



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 11:22 AM UTC

PDB ID : 1AFR / pdb_00001afr
Title : STEAROYL-ACYL CARRIER PROTEIN DESATURASE FROM CASTOR SEEDS
Authors : Lindqvist, Y.; Huang, W.; Schneider, G.
Deposited on : 1997-03-13
Resolution : 2.40 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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

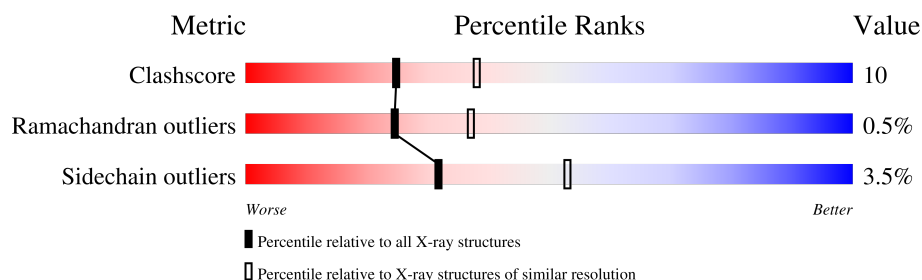
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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))
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	345	76% 22% .
1	B	345	78% 20% .
1	C	345	73% 24% .
1	D	345	73% 25% .
1	E	345	74% 23% .
1	F	345	73% 24% .

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 17326 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 DELTA9 STEAROYL-ACYL CARRIER PROTEIN DESATURASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	345	Total	C	N	O	S	34	0	0
			2796	1771	486	525	14			
1	B	345	Total	C	N	O	S	64	0	0
			2796	1771	486	525	14			
1	C	345	Total	C	N	O	S	46	0	0
			2796	1771	486	525	14			
1	D	345	Total	C	N	O	S	62	0	0
			2796	1771	486	525	14			
1	E	345	Total	C	N	O	S	71	0	0
			2796	1771	486	525	14			
1	F	345	Total	C	N	O	S	73	0	0
			2796	1771	486	525	14			

- Molecule 2 is FE (II) ION (CCD ID: FE2) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Fe	0	0
			2	2		
2	B	2	Total	Fe	0	0
			2	2		
2	C	2	Total	Fe	0	0
			2	2		
2	D	2	Total	Fe	0	0
			2	2		
2	E	2	Total	Fe	0	0
			2	2		
2	F	2	Total	Fe	0	0
			2	2		

- Molecule 3 is water.

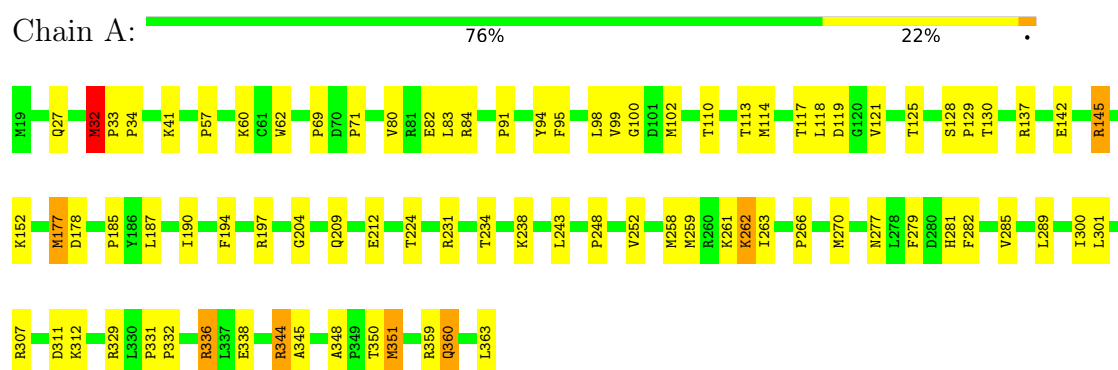
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	84	Total 84	O 84	0	0
3	B	102	Total 102	O 102	0	0
3	C	87	Total 87	O 87	0	0
3	D	95	Total 95	O 95	0	0
3	E	90	Total 90	O 90	0	0
3	F	80	Total 80	O 80	0	0

3 Residue-property plots

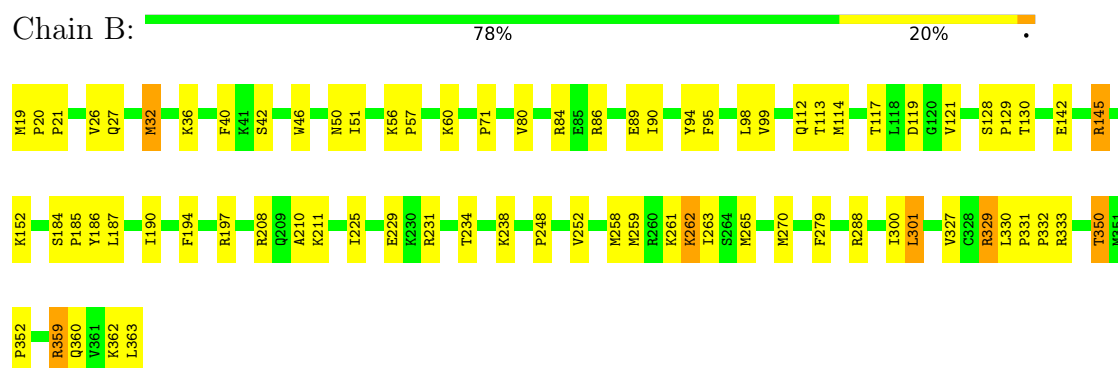
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

Note EDS was not executed.

