



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 11:02 AM UTC

PDB ID : 1FJ4 / pdb_00001fj4
Title : THE STRUCTURE OF BETA-KETOACYL-[ACYL CARRIER PROTEIN] SYNTHASE I IN COMPLEX WITH THIOLACTOMYCIN, IMPLICATIONS FOR DRUG DESIGN
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Deposited on : 2000-08-07
Resolution : 2.35 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

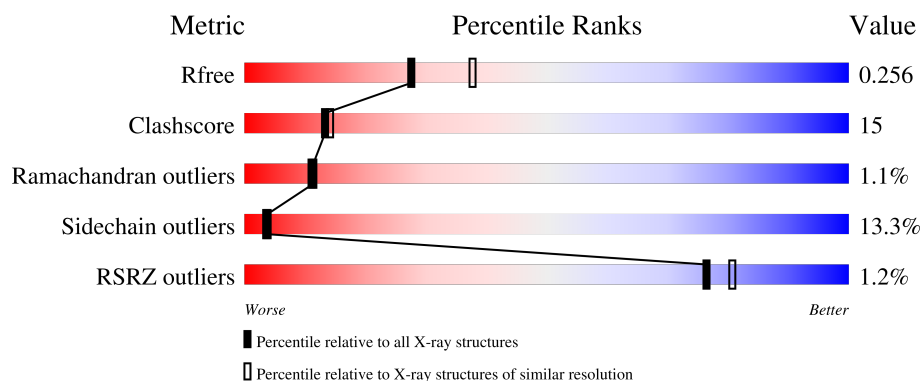
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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	1596 (2.36-2.36)
Clashscore	190562	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)
RSRZ outliers	180081	1598 (2.36-2.36)

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	
1	B	406	
1	C	406	
1	D	406	

2 Entry composition [i](#)

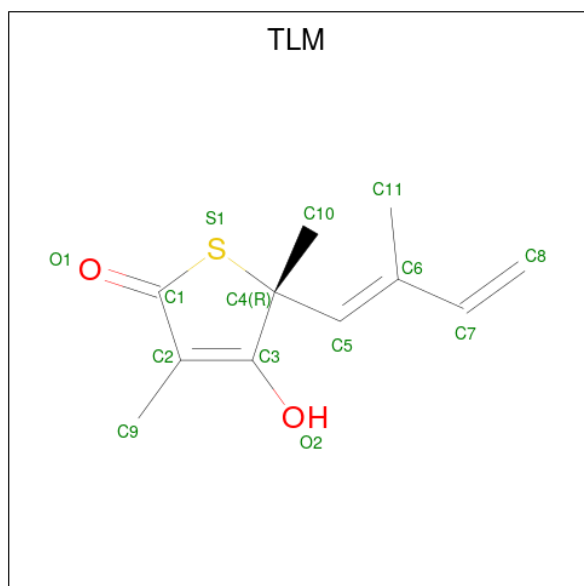
There are 3 unique types of molecules in this entry. The entry contains 12182 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 THIOLACTOMYCIN (CCD ID: TLM) (formula: $C_{11}H_{14}O_2S$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	S	0	0
			14	11	2	1		
2	B	1	Total	C	O	S	0	0
			14	11	2	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	C	1	Total	C	O	S	0	0
			14	11	2	1		
2	D	1	Total	C	O	S	0	0
			14	11	2	1		

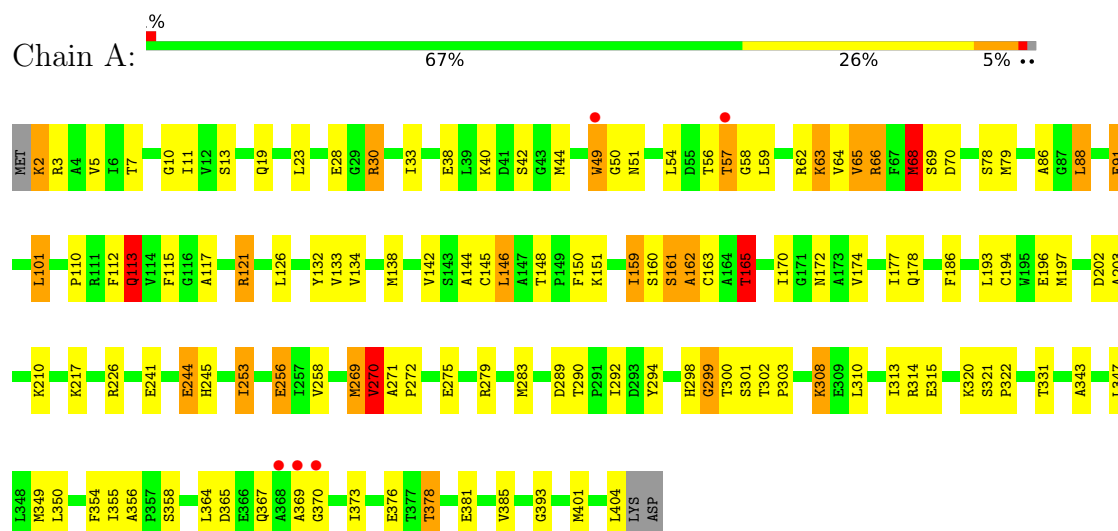
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	79	Total	O	0	0
			79	79		
3	B	83	Total	O	0	0
			83	83		
3	C	65	Total	O	0	0
			65	65		
3	D	79	Total	O	0	0
			79	79		

