



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:08 PM UTC

PDB ID : 2J2F / pdb_00002j2f
Title : The T199D Mutant of Stearoyl Acyl Carrier Protein Desaturase from Ricinus Communis (Castor Bean)
Authors : Guy, J.E.; Abreu, I.A.; Moche, M.; Lindqvist, Y.; Whittle, E.; Shanklin, J.
Deposited on : 2006-08-16
Resolution : 2.65 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:

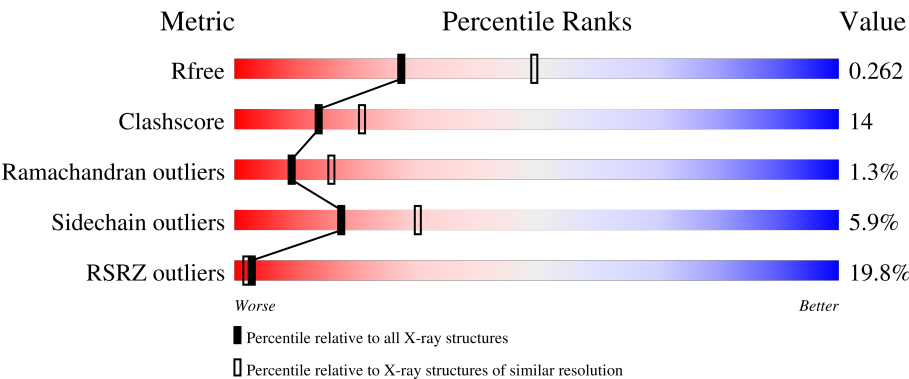
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)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

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.65 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	1110 (2.66-2.66)
Clashscore	190562	1141 (2.66-2.66)
Ramachandran outliers	187476	1126 (2.66-2.66)
Sidechain outliers	187428	1126 (2.66-2.66)
RSRZ outliers	180081	1110 (2.66-2.66)

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	363	36% 67% 25% . .
1	B	363	5% 72% 20% . .
1	C	363	11% 69% 23% . 5%
1	D	363	8% 68% 24% . .
1	E	363	12% 70% 23% . .

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Mol	Chain	Length	Quality of chain
1	F	363	41% 71% 21% • 5%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 17055 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 ACYL-[ACYL-CARRIER-PROTEIN] DESATURASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	348	Total	C	N	O	S	0	0	0
			2824	1791	490	529	14			
1	B	347	Total	C	N	O	S	0	0	0
			2815	1785	488	528	14			
1	C	346	Total	C	N	O	S	0	0	0
			2808	1780	487	527	14			
1	D	347	Total	C	N	O	S	0	0	0
			2815	1785	488	528	14			
1	E	347	Total	C	N	O	S	0	0	0
			2815	1785	488	528	14			
1	F	346	Total	C	N	O	S	0	0	0
			2808	1780	487	527	14			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	199	ASP	THR	engineered mutation	UNP P22337
B	199	ASP	THR	engineered mutation	UNP P22337
C	199	ASP	THR	engineered mutation	UNP P22337
D	199	ASP	THR	engineered mutation	UNP P22337
E	199	ASP	THR	engineered mutation	UNP P22337
F	199	ASP	THR	engineered mutation	UNP P22337

- Molecule 2 is FE (III) ION (CCD ID: FE) (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		