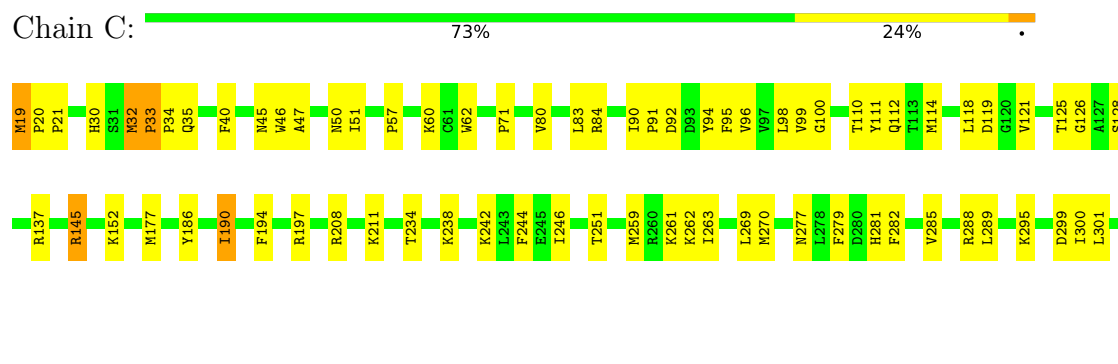
• Molecule 1: DELTA9 STEAROYL-ACYL CARRIER PROTEIN DESATURASE

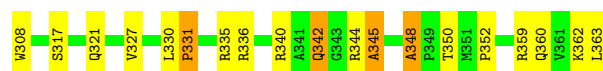


• Molecule 1: DELTA9 STEAROYL-ACYL CARRIER PROTEIN DESATURASE



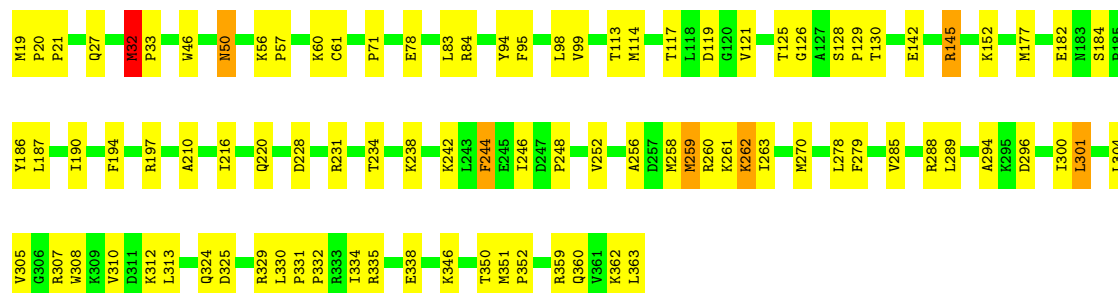
• Molecule 1: DELTA9 STEAROYL-ACYL CARRIER PROTEIN DESATURASE





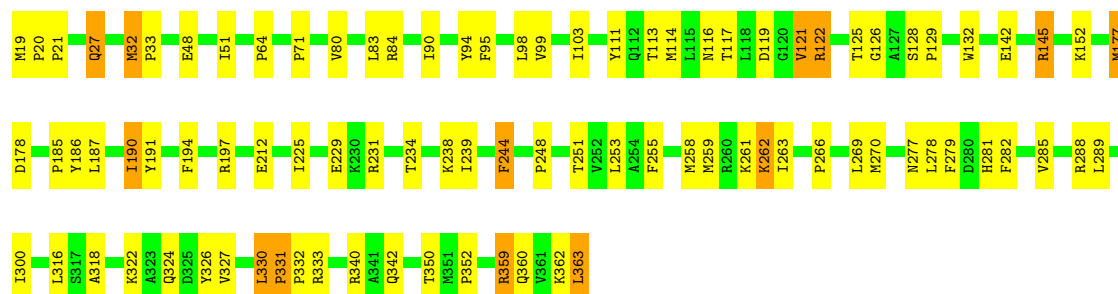
• Molecule 1: DELTA9 STEAROYL-ACYL CARRIER PROTEIN DESATURASE

Chain D: 73% 25% .



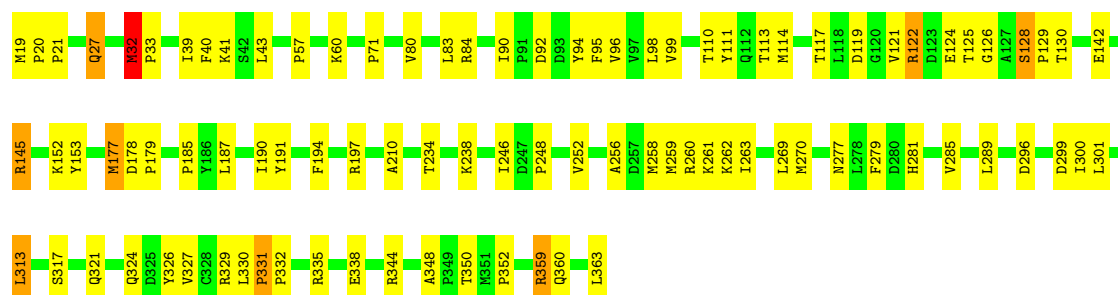
• Molecule 1: DELTA9 STEAROYL-ACYL CARRIER PROTEIN DESATURASE

Chain E: 74% 23% .



• Molecule 1: DELTA9 STEAROYL-ACYL CARRIER PROTEIN DESATURASE

Chain F: 73% 24% .



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	82.20Å 147.80Å 198.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	7.00 – 2.40	Depositor
% Data completeness (in resolution range)	87.0 (7.00-2.40)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.220 , 0.285	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	17326	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FE2

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	0.54	1/2863 (0.0%)	1.02	9/3876 (0.2%)
1	B	0.54	0/2863	1.01	9/3876 (0.2%)
1	C	0.51	0/2863	1.03	13/3876 (0.3%)
1	D	0.55	0/2863	1.02	13/3876 (0.3%)
1	E	0.51	0/2863	1.01	11/3876 (0.3%)
1	F	0.53	0/2863	1.05	16/3876 (0.4%)
All	All	0.53	1/17178 (0.0%)	1.02	71/23256 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	F	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	102	MET	SD-CE	-5.96	1.64	1.79