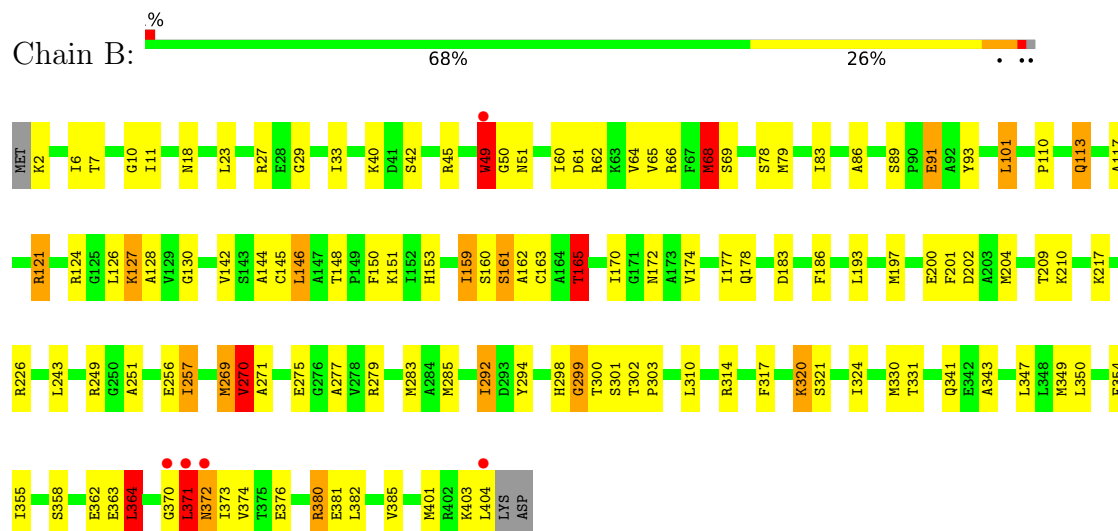
3 Residue-property plots

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

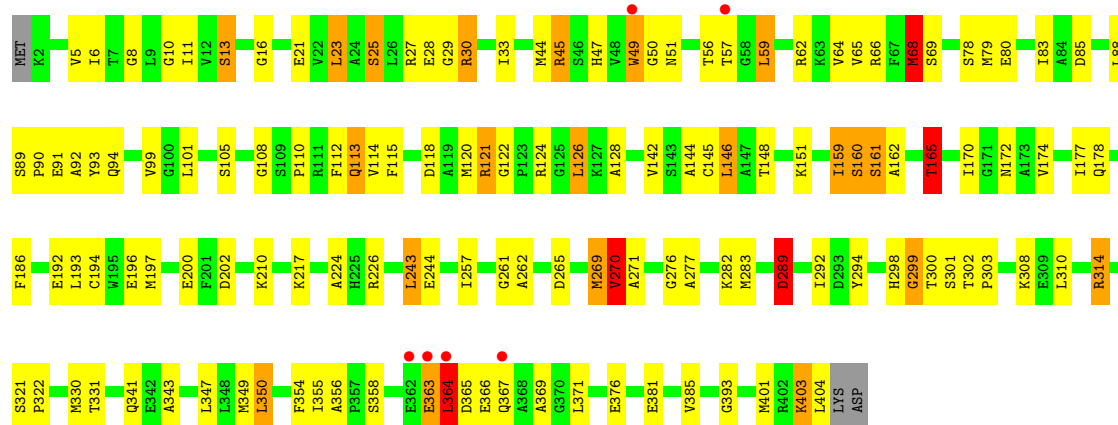


• Molecule 1: BETA-KETOACYL-[ACYL CARRIER PROTEIN] SYNTHASE I

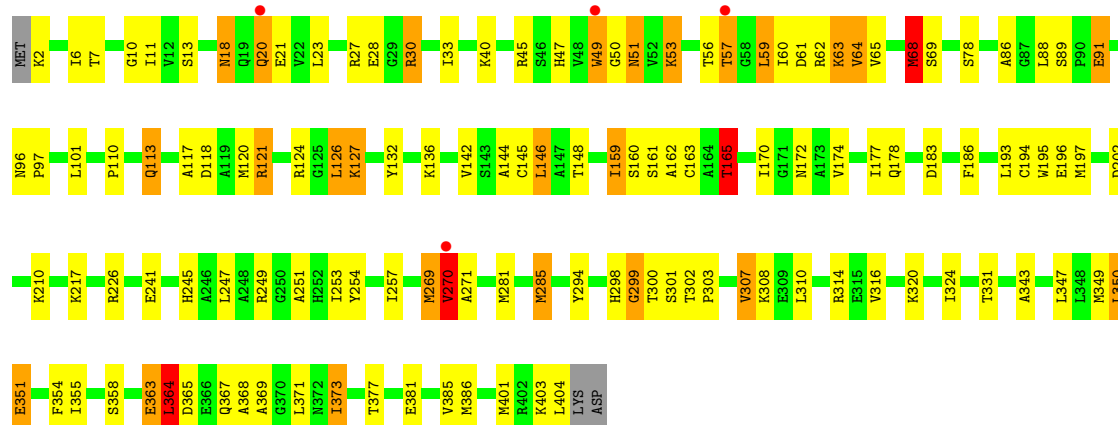


• Molecule 1: BETA-KETOACYL-[ACYL CARRIER PROTEIN] SYNTHASE I





● 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	59.07Å 138.97Å 211.85Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.35 20.00 – 2.35	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-2.35) 88.9 (20.00-2.35)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.16 (at 2.30Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.197 , 0.253 0.205 , 0.256	Depositor DCC
R_{free} test set	5720 reflections (7.61%)	wwPDB-VP
Wilson B-factor (Å ²)	19.7	Xtriage
Anisotropy	0.188	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 42.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	12182	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.21% 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 ⓘ

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

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	0.47	0/3003	0.97	16/4058 (0.4%)
1	B	0.48	0/3003	0.99	18/4058 (0.4%)
1	C	0.47	0/3003	0.98	17/4058 (0.4%)
1	D	0.49	0/3003	0.99	16/4058 (0.4%)
All	All	0.48	0/12012	0.98	67/16232 (0.4%)

There are no bond length outliers.