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

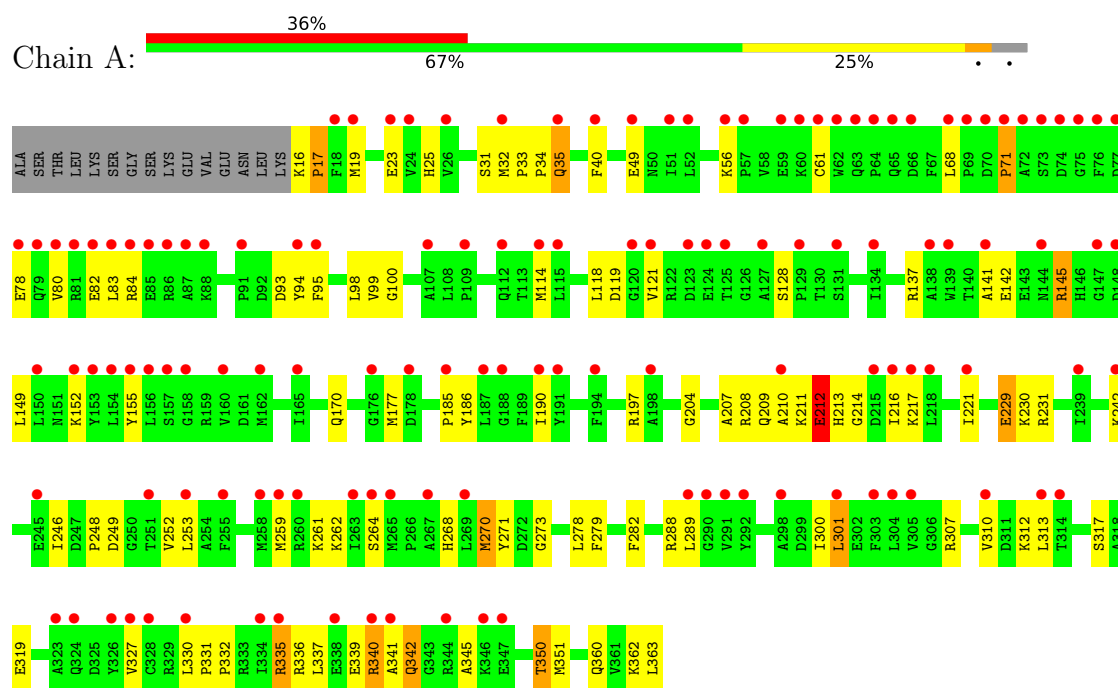
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	20	Total 20	O 20	0	0
3	B	38	Total 38	O 38	0	0
3	C	27	Total 27	O 27	0	0
3	D	33	Total 33	O 33	0	0
3	E	20	Total 20	O 20	0	0
3	F	20	Total 20	O 20	0	0

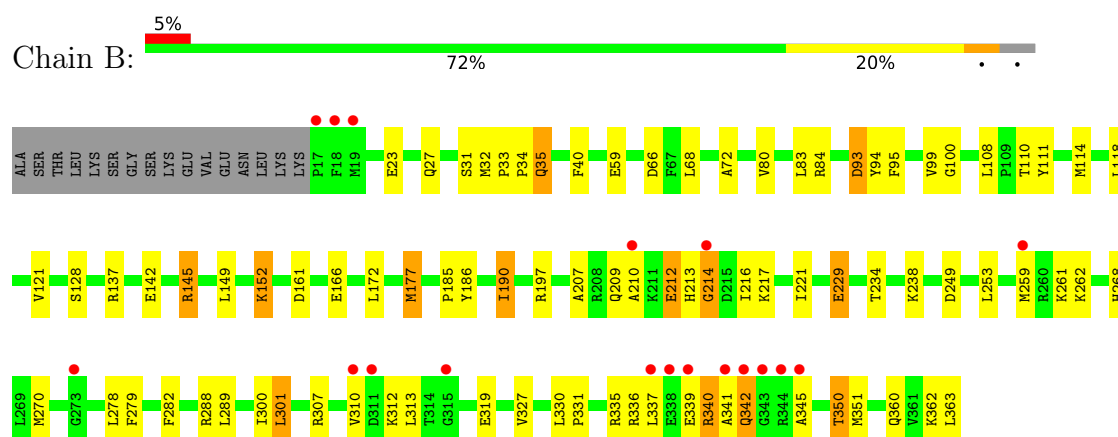
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

