



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:39 PM UTC

PDB ID : 6ZU0 / pdb_00006zu0
Title : Crystal structure of citrate synthase (GltA) from *Pseudomonas aeruginosa*
Authors : Wijaya, A.J.; Brear, P.; Dolan, S.K.; Welch, M.
Deposited on : 2020-07-21
Resolution : 3.40 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

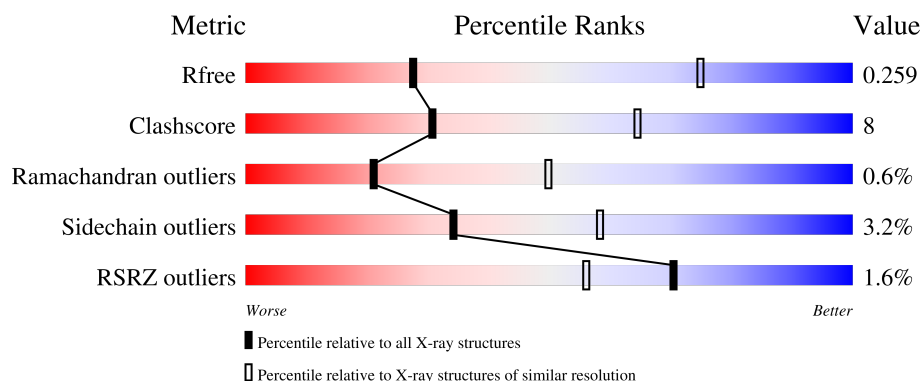
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 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	1001 (3.44-3.36)
Clashscore	190562	1022 (3.44-3.36)
Ramachandran outliers	187476	1012 (3.44-3.36)
Sidechain outliers	187428	1012 (3.44-3.36)
RSRZ outliers	180081	1001 (3.44-3.36)

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	428	% 87% 12% .
1	B	428	% 84% 15% ..
1	C	428	 81% 17% .
1	D	428	% 79% 18% ..
1	E	428	4% 83% 14% ..

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Mol	Chain	Length	Quality of chain
1	F	428	2% 81% 16% ..

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 19923 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.

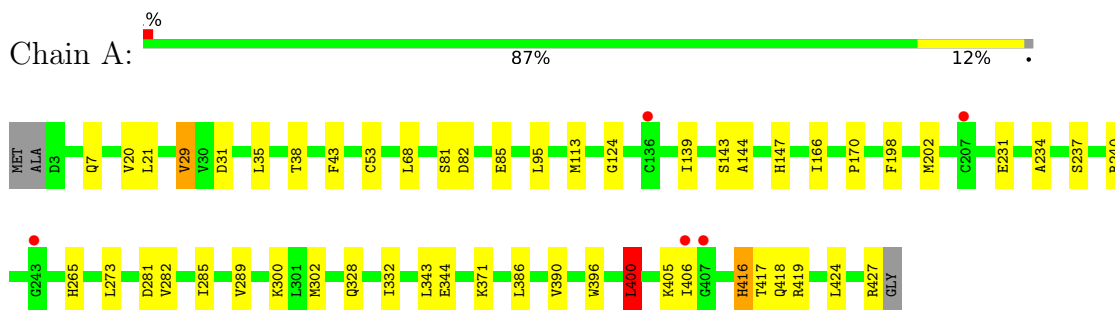
- Molecule 1 is a protein called Citrate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	425	Total	C	N	O	S	0	0	0
			3332	2123	573	612	24			
1	B	424	Total	C	N	O	S	0	0	0
			3326	2120	572	611	23			
1	C	426	Total	C	N	O	S	0	0	0
			3336	2125	574	613	24			
1	D	424	Total	C	N	O	S	0	0	0
			3321	2117	569	611	24			
1	E	422	Total	C	N	O	S	0	0	0
			3304	2108	567	605	24			
1	F	422	Total	C	N	O	S	0	0	0
			3304	2107	566	607	24			

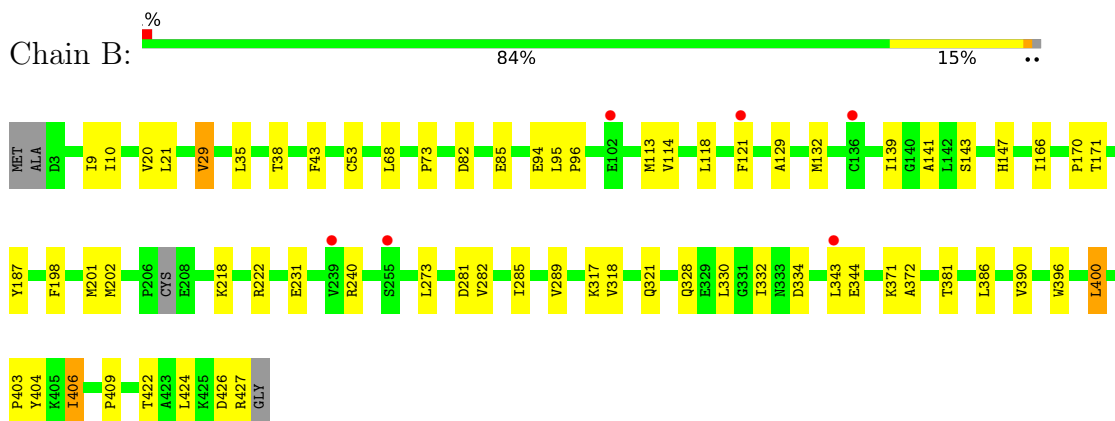
3 Residue-property plots

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.