All (67) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	113	GLN	N-CA-C	-10.19	100.13	111.14
1	B	275	GLU	N-CA-C	-7.91	98.57	110.28
1	D	113	GLN	N-CA-C	-7.28	103.27	111.14
1	D	165	THR	N-CA-C	7.21	119.76	111.11
1	C	165	THR	N-CA-C	7.08	119.61	111.11
1	B	165	THR	N-CA-C	6.96	119.51	111.02
1	A	113	GLN	N-CA-C	-6.95	103.78	111.36
1	B	113	GLN	N-CA-C	-6.93	103.81	111.36
1	A	165	THR	N-CA-C	6.81	119.32	111.02
1	C	269	MET	N-CA-C	-6.73	100.56	110.52
1	B	68	MET	N-CA-C	6.66	120.74	110.42
1	D	68	MET	N-CA-C	6.52	120.17	110.52
1	D	269	MET	N-CA-C	-6.44	100.99	110.52
1	B	269	MET	N-CA-C	-6.44	100.99	110.52
1	A	68	MET	N-CA-C	6.39	119.98	110.52
1	A	269	MET	N-CA-C	-6.34	101.14	110.52
1	C	243	LEU	N-CA-C	6.33	118.74	111.02
1	A	253	ILE	N-CA-C	6.00	116.25	107.37
1	C	69	SER	N-CA-C	-5.96	101.37	109.95
1	C	68	MET	N-CA-C	5.94	119.62	110.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	343	ALA	N-CA-C	-5.92	104.91	111.36
1	C	159	ILE	N-CA-C	-5.74	100.21	108.48
1	B	243	LEU	N-CA-C	5.71	117.99	111.02
1	B	277	ALA	N-CA-C	-5.69	105.06	112.23
1	D	69	SER	N-CA-C	-5.65	101.81	109.95
1	B	69	SER	N-CA-C	-5.64	101.83	109.95
1	D	159	ILE	N-CA-C	-5.64	100.36	108.48
1	A	133	VAL	N-CA-C	5.60	116.33	110.62
1	A	159	ILE	N-CA-C	-5.60	100.42	108.48
1	A	50	GLY	N-CA-C	-5.58	99.94	113.18
1	D	343	ALA	N-CA-C	-5.57	105.29	111.36
1	B	159	ILE	N-CA-C	-5.56	100.47	108.48
1	D	50	GLY	N-CA-C	-5.56	100.00	113.18
1	B	50	GLY	N-CA-C	-5.55	100.03	113.18
1	C	50	GLY	N-CA-C	-5.54	100.05	113.18
1	A	343	ALA	N-CA-C	-5.47	105.40	111.36
1	D	331	THR	N-CA-C	5.47	120.06	112.90
1	C	343	ALA	N-CA-C	-5.45	105.42	111.36
1	A	69	SER	N-CA-C	-5.43	102.13	109.95
1	A	13	SER	N-CA-C	5.38	116.45	108.86
1	D	368	ALA	N-CA-C	-5.35	105.43	113.89
1	C	122	GLY	CA-C-N	5.35	125.02	119.56
1	C	122	GLY	C-N-CA	5.35	125.02	119.56
1	D	30	ARG	N-CA-C	5.33	117.41	109.25
1	D	51	ASN	N-CA-C	5.32	117.73	110.55
1	C	11	ILE	N-CA-C	5.30	114.85	108.06
1	D	13	SER	N-CA-C	5.29	116.33	108.86
1	A	11	ILE	N-CA-C	5.29	114.83	108.06
1	D	11	ILE	N-CA-C	5.29	114.83	108.06
1	B	11	ILE	N-CA-C	5.28	114.81	108.06
1	B	51	ASN	N-CA-C	5.28	118.29	110.48
1	D	57	THR	N-CA-C	5.27	122.02	110.80
1	C	331	THR	N-CA-C	5.26	119.78	112.90
1	C	51	ASN	N-CA-C	5.19	118.16	110.48
1	C	80	GLU	N-CA-C	-5.18	105.52	111.07
1	C	13	SER	N-CA-C	5.17	116.16	108.86
1	A	51	ASN	N-CA-C	5.17	117.53	110.55
1	A	70	ASP	N-CA-C	5.16	116.91	111.28
1	B	183	ASP	N-CA-C	-5.16	107.12	113.41
1	B	331	THR	N-CA-C	5.12	119.61	112.90
1	B	371	LEU	N-CA-C	5.10	121.67	110.80
1	D	183	ASP	N-CA-C	-5.09	107.20	113.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	49	TRP	N-CA-C	5.05	117.81	109.72
1	A	331	THR	N-CA-C	5.01	119.47	112.90
1	A	162	ALA	CB-CA-C	-5.01	110.42	117.23
1	C	289	ASP	N-CA-C	5.01	119.15	113.19
1	B	292	ILE	N-CA-C	-5.01	100.57	108.23

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	88	0
1	B	2955	0	2910	87	0
1	C	2955	0	2910	107	0
1	D	2955	0	2910	101	0
2	A	14	0	13	0	0
2	B	14	0	13	0	0
2	C	14	0	13	0	0
2	D	14	0	13	1	0
3	A	79	0	0	4	0
3	B	83	0	0	5	0
3	C	65	0	0	5	0
3	D	79	0	0	4	0
All	All	12182	0	11692	348	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 15.