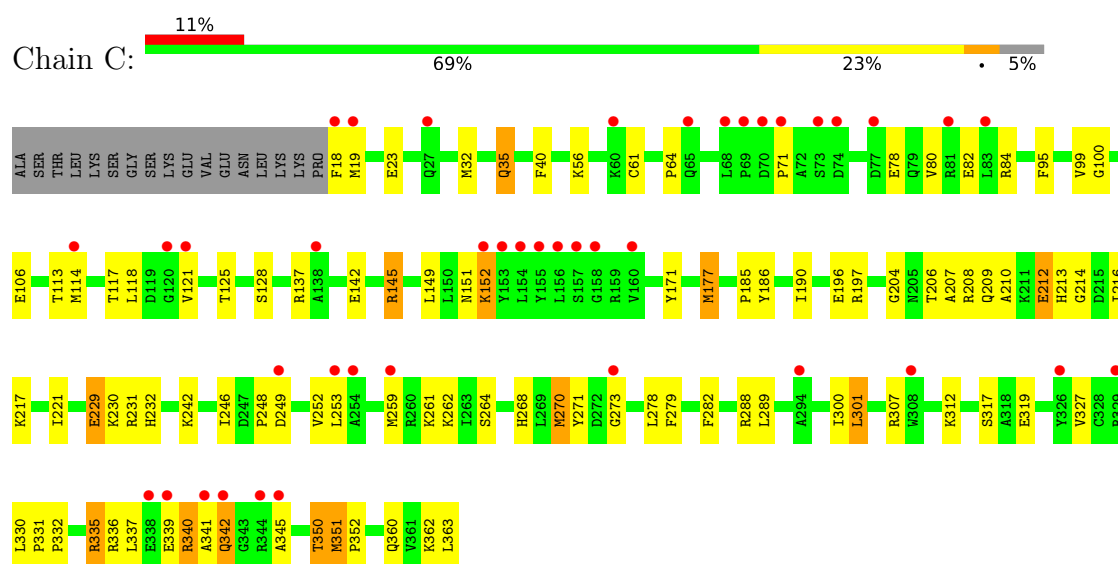
• Molecule 1: ACYL-[ACYL-CARRIER-PROTEIN] DESATURASE



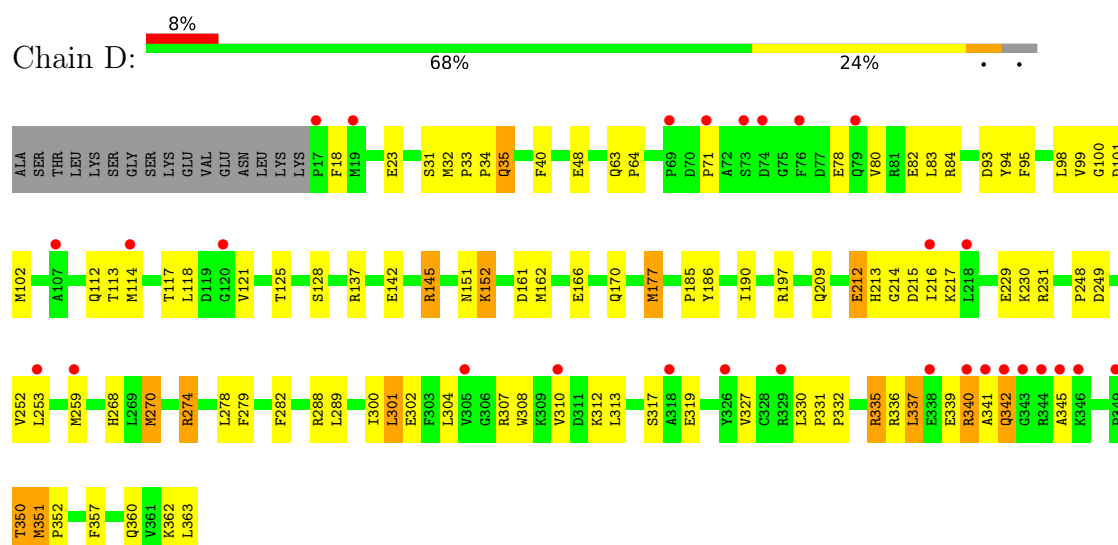
• Molecule 1: ACYL-[ACYL-CARRIER-PROTEIN] DESATURASE



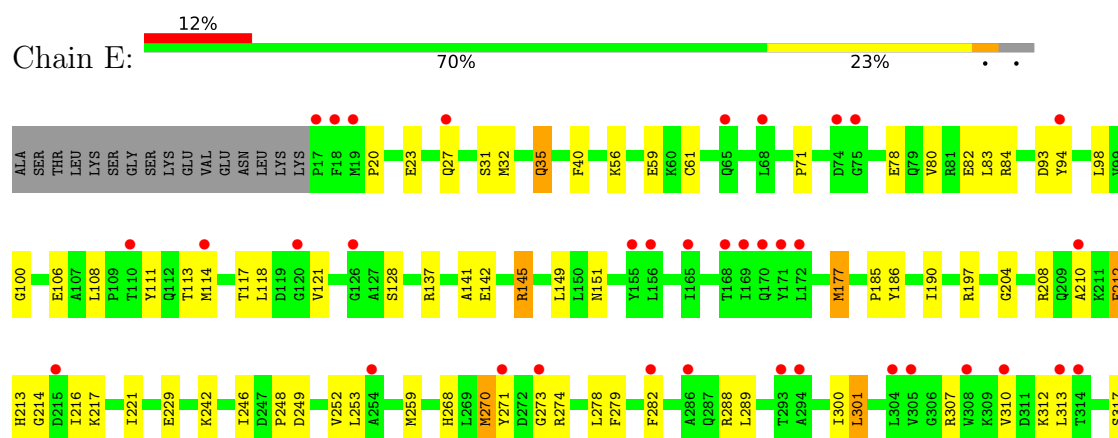
• Molecule 1: ACYL-[ACYL-CARRIER-PROTEIN] DESATURASE