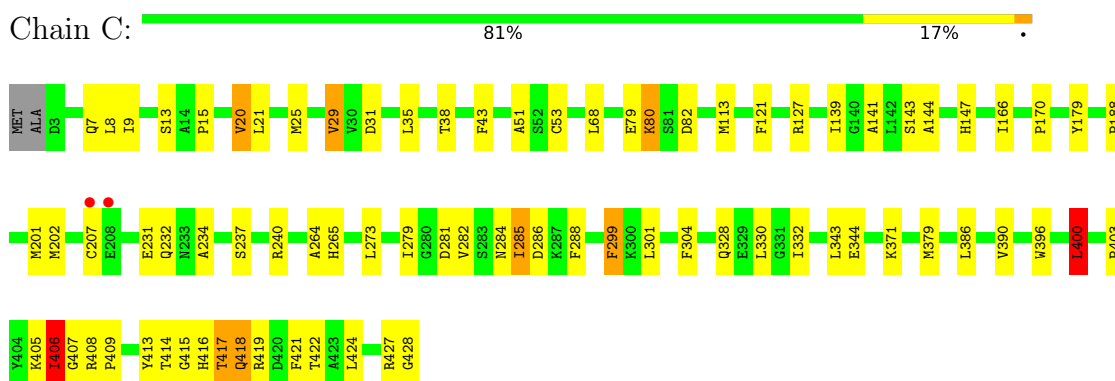
• Molecule 1: Citrate synthase



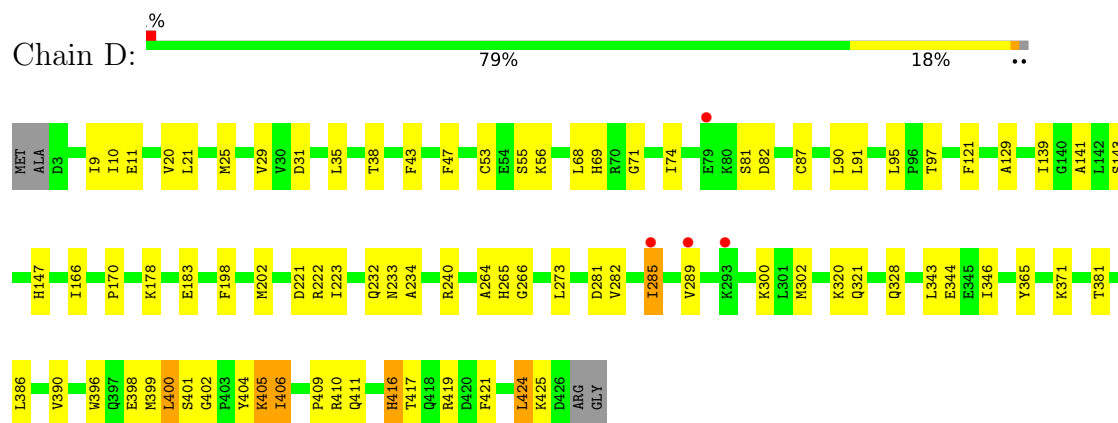
• Molecule 1: Citrate synthase



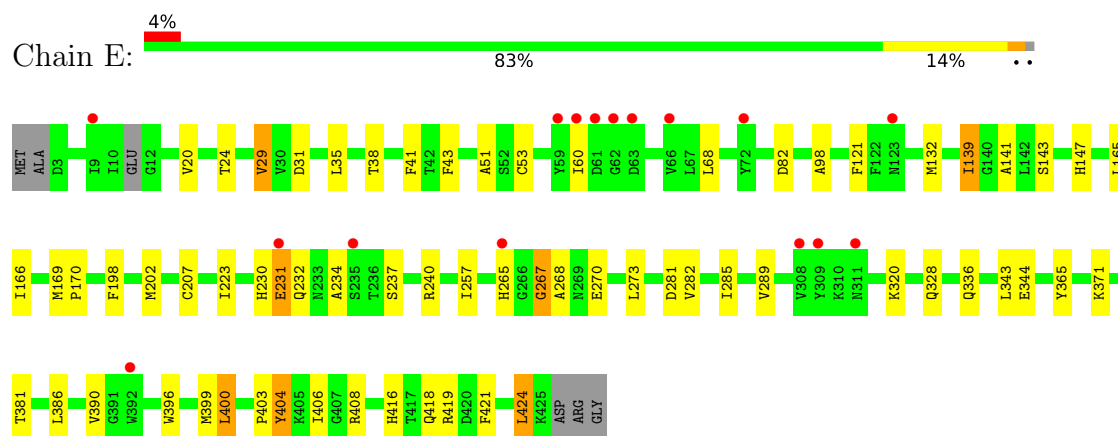
• Molecule 1: Citrate synthase



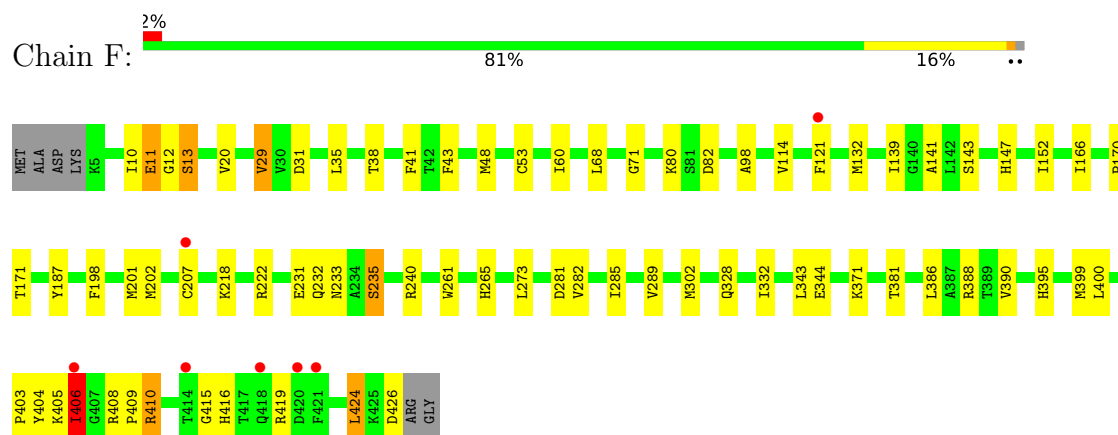
- Molecule 1: Citrate synthase



- Molecule 1: Citrate synthase



- Molecule 1: Citrate synthase



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	216.75Å 80.18Å 196.66Å 90.00° 121.89° 90.00°	Depositor
Resolution (Å)	83.49 – 3.40 83.49 – 3.40	Depositor EDS
% Data completeness (in resolution range)	99.0 (83.49-3.40) 99.1 (83.49-3.40)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.74 (at 3.41Å)	Xtriage
Refinement program	PHENIX 1.12_2829	Depositor
R, R_{free}	0.238 , 0.267 (Not available) , 0.259	Depositor DCC
R_{free} test set	1908 reflections (4.78%)	wwPDB-VP
Wilson B-factor (Å ²)	82.7	Xtriage
Anisotropy	0.432	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 41.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.000 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	19923	wwPDB-VP
Average B, all atoms (Å ²)	92.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.49% 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	0.47	0/3413	0.98	2/4619 (0.0%)
1	B	0.48	0/3406	0.99	3/4608 (0.1%)
1	C	0.53	0/3417	1.09	10/4624 (0.2%)
1	D	0.52	1/3402 (0.0%)	1.01	4/4605 (0.1%)
1	E	0.50	0/3384	1.01	5/4579 (0.1%)
1	F	0.49	0/3385	0.99	4/4583 (0.1%)
All	All	0.50	1/20407 (0.0%)	1.01	28/27618 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	405	LYS	CA-C	5.95	1.61	1.53