All (348) 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:C:56:THR:HA	1:C:59:LEU:HD22	1.33	1.11
1:D:349:MET:HE3	1:D:355:ILE:HA	1.33	1.10
1:C:349:MET:HE3	1:C:355:ILE:HA	1.36	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:349:MET:HE3	1:B:355:ILE:HA	1.36	1.05
1:A:349:MET:HE3	1:A:355:ILE:HA	1.38	1.05
1:A:269:MET:HE1	1:B:145:CYS:HA	1.40	1.04
1:C:269:MET:HE1	1:D:145:CYS:HA	1.36	1.04
1:C:262:ALA:H	1:C:283:MET:HE3	1.25	0.97
1:A:56:THR:HA	1:A:59:LEU:HD22	1.46	0.97
1:B:314:ARG:HH22	1:B:370:GLY:H	1.03	0.96
1:C:161:SER:H	1:C:165:THR:HG22	1.32	0.94
1:A:148:THR:HB	1:B:269:MET:HE2	1.49	0.94
1:B:161:SER:H	1:B:165:THR:HG22	1.34	0.93
1:D:18:ASN:HD21	1:D:20:GLN:HG3	1.30	0.92
1:A:161:SER:H	1:A:165:THR:HG22	1.35	0.91
1:C:145:CYS:HA	1:D:269:MET:HE1	1.49	0.91
1:C:162:ALA:O	1:C:165:THR:HG23	1.72	0.90
1:D:161:SER:H	1:D:165:THR:HG22	1.35	0.89
1:A:269:MET:HE2	1:B:148:THR:HB	1.54	0.89
1:A:145:CYS:HA	1:B:269:MET:HE1	1.54	0.88
1:C:148:THR:HB	1:D:269:MET:HE2	1.54	0.88
1:A:162:ALA:O	1:A:165:THR:HG23	1.74	0.88
1:A:64:VAL:HG12	1:A:68:MET:HE3	1.53	0.87
1:D:162:ALA:O	1:D:165:THR:HG23	1.75	0.87
1:D:56:THR:HA	1:D:59:LEU:HD22	1.58	0.85
1:B:162:ALA:O	1:B:165:THR:HG23	1.77	0.85
1:C:262:ALA:N	1:C:283:MET:HE3	1.93	0.83
1:A:117:ALA:O	1:A:121:ARG:HD2	1.80	0.82
1:D:18:ASN:ND2	1:D:21:GLU:H	1.79	0.81
1:C:159:ILE:HD13	1:D:159:ILE:HD13	1.62	0.81
1:C:269:MET:HE2	1:D:148:THR:HB	1.61	0.80
1:B:314:ARG:HH22	1:B:370:GLY:N	1.78	0.79
1:B:117:ALA:O	1:B:121:ARG:HD2	1.83	0.78
1:C:45:ARG:HB2	1:C:45:ARG:HH11	1.46	0.78
1:C:110:PRO:HG2	1:C:197:MET:HB2	1.65	0.78
1:A:159:ILE:HD13	1:B:159:ILE:HD13	1.64	0.77
1:A:279:ARG:NH2	1:B:153:HIS:O	2.17	0.77
1:B:314:ARG:NH2	1:B:370:GLY:H	1.80	0.77
1:D:64:VAL:HG23	1:D:68:MET:HE3	1.67	0.76
1:D:18:ASN:ND2	1:D:20:GLN:HG3	2.01	0.75
1:B:65:VAL:HA	1:B:68:MET:HG3	1.69	0.74
1:B:45:ARG:HB2	1:B:45:ARG:HH11	1.52	0.73
1:D:65:VAL:HA	1:D:68:MET:HG3	1.71	0.73
1:C:124:ARG:HB2	1:C:128:ALA:HB2	1.72	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:6:ILE:HD11	1:C:257:ILE:HD11	1.71	0.72
1:D:241:GLU:OE1	1:D:245:HIS:HD2	1.73	0.72
1:A:226:ARG:NH2	1:A:365:ASP:OD1	2.23	0.72
1:D:18:ASN:C	1:D:18:ASN:HD22	1.97	0.71
1:D:28:GLU:HG3	1:D:30:ARG:HH21	1.54	0.71
1:C:385:VAL:HG23	1:C:401:MET:HE3	1.74	0.69
1:A:148:THR:CB	1:B:269:MET:HE2	2.22	0.69
1:C:110:PRO:HB3	1:D:113:GLN:CD	2.19	0.68
1:C:261:GLY:HA2	1:C:283:MET:HG2	1.75	0.68
1:C:118:ASP:CG	1:D:121:ARG:HH22	2.01	0.68
1:C:262:ALA:H	1:C:283:MET:CE	2.05	0.67
1:B:317:PHE:O	1:B:320:LYS:HG3	1.95	0.67
1:D:120:MET:HE1	1:D:126:LEU:HD13	1.77	0.66
1:C:65:VAL:HA	1:C:68:MET:HG3	1.77	0.66
1:D:254:TYR:HD1	1:D:351:GLU:HG3	1.58	0.66
1:C:101:LEU:HD23	1:C:186:PHE:HB2	1.77	0.66
1:B:110:PRO:HG2	1:B:197:MET:HB2	1.78	0.66
1:D:101:LEU:HD23	1:D:186:PHE:HB2	1.78	0.65
1:B:385:VAL:HG23	1:B:401:MET:HE3	1.78	0.65
1:C:161:SER:N	1:C:165:THR:HG22	2.09	0.65
1:B:161:SER:N	1:B:165:THR:HG22	2.10	0.65
1:A:101:LEU:HD23	1:A:186:PHE:HB2	1.79	0.65
1:D:385:VAL:HG23	1:D:401:MET:HE3	1.77	0.65
1:D:161:SER:N	1:D:165:THR:HG22	2.11	0.65
1:D:132:TYR:O	1:D:136:LYS:HG3	1.97	0.65
1:A:385:VAL:HG23	1:A:401:MET:HE3	1.79	0.64
1:D:307:VAL:HG22	1:D:367:GLN:HB2	1.80	0.64
1:A:283:MET:HE2	3:B:525:HOH:O	1.97	0.64
1:A:275:GLU:OE1	1:A:279:ARG:NH1	2.30	0.64
1:B:101:LEU:HD23	1:B:186:PHE:HB2	1.78	0.64
1:B:64:VAL:HG12	1:B:68:MET:HE3	1.80	0.64
1:A:161:SER:N	1:A:165:THR:HG22	2.12	0.63
1:C:118:ASP:OD1	1:D:121:ARG:NH2	2.32	0.63
1:C:314:ARG:NH1	1:C:369:ALA:O	2.32	0.62
1:C:148:THR:CB	1:D:269:MET:HE2	2.28	0.61
1:A:134:VAL:HG12	1:A:138:MET:HE3	1.82	0.61
1:A:269:MET:O	1:A:270:VAL:HG22	2.01	0.61
1:C:350:LEU:HD22	1:C:403:LYS:HD2	1.82	0.61
1:D:310:LEU:HD13	1:D:371:LEU:HD12	1.81	0.60
1:C:79:MET:O	1:C:83:ILE:HG13	2.00	0.60
1:C:269:MET:CE	1:D:145:CYS:HA	2.22	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:224:ALA:HB2	1:C:363:GLU:HG2	1.84	0.60