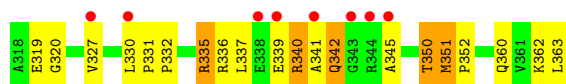


• Molecule 1: ACYL-[ACYL-CARRIER-PROTEIN] DESATURASE

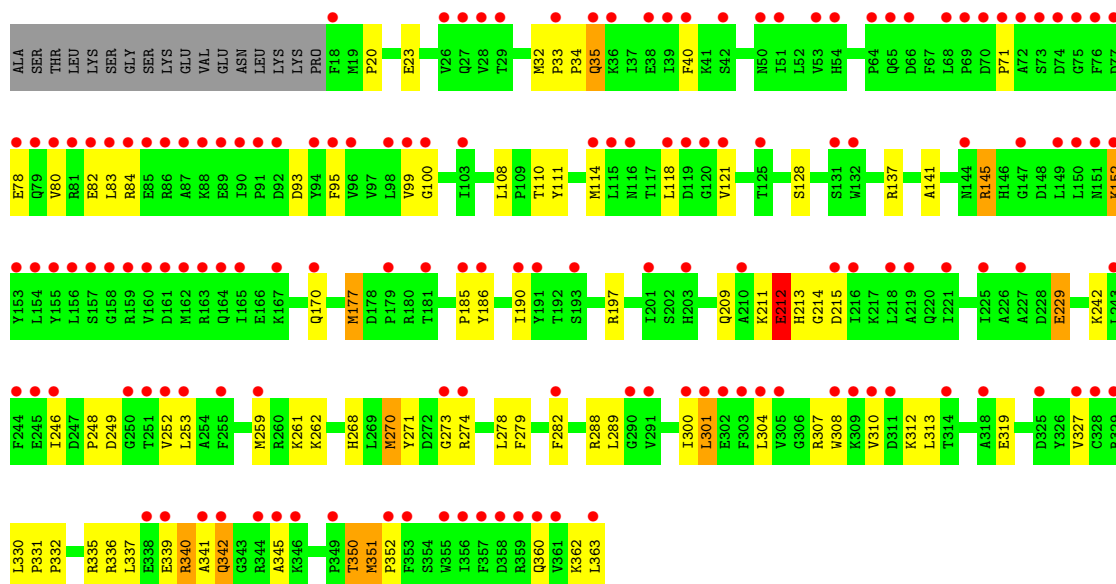
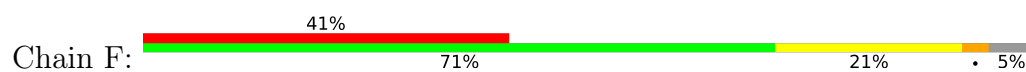


• Molecule 1: ACYL-[ACYL-CARRIER-PROTEIN] DESATURASE





● Molecule 1: ACYL-[ACYL-CARRIER-PROTEIN] DESATURASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	82.05Å 145.77Å 193.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.65 40.00 – 2.65	Depositor EDS
% Data completeness (in resolution range)	98.4 (40.00-2.65) 97.9 (40.00-2.65)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.10 (at 2.65Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.240 , 0.272 0.232 , 0.262	Depositor DCC
R_{free} test set	3388 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	43.2	Xtriage
Anisotropy	0.476	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 63.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	17055	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 16.93% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.81	2/2893 (0.1%)	0.97	1/3916 (0.0%)
1	B	0.99	3/2884 (0.1%)	1.01	3/3904 (0.1%)
1	C	0.92	0/2876	0.99	0/3893
1	D	0.96	1/2884 (0.0%)	1.02	2/3904 (0.1%)
1	E	0.87	0/2884	0.97	1/3904 (0.0%)
1	F	0.85	1/2876 (0.0%)	0.98	1/3893 (0.0%)
All	All	0.90	7/17297 (0.0%)	0.99	8/23414 (0.0%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	71	PRO	C-O	-6.44	1.16	1.24
1	B	66	ASP	C-O	-5.45	1.17	1.24
1	B	72	ALA	CA-CB	-5.43	1.45	1.53
1	F	20	PRO	CA-C	5.33	1.55	1.52
1	D	101	ASP	CA-C	-5.24	1.46	1.52
1	B	68	LEU	C-O	-5.23	1.18	1.24
1	A	68	LEU	C-O	-5.15	1.18	1.24