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	279	ILE	N-CA-C	-9.94	101.08	110.42
1	C	279	ILE	N-CA-CB	9.18	121.02	110.65
1	D	223	ILE	N-CA-CB	8.04	119.96	110.55
1	F	424	LEU	N-CA-C	-7.73	102.94	111.36
1	C	80	LYS	N-CA-C	7.44	122.25	112.72
1	D	223	ILE	N-CA-C	-7.23	103.48	110.42
1	B	21	LEU	N-CA-C	6.69	120.72	109.76
1	C	406	ILE	N-CA-C	6.68	123.23	109.34
1	D	21	LEU	N-CA-C	6.45	120.33	109.76
1	C	406	ILE	N-CA-CB	-6.39	100.68	111.23
1	A	21	LEU	N-CA-C	6.36	120.19	109.76
1	E	231	GLU	CB-CA-C	-6.08	109.55	116.54
1	C	21	LEU	N-CA-C	6.01	119.62	109.76
1	C	400	LEU	N-CA-CB	5.94	118.95	110.16
1	C	79	GLU	N-CA-C	5.92	117.73	111.28
1	D	221	ASP	N-CA-C	5.71	117.97	111.11
1	E	403	PRO	N-CA-C	-5.66	100.82	112.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	406	ILE	N-CA-CB	-5.41	102.30	111.23
1	C	299	PHE	CA-C-N	5.38	128.73	120.82
1	C	299	PHE	C-N-CA	5.38	128.73	120.82
1	B	334	ASP	N-CA-C	5.36	117.20	109.48
1	F	406	ILE	N-CA-C	5.31	120.38	109.34
1	E	424	LEU	N-CA-C	-5.22	106.69	113.16
1	F	426	ASP	N-CA-CB	-5.18	101.69	110.50
1	E	223	ILE	N-CA-CB	5.18	116.61	110.55
1	E	404	TYR	CB-CA-C	-5.12	102.78	111.02
1	B	426	ASP	CB-CA-C	5.06	119.19	110.79
1	A	400	LEU	N-CA-CB	5.01	117.58	110.16

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	3332	0	3300	41	0
1	B	3326	0	3294	69	0
1	C	3336	0	3303	95	0
1	D	3321	0	3287	91	0
1	E	3304	0	3276	59	0
1	F	3304	0	3270	66	0
All	All	19923	0	19730	329	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 8.