1:B:124:ARG:HB2	1:B:128:ALA:HB2	1.82	0.59
1:D:269:MET:O	1:D:270:VAL:HG22	2.02	0.59
1:A:269:MET:CE	1:B:145:CYS:HA	2.26	0.59
1:A:294:TYR:CZ	1:A:349:MET:HE1	2.38	0.59
1:D:363:GLU:O	1:D:364:LEU:CB	2.51	0.58
1:A:42:SER:OG	1:A:44:MET:HG3	2.03	0.58
1:C:121:ARG:HH22	1:D:118:ASP:CG	2.12	0.58
1:B:269:MET:O	1:B:270:VAL:HG22	2.03	0.58
1:D:18:ASN:HD21	1:D:21:GLU:H	1.48	0.58
1:D:162:ALA:HB1	3:D:574:HOH:O	2.03	0.58
1:D:253:ILE:HG21	1:D:404:LEU:HD12	1.86	0.57
1:C:349:MET:HE3	1:C:355:ILE:CA	2.25	0.57
1:C:269:MET:O	1:C:270:VAL:HG22	2.06	0.56
1:C:294:TYR:CZ	1:C:349:MET:HE1	2.40	0.56
1:C:363:GLU:O	1:C:364:LEU:CB	2.53	0.56
1:A:65:VAL:HA	1:A:68:MET:HG3	1.88	0.56
1:A:144:ALA:O	1:B:269:MET:HE1	2.05	0.56
1:B:163:CYS:SG	3:B:516:HOH:O	2.43	0.56
1:B:294:TYR:CZ	1:B:349:MET:HE1	2.40	0.56
1:C:45:ARG:NH1	1:C:202:ASP:OD1	2.39	0.56
1:D:294:TYR:CZ	1:D:349:MET:HE1	2.40	0.56
1:C:174:VAL:O	1:C:178:GLN:HG3	2.06	0.56
1:D:254:TYR:CD1	1:D:351:GLU:HG3	2.41	0.56
1:A:161:SER:OG	1:A:165:THR:HA	2.07	0.55
1:B:174:VAL:O	1:B:178:GLN:HG3	2.07	0.55
1:D:142:VAL:O	1:D:146:LEU:HG	2.07	0.55
1:A:63:LYS:HA	1:A:66:ARG:HD3	1.89	0.55
1:D:174:VAL:O	1:D:178:GLN:HG3	2.06	0.55
1:B:363:GLU:O	1:B:364:LEU:CB	2.54	0.54
1:C:45:ARG:HH11	1:C:45:ARG:CB	2.18	0.54
1:C:121:ARG:HD2	1:D:195:TRP:HH2	1.72	0.54
1:D:161:SER:OG	1:D:165:THR:HA	2.07	0.54
1:A:174:VAL:O	1:A:178:GLN:HG3	2.07	0.54
1:B:45:ARG:HB2	1:B:45:ARG:NH1	2.21	0.54
1:A:269:MET:HE2	1:B:148:THR:CB	2.33	0.54
1:D:373:ILE:HD13	1:D:373:ILE:O	2.06	0.54
1:D:349:MET:CE	1:D:355:ILE:HA	2.23	0.54
1:A:289:ASP:OD1	1:A:290:THR:HG23	2.08	0.54
1:D:45:ARG:NH2	1:D:202:ASP:O	2.40	0.54
1:D:300:THR:OG1	1:D:302:THR:HG23	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:324:ILE:O	1:D:373:ILE:HA	2.07	0.54
1:B:314:ARG:HH12	1:B:370:GLY:HA3	1.73	0.54
1:C:142:VAL:O	1:C:146:LEU:HG	2.08	0.54
1:D:117:ALA:O	1:D:121:ARG:HD2	2.08	0.53
1:D:310:LEU:O	1:D:314:ARG:HG3	2.07	0.53
1:D:241:GLU:OE1	1:D:245:HIS:CD2	2.57	0.53
1:C:8:GLY:HA2	1:C:85:ASP:OD2	2.09	0.53
1:C:200:GLU:OE2	1:D:113:GLN:NE2	2.41	0.53
1:A:244:GLU:OE1	1:A:244:GLU:HA	2.08	0.53
1:C:269:MET:HE3	3:D:539:HOH:O	2.07	0.53
1:B:142:VAL:O	1:B:146:LEU:HG	2.08	0.53
1:B:161:SER:OG	1:B:165:THR:HA	2.08	0.53
1:C:90:PRO:HB3	1:C:94:GLN:NE2	2.24	0.53
1:C:341:GLN:NE2	3:C:543:HOH:O	2.42	0.53
1:A:349:MET:CE	1:A:355:ILE:HA	2.26	0.53
1:B:226:ARG:NH1	1:B:303:PRO:HA	2.25	0.52
1:A:142:VAL:O	1:A:146:LEU:HG	2.08	0.52
1:C:161:SER:OG	1:C:165:THR:HA	2.10	0.52
1:A:253:ILE:HG21	1:A:404:LEU:HD12	1.92	0.52
1:A:226:ARG:NH1	1:A:303:PRO:HA	2.24	0.52
1:D:226:ARG:NH1	1:D:303:PRO:HA	2.24	0.52
1:C:244:GLU:OE2	1:C:244:GLU:HA	2.10	0.52
1:D:110:PRO:HG2	1:D:197:MET:HB2	1.91	0.52
1:A:300:THR:OG1	1:A:302:THR:HG23	2.10	0.52
1:B:285:MET:CE	1:B:292:ILE:HG12	2.40	0.52
1:D:349:MET:HE3	1:D:355:ILE:CA	2.24	0.52
1:D:18:ASN:HD21	1:D:21:GLU:HG3	1.75	0.51
1:D:51:ASN:O	1:D:53:LYS:HE3	2.09	0.51
1:A:376:GLU:O	1:A:378:THR:HG23	2.10	0.51
1:D:300:THR:O	1:D:301:SER:HB3	2.10	0.51
1:A:300:THR:O	1:A:301:SER:HB3	2.10	0.51
1:A:365:ASP:OD2	1:A:367:GLN:HB2	2.09	0.51
1:D:60:ILE:HG22	1:D:64:VAL:HG22	1.92	0.51
1:C:162:ALA:HB1	3:C:559:HOH:O	2.11	0.51
1:B:45:ARG:HH11	1:B:45:ARG:CB	2.23	0.51
1:D:163:CYS:SG	3:D:573:HOH:O	2.43	0.51
1:D:310:LEU:HD22	1:D:371:LEU:CD1	2.41	0.51
1:D:363:GLU:O	1:D:364:LEU:HB2	2.10	0.51
1:C:349:MET:CE	1:C:355:ILE:HA	2.24	0.51
1:B:380:ARG:HG2	1:B:382:LEU:HD23	1.92	0.50
1:B:6:ILE:HD11	1:B:257:ILE:HD11	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:310:LEU:O	1:B:314:ARG:HG3	2.11	0.50
1:C:226:ARG:NH1	1:C:303:PRO:HA	2.27	0.50
1:C:310:LEU:HD22	1:C:371:LEU:HD12	1.94	0.50
1:C:112:PHE:HA	1:C:115:PHE:HB3	1.94	0.50
1:C:300:THR:O	1:C:301:SER:HB3	2.11	0.50
1:B:89:SER:OG	1:B:91:GLU:HG2	2.12	0.49
1:A:203:ALA:HB1	1:B:130:GLY:O	2.11	0.49
1:D:6:ILE:HD11	1:D:257:ILE:HD11	1.94	0.49