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	215	ASP	N-CA-C	5.95	119.43	107.41
1	B	190	ILE	N-CA-C	-5.43	105.20	110.42
1	D	112	GLN	N-CA-C	-5.43	105.44	111.36
1	F	215	ASP	N-CA-C	5.42	118.35	107.41
1	B	214	GLY	N-CA-C	5.16	122.95	115.32
1	A	119	ASP	N-CA-C	5.11	116.54	111.07
1	E	20	PRO	O-C-N	5.04	123.52	121.15
1	B	172	LEU	N-CA-C	5.01	117.12	111.11

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	2824	0	2765	89	2
1	B	2815	0	2753	73	1
1	C	2808	0	2745	91	0
1	D	2815	0	2753	85	0
1	E	2815	0	2753	84	0
1	F	2808	0	2745	78	1
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	20	0	0	1	0
3	B	38	0	0	2	0
3	C	27	0	0	4	0
3	D	33	0	0	2	0
3	E	20	0	0	5	0
3	F	20	0	0	9	0
All	All	17055	0	16514	482	3

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 14.

All (482) 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:A:16:LYS:HG2	1:A:19:MET:HE3	1.38	1.06
1:A:16:LYS:HG2	1:A:19:MET:CE	1.90	1.02
1:D:114:MET:CE	1:D:177:MET:HB3	1.96	0.95
1:E:217:LYS:HE2	3:E:2018:HOH:O	1.67	0.95
1:B:59:GLU:HG3	1:C:18:PHE:CD2	2.03	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:114:MET:HB3	3:C:2010:HOH:O	1.66	0.94
1:C:114:MET:CE	1:C:177:MET:HB3	1.99	0.91
1:F:114:MET:CE	1:F:177:MET:HB3	2.02	0.90
1:B:114:MET:CE	1:B:177:MET:HB3	2.04	0.86
1:E:114:MET:CE	1:E:177:MET:HB3	2.07	0.84
1:D:342:GLN:HA	1:D:342:GLN:HE21	1.44	0.83
1:B:212:GLU:O	1:B:214:GLY:N	2.12	0.82
1:B:259:MET:SD	1:B:330:LEU:HD23	2.20	0.81
1:A:114:MET:CE	1:A:177:MET:HB3	2.09	0.81
1:D:259:MET:SD	1:D:330:LEU:HD23	2.20	0.81
1:B:342:GLN:HE21	1:B:342:GLN:HA	1.45	0.80
1:C:259:MET:SD	1:C:301:LEU:HD11	2.22	0.80
1:A:114:MET:HE1	1:A:177:MET:SD	2.23	0.79
1:A:212:GLU:O	1:A:214:GLY:N	2.16	0.79
1:B:253:LEU:HD21	1:B:319:GLU:HG3	1.64	0.78
1:A:16:LYS:HD2	1:A:17:PRO:HD2	1.63	0.78
1:B:270:MET:HE3	1:B:278:LEU:HG	1.67	0.76
1:F:342:GLN:HE21	1:F:342:GLN:HA	1.51	0.76
1:A:270:MET:HE2	1:A:279:PHE:HA	1.68	0.76
1:E:342:GLN:HE21	1:E:342:GLN:HA	1.50	0.76
1:D:274:ARG:NE	3:D:2031:HOH:O	2.19	0.76
1:E:114:MET:HE1	1:E:177:MET:SD	2.26	0.76
1:B:114:MET:HE1	1:B:177:MET:SD	2.26	0.75
1:F:336:ARG:O	1:F:339:GLU:HB3	1.86	0.75
1:C:336:ARG:O	1:C:339:GLU:HB3	1.87	0.74