All (71) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	119	ASP	N-CA-C	8.86	121.74	111.11
1	E	190	ILE	N-CA-C	-8.54	102.54	110.82
1	F	190	ILE	N-CA-C	-8.46	102.62	110.82
1	C	190	ILE	N-CA-C	-8.45	102.63	110.82
1	E	119	ASP	N-CA-C	8.45	121.24	111.11
1	F	119	ASP	N-CA-C	8.43	121.22	111.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	190	ILE	N-CA-C	-7.95	103.11	110.82
1	F	348	ALA	N-CA-C	7.76	119.11	109.57
1	A	190	ILE	N-CA-C	-7.69	103.36	110.82
1	D	190	ILE	N-CA-C	-7.13	103.23	111.00
1	F	33	PRO	CA-C-N	7.02	128.61	119.84
1	F	33	PRO	C-N-CA	7.02	128.61	119.84
1	C	33	PRO	CA-C-N	6.74	128.26	119.84
1	C	33	PRO	C-N-CA	6.74	128.26	119.84
1	C	119	ASP	N-CA-C	6.60	122.26	111.37
1	D	32	MET	CA-C-N	6.55	127.12	120.38
1	D	32	MET	C-N-CA	6.55	127.12	120.38
1	D	33	PRO	CA-C-N	6.51	127.97	119.84
1	D	33	PRO	C-N-CA	6.51	127.97	119.84
1	B	210	ALA	N-CA-C	-6.44	104.27	111.28
1	E	121	VAL	N-CA-C	6.42	120.43	113.43
1	B	119	ASP	N-CA-C	6.37	121.88	111.37
1	E	90	ILE	CA-C-N	6.30	126.27	119.78
1	E	90	ILE	C-N-CA	6.30	126.27	119.78
1	B	121	VAL	N-CA-C	6.13	118.07	112.43
1	A	32	MET	CA-C-N	6.12	126.68	120.38
1	A	32	MET	C-N-CA	6.12	126.68	120.38
1	C	348	ALA	CA-C-N	6.11	126.07	120.21
1	C	348	ALA	C-N-CA	6.11	126.07	120.21
1	F	246	ILE	N-CA-C	6.08	116.83	110.62
1	B	359	ARG	N-CA-C	-6.07	102.52	110.53
1	D	119	ASP	N-CA-C	6.01	121.23	111.37
1	C	359	ARG	N-CA-C	-5.95	102.67	110.53
1	B	90	ILE	CA-C-N	5.78	125.68	119.85
1	B	90	ILE	C-N-CA	5.78	125.68	119.85
1	D	359	ARG	N-CA-C	-5.75	102.40	110.50
1	D	126	GLY	N-CA-C	-5.72	106.77	115.00
1	D	210	ALA	N-CA-C	-5.68	104.99	111.07
1	F	359	ARG	N-CA-C	-5.68	103.03	110.53
1	F	126	GLY	N-CA-C	-5.59	106.95	115.00
1	F	121	VAL	N-CA-C	5.57	118.25	112.90
1	F	90	ILE	CA-C-N	5.57	125.54	120.03
1	F	90	ILE	C-N-CA	5.57	125.54	120.03
1	E	359	ARG	N-CA-C	-5.55	103.20	110.53
1	D	121	VAL	N-CA-C	5.51	119.43	113.43
1	C	246	ILE	CB-CA-C	-5.50	104.87	112.24
1	B	112	GLN	N-CA-C	-5.49	105.37	111.36
1	C	331	PRO	N-CA-C	5.40	117.29	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	33	PRO	CA-C-N	5.38	125.46	119.32
1	E	33	PRO	C-N-CA	5.38	125.46	119.32
1	C	112	GLN	N-CA-C	-5.38	105.58	111.82
1	B	46	TRP	N-CA-C	-5.37	105.43	111.28
1	F	331	PRO	N-CA-C	5.37	117.25	110.70
1	A	351	MET	CA-C-N	5.37	125.78	119.99
1	A	351	MET	C-N-CA	5.37	125.78	119.99
1	E	126	GLY	N-CA-C	-5.36	107.29	115.00
1	A	359	ARG	N-CA-C	-5.35	103.47	110.53
1	C	62	TRP	N-CA-C	-5.34	103.34	110.55
1	E	331	PRO	N-CA-C	5.29	117.15	110.70
1	D	184	SER	CA-C-N	5.25	125.05	119.28
1	D	184	SER	C-N-CA	5.25	125.05	119.28
1	F	128	SER	CA-C-N	5.19	126.32	119.84
1	F	128	SER	C-N-CA	5.19	126.32	119.84
1	D	182	GLU	N-CA-C	5.15	118.55	111.54
1	F	32	MET	CA-C-N	5.14	125.67	120.38
1	F	32	MET	C-N-CA	5.14	125.67	120.38
1	A	360	GLN	N-CA-C	5.09	117.79	109.59
1	A	338	GLU	N-CA-C	5.09	119.20	112.89
1	C	30	HIS	N-CA-C	5.04	118.35	111.39
1	C	126	GLY	N-CA-C	-5.04	107.84	114.95
1	E	342	GLN	N-CA-C	-5.01	106.52	113.18

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	F	153	TYR	Sidechain

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	2796	0	2739	52	0
1	B	2796	0	2739	53	0
1	C	2796	0	2739	58	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	2796	0	2739	58	0
1	E	2796	0	2739	57	0
1	F	2796	0	2739	53	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
3	A	84	0	0	3	0
3	B	102	0	0	2	0
3	C	87	0	0	2	0
3	D	95	0	0	2	0
3	E	90	0	0	1	0
3	F	80	0	0	0	0
All	All	17326	0	16434	318	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 10.

