
1	B	396	ASN
1	B	398	THR
1	B	403	LYS
1	B	404	LEU
1	C	2	LYS
1	C	23	LEU
1	C	25	SER
1	C	30	ARG
1	C	49	TRP
1	C	53	LYS
1	C	59	LEU
1	C	68	MET
1	C	81	GLN
1	C	88	LEU
1	C	91	GLU
1	C	101	LEU
1	C	113	GLN
1	C	121	ARG
1	C	126	LEU
1	C	127	LYS
1	C	146	LEU
1	C	151	LYS
1	C	160	SER
1	C	161	SER
1	C	163	CYS
1	C	165	THR
1	C	172	ASN
1	C	217	LYS
1	C	219	SER
1	C	226	ARG

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Mol	Chain	Res	Type
1	C	244	GLU
1	C	257	ILE
1	C	307	VAL
1	C	308	LYS
1	C	314	ARG
1	C	321	SER
1	C	347	LEU
1	C	350	LEU
1	C	358	SER
1	C	362	GLU
1	C	363	GLU
1	C	364	LEU
1	C	366	GLU
1	C	367	GLN
1	C	396	ASN
1	C	398	THR
1	C	403	LYS
1	D	2	LYS
1	D	18	ASN
1	D	20	GLN
1	D	23	LEU
1	D	42	SER
1	D	49	TRP
1	D	53	LYS
1	D	59	LEU
1	D	68	MET
1	D	88	LEU
1	D	91	GLU
1	D	94	GLN
1	D	101	LEU
1	D	113	GLN
1	D	121	ARG
1	D	124	ARG
1	D	126	LEU
1	D	127	LYS
1	D	146	LEU
1	D	160	SER
1	D	161	SER
1	D	165	THR
1	D	172	ASN
1	D	217	LYS
1	D	219	SER

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Mol	Chain	Res	Type
1	D	226	ARG
1	D	275	GLU
1	D	285	MET
1	D	315	GLU
1	D	320	LYS
1	D	347	LEU
1	D	350	LEU
1	D	358	SER
1	D	364	LEU
1	D	367	GLN
1	D	371	LEU
1	D	373	ILE
1	D	376	GLU
1	D	398	THR
1	D	404	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	95	ASN
1	A	225	HIS
1	A	252	HIS
1	A	341	GLN
1	A	352	HIS
1	A	367	GLN
1	A	372	ASN
1	B	19	GLN
1	B	95	ASN
1	B	245	HIS
1	B	286	HIS
1	B	341	GLN
1	B	372	ASN
1	C	341	GLN
1	C	372	ASN
1	D	18	ASN
1	D	37	GLN
1	D	341	GLN
1	D	396	ASN

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	403/406 (99%)	-0.06	4 (0%) 79 80	9, 19, 37, 48	0
1	B	403/406 (99%)	-0.15	4 (0%) 79 80	8, 16, 31, 44	0
1	C	403/406 (99%)	-0.06	8 (1%) 65 66	9, 18, 32, 54	0
1	D	403/406 (99%)	-0.09	9 (2%) 62 64	6, 17, 32, 46	0
All	All	1612/1624 (99%)	-0.09	25 (1%) 70 73	6, 18, 33, 54	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	270	VAL	4.6
1	D	270	VAL	4.2
1	D	371	LEU	3.8
1	B	273	SER	3.5
1	D	57	THR	3.4
1	B	49	TRP	3.2
1	D	368	ALA	3.2
1	B	370	GLY	3.1
1	D	49	TRP	3.0
1	C	273	SER	2.8
1	D	273	SER	2.7
1	C	268	ASP	2.7
1	A	371	LEU	2.5
1	C	369	ALA	2.5
1	C	267	ALA	2.5
1	C	49	TRP	2.4
1	D	62	ARG	2.3
1	D	392	PHE	2.3
1	A	273	SER	2.3
1	A	49	TRP	2.2
1	C	271	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	371	LEU	2.2
1	A	113	GLN	2.1
1	D	268	ASP	2.1
1	C	392	PHE	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.