1:C:253:LEU:HD21	1:C:319:GLU:HG3	1.69	0.74
1:B:301:LEU:HD23	1:B:331:PRO:HG3	1.70	0.74
1:C:270:MET:HE3	1:C:278:LEU:HG	1.70	0.74
1:B:270:MET:HE2	1:B:279:PHE:HA	1.70	0.73
1:E:114:MET:HE2	1:E:177:MET:HB3	1.70	0.73
1:D:336:ARG:O	1:D:339:GLU:HB3	1.88	0.73
1:B:114:MET:HB3	3:B:2016:HOH:O	1.88	0.72
1:A:229:GLU:HA	1:A:229:GLU:OE1	1.88	0.72
1:C:114:MET:HE2	1:C:177:MET:HB3	1.70	0.72
1:C:259:MET:SD	1:C:330:LEU:HD23	2.29	0.71
1:D:253:LEU:HD21	1:D:319:GLU:HG3	1.71	0.71
1:A:342:GLN:HE21	1:A:342:GLN:HA	1.56	0.71
1:D:270:MET:HE3	1:D:278:LEU:HG	1.72	0.71
1:B:336:ARG:O	1:B:339:GLU:HB3	1.91	0.70
1:F:253:LEU:HD21	1:F:319:GLU:HG3	1.71	0.70
1:B:59:GLU:HG3	1:C:18:PHE:CE2	2.28	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:118:LEU:HB2	1:A:121:VAL:CG2	2.23	0.69
1:B:229:GLU:OE1	1:B:229:GLU:HA	1.92	0.69
1:E:336:ARG:O	1:E:339:GLU:HB3	1.92	0.69
1:F:301:LEU:HD23	1:F:331:PRO:HG3	1.75	0.69
1:A:259:MET:HE1	1:A:327:VAL:HG13	1.74	0.69
1:F:118:LEU:HB2	1:F:121:VAL:CG2	2.21	0.69
1:D:270:MET:HE2	1:D:279:PHE:HA	1.75	0.69
1:A:253:LEU:HD21	1:A:319:GLU:HG3	1.74	0.68
1:C:229:GLU:HA	1:C:229:GLU:OE1	1.92	0.68
1:E:217:LYS:HE3	3:E:2002:HOH:O	1.93	0.68
1:F:270:MET:HE3	1:F:278:LEU:HG	1.74	0.68
1:F:259:MET:SD	1:F:330:LEU:HD23	2.33	0.68
1:F:350:THR:HG23	1:F:360:GLN:HB3	1.75	0.68
1:A:336:ARG:O	1:A:339:GLU:HB3	1.94	0.68
1:D:212:GLU:O	1:D:214:GLY:N	2.26	0.68
1:D:301:LEU:HD23	1:D:331:PRO:HG3	1.74	0.68
1:E:212:GLU:O	1:E:214:GLY:N	2.26	0.68
1:E:253:LEU:HD21	1:E:319:GLU:HG3	1.75	0.68
1:C:259:MET:SD	1:C:301:LEU:HD21	2.34	0.67
1:E:118:LEU:HB2	1:E:121:VAL:CG2	2.24	0.67
1:E:350:THR:HG23	1:E:360:GLN:HB3	1.73	0.67
1:D:229:GLU:OE1	1:D:229:GLU:HA	1.93	0.67
1:E:197:ARG:HG2	1:E:300:ILE:HG12	1.75	0.67
1:E:307:ARG:HD3	1:E:307:ARG:O	1.95	0.67
1:A:155:TYR:CG	3:F:2008:HOH:O	2.46	0.67
1:F:212:GLU:O	1:F:214:GLY:N	2.27	0.67
1:A:259:MET:SD	1:A:330:LEU:HD23	2.34	0.67
1:B:259:MET:HE1	1:B:327:VAL:HG13	1.75	0.67
1:D:114:MET:HE1	1:D:177:MET:SD	2.35	0.67
1:D:331:PRO:HB2	1:D:332:PRO:HD3	1.76	0.66
1:A:80:VAL:O	1:A:84:ARG:HG3	1.95	0.66
1:C:350:THR:HG23	1:C:360:GLN:HB3	1.78	0.65
1:F:229:GLU:OE1	1:F:229:GLU:HA	1.96	0.65
1:B:128:SER:O	1:B:137:ARG:NH2	2.30	0.65