1:D:281:MET:O	1:D:285:MET:HG2	2.13	0.49
1:A:33:ILE:HA	1:A:49:TRP:O	2.13	0.49
1:A:161:SER:H	1:A:165:THR:CG2	2.17	0.49
1:C:292:ILE:O	1:C:322:PRO:HB3	2.12	0.49
1:B:300:THR:O	1:B:301:SER:HB3	2.13	0.48
1:D:20:GLN:HG3	1:D:21:GLU:N	2.28	0.48
1:D:285:MET:SD	1:D:386:MET:HE1	2.53	0.48
1:A:203:ALA:HA	1:B:126:LEU:HD22	1.95	0.48
1:B:33:ILE:HA	1:B:49:TRP:O	2.14	0.48
1:D:161:SER:H	1:D:165:THR:CG2	2.17	0.48
1:A:367:GLN:HA	1:A:367:GLN:NE2	2.27	0.48
1:B:300:THR:OG1	1:B:302:THR:HG23	2.14	0.48
1:C:393:GLY:HA3	1:D:144:ALA:HB1	1.95	0.48
1:D:350:LEU:HD22	1:D:403:LYS:HE2	1.96	0.48
1:A:79:MET:HE2	1:A:150:PHE:CG	2.48	0.48
1:B:256:GLU:HB2	1:B:404:LEU:HD11	1.95	0.48
1:C:310:LEU:HD22	1:C:371:LEU:CD1	2.42	0.48
1:D:349:MET:HB3	1:D:354:PHE:O	2.14	0.48
1:B:349:MET:HE3	1:B:355:ILE:CA	2.26	0.48
1:D:33:ILE:HA	1:D:49:TRP:O	2.13	0.47
1:B:170:ILE:O	1:B:174:VAL:HG23	2.15	0.47
1:C:144:ALA:O	1:D:269:MET:HE1	2.13	0.47
1:B:7:THR:O	1:B:86:ALA:HA	2.14	0.47
1:D:40:LYS:HG3	1:D:47:HIS:CE1	2.50	0.47
1:D:124:ARG:NH2	1:D:127:LYS:HB3	2.29	0.47
1:C:121:ARG:NH2	1:D:118:ASP:OD1	2.47	0.47
1:C:269:MET:HE2	1:D:148:THR:CB	2.41	0.47
1:A:298:HIS:O	1:A:299:GLY:C	2.58	0.47
1:B:294:TYR:HB3	1:B:385:VAL:HG12	1.97	0.47
1:C:33:ILE:HA	1:C:49:TRP:O	2.13	0.47
1:C:300:THR:OG1	1:C:302:THR:HG23	2.13	0.47
1:A:269:MET:HE1	1:B:144:ALA:O	2.15	0.47
1:C:145:CYS:HA	1:D:269:MET:CE	2.35	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:5:VAL:HG12	1:A:256:GLU:HB2	1.96	0.47
1:C:160:SER:HB3	3:C:518:HOH:O	2.15	0.47
1:D:28:GLU:HG3	1:D:30:ARG:NH2	2.27	0.47
1:B:314:ARG:NH1	1:B:370:GLY:HA3	2.30	0.47
1:A:113:GLN:NE2	1:B:200:GLU:OE2	2.48	0.46
1:A:349:MET:HE3	1:A:355:ILE:CA	2.27	0.46
1:B:161:SER:H	1:B:165:THR:CG2	2.16	0.46
1:B:371:LEU:HB3	1:B:372:ASN:H	1.38	0.46
1:C:243:LEU:HD11	1:C:404:LEU:HD21	1.96	0.46
1:A:349:MET:HB3	1:A:354:PHE:O	2.15	0.46
1:B:363:GLU:O	1:B:364:LEU:HB2	2.15	0.46
1:B:127:LYS:HE3	1:B:127:LYS:HB2	1.77	0.46
1:D:310:LEU:HD22	1:D:371:LEU:HD13	1.98	0.46
1:A:5:VAL:HG12	1:A:256:GLU:CB	2.46	0.46
1:A:163:CYS:SG	3:A:502:HOH:O	2.51	0.46
1:A:269:MET:HE3	3:B:571:HOH:O	2.16	0.46
1:A:292:ILE:O	1:A:322:PRO:HB3	2.16	0.46
1:B:226:ARG:HH11	1:B:303:PRO:HA	1.81	0.46
1:D:226:ARG:HH11	1:D:303:PRO:HA	1.79	0.46
1:A:226:ARG:HH11	1:A:303:PRO:HA	1.81	0.45
1:A:112:PHE:HA	1:A:115:PHE:HB3	1.99	0.45
1:A:269:MET:O	1:A:271:ALA:N	2.49	0.45
1:B:324:ILE:O	1:B:373:ILE:HA	2.16	0.45
1:C:89:SER:O	1:C:92:ALA:HB3	2.15	0.45
1:B:79:MET:HE2	1:B:150:PHE:CG	2.52	0.45
1:C:83:ILE:HD13	1:C:93:TYR:CZ	2.52	0.45
1:D:117:ALA:O	1:D:121:ARG:CD	2.65	0.45
1:B:341:GLN:NE2	3:B:502:HOH:O	2.49	0.45
1:D:64:VAL:CG2	1:D:65:VAL:N	2.80	0.45
1:C:64:VAL:HG12	1:C:68:MET:HE3	1.99	0.45
1:B:65:VAL:HG22	1:B:65:VAL:O	2.17	0.45
2:D:503:TLM:H111	3:D:570:HOH:O	2.15	0.45
1:C:162:ALA:O	1:C:165:THR:CG2	2.56	0.45
1:A:2:LYS:O	1:A:178:GLN:HG2	2.17	0.45
1:A:308:LYS:HA	1:A:308:LYS:HD3	1.56	0.45
1:B:2:LYS:N	3:B:550:HOH:O	2.49	0.45
1:B:349:MET:HB3	1:B:354:PHE:O	2.17	0.45
1:B:349:MET:CE	1:B:355:ILE:HA	2.26	0.45
1:A:57:THR:HG22	1:A:58:GLY:N	2.31	0.44
1:B:10:GLY:HA3	1:B:78:SER:O	2.17	0.44
1:C:363:GLU:O	1:C:364:LEU:HB2	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:49:TRP:NE1	1:C:193:LEU:HG	2.33	0.44
1:A:66:ARG:HG3	1:A:132:TYR:CE1	2.52	0.44
1:A:272:PRO:HD3	3:A:567:HOH:O	2.17	0.44
1:B:279:ARG:O	1:B:283:MET:HB2	2.17	0.44
1:C:298:HIS:O	1:C:299:GLY:C	2.60	0.44
1:D:10:GLY:HA3	1:D:78:SER:O	2.18	0.44
1:C:10:GLY:HA3	1:C:78:SER:O	2.17	0.44
1:C:224:ALA:H	1:C:363:GLU:HB3	1.82	0.44
1:C:269:MET:HE1	1:D:144:ALA:O	2.17	0.44
1:B:269:MET:O	1:B:271:ALA:N	2.51	0.44
1:C:110:PRO:HD2	1:C:192:GLU:OE2	2.17	0.44
1:C:56:THR:HA	1:C:59:LEU:CD2	2.23	0.44
1:A:86:ALA:CB	1:A:88:LEU:HD22	2.47	0.44
1:A:393:GLY:HA3	1:B:144:ALA:HB1	2.00	0.44
1:C:5:VAL:HG11	1:C:243:LEU:HD13	2.00	0.44
1:C:29:GLY:HA2	1:C:330:MET:SD	2.58	0.44