All (329) 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:264:ALA:HB1	1:D:406:ILE:CD1	1.72	1.18
1:C:264:ALA:CB	1:D:406:ILE:HD11	1.74	1.16
1:C:264:ALA:HB1	1:D:406:ILE:HD11	1.03	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:413:TYR:CZ	1:C:415:GLY:HA3	1.94	1.01
1:E:60:ILE:HD12	1:E:231:GLU:CD	1.87	0.99
1:C:80:LYS:CB	1:D:421:PHE:HE2	1.78	0.96
1:C:413:TYR:CE1	1:C:415:GLY:HA3	2.00	0.96
1:C:413:TYR:CZ	1:C:415:GLY:CA	2.49	0.95
1:C:427:ARG:NH1	1:D:95:LEU:HB3	1.85	0.92
1:C:80:LYS:HB2	1:D:421:PHE:CE2	2.05	0.91
1:D:416:HIS:CD2	1:D:419:ARG:HE	1.90	0.90
1:B:424:LEU:HA	1:B:427:ARG:HH21	1.35	0.89
1:D:416:HIS:HD2	1:D:419:ARG:NE	1.69	0.89
1:C:422:THR:HG23	1:C:427:ARG:HD3	1.55	0.88
1:C:80:LYS:CB	1:D:421:PHE:CE2	2.56	0.87
1:C:406:ILE:HD12	1:D:264:ALA:HB1	1.55	0.87
1:B:406:ILE:HD13	1:B:406:ILE:N	1.89	0.87
1:B:424:LEU:CA	1:B:427:ARG:HH21	1.88	0.86
1:F:231:GLU:HG2	1:F:232:GLN:H	1.40	0.86
1:C:80:LYS:HB3	1:D:421:PHE:HE2	1.40	0.85
1:E:121:PHE:CZ	1:F:121:PHE:CZ	2.65	0.85
1:A:424:LEU:HD12	1:A:424:LEU:O	1.81	0.80
1:C:413:TYR:OH	1:C:415:GLY:C	2.24	0.80
1:B:424:LEU:HD23	1:B:424:LEU:O	1.83	0.79
1:E:60:ILE:HD12	1:E:231:GLU:OE2	1.84	0.78
1:B:406:ILE:HD13	1:B:406:ILE:H	1.47	0.77
1:C:20:VAL:HG21	1:D:10:ILE:HD11	1.68	0.76
1:E:234:ALA:HB3	1:E:265:HIS:CD2	2.22	0.75
1:C:121:PHE:CZ	1:D:121:PHE:CE2	2.76	0.74
1:D:416:HIS:HD2	1:D:419:ARG:HE	1.25	0.74
1:A:417:THR:O	1:A:419:ARG:HG3	1.88	0.73
1:D:404:TYR:CD1	1:D:405:LYS:N	2.56	0.73
1:C:413:TYR:CZ	1:C:415:GLY:C	2.67	0.73
1:A:273:LEU:HD11	1:A:371:LYS:HD3	1.68	0.73
1:E:121:PHE:CZ	1:F:121:PHE:CE2	2.76	0.72
1:E:273:LEU:HD11	1:E:371:LYS:HD3	1.71	0.72
1:C:121:PHE:CE2	1:D:121:PHE:CZ	2.78	0.72
1:A:427:ARG:HH21	1:B:95:LEU:HD13	1.54	0.72
1:D:234:ALA:HB3	1:D:265:HIS:CD2	2.24	0.71
1:E:121:PHE:CE2	1:F:121:PHE:CZ	2.77	0.71
1:B:273:LEU:HD11	1:B:371:LYS:HD3	1.73	0.71
1:A:237:SER:OG	1:B:409:PRO:CG	2.39	0.70
1:C:427:ARG:HH11	1:D:95:LEU:HB3	1.56	0.70
1:A:237:SER:OG	1:B:409:PRO:HG2	1.90	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:113:MET:HE3	1:C:207:CYS:HB2	1.74	0.70
1:C:9:ILE:CG1	1:C:15:PRO:HG3	2.23	0.69
1:C:121:PHE:CZ	1:D:121:PHE:CZ	2.81	0.69
1:B:10:ILE:HG22	1:B:10:ILE:O	1.92	0.68
1:C:80:LYS:HB3	1:D:421:PHE:CE2	2.27	0.68
1:E:230:HIS:O	1:E:231:GLU:HG2	1.93	0.68
1:C:188:PRO:HB3	1:C:201:MET:HE3	1.75	0.67
1:D:273:LEU:HD11	1:D:371:LYS:HD3	1.74	0.67
1:C:53:CYS:SG	1:C:240:ARG:NH1	2.68	0.67
1:B:53:CYS:SG	1:B:240:ARG:NH1	2.68	0.67
1:C:188:PRO:HB3	1:C:201:MET:CE	2.25	0.66
1:F:273:LEU:HD11	1:F:371:LYS:HD3	1.76	0.66
1:A:53:CYS:SG	1:A:240:ARG:NH1	2.68	0.66
1:E:408:ARG:H	1:F:48:MET:HE2	1.59	0.66
1:C:25:MET:CE	1:D:417:THR:HG23	2.25	0.66
1:E:53:CYS:SG	1:E:240:ARG:NH1	2.69	0.66
1:F:424:LEU:O	1:F:424:LEU:HD23	1.96	0.66
1:F:53:CYS:SG	1:F:240:ARG:NH1	2.68	0.65
1:B:118:LEU:O	1:B:121:PHE:HB2	1.96	0.65
1:B:424:LEU:HA	1:B:427:ARG:NH2	2.09	0.65
1:D:53:CYS:SG	1:D:240:ARG:NH1	2.69	0.65
1:D:198:PHE:CZ	1:D:202:MET:HE3	2.32	0.65
1:F:231:GLU:HG2	1:F:232:GLN:N	2.09	0.65
1:B:222:ARG:HH12	1:B:321:GLN:NE2	1.95	0.65
1:F:198:PHE:CZ	1:F:202:MET:HE3	2.32	0.64
1:E:198:PHE:CZ	1:E:202:MET:HE3	2.32	0.64
1:E:424:LEU:HD21	1:F:98:ALA:HB2	1.78	0.64
1:B:198:PHE:CZ	1:B:202:MET:HE3	2.32	0.64
1:C:202:MET:HE1	1:C:379:MET:HE2	1.79	0.64
1:D:416:HIS:CD2	1:D:419:ARG:NE	2.53	0.64
1:E:98:ALA:HB2	1:F:424:LEU:HD21	1.79	0.64
1:B:132:MET:CG	1:B:381:THR:HG23	2.28	0.63
1:C:406:ILE:HD12	1:D:264:ALA:CB	2.26	0.63
1:A:198:PHE:CZ	1:A:202:MET:HE3	2.33	0.63
1:C:231:GLU:OE2	1:D:411:GLN:HG2	1.98	0.63
1:C:273:LEU:HD11	1:C:371:LYS:HD3	1.80	0.63
1:F:10:ILE:O	1:F:12:GLY:N	2.32	0.62
1:F:404:TYR:O	1:F:405:LYS:HD3	1.99	0.62
1:B:132:MET:CG	1:B:381:THR:CG2	2.78	0.61
1:A:124:GLY:O	1:B:121:PHE:CE2	2.54	0.61
1:D:424:LEU:HD12	1:D:424:LEU:O	1.99	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:267:GLY:O	1:E:270:GLU:N	2.33	0.61
1:C:51:ALA:HA	1:D:410:ARG:O	2.00	0.61
1:D:404:TYR:CG	1:D:405:LYS:N	2.65	0.61
1:F:171:THR:HG23	1:F:201:MET:HE1	1.81	0.61
1:E:424:LEU:HD23	1:E:424:LEU:O	2.01	0.60
1:F:416:HIS:ND1	1:F:419:ARG:NH2	2.48	0.60
1:B:406:ILE:N	1:B:406:ILE:CD1	2.60	0.60
1:C:9:ILE:HG13	1:C:15:PRO:HG3	1.84	0.60
1:A:281:ASP:OD1	1:A:282:VAL:N	2.35	0.60
1:F:405:LYS:C	1:F:406:ILE:HG22	2.27	0.60
1:B:424:LEU:CB	1:B:427:ARG:HH21	2.14	0.60
1:D:281:ASP:OD1	1:D:282:VAL:N	2.35	0.60
1:E:320:LYS:HD3	1:E:365:TYR:OH	2.02	0.60
1:C:281:ASP:OD1	1:C:282:VAL:N	2.35	0.59
1:D:320:LYS:HD3	1:D:365:TYR:OH	2.02	0.59
1:F:281:ASP:OD1	1:F:282:VAL:N	2.35	0.59
1:B:281:ASP:OD1	1:B:282:VAL:N	2.35	0.59
1:A:417:THR:O	1:A:418:GLN:C	2.45	0.59
1:F:10:ILE:O	1:F:10:ILE:HG22	2.02	0.59
1:C:413:TYR:OH	1:C:416:HIS:N	2.35	0.59
1:F:235:SER:OG	1:F:265:HIS:NE2	2.27	0.59
1:A:95:LEU:HB2	1:B:427:ARG:HD3	1.84	0.59
1:E:281:ASP:OD1	1:E:282:VAL:N	2.35	0.59
1:E:231:GLU:HG3	1:E:232:GLN:N	2.17	0.59
1:E:230:HIS:C	1:E:231:GLU:HG2	2.28	0.58
1:E:267:GLY:O	1:E:268:ALA:C	2.46	0.58
1:C:332:ILE:HG22	1:C:332:ILE:O	2.02	0.58