All (318) 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:259:MET:SD	1:C:301:LEU:HD11	2.02	0.99
1:D:248:PRO:O	1:D:252:VAL:HG23	1.78	0.84
1:A:27:GLN:HG3	1:F:125:THR:HG21	1.62	0.82
1:C:110:THR:HG22	1:C:114:MET:HE3	1.62	0.81
1:F:114:MET:SD	1:F:179:PRO:HD3	2.22	0.80
1:E:244:PHE:O	1:E:248:PRO:HG3	1.83	0.79
1:A:344:ARG:O	1:A:348:ALA:HB2	1.84	0.78
1:E:331:PRO:HB2	1:E:332:PRO:HD3	1.64	0.78
1:F:259:MET:HE1	1:F:327:VAL:HG13	1.65	0.78
1:D:259:MET:SD	1:D:330:LEU:HD22	2.24	0.77
1:D:114:MET:HB3	3:D:682:HOH:O	1.84	0.76
1:D:27:GLN:HG3	1:E:125:THR:HG21	1.69	0.75
1:B:331:PRO:HB2	1:B:332:PRO:HD3	1.68	0.74
1:D:331:PRO:HB2	1:D:332:PRO:HD3	1.70	0.73
1:B:32:MET:HE3	1:B:186:TYR:CE1	2.23	0.73
1:E:234:THR:O	1:E:238:LYS:HG2	1.87	0.73
1:E:177:MET:SD	1:E:266:PRO:HA	2.31	0.70
1:B:114:MET:HB3	3:B:488:HOH:O	1.92	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:110:THR:HG22	1:F:114:MET:HE2	1.72	0.69
1:C:234:THR:O	1:C:238:LYS:HG2	1.93	0.69
1:A:234:THR:O	1:A:238:LYS:HG2	1.93	0.68
1:F:234:THR:O	1:F:238:LYS:HG2	1.94	0.68
1:F:248:PRO:O	1:F:252:VAL:HG23	1.93	0.68
1:A:209:GLN:O	1:A:212:GLU:HG2	1.94	0.68
1:F:326:TYR:CE1	1:F:330:LEU:HD13	2.30	0.67
1:B:27:GLN:HG3	1:C:125:THR:HG21	1.77	0.67
1:A:332:PRO:O	1:A:336:ARG:HG2	1.94	0.67
1:B:234:THR:O	1:B:238:LYS:HG2	1.95	0.66
1:A:125:THR:HG21	1:F:27:GLN:HG2	1.78	0.66
1:A:248:PRO:O	1:A:252:VAL:HG23	1.94	0.66
1:F:94:TYR:HE1	1:F:98:LEU:HD22	1.60	0.66
1:A:95:PHE:O	1:A:99:VAL:HG23	1.96	0.65
1:F:329:ARG:O	1:F:332:PRO:HD2	1.95	0.65
1:B:32:MET:HE2	1:B:36:LYS:HB3	1.78	0.65
1:B:248:PRO:O	1:B:252:VAL:HG23	1.96	0.65
1:C:114:MET:HB3	3:C:592:HOH:O	1.96	0.65
1:F:177:MET:HE1	1:F:191:TYR:OH	1.99	0.63
1:A:94:TYR:HE1	1:A:98:LEU:HD22	1.63	0.63
1:A:331:PRO:HB2	1:A:332:PRO:HD3	1.81	0.63
1:C:94:TYR:HE1	1:C:98:LEU:HD22	1.64	0.63
1:B:113:THR:O	1:B:117:THR:HG23	1.98	0.63
1:C:299:ASP:CG	1:C:335:ARG:HH21	2.06	0.63
1:B:95:PHE:O	1:B:99:VAL:HG23	1.98	0.62
1:D:94:TYR:HE1	1:D:98:LEU:HD22	1.64	0.62
1:C:46:TRP:CZ2	1:C:242:LYS:HG3	2.35	0.62
1:A:71:PRO:O	1:F:84:ARG:NH2	2.32	0.62
1:A:350:THR:HG22	1:A:360:GLN:HB3	1.81	0.61
1:B:50:ASN:O	1:B:51:ILE:HD13	2.00	0.61
1:C:95:PHE:O	1:C:99:VAL:HG23	2.00	0.61
1:D:259:MET:SD	1:D:330:LEU:CD2	2.89	0.61
1:D:234:THR:O	1:D:238:LYS:HG2	1.99	0.60
1:B:32:MET:HE1	1:B:40:PHE:HE2	1.66	0.60
1:A:84:ARG:NH2	1:F:71:PRO:O	2.35	0.60
1:B:32:MET:HE3	1:B:186:TYR:CD1	2.37	0.60
1:D:84:ARG:NH2	1:E:71:PRO:O	2.34	0.60
1:A:80:VAL:O	1:A:84:ARG:HG3	2.02	0.59
1:A:110:THR:HG22	1:A:114:MET:CE	2.33	0.59
1:B:259:MET:HG2	1:B:330:LEU:HD23	1.83	0.59
1:D:114:MET:HE2	1:D:177:MET:SD	2.43	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:228:ASP:HA	1:D:231:ARG:HH11	1.68	0.59
1:F:19:MET:N	1:F:20:PRO:HD3	2.18	0.58
1:E:270:MET:HE2	1:E:279:PHE:HA	1.85	0.58
1:E:145:ARG:HG3	1:E:145:ARG:HH11	1.69	0.58
1:C:145:ARG:HH11	1:C:145:ARG:HG3	1.69	0.58
1:A:57:PRO:HG2	1:A:60:LYS:HG3	1.85	0.58
1:D:312:LYS:HA	1:D:312:LYS:HE2	1.86	0.57
1:A:177:MET:SD	1:A:266:PRO:HA	2.44	0.57
1:C:197:ARG:HG2	1:C:300:ILE:HG12	1.87	0.57
1:D:261:LYS:O	1:D:262:LYS:HB2	2.03	0.57
1:B:145:ARG:HG3	1:B:145:ARG:HH11	1.68	0.57
1:C:259:MET:SD	1:C:301:LEU:CD1	2.88	0.57
1:F:80:VAL:O	1:F:84:ARG:HG3	2.04	0.56
1:B:84:ARG:NH2	1:C:71:PRO:O	2.38	0.56
1:D:71:PRO:O	1:E:84:ARG:NH2	2.39	0.56
1:E:48:GLU:O	1:E:48:GLU:HG2	2.05	0.56
1:B:32:MET:HE3	1:B:186:TYR:HE1	1.71	0.56
1:C:80:VAL:O	1:C:84:ARG:HG3	2.05	0.56
1:A:187:LEU:HD22	1:A:258:MET:SD	2.45	0.56
1:E:114:MET:HB3	3:E:784:HOH:O	2.05	0.56
1:F:94:TYR:CE1	1:F:98:LEU:HD22	2.40	0.56
1:B:270:MET:HE2	1:B:279:PHE:HA	1.88	0.56