1:E:229:GLU:HA	1:E:229:GLU:OE1	1.97	0.65
1:C:301:LEU:HD23	1:C:331:PRO:HG3	1.77	0.65
1:B:212:GLU:C	1:B:214:GLY:H	2.05	0.64
1:C:270:MET:HE2	1:C:279:PHE:HA	1.78	0.64
1:B:32:MET:HE2	1:B:186:TYR:CE1	2.32	0.64
1:B:350:THR:HG23	1:B:360:GLN:HB3	1.79	0.64
1:C:342:GLN:HE21	1:C:342:GLN:HA	1.62	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:259:MET:SD	1:A:301:LEU:HD11	2.38	0.64
1:B:259:MET:CE	1:B:327:VAL:HG13	2.27	0.64
1:E:270:MET:HE3	1:E:278:LEU:HG	1.80	0.64
1:C:118:LEU:HB2	1:C:121:VAL:CG2	2.27	0.63
1:D:118:LEU:HB2	1:D:121:VAL:CG2	2.29	0.63
1:D:350:THR:HG23	1:D:360:GLN:HB3	1.79	0.63
1:D:307:ARG:O	1:D:307:ARG:HD3	1.98	0.63
1:F:270:MET:HE2	1:F:279:PHE:HA	1.80	0.63
1:A:350:THR:HG23	1:A:360:GLN:HB3	1.79	0.63
1:E:32:MET:HE2	1:E:186:TYR:HE1	1.63	0.63
1:A:259:MET:CE	1:A:327:VAL:HG13	2.29	0.63
1:D:259:MET:HE1	1:D:327:VAL:HG13	1.81	0.63
1:F:259:MET:SD	1:F:301:LEU:HD11	2.39	0.63
1:E:259:MET:SD	1:E:330:LEU:HD23	2.39	0.62
1:E:270:MET:HE2	1:E:279:PHE:HA	1.80	0.62
1:E:145:ARG:HG3	1:E:145:ARG:HH11	1.64	0.62
1:C:288:ARG:NH1	1:C:362:LYS:O	2.33	0.62
1:F:80:VAL:O	1:F:84:ARG:HG3	2.00	0.61
1:F:114:MET:HE2	1:F:177:MET:HB3	1.79	0.61
1:C:128:SER:O	1:C:137:ARG:NH2	2.34	0.61
1:E:259:MET:HE1	1:E:327:VAL:HG13	1.81	0.61
1:A:270:MET:HE3	1:A:278:LEU:HG	1.81	0.61
1:D:114:MET:HE1	1:D:177:MET:HB3	1.82	0.61
1:E:32:MET:HE2	1:E:186:TYR:CE1	2.35	0.61
1:E:114:MET:CE	1:E:177:MET:SD	2.89	0.61
1:D:80:VAL:O	1:D:84:ARG:HG3	2.01	0.61
1:F:114:MET:HE1	1:F:177:MET:SD	2.41	0.61
1:A:155:TYR:CB	3:F:2008:HOH:O	2.48	0.61
1:B:114:MET:HE1	1:B:177:MET:HB3	1.83	0.60
1:A:301:LEU:HD23	1:A:331:PRO:HG3	1.81	0.60
1:E:128:SER:O	1:E:137:ARG:NH2	2.34	0.60
1:C:212:GLU:O	1:C:214:GLY:N	2.34	0.60
1:E:80:VAL:O	1:E:84:ARG:HG3	2.02	0.60
1:E:331:PRO:HB2	1:E:332:PRO:HD3	1.83	0.60
1:B:307:ARG:O	1:B:307:ARG:HD3	2.01	0.60
1:A:270:MET:CE	1:A:279:PHE:HA	2.32	0.60
1:B:118:LEU:HB2	1:B:121:VAL:CG2	2.32	0.60
1:A:32:MET:HE2	1:A:186:TYR:HE1	1.67	0.59
1:D:128:SER:O	1:D:137:ARG:NH2	2.34	0.59
1:B:32:MET:HE2	1:B:186:TYR:HE1	1.67	0.59
1:A:71:PRO:O	1:F:84:ARG:NH2	2.31	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:197:ARG:HG2	1:A:300:ILE:HG12	1.85	0.59