1:D:91:LEU:HD21	1:D:390:VAL:HG23	1.85	0.58
1:C:234:ALA:HB3	1:C:265:HIS:CD2	2.38	0.58
1:E:170:PRO:HA	1:E:386:LEU:HD11	1.85	0.58
1:B:10:ILE:O	1:B:10:ILE:CG2	2.52	0.58
1:B:171:THR:HG23	1:B:201:MET:HE1	1.86	0.57
1:C:9:ILE:HD12	1:C:15:PRO:HG3	1.86	0.57
1:E:147:HIS:CE1	1:F:261:TRP:CZ2	2.93	0.57
1:F:170:PRO:HA	1:F:386:LEU:HD11	1.87	0.57
1:E:165:LEU:O	1:E:169:MET:HG2	2.04	0.57
1:A:170:PRO:HA	1:A:386:LEU:HD11	1.86	0.57
1:C:170:PRO:HA	1:C:386:LEU:HD11	1.87	0.56
1:A:237:SER:OG	1:B:409:PRO:HG3	2.06	0.56
1:F:424:LEU:HD23	1:F:424:LEU:C	2.31	0.56
1:B:170:PRO:HA	1:B:386:LEU:HD11	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:285:ILE:HD13	1:D:346:ILE:HD11	1.88	0.56
1:D:170:PRO:HA	1:D:386:LEU:HD11	1.87	0.56
1:A:95:LEU:CB	1:B:427:ARG:HD3	2.36	0.55
1:D:232:GLN:HE22	1:D:240:ARG:NH1	2.03	0.55
1:D:266:GLY:O	1:D:381:THR:HG22	2.06	0.55
1:E:234:ALA:HB3	1:E:265:HIS:HD2	1.70	0.55
1:C:414:THR:OG1	1:D:56:LYS:HE2	2.06	0.55
1:C:414:THR:HG1	1:D:56:LYS:HE2	1.72	0.55
1:C:424:LEU:HA	1:C:427:ARG:HH21	1.71	0.55
1:C:25:MET:HE3	1:D:417:THR:HG23	1.88	0.54
1:C:299:PHE:O	1:C:299:PHE:CD2	2.60	0.54
1:D:417:THR:O	1:D:419:ARG:HG3	2.08	0.54
1:F:152:ILE:CG1	1:F:400:LEU:HD21	2.37	0.54
1:B:132:MET:HG3	1:B:381:THR:HG21	1.90	0.54
1:C:9:ILE:CD1	1:C:15:PRO:HG3	2.38	0.54
1:C:285:ILE:HG22	1:C:286:ASP:N	2.23	0.54
1:D:273:LEU:HD11	1:D:371:LYS:CD	2.38	0.54
1:D:266:GLY:O	1:D:381:THR:CG2	2.55	0.54
1:F:232:GLN:NE2	1:F:395:HIS:CE1	2.76	0.54
1:E:421:PHE:CE2	1:F:80:LYS:HB3	2.43	0.53
1:C:413:TYR:CE1	1:C:415:GLY:CA	2.82	0.53
1:F:232:GLN:HE21	1:F:395:HIS:CE1	2.27	0.53
1:B:273:LEU:HD11	1:B:371:LYS:CD	2.39	0.52
1:C:7:GLN:HB3	1:D:9:ILE:HG13	1.91	0.52
1:C:273:LEU:HD11	1:C:371:LYS:CD	2.40	0.52
1:E:237:SER:OG	1:F:409:PRO:HG3	2.09	0.52
1:A:35:LEU:O	1:A:38:THR:HG22	2.10	0.52
1:B:35:LEU:O	1:B:38:THR:HG22	2.10	0.52
1:C:35:LEU:O	1:C:38:THR:HG22	2.10	0.52
1:C:427:ARG:HH11	1:D:95:LEU:CB	2.20	0.52
1:C:427:ARG:HH12	1:D:95:LEU:HB3	1.74	0.52
1:F:10:ILE:O	1:F:13:SER:N	2.43	0.52
1:C:8:LEU:O	1:C:15:PRO:HA	2.09	0.52
1:C:264:ALA:CB	1:D:406:ILE:CD1	2.56	0.52
1:D:166:ILE:HD11	1:D:390:VAL:HG23	1.92	0.52
1:A:166:ILE:HD11	1:A:390:VAL:HG23	1.92	0.52
1:F:35:LEU:O	1:F:38:THR:HG22	2.10	0.52
1:E:273:LEU:HD11	1:E:371:LYS:CD	2.37	0.52
1:F:273:LEU:HD11	1:F:371:LYS:CD	2.39	0.52
1:E:35:LEU:O	1:E:38:THR:HG22	2.09	0.52
1:D:35:LEU:O	1:D:38:THR:HG22	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:406:ILE:HG23	1:F:406:ILE:O	2.10	0.51
1:B:166:ILE:HD11	1:B:390:VAL:HG23	1.92	0.51
1:C:166:ILE:HD11	1:C:390:VAL:HG23	1.92	0.51
1:E:51:ALA:HA	1:F:410:ARG:O	2.11	0.51
1:F:218:LYS:HZ3	1:F:222:ARG:HH21	1.59	0.51
1:A:234:ALA:HB3	1:A:265:HIS:CD2	2.45	0.51
1:C:413:TYR:OH	1:C:415:GLY:HA3	2.10	0.51
1:C:25:MET:HE1	1:D:417:THR:HG23	1.92	0.51
1:E:166:ILE:HD11	1:E:390:VAL:HG23	1.92	0.51
1:E:29:VAL:HG13	1:F:41:PHE:HB2	1.93	0.51
1:B:400:LEU:HD23	1:B:404:TYR:CE2	2.46	0.51
1:F:166:ILE:HD11	1:F:390:VAL:HG23	1.93	0.51
1:B:114:VAL:HG23	1:B:171:THR:HG21	1.92	0.51
1:C:80:LYS:HB2	1:D:421:PHE:CD2	2.45	0.51
1:C:413:TYR:OH	1:C:415:GLY:CA	2.58	0.51
1:E:231:GLU:HG3	1:E:232:GLN:H	1.75	0.50
1:D:69:HIS:CE1	1:D:74:ILE:HD13	2.45	0.50
1:C:237:SER:OG	1:D:409:PRO:HG2	2.11	0.50
1:A:95:LEU:HB3	1:B:427:ARG:HH11	1.76	0.50
1:B:222:ARG:NH1	1:B:321:GLN:NE2	2.59	0.50
1:A:406:ILE:HG23	1:A:406:ILE:O	2.11	0.50
1:D:222:ARG:HH12	1:D:321:GLN:NE2	2.10	0.50
1:F:233:ASN:HD22	1:F:388:ARG:HH12	1.60	0.49
1:B:132:MET:HG2	1:B:381:THR:HG23	1.94	0.49
1:B:170:PRO:CA	1:B:386:LEU:HD11	2.43	0.49
1:B:132:MET:HG2	1:B:381:THR:CG2	2.41	0.49
1:F:404:TYR:O	1:F:405:LYS:CD	2.61	0.49
1:A:237:SER:CB	1:B:409:PRO:HG3	2.42	0.49
1:C:144:ALA:HB1	1:D:129:ALA:HB1	1.95	0.49
1:C:231:GLU:CD	1:C:232:GLN:H	2.20	0.49
1:D:399:MET:O	1:D:402:GLY:O	2.30	0.49
1:A:273:LEU:HD11	1:A:371:LYS:CD	2.39	0.49
1:E:237:SER:OG	1:F:409:PRO:CG	2.61	0.49
1:E:170:PRO:CA	1:E:386:LEU:HD11	2.43	0.48
1:B:132:MET:SD	1:B:381:THR:HG23	2.54	0.48
1:B:424:LEU:HA	1:B:427:ARG:HE	1.78	0.48
1:C:113:MET:HE3	1:F:207:CYS:HB2	1.95	0.48
1:A:144:ALA:HB1	1:B:129:ALA:HB1	1.95	0.48
1:A:170:PRO:CA	1:A:386:LEU:HD11	2.43	0.48
1:C:80:LYS:HD2	1:D:421:PHE:CD2	2.49	0.48
1:C:417:THR:O	1:C:419:ARG:N	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:170:PRO:CA	1:D:386:LEU:HD11	2.43	0.48
1:C:170:PRO:CA	1:C:386:LEU:HD11	2.43	0.48
1:C:408:ARG:O	1:C:408:ARG:HG3	2.12	0.48
1:E:60:ILE:HD12	1:E:231:GLU:CG	2.43	0.48
1:A:427:ARG:HD3	1:B:96:PRO:O	2.14	0.48
1:F:170:PRO:CA	1:F:386:LEU:HD11	2.43	0.48
1:A:7:GLN:HB3	1:B:9:ILE:CG1	2.44	0.47
1:A:113:MET:HE3	1:E:207:CYS:HB2	1.96	0.47
1:C:427:ARG:O	1:D:97:THR:HG22	2.14	0.47
1:A:416:HIS:HE1	1:B:94:GLU:OE1	1.97	0.47
1:D:398:GLU:O	1:D:401:SER:OG	2.33	0.47
1:C:7:GLN:HB3	1:D:9:ILE:CG1	2.45	0.47
1:C:418:GLN:HA	1:D:71:GLY:O	2.15	0.47
1:C:20:VAL:CG2	1:D:10:ILE:HD11	2.43	0.47
1:C:284:ASN:O	1:C:288:PHE:HD2	1.97	0.47
1:E:132:MET:CE	1:E:257:ILE:HG23	2.45	0.47
1:C:143:SER:O	1:C:147:HIS:HB2	2.15	0.47