1:C:259:MET:SD	1:C:301:LEU:HD21	2.46	0.56
1:F:95:PHE:O	1:F:99:VAL:HG23	2.06	0.55
1:C:301:LEU:HD23	1:C:331:PRO:HG3	1.88	0.55
1:F:256:ALA:O	1:F:260:ARG:HG3	2.07	0.55
1:F:350:THR:HG22	1:F:360:GLN:HB3	1.88	0.55
1:A:301:LEU:HG	1:A:331:PRO:HG3	1.89	0.55
1:B:261:LYS:O	1:B:262:LYS:HB2	2.07	0.55
1:C:57:PRO:HG2	1:C:60:LYS:HB2	1.89	0.55
1:B:259:MET:SD	1:B:330:LEU:HD23	2.48	0.54
1:B:208:ARG:O	1:B:211:LYS:HB3	2.06	0.54
1:E:80:VAL:O	1:E:84:ARG:HG3	2.08	0.54
1:E:330:LEU:O	1:E:333:ARG:HB3	2.08	0.54
1:C:270:MET:HE2	1:C:279:PHE:HA	1.88	0.54
1:A:128:SER:O	1:A:137:ARG:NH2	2.41	0.53
1:C:342:GLN:HA	1:C:345:ALA:HB3	1.89	0.53
1:B:259:MET:HG2	1:B:330:LEU:CD2	2.38	0.53
1:F:145:ARG:HG3	1:F:145:ARG:HH11	1.73	0.53
1:E:94:TYR:HE1	1:E:98:LEU:HD22	1.73	0.53
1:A:82:GLU:HG2	3:A:438:HOH:O	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:350:THR:HG22	1:D:360:GLN:HB3	1.90	0.52
1:D:187:LEU:HD22	1:D:258:MET:SD	2.50	0.52
1:E:32:MET:HE3	1:E:185:PRO:HD2	1.91	0.52
1:E:255:PHE:CE1	1:E:259:MET:HE3	2.45	0.52
1:A:110:THR:HG22	1:A:114:MET:HE2	1.92	0.52
1:A:145:ARG:HG3	1:A:145:ARG:HH11	1.74	0.52
1:D:32:MET:HE2	1:D:186:TYR:HE1	1.74	0.52
1:D:270:MET:HE2	1:D:279:PHE:HA	1.91	0.52
1:A:113:THR:O	1:A:117:THR:HG23	2.09	0.52
1:E:197:ARG:HG2	1:E:300:ILE:HG12	1.92	0.52
1:D:95:PHE:O	1:D:99:VAL:HG23	2.09	0.51
1:C:32:MET:HE2	1:C:186:TYR:HE2	1.75	0.51
1:E:95:PHE:O	1:E:99:VAL:HG23	2.10	0.51
1:B:32:MET:HE2	1:B:36:LYS:CB	2.41	0.51
1:D:145:ARG:HG3	1:D:145:ARG:HH11	1.76	0.51
1:F:270:MET:HE2	1:F:279:PHE:HA	1.93	0.51
1:B:187:LEU:HD22	1:B:258:MET:SD	2.51	0.50
1:B:350:THR:HG22	1:B:360:GLN:OE1	2.11	0.50
1:F:32:MET:HE3	1:F:185:PRO:HD2	1.93	0.50
1:D:259:MET:HE2	1:D:301:LEU:HG	1.93	0.50
1:B:259:MET:HE1	1:B:327:VAL:HG13	1.93	0.50
1:D:125:THR:HG21	1:E:27:GLN:HG2	1.93	0.50
1:C:261:LYS:O	1:C:262:LYS:HB2	2.12	0.50
1:F:40:PHE:CZ	1:F:185:PRO:HB2	2.47	0.50
1:B:94:TYR:HE1	1:B:98:LEU:HD22	1.76	0.50
1:F:331:PRO:HB2	1:F:332:PRO:HD3	1.94	0.50
1:F:21:PRO:O	1:F:269:LEU:HD22	2.11	0.50
1:F:299:ASP:OD1	1:F:335:ARG:NH2	2.45	0.50
1:C:47:ALA:HA	1:C:51:ILE:HG12	1.93	0.50
1:D:128:SER:OG	1:D:130:THR:HG23	2.12	0.50
1:E:261:LYS:O	1:E:262:LYS:HB2	2.11	0.50
1:C:21:PRO:O	1:C:269:LEU:HD22	2.12	0.49
1:E:318:ALA:O	1:E:322:LYS:HG3	2.11	0.49
1:B:259:MET:SD	1:B:330:LEU:CD2	3.00	0.49
1:F:277:ASN:HB2	1:F:281:HIS:CE1	2.46	0.49
1:E:21:PRO:O	1:E:269:LEU:HD22	2.13	0.49
1:A:204:GLY:HA3	3:A:441:HOH:O	2.12	0.49
1:C:259:MET:HE1	1:C:327:VAL:HG13	1.95	0.49
1:E:113:THR:O	1:E:117:THR:HG23	2.13	0.49
1:E:244:PHE:CE1	1:E:251:THR:HB	2.48	0.49
1:A:197:ARG:HG2	1:A:300:ILE:HG12	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:352:PRO:HB3	1:E:360:GLN:HG2	1.94	0.49
1:F:317:SER:O	1:F:321:GLN:HG3	2.13	0.48
1:B:128:SER:OG	1:B:130:THR:HG23	2.13	0.48
1:E:259:MET:HE1	1:E:327:VAL:HG13	1.94	0.48
1:A:270:MET:HE2	1:A:279:PHE:HA	1.95	0.48
1:D:94:TYR:CE1	1:D:98:LEU:HD22	2.47	0.48
1:D:330:LEU:O	1:D:334:ILE:HG13	2.14	0.48
1:C:94:TYR:CE1	1:C:98:LEU:HD22	2.46	0.48
1:F:259:MET:HG2	1:F:301:LEU:HD21	1.95	0.48
1:D:197:ARG:HG2	1:D:300:ILE:HG12	1.96	0.48
1:E:19:MET:N	1:E:20:PRO:HD3	2.29	0.48
1:F:261:LYS:O	1:F:262:LYS:HB2	2.13	0.48
1:F:313:LEU:HB2	1:F:324:GLN:NE2	2.29	0.47
1:C:19:MET:N	1:C:20:PRO:HD3	2.30	0.47
1:C:244:PHE:CD1	1:C:251:THR:HB	2.49	0.47
1:C:299:ASP:CG	1:C:335:ARG:NH2	2.72	0.47
1:E:142:GLU:O	1:E:145:ARG:HG3	2.14	0.47
1:F:187:LEU:HD22	1:F:258:MET:SD	2.55	0.47
1:F:259:MET:CE	1:F:327:VAL:HG13	2.42	0.47
1:B:80:VAL:O	1:B:84:ARG:HG3	2.14	0.47
1:A:94:TYR:CE1	1:A:98:LEU:HD22	2.48	0.47
1:B:32:MET:CE	1:B:186:TYR:HE1	2.27	0.47