1:C:105:SER:OG	1:C:108:GLY:HA2	2.18	0.44
1:D:18:ASN:ND2	1:D:18:ASN:C	2.69	0.44
1:C:23:LEU:O	1:C:27:ARG:HG3	2.18	0.43
1:A:113:GLN:NE2	1:A:113:GLN:HA	2.31	0.43
1:C:294:TYR:HB3	1:C:385:VAL:HG12	2.00	0.43
1:D:120:MET:CE	1:D:126:LEU:HD13	2.47	0.43
1:B:61:ASP:O	1:B:65:VAL:HG12	2.18	0.43
1:D:194:CYS:HB2	1:D:196:GLU:OE1	2.18	0.43
1:A:256:GLU:HG3	1:A:258:VAL:HG13	2.00	0.43
1:C:79:MET:HE3	1:C:186:PHE:CD1	2.53	0.43
1:C:170:ILE:O	1:C:174:VAL:HG23	2.18	0.43
1:C:269:MET:O	1:C:271:ALA:N	2.51	0.43
1:A:275:GLU:OE2	1:A:279:ARG:HD3	2.19	0.43
1:B:49:TRP:NE1	1:B:193:LEU:HG	2.34	0.43
1:B:79:MET:O	1:B:83:ILE:HG13	2.19	0.43
1:C:265:ASP:OD1	1:C:276:GLY:HA3	2.19	0.43
1:C:349:MET:HB3	1:C:354:PHE:O	2.18	0.43
1:B:298:HIS:O	1:B:299:GLY:C	2.62	0.43
1:C:161:SER:H	1:C:165:THR:CG2	2.15	0.43
1:D:281:MET:O	1:D:285:MET:CG	2.67	0.43
1:D:89:SER:OG	1:D:91:GLU:HG2	2.18	0.43
1:A:91:GLU:CD	1:A:91:GLU:H	2.26	0.42
1:D:170:ILE:O	1:D:174:VAL:HG23	2.19	0.42
1:A:300:THR:O	1:A:301:SER:CB	2.68	0.42
1:B:45:ARG:NH1	1:B:202:ASP:OD1	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:289:ASP:OD1	1:C:289:ASP:N	2.39	0.42
1:A:44:MET:HE3	1:A:202:ASP:HB2	2.00	0.42
1:D:63:LYS:HZ3	1:D:63:LYS:HG3	1.73	0.42
1:D:298:HIS:O	1:D:299:GLY:C	2.62	0.42
1:D:300:THR:O	1:D:301:SER:CB	2.67	0.42
1:C:110:PRO:O	1:C:114:VAL:HG23	2.19	0.42
1:C:226:ARG:HH22	1:C:365:ASP:CG	2.28	0.42
1:C:224:ALA:CB	1:C:363:GLU:HG2	2.47	0.42
1:D:269:MET:O	1:D:271:ALA:N	2.52	0.42
1:B:201:PHE:O	1:B:204:MET:HG2	2.20	0.42
1:C:25:SER:HB3	1:C:30:ARG:HB3	2.00	0.42
1:C:120:MET:SD	1:C:126:LEU:HD13	2.59	0.42
1:A:110:PRO:HG2	1:A:197:MET:HB2	2.01	0.42
1:A:162:ALA:O	1:A:165:THR:CG2	2.57	0.42
1:C:226:ARG:NH2	1:C:365:ASP:HB2	2.35	0.42
1:A:3:ARG:N	3:A:547:HOH:O	2.46	0.42
1:C:226:ARG:HH11	1:C:303:PRO:HA	1.84	0.42
1:A:28:GLU:HG2	1:A:30:ARG:HH21	1.84	0.41
1:D:281:MET:HE3	1:D:316:VAL:HG21	2.02	0.41
1:C:90:PRO:HA	1:C:93:TYR:CE2	2.55	0.41
1:D:294:TYR:HB3	1:D:385:VAL:HG12	2.01	0.41
1:A:49:TRP:NE1	1:A:193:LEU:HG	2.36	0.41
3:A:570:HOH:O	1:B:269:MET:HE3	2.19	0.41
1:A:349:MET:HE3	1:A:356:ALA:H	1.85	0.41
1:A:113:GLN:NE2	1:A:113:GLN:CA	2.83	0.41
1:A:194:CYS:HB2	1:A:196:GLU:OE1	2.21	0.41
1:A:241:GLU:OE1	1:A:245:HIS:ND1	2.46	0.41
1:C:194:CYS:HB2	1:C:196:GLU:OE1	2.20	0.41
1:C:261:GLY:CA	1:C:283:MET:HG2	2.47	0.41
1:A:7:THR:O	1:A:86:ALA:HA	2.21	0.41
1:C:93:TYR:HB2	1:C:99:VAL:HG11	2.03	0.41
1:A:145:CYS:HA	1:B:269:MET:CE	2.38	0.41
1:B:83:ILE:HD13	1:B:93:TYR:CZ	2.56	0.41
1:D:7:THR:O	1:D:86:ALA:HA	2.20	0.41
1:D:49:TRP:NE1	1:D:193:LEU:HG	2.36	0.41
1:D:249:ARG:CZ	1:D:251:ALA:HB2	2.51	0.41
1:B:29:GLY:HA2	1:B:330:MET:SD	2.61	0.41
1:C:277:ALA:HB2	3:C:558:HOH:O	2.21	0.41
1:C:300:THR:O	1:C:301:SER:CB	2.69	0.41
1:B:18:ASN:OD1	1:B:18:ASN:C	2.64	0.40
1:B:146:LEU:O	1:B:150:PHE:HB2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:249:ARG:CZ	1:B:251:ALA:HB2	2.51	0.40
1:C:16:GLY:HA2	1:C:21:GLU:HB3	2.03	0.40
1:C:121:ARG:HD2	1:D:195:TRP:CH2	2.54	0.40
1:D:96:ASN:HA	1:D:97:PRO:HD2	1.88	0.40
1:D:226:ARG:HH21	1:D:365:ASP:HB2	1.86	0.40
1:A:10:GLY:HA3	1:A:78:SER:O	2.21	0.40
1:A:170:ILE:O	1:A:174:VAL:HG23	2.21	0.40
1:B:60:ILE:O	1:B:61:ASP:C	2.62	0.40
1:A:28:GLU:HG2	1:A:30:ARG:NH2	2.37	0.40
1:A:162:ALA:N	1:A:165:THR:HG22	2.36	0.40
1:C:13:SER:HB2	3:C:527:HOH:O	2.20	0.40
1:C:349:MET:HE3	1:C:356:ALA:H	1.86	0.40
1:B:45:ARG:HH11	1:B:209:THR:HG21	1.86	0.40
1:B:380:ARG:HE	1:B:380:ARG:HB2	1.68	0.40
1:C:44:MET:O	1:C:47:HIS:NE2	2.54	0.40
1:C:401:MET:HE3	1:C:401:MET:HB2	1.95	0.40
1:A:294:TYR:HB3	1:A:385:VAL:HG12	2.03	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	401/406 (99%)	380 (95%)	16 (4%)	5 (1%)	10	9
1	B	401/406 (99%)	377 (94%)	20 (5%)	4 (1%)	12	12
1	C	401/406 (99%)	377 (94%)	20 (5%)	4 (1%)	12	12
1	D	401/406 (99%)	373 (93%)	23 (6%)	5 (1%)	10	9
All	All	1604/1624 (99%)	1507 (94%)	79 (5%)	18 (1%)	11	11