1:E:24:THR:HG21	1:F:415:GLY:O	2.15	0.47
1:E:230:HIS:O	1:E:231:GLU:CG	2.62	0.47
1:E:231:GLU:CD	1:F:408:ARG:NH2	2.73	0.47
1:A:143:SER:O	1:A:147:HIS:HB2	2.15	0.46
1:B:143:SER:O	1:B:147:HIS:HB2	2.15	0.46
1:D:143:SER:O	1:D:147:HIS:HB2	2.16	0.46
1:C:188:PRO:CB	1:C:201:MET:HE3	2.45	0.46
1:E:404:TYR:O	1:E:404:TYR:CD2	2.69	0.46
1:A:427:ARG:NH2	1:B:85:GLU:OE2	2.49	0.46
1:F:218:LYS:NZ	1:F:222:ARG:HH21	2.13	0.46
1:B:403:PRO:HG2	1:B:403:PRO:O	2.16	0.46
1:E:41:PHE:HB2	1:F:29:VAL:HG13	1.98	0.46
1:F:152:ILE:HG12	1:F:400:LEU:HD21	1.98	0.46
1:A:81:SER:HB2	1:A:85:GLU:OE1	2.15	0.46
1:E:143:SER:O	1:E:147:HIS:HB2	2.15	0.45
1:F:143:SER:O	1:F:147:HIS:HB2	2.15	0.45
1:A:7:GLN:HB3	1:B:9:ILE:HG13	1.97	0.45
1:B:222:ARG:HH12	1:B:321:GLN:HE21	1.64	0.45
1:B:317:LYS:HG3	1:B:318:VAL:N	2.31	0.45
1:C:413:TYR:CE2	1:C:415:GLY:O	2.69	0.45
1:D:87:CYS:O	1:D:91:LEU:HD23	2.16	0.45
1:A:427:ARG:NH2	1:B:95:LEU:HD13	2.27	0.45
1:B:422:THR:O	1:B:422:THR:OG1	2.35	0.45
1:B:424:LEU:HD23	1:B:424:LEU:C	2.39	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:127:ARG:HG2	1:C:179:TYR:CE1	2.51	0.45
1:D:240:ARG:HA	1:D:399:MET:HE1	1.99	0.45
1:B:132:MET:CG	1:B:381:THR:HG21	2.44	0.45
1:C:31:ASP:HA	1:D:43:PHE:HB3	1.99	0.45
1:C:264:ALA:HB1	1:D:406:ILE:CG1	2.41	0.45
1:D:416:HIS:HD2	1:D:419:ARG:CZ	2.25	0.44
1:E:418:GLN:HA	1:F:71:GLY:O	2.18	0.44
1:C:408:ARG:HB2	1:D:233:ASN:HA	1.98	0.44
1:A:43:PHE:HB2	1:B:29:VAL:HG12	1.99	0.44
1:C:299:PHE:O	1:C:299:PHE:CG	2.71	0.44
1:B:396:TRP:CE2	1:B:400:LEU:CD1	3.01	0.44
1:C:417:THR:HB	1:D:25:MET:HE3	2.00	0.44
1:D:69:HIS:CD2	1:D:90:LEU:HD21	2.53	0.44
1:D:416:HIS:CD2	1:D:419:ARG:HH21	2.36	0.44
1:F:240:ARG:HD3	1:F:399:MET:HE2	2.00	0.44
1:D:234:ALA:HB3	1:D:265:HIS:HD2	1.81	0.43
1:D:396:TRP:CE2	1:D:400:LEU:CD1	3.01	0.43
1:F:187:TYR:C	1:F:201:MET:HE3	2.43	0.43
1:B:187:TYR:C	1:B:201:MET:HE3	2.43	0.43
1:B:330:LEU:CD2	1:B:372:ALA:O	2.67	0.43
1:D:91:LEU:CD2	1:D:390:VAL:CG2	2.96	0.43
1:E:231:GLU:OE2	1:F:408:ARG:NH2	2.52	0.43
1:C:428:GLY:HA2	1:D:97:THR:HB	2.01	0.43
1:C:301:LEU:HB3	1:C:304:PHE:CD2	2.54	0.42
1:C:396:TRP:CE2	1:C:400:LEU:CD1	3.02	0.42
1:B:218:LYS:HD3	1:B:222:ARG:HH21	1.85	0.42
1:D:300:LYS:HG3	1:D:302:MET:HE3	2.01	0.42
1:E:399:MET:O	1:E:404:TYR:HB3	2.19	0.42
1:C:121:PHE:CZ	1:C:141:ALA:HB2	2.55	0.42
1:C:421:PHE:CE2	1:D:81:SER:HB3	2.55	0.42
1:B:121:PHE:CZ	1:B:141:ALA:HB1	2.54	0.42
1:B:132:MET:HG3	1:B:381:THR:CG2	2.46	0.42
1:C:409:PRO:HA	1:D:47:PHE:O	2.19	0.42
1:C:424:LEU:HA	1:C:427:ARG:NH2	2.34	0.42
1:E:132:MET:HE1	1:E:257:ILE:HG23	2.01	0.42
1:A:418:GLN:HE22	1:B:73:PRO:CG	2.32	0.42
1:E:336:GLN:HE21	1:E:371:LYS:HE2	1.85	0.42
1:F:114:VAL:HG23	1:F:171:THR:HG21	2.00	0.42
1:A:396:TRP:CE2	1:A:400:LEU:CD1	3.02	0.42
1:E:231:GLU:CD	1:F:408:ARG:HH21	2.27	0.42
1:E:396:TRP:CE2	1:E:400:LEU:CD1	3.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:264:ALA:CB	1:D:406:ILE:CG1	2.96	0.42
1:E:121:PHE:CZ	1:E:141:ALA:HB2	2.55	0.42
1:F:302:MET:HE2	1:F:302:MET:HA	2.02	0.42
1:A:29:VAL:HG12	1:B:43:PHE:HB2	2.02	0.41
1:E:43:PHE:HB3	1:F:31:ASP:HA	2.01	0.41
1:E:421:PHE:CE2	1:F:80:LYS:CB	3.03	0.41
1:C:29:VAL:HG12	1:D:43:PHE:HB2	2.01	0.41
1:C:408:ARG:NH2	1:D:232:GLN:O	2.53	0.41
1:D:121:PHE:CZ	1:D:141:ALA:HB2	2.55	0.41
1:F:405:LYS:C	1:F:406:ILE:CG2	2.92	0.41
1:E:285:ILE:O	1:E:289:VAL:HG23	2.21	0.41
1:F:121:PHE:CZ	1:F:141:ALA:HB2	2.55	0.41
1:A:300:LYS:HG3	1:A:302:MET:HE3	2.01	0.41
1:A:31:ASP:HA	1:B:43:PHE:HB3	2.02	0.41
1:B:330:LEU:HD22	1:B:372:ALA:O	2.20	0.41
1:C:43:PHE:HB3	1:D:31:ASP:HA	2.02	0.41
1:E:416:HIS:CG	1:E:419:ARG:NH2	2.89	0.41
1:B:118:LEU:HA	1:B:121:PHE:HD2	1.86	0.41
1:D:285:ILE:O	1:D:289:VAL:HG23	2.21	0.41
1:F:60:ILE:HD12	1:F:231:GLU:HB2	2.03	0.41
1:B:285:ILE:O	1:B:289:VAL:HG23	2.21	0.41
1:C:424:LEU:CD1	1:C:427:ARG:HH21	2.34	0.41
1:A:285:ILE:O	1:A:289:VAL:HG23	2.21	0.41
1:C:406:ILE:HG23	1:C:407:GLY:H	1.86	0.41
1:C:413:TYR:HA	1:D:55:SER:O	2.21	0.41
1:D:178:LYS:NZ	1:D:183:GLU:OE1	2.45	0.41
1:D:302:MET:HE2	1:D:302:MET:HA	2.03	0.41
1:D:416:HIS:CD2	1:D:419:ARG:NH2	2.89	0.41
1:D:425:LYS:HD2	1:D:425:LYS:HA	1.92	0.41
1:E:31:ASP:HA	1:F:43:PHE:HB3	2.03	0.41
1:F:404:TYR:O	1:F:405:LYS:CG	2.69	0.41
1:A:302:MET:HE2	1:A:302:MET:HA	2.03	0.41
1:F:132:MET:HG2	1:F:381:THR:HG23	2.03	0.40
1:F:403:PRO:O	1:F:403:PRO:HG2	2.21	0.40
1:F:235:SER:HG	1:F:265:HIS:CD2	2.30	0.40
1:F:285:ILE:O	1:F:289:VAL:HG23	2.21	0.40
1:E:132:MET:HG2	1:E:381:THR:HG23	2.03	0.40
1:E:139:ILE:HD11	1:E:257:ILE:HD12	2.04	0.40
1:E:408:ARG:N	1:F:48:MET:HE2	2.32	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	423/428 (99%)	404 (96%)	17 (4%)	2 (0%)	24	54
1	B	420/428 (98%)	401 (96%)	19 (4%)	0	100	100
1	C	424/428 (99%)	397 (94%)	23 (5%)	4 (1%)	14	42
1	D	422/428 (99%)	402 (95%)	17 (4%)	3 (1%)	18	47
1	E	418/428 (98%)	398 (95%)	18 (4%)	2 (0%)	24	54
1	F	420/428 (98%)	401 (96%)	16 (4%)	3 (1%)	18	47
All	All	2527/2568 (98%)	2403 (95%)	110 (4%)	14 (1%)	21	50