1:B:352:PRO:HB3	1:B:360:GLN:HG2	1.96	0.47
1:C:285:VAL:O	1:C:289:LEU:HD13	2.15	0.47
1:E:270:MET:HE1	1:E:282:PHE:CD2	2.50	0.47
1:F:128:SER:OG	1:F:130:THR:HG23	2.15	0.47
1:C:277:ASN:HB2	1:C:281:HIS:CE1	2.49	0.47
1:D:32:MET:HE2	1:D:186:TYR:CE1	2.50	0.47
1:D:56:LYS:HB3	1:D:61:CYS:SG	2.55	0.46
1:F:122:ARG:HD3	1:F:124:GLU:CD	2.40	0.46
1:A:178:ASP:OD1	1:F:125:THR:HB	2.15	0.46
1:B:259:MET:CG	1:B:330:LEU:HD23	2.45	0.46
1:B:350:THR:CG2	1:B:360:GLN:HB3	2.45	0.46
1:E:121:VAL:HB	1:E:132:TRP:HB3	1.96	0.46
1:B:194:PHE:HE2	1:B:301:LEU:HD13	1.80	0.46
1:E:225:ILE:O	1:E:229:GLU:HG2	2.14	0.46
1:B:71:PRO:O	1:C:84:ARG:NH2	2.48	0.46
1:B:350:THR:HG23	1:B:360:GLN:HB3	1.98	0.46
1:B:225:ILE:O	1:B:229:GLU:HG2	2.15	0.46
1:D:78:GLU:HG2	3:D:654:HOH:O	2.15	0.46
1:D:194:PHE:HE2	1:D:301:LEU:HD13	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:304:LEU:HB3	1:D:308:TRP:CZ3	2.51	0.46
1:F:113:THR:O	1:F:117:THR:HG23	2.15	0.46
1:D:46:TRP:CZ2	1:D:242:LYS:HB2	2.51	0.46
1:E:187:LEU:HD22	1:E:258:MET:SD	2.56	0.46
1:A:118:LEU:HB2	1:A:121:VAL:CG2	2.46	0.46
1:C:114:MET:HE2	1:C:177:MET:HB3	1.98	0.46
1:D:194:PHE:CD1	1:D:263:ILE:HG21	2.51	0.46
1:E:116:ASN:O	1:E:122:ARG:HB2	2.16	0.46
1:E:186:TYR:O	1:E:190:ILE:HG12	2.15	0.45
1:F:197:ARG:HG2	1:F:300:ILE:HG12	1.98	0.45
1:A:311:ASP:OD2	1:A:312:LYS:HG3	2.17	0.45
1:E:142:GLU:OE1	1:E:231:ARG:NH2	2.50	0.45
1:B:56:LYS:H	1:B:231:ARG:NH2	2.13	0.45
1:A:110:THR:HG22	1:A:114:MET:HE3	1.97	0.45
1:A:194:PHE:CD1	1:A:263:ILE:HG21	2.50	0.45
1:D:57:PRO:HG2	1:D:60:LYS:HB2	1.98	0.45
1:E:111:TYR:CD1	1:E:111:TYR:N	2.84	0.45
1:C:32:MET:HE2	1:C:186:TYR:CE2	2.51	0.45
1:D:113:THR:O	1:D:117:THR:HG23	2.17	0.45
1:F:285:VAL:O	1:F:289:LEU:HD13	2.17	0.45
1:B:259:MET:HE2	1:B:301:LEU:HG	1.99	0.45
1:E:99:VAL:O	1:E:103:ILE:HG13	2.16	0.45
1:A:142:GLU:CD	1:A:231:ARG:HH22	2.25	0.45
1:C:32:MET:HE1	1:C:40:PHE:CE2	2.52	0.45
1:C:259:MET:CE	1:C:327:VAL:HG22	2.46	0.45
1:E:277:ASN:HB2	1:E:281:HIS:CE1	2.52	0.45
1:C:317:SER:O	1:C:321:GLN:HG3	2.17	0.45
1:E:285:VAL:O	1:E:289:LEU:HD13	2.17	0.45
1:D:325:ASP:O	1:D:329:ARG:HG3	2.17	0.44
1:F:114:MET:HE1	1:F:177:MET:SD	2.58	0.44
1:A:238:LYS:HD3	1:A:307:ARG:HH22	1.81	0.44
1:D:242:LYS:HE3	1:D:246:ILE:HD11	1.98	0.44
1:B:142:GLU:O	1:B:145:ARG:HG3	2.17	0.44
1:B:288:ARG:NH1	1:B:362:LYS:O	2.50	0.44
1:A:277:ASN:HB2	1:A:281:HIS:CE1	2.52	0.44
1:E:352:PRO:HA	1:E:359:ARG:O	2.17	0.44
1:C:20:PRO:HA	1:C:21:PRO:HD3	1.86	0.44
1:C:33:PRO:HA	1:C:34:PRO:HD3	1.82	0.44
1:B:20:PRO:HA	1:B:21:PRO:HD3	1.81	0.44
1:E:128:SER:HA	1:E:129:PRO:HD3	1.81	0.44
1:B:265:MET:HB3	3:B:511:HOH:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:329:ARG:O	1:B:333:ARG:HG3	2.18	0.44
1:C:244:PHE:CE2	1:C:308:TRP:HB3	2.52	0.44
1:A:100:GLY:HA3	1:A:282:PHE:CE1	2.53	0.43
1:C:83:LEU:C	1:C:83:LEU:HD23	2.43	0.43
1:D:294:ALA:HB1	1:D:338:GLU:HB3	2.00	0.43
1:C:259:MET:HE3	1:C:327:VAL:HG22	1.99	0.43
1:A:41:LYS:HA	1:A:41:LYS:HD3	1.83	0.43
1:C:186:TYR:O	1:C:190:ILE:HG12	2.18	0.43
1:C:194:PHE:CD1	1:C:263:ILE:HG21	2.53	0.43
1:B:57:PRO:HG2	1:B:60:LYS:HB2	2.01	0.43
1:C:208:ARG:O	1:C:211:LYS:HB3	2.18	0.43
1:C:288:ARG:NH1	1:C:362:LYS:O	2.51	0.43
1:D:114:MET:CE	1:D:177:MET:SD	3.06	0.43
1:D:142:GLU:O	1:D:145:ARG:HG3	2.18	0.43
1:B:197:ARG:HG2	1:B:300:ILE:HG12	1.98	0.43
1:C:92:ASP:O	1:C:96:VAL:HG23	2.18	0.43
1:E:20:PRO:HA	1:E:21:PRO:HD3	1.85	0.43
1:D:296:ASP:O	1:D:300:ILE:HG13	2.19	0.43
1:D:128:SER:HA	1:D:129:PRO:HD3	1.74	0.43
1:D:256:ALA:O	1:D:260:ARG:HG3	2.19	0.43
1:D:294:ALA:CB	1:D:338:GLU:HB3	2.49	0.43
1:E:51:ILE:CD1	1:E:239:ILE:HG12	2.48	0.43