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	369	ALA
1	B	371	LEU
1	C	57	THR
1	D	57	THR
1	A	57	THR
1	A	270	VAL
1	A	299	GLY
1	A	370	GLY
1	B	270	VAL
1	B	299	GLY
1	C	270	VAL
1	C	299	GLY
1	D	270	VAL
1	D	299	GLY
1	D	364	LEU
1	D	369	ALA
1	C	364	LEU
1	B	364	LEU

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%)	261 (85%)	45 (15%)	3	2
1	B	306/309 (99%)	268 (88%)	38 (12%)	4	4
1	C	306/309 (99%)	266 (87%)	40 (13%)	4	4
1	D	306/309 (99%)	266 (87%)	40 (13%)	4	4
All	All	1224/1236 (99%)	1061 (87%)	163 (13%)	4	3

All (163) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	LYS
1	A	19	GLN
1	A	23	LEU
1	A	30	ARG

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Mol	Chain	Res	Type
1	A	38	GLU
1	A	40	LYS
1	A	49	TRP
1	A	54	LEU
1	A	62	ARG
1	A	63	LYS
1	A	65	VAL
1	A	66	ARG
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	146	LEU
1	A	151	LYS
1	A	160	SER
1	A	161	SER
1	A	165	THR
1	A	172	ASN
1	A	177	ILE
1	A	210	LYS
1	A	217	LYS
1	A	244	GLU
1	A	256	GLU
1	A	270	VAL
1	A	308	LYS
1	A	310	LEU
1	A	313	ILE
1	A	314	ARG
1	A	315	GLU
1	A	320	LYS
1	A	321	SER
1	A	347	LEU
1	A	350	LEU
1	A	358	SER
1	A	364	LEU
1	A	373	ILE
1	A	378	THR
1	A	381	GLU
1	B	23	LEU

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Mol	Chain	Res	Type
1	B	27	ARG
1	B	40	LYS
1	B	42	SER
1	B	49	TRP
1	B	62	ARG
1	B	66	ARG
1	B	68	MET
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	151	LYS
1	B	160	SER
1	B	161	SER
1	B	165	THR
1	B	172	ASN
1	B	177	ILE
1	B	210	LYS
1	B	217	LYS
1	B	257	ILE
1	B	270	VAL
1	B	320	LYS
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	371	LEU
1	B	372	ASN
1	B	374	VAL
1	B	376	GLU
1	B	380	ARG
1	B	381	GLU
1	B	403	LYS
1	C	23	LEU
1	C	25	SER
1	C	28	GLU
1	C	30	ARG
1	C	45	ARG

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Mol	Chain	Res	Type
1	C	49	TRP
1	C	59	LEU
1	C	62	ARG
1	C	66	ARG
1	C	68	MET
1	C	88	LEU
1	C	91	GLU
1	C	113	GLN
1	C	121	ARG
1	C	126	LEU
1	C	146	LEU
1	C	151	LYS
1	C	160	SER
1	C	161	SER
1	C	165	THR
1	C	172	ASN
1	C	177	ILE
1	C	210	LYS
1	C	217	LYS
1	C	270	VAL
1	C	282	LYS
1	C	289	ASP
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	363	GLU
1	C	364	LEU
1	C	366	GLU
1	C	367	GLN
1	C	376	GLU
1	C	381	GLU
1	C	403	LYS
1	D	2	LYS
1	D	18	ASN
1	D	20	GLN
1	D	23	LEU
1	D	27	ARG
1	D	49	TRP
1	D	53	LYS

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Mol	Chain	Res	Type
1	D	59	LEU
1	D	61	ASP
1	D	62	ARG
1	D	63	LYS
1	D	64	VAL
1	D	68	MET
1	D	88	LEU
1	D	91	GLU
1	D	121	ARG
1	D	126	LEU
1	D	127	LYS
1	D	146	LEU
1	D	160	SER
1	D	165	THR
1	D	172	ASN
1	D	177	ILE
1	D	210	LYS
1	D	217	LYS
1	D	247	LEU
1	D	270	VAL
1	D	285	MET
1	D	307	VAL
1	D	308	LYS
1	D	320	LYS
1	D	347	LEU
1	D	350	LEU
1	D	351	GLU
1	D	358	SER
1	D	363	GLU
1	D	364	LEU
1	D	373	ILE
1	D	377	THR
1	D	381	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	19	GLN
1	A	113	GLN
1	A	296	ASN
1	A	341	GLN
1	A	352	HIS

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Mol	Chain	Res	Type
1	A	367	GLN
1	A	372	ASN
1	B	95	ASN
1	B	341	GLN
1	B	372	ASN
1	C	19	GLN
1	C	37	GLN
1	C	172	ASN
1	C	296	ASN
1	C	341	GLN
1	C	367	GLN
1	C	372	ASN
1	D	18	ASN
1	D	20	GLN
1	D	153	HIS
1	D	172	ASN
1	D	245	HIS
1	D	341	GLN
1	D	372	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	TLM	A	500	-	5,14,14	0.52	0	5,21,21	0.68	0
2	TLM	D	503	-	5,14,14	0.46	0	5,21,21	0.69	0
2	TLM	B	501	-	5,14,14	0.51	0	5,21,21	0.68	0
2	TLM	C	502	-	5,14,14	0.52	0	5,21,21	0.66	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
2	TLM	A	500	-	-	0/4/26/26	0/1/1/1
2	TLM	D	503	-	-	0/4/26/26	0/1/1/1
2	TLM	B	501	-	-	0/4/26/26	0/1/1/1
2	TLM	C	502	-	-	0/4/26/26	0/1/1/1

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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	503	TLM	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	403/406 (99%)	-0.04	5 (1%) 76 81	8, 17, 31, 50	0
1	B	403/406 (99%)	-0.10	5 (1%) 76 81	9, 16, 27, 40	0
1	C	403/406 (99%)	-0.04	6 (1%) 72 77	10, 18, 28, 48	0
1	D	403/406 (99%)	-0.12	4 (0%) 79 83	9, 16, 27, 39	0
All	All	1612/1624 (99%)	-0.07	20 (1%) 76 81	8, 17, 29, 50	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	370	GLY	5.3
1	A	49	TRP	4.2
1	B	371	LEU	3.8
1	B	49	TRP	3.2
1	C	49	TRP	3.0
1	D	49	TRP	2.9
1	A	368	ALA	2.9
1	A	370	GLY	2.6
1	C	367	GLN	2.5
1	C	362	GLU	2.4
1	B	404	LEU	2.4
1	D	57	THR	2.3
1	C	363	GLU	2.3
1	C	57	THR	2.3
1	D	270	VAL	2.3
1	A	369	ALA	2.3
1	A	57	THR	2.2
1	C	364	LEU	2.2
1	D	20	GLN	2.2
1	B	372	ASN	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](#)

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. 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	B-factors($\text{\AA}^2$)	Q<0.9
2	TLM	A	500	14/14	0.94	0.08	9,17,19,20	0
2	TLM	C	502	14/14	0.94	0.09	11,15,19,21	0
2	TLM	D	503	14/14	0.95	0.08	11,16,19,21	0
2	TLM	B	501	14/14	0.96	0.07	3,12,16,18	0

6.5 Other polymers [i](#)

There are no such residues in this entry.