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	406	ILE
1	C	418	GLN
1	D	406	ILE
1	F	11	GLU
1	A	416	HIS
1	C	405	LYS
1	D	416	HIS
1	C	403	PRO
1	E	267	GLY
1	E	406	ILE
1	F	406	ILE
1	A	332	ILE
1	D	11	GLU
1	F	332	ILE

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	357/358 (100%)	346 (97%)	11 (3%)	35	59
1	B	356/358 (99%)	344 (97%)	12 (3%)	32	57
1	C	357/358 (100%)	344 (96%)	13 (4%)	31	56
1	D	356/358 (99%)	345 (97%)	11 (3%)	35	59
1	E	354/358 (99%)	345 (98%)	9 (2%)	42	62
1	F	354/358 (99%)	342 (97%)	12 (3%)	32	57
All	All	2134/2148 (99%)	2066 (97%)	68 (3%)	34	58

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	VAL
1	A	29	VAL
1	A	68	LEU
1	A	82	ASP
1	A	139	ILE
1	A	231	GLU
1	A	328	GLN
1	A	343	LEU
1	A	344	GLU
1	A	400	LEU
1	A	405	LYS
1	B	20	VAL
1	B	29	VAL
1	B	68	LEU
1	B	82	ASP
1	B	139	ILE
1	B	231	GLU
1	B	328	GLN
1	B	332	ILE
1	B	343	LEU
1	B	344	GLU
1	B	400	LEU
1	B	406	ILE
1	C	13	SER
1	C	20	VAL
1	C	29	VAL
1	C	68	LEU