1:A:285:VAL:O	1:A:289:LEU:HD13	2.19	0.43
1:D:313:LEU:HB2	1:D:324:GLN:HE21	1.83	0.43
1:E:330:LEU:HD12	1:E:333:ARG:HD3	2.01	0.43
1:F:194:PHE:CD1	1:F:263:ILE:HG21	2.54	0.43
1:E:350:THR:HG22	1:E:360:GLN:HB3	2.00	0.43
1:A:128:SER:OG	1:A:130:THR:HG23	2.19	0.43
1:D:352:PRO:HB3	1:D:360:GLN:HG2	2.01	0.43
1:A:128:SER:HA	1:A:129:PRO:HD3	1.73	0.42
1:A:261:LYS:O	1:A:262:LYS:HB2	2.19	0.42
1:C:111:TYR:CD1	1:C:111:TYR:N	2.85	0.42
1:E:288:ARG:NH1	1:E:362:LYS:O	2.52	0.42
1:A:118:LEU:HB2	1:A:121:VAL:HG22	2.01	0.42
1:A:329:ARG:O	1:A:332:PRO:HD2	2.20	0.42
1:F:128:SER:HA	1:F:129:PRO:HD3	1.79	0.42
1:F:142:GLU:O	1:F:145:ARG:HG3	2.19	0.42
1:E:83:LEU:C	1:E:83:LEU:HD23	2.44	0.42
1:F:352:PRO:HB3	1:F:360:GLN:HG2	2.00	0.42
1:D:27:GLN:HG3	1:E:125:THR:CG2	2.46	0.42
1:D:288:ARG:NH1	1:D:362:LYS:O	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:177:MET:HE1	1:E:191:TYR:OH	2.20	0.42
1:D:307:ARG:O	1:D:307:ARG:HD3	2.19	0.42
1:F:177:MET:HG2	1:F:178:ASP:N	2.34	0.42
1:C:128:SER:O	1:C:137:ARG:NH2	2.53	0.42
1:C:344:ARG:O	1:C:348:ALA:N	2.52	0.42
1:A:33:PRO:HA	1:A:34:PRO:HD3	1.92	0.41
1:D:270:MET:HE3	1:D:278:LEU:HG	2.02	0.41
1:F:57:PRO:HG2	1:F:60:LYS:HB2	2.02	0.41
1:A:32:MET:HE3	1:A:185:PRO:HD2	2.01	0.41
1:C:90:ILE:HA	1:C:91:PRO:HD2	1.89	0.41
1:A:114:MET:HB3	3:A:398:HOH:O	2.19	0.41
1:B:352:PRO:HA	1:B:359:ARG:O	2.20	0.41
1:D:19:MET:N	1:D:20:PRO:HD3	2.34	0.41
1:D:244:PHE:HE1	1:D:252:VAL:HG22	1.86	0.41
1:F:352:PRO:HA	1:F:359:ARG:O	2.20	0.41
1:C:270:MET:HE1	1:C:282:PHE:CD2	2.56	0.41
1:C:281:HIS:O	1:C:285:VAL:HG23	2.21	0.41
1:D:50:ASN:HD22	1:D:50:ASN:N	2.18	0.41
1:B:86:ARG:O	1:B:89:GLU:HB2	2.21	0.41
1:C:32:MET:HE1	1:C:40:PHE:HE2	1.85	0.41
1:D:285:VAL:O	1:D:289:LEU:HD13	2.20	0.41
1:F:94:TYR:OH	1:F:210:ALA:HB2	2.21	0.41
1:A:243:LEU:HD23	1:A:243:LEU:HA	1.86	0.41
1:E:142:GLU:O	1:E:145:ARG:NH1	2.52	0.41
1:E:326:TYR:CE1	1:E:330:LEU:HD13	2.56	0.41
1:A:62:TRP:NE1	1:A:224:THR:HG22	2.35	0.41
1:C:352:PRO:HB3	1:C:360:GLN:HG2	2.03	0.41
1:D:305:VAL:HG13	1:D:310:VAL:HB	2.03	0.41
1:E:114:MET:HE1	1:E:177:MET:SD	2.61	0.41
1:F:92:ASP:O	1:F:96:VAL:HG23	2.21	0.41
1:B:19:MET:N	1:B:20:PRO:HD3	2.36	0.41
1:E:177:MET:HG2	1:E:178:ASP:N	2.36	0.41
1:F:111:TYR:N	1:F:111:TYR:CD1	2.87	0.41
1:A:259:MET:HE2	1:A:301:LEU:HD22	2.02	0.40
1:C:118:LEU:HB2	1:C:121:VAL:CG2	2.51	0.40
1:C:295:LYS:HD2	3:C:628:HOH:O	2.20	0.40
1:D:20:PRO:HA	1:D:21:PRO:HD3	1.84	0.40
1:D:83:LEU:HD23	1:D:83:LEU:C	2.46	0.40
1:E:316:LEU:HD12	1:E:324:GLN:OE1	2.22	0.40
1:F:296:ASP:O	1:F:300:ILE:HG13	2.19	0.40
1:A:83:LEU:C	1:A:83:LEU:HD23	2.46	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:100:GLY:HA3	1:C:282:PHE:CE1	2.57	0.40
1:E:363:LEU:HD12	1:E:363:LEU:HA	1.93	0.40
1:F:39:ILE:O	1:F:43:LEU:HG	2.22	0.40
1:F:83:LEU:HD23	1:F:83:LEU:C	2.46	0.40
1:B:40:PHE:CZ	1:B:185:PRO:HB2	2.56	0.40
1:B:194:PHE:CD1	1:B:263:ILE:HG21	2.57	0.40
1:E:270:MET:HE3	1:E:278:LEU:HG	2.04	0.40
1:B:32:MET:HE1	1:B:40:PHE:CE2	2.51	0.40
1:C:46:TRP:CD1	1:C:50:ASN:ND2	2.89	0.40
1:D:216:ILE:O	1:D:220:GLN:HG3	2.22	0.40
1:E:194:PHE:CD1	1:E:263:ILE:HG21	2.56	0.40
1:A:32:MET:HA	1:A:33:PRO:HD3	1.89	0.40
1:B:184:SER:HA	1:B:185:PRO:HD3	1.94	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	343/345 (99%)	328 (96%)	13 (4%)	2 (1%)	21	32
1	B	343/345 (99%)	325 (95%)	16 (5%)	2 (1%)	21	32
1	C	343/345 (99%)	327 (95%)	14 (4%)	2 (1%)	21	32
1	D	343/345 (99%)	325 (95%)	17 (5%)	1 (0%)	36	50
1	E	343/345 (99%)	323 (94%)	18 (5%)	2 (1%)	21	32
1	F	343/345 (99%)	322 (94%)	20 (6%)	1 (0%)	36	50
All	All	2058/2070 (99%)	1950 (95%)	98 (5%)	10 (0%)	24	37

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	340	ARG
1	A	345	ALA
1	F	313	LEU
1	C	345	ALA
1	E	340	ARG
1	B	262	LYS
1	D	262	LYS
1	E	262	LYS
1	A	262	LYS
1	B	129	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	299/299 (100%)	289 (97%)	10 (3%)	33	55
1	B	299/299 (100%)	290 (97%)	9 (3%)	36	58
1	C	299/299 (100%)	288 (96%)	11 (4%)	30	51
1	D	299/299 (100%)	288 (96%)	11 (4%)	30	51
1	E	299/299 (100%)	287 (96%)	12 (4%)	28	47
1	F	299/299 (100%)	289 (97%)	10 (3%)	33	55
All	All	1794/1794 (100%)	1731 (96%)	63 (4%)	32	53

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	MET
1	A	69	PRO
1	A	91	PRO
1	A	145	ARG
1	A	152	LYS
1	A	177	MET
1	A	336	ARG
1	A	344	ARG
1	A	351	MET

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Mol	Chain	Res	Type
1	A	363	LEU
1	B	26	VAL
1	B	32	MET
1	B	42	SER
1	B	145	ARG
1	B	152	LYS
1	B	301	LEU
1	B	329	ARG
1	B	350	THR
1	B	363	LEU
1	C	19	MET
1	C	32	MET
1	C	35	GLN
1	C	45	ASN
1	C	145	ARG
1	C	152	LYS
1	C	330	LEU
1	C	336	ARG
1	C	342	GLN
1	C	350	THR
1	C	363	LEU
1	D	32	MET
1	D	50	ASN
1	D	145	ARG
1	D	152	LYS
1	D	244	PHE
1	D	259	MET
1	D	301	LEU
1	D	335	ARG
1	D	346	LYS
1	D	351	MET
1	D	363	LEU
1	E	27	GLN
1	E	32	MET
1	E	64	PRO
1	E	122	ARG
1	E	145	ARG
1	E	152	LYS
1	E	177	MET
1	E	212	GLU
1	E	244	PHE
1	E	253	LEU

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Mol	Chain	Res	Type
1	E	330	LEU
1	E	363	LEU
1	F	27	GLN
1	F	32	MET
1	F	41	LYS
1	F	122	ARG
1	F	145	ARG
1	F	152	LYS
1	F	177	MET
1	F	338	GLU
1	F	344	ARG
1	F	363	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	GLN
1	A	112	GLN
1	B	112	GLN
1	B	213	HIS
1	C	27	GLN
1	C	30	HIS
1	C	35	GLN
1	C	112	GLN
1	C	342	GLN
1	D	27	GLN
1	D	50	ASN
1	D	112	GLN
1	D	213	HIS
1	D	324	GLN
1	E	25	HIS
1	E	112	GLN
1	F	324	GLN

5.3.3 RNA ⓘ

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](#)

Of 12 ligands modelled in this entry, 12 are monoatomic - leaving 0 for Mogul analysis.

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.

No monomer is involved in short contacts.

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

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.