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Mol	Chain	Res	Type
1	C	82	ASP
1	C	139	ILE
1	C	285	ILE
1	C	328	GLN
1	C	330	LEU
1	C	343	LEU
1	C	344	GLU
1	C	400	LEU
1	C	417	THR
1	D	20	VAL
1	D	29	VAL
1	D	68	LEU
1	D	82	ASP
1	D	139	ILE
1	D	285	ILE
1	D	328	GLN
1	D	343	LEU
1	D	344	GLU
1	D	400	LEU
1	D	424	LEU
1	E	20	VAL
1	E	29	VAL
1	E	68	LEU
1	E	82	ASP
1	E	139	ILE
1	E	328	GLN
1	E	343	LEU
1	E	344	GLU
1	E	400	LEU
1	F	11	GLU
1	F	13	SER
1	F	20	VAL
1	F	29	VAL
1	F	68	LEU
1	F	82	ASP
1	F	139	ILE
1	F	235	SER
1	F	328	GLN
1	F	343	LEU
1	F	344	GLU
1	F	410	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	230	HIS
1	A	296	ASN
1	A	328	GLN
1	A	336	GLN
1	A	416	HIS
1	B	230	HIS
1	B	296	ASN
1	B	321	GLN
1	B	328	GLN
1	B	336	GLN
1	C	7	GLN
1	C	153	ASN
1	C	230	HIS
1	C	296	ASN
1	C	328	GLN
1	C	416	HIS
1	D	69	HIS
1	D	296	ASN
1	D	321	GLN
1	D	328	GLN
1	D	416	HIS
1	E	230	HIS
1	E	296	ASN
1	E	328	GLN
1	E	336	GLN
1	F	232	GLN
1	F	233	ASN
1	F	296	ASN
1	F	328	GLN
1	F	336	GLN
1	F	411	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates [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	425/428 (99%)	-0.08	5 (1%) 76 63	46, 75, 121, 137	0
1	B	424/428 (99%)	-0.06	6 (1%) 73 59	49, 78, 130, 152	0
1	C	426/428 (99%)	-0.21	2 (0%) 87 78	58, 90, 129, 159	0
1	D	424/428 (99%)	-0.18	4 (0%) 81 68	50, 83, 149, 177	0
1	E	422/428 (98%)	0.04	16 (3%) 44 31	59, 101, 139, 170	0
1	F	422/428 (98%)	-0.09	7 (1%) 69 54	61, 107, 150, 174	0
All	All	2543/2568 (99%)	-0.10	40 (1%) 70 56	46, 89, 139, 177	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	418	GLN	4.9
1	E	62	GLY	4.5
1	E	59	TYR	4.1
1	A	407	GLY	4.0
1	A	406	ILE	3.9
1	E	235	SER	3.8
1	A	136	CYS	3.7
1	E	309	TYR	3.4
1	A	207	CYS	3.4
1	C	208	GLU	3.4
1	E	308	VAL	3.3
1	E	60	ILE	3.2
1	D	289	VAL	3.2
1	F	207	CYS	3.1
1	E	72	TYR	3.1
1	E	231	GLU	3.0
1	E	392	TRP	2.9
1	C	207	CYS	2.9
1	B	102	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
1	F	406	ILE	2.7
1	E	61	ASP	2.7
1	E	63	ASP	2.6
1	E	123	ASN	2.6
1	B	343	LEU	2.6
1	E	265	HIS	2.5
1	E	66	VAL	2.5
1	B	239	VAL	2.4
1	E	311	ASN	2.4
1	E	9	ILE	2.4
1	D	79	GLU	2.3
1	F	420	ASP	2.3
1	B	255	SER	2.2
1	F	421	PHE	2.2
1	B	121	PHE	2.2
1	A	243	GLY	2.2
1	D	293	LYS	2.1
1	B	136	CYS	2.1
1	F	414	THR	2.1
1	F	121	PHE	2.0
1	D	285	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.