1:C:114:MET:HE1	1:C:177:MET:SD	2.42	0.59
1:F:152:LYS:CD	3:F:2008:HOH:O	2.50	0.59
1:A:32:MET:HE2	1:A:186:TYR:CE1	2.37	0.59
1:E:270:MET:HE1	1:E:282:PHE:HB3	1.84	0.59
1:C:271:TYR:CE2	1:C:273:GLY:HA2	2.38	0.59
1:A:307:ARG:O	1:A:307:ARG:HD3	2.02	0.59
1:D:71:PRO:O	1:E:84:ARG:NH2	2.33	0.59
1:D:270:MET:CE	1:D:279:PHE:HA	2.32	0.59
1:B:84:ARG:NH2	1:C:71:PRO:O	2.34	0.59
1:A:16:LYS:CG	1:A:19:MET:HE3	2.23	0.58
1:F:259:MET:HE1	1:F:327:VAL:HG13	1.85	0.58
1:B:341:ALA:HB1	1:B:345:ALA:HB2	1.84	0.58
1:D:341:ALA:HB1	1:D:345:ALA:HB2	1.86	0.58
1:E:100:GLY:HA3	1:E:282:PHE:CE1	2.39	0.58
1:E:186:TYR:O	1:E:190:ILE:HG12	2.04	0.58
1:C:100:GLY:HA3	1:C:282:PHE:CE1	2.39	0.57
1:A:212:GLU:C	1:A:214:GLY:H	2.13	0.57
1:B:270:MET:CE	1:B:279:PHE:HA	2.32	0.57
1:F:197:ARG:HG2	1:F:300:ILE:HG12	1.86	0.57
1:A:35:GLN:H	1:A:35:GLN:HE21	1.51	0.57
1:C:270:MET:CE	1:C:279:PHE:HA	2.35	0.57
1:E:35:GLN:H	1:E:35:GLN:HE21	1.52	0.56
1:D:212:GLU:C	1:D:214:GLY:H	2.13	0.56
1:E:301:LEU:HD23	1:E:331:PRO:HG3	1.86	0.56
1:F:259:MET:CE	1:F:327:VAL:HG13	2.35	0.56
1:B:161:ASP:OD2	1:D:78:GLU:OE2	2.23	0.56
1:E:106:GLU:HB3	3:E:2010:HOH:O	2.06	0.56
1:B:197:ARG:HG2	1:B:300:ILE:HG12	1.87	0.56
1:A:128:SER:O	1:A:137:ARG:NH2	2.38	0.56
1:A:186:TYR:O	1:A:190:ILE:HG12	2.05	0.56
1:D:94:TYR:HE1	1:D:98:LEU:HD22	1.71	0.56
1:D:197:ARG:HG2	1:D:300:ILE:HG12	1.86	0.56
1:E:212:GLU:C	1:E:214:GLY:H	2.13	0.55
1:B:341:ALA:O	1:B:345:ALA:HB3	2.06	0.55
1:B:95:PHE:O	1:B:99:VAL:HG23	2.07	0.55
1:D:259:MET:CE	1:D:327:VAL:HG13	2.36	0.55
1:C:32:MET:HE2	1:C:186:TYR:HE1	1.72	0.55
1:D:84:ARG:NH2	1:E:71:PRO:O	2.35	0.55
1:B:35:GLN:H	1:B:35:GLN:HE21	1.55	0.55
1:F:212:GLU:C	1:F:214:GLY:H	2.13	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:95:PHE:O	1:D:99:VAL:HG23	2.06	0.55
1:A:331:PRO:HB2	1:A:332:PRO:HD3	1.89	0.55
1:C:271:TYR:CZ	1:C:273:GLY:HA2	2.41	0.55
1:C:341:ALA:HB1	1:C:345:ALA:HB2	1.86	0.55
1:E:270:MET:CE	1:E:279:PHE:HA	2.36	0.55
1:D:186:TYR:O	1:D:190:ILE:HG12	2.06	0.54
1:A:84:ARG:NH2	1:F:71:PRO:O	2.35	0.54
1:A:114:MET:HE1	1:A:177:MET:HB3	1.89	0.54
1:E:106:GLU:CD	3:E:2010:HOH:O	2.49	0.54
1:A:288:ARG:NH1	1:A:362:LYS:O	2.38	0.54
1:C:35:GLN:H	1:C:35:GLN:HE21	1.55	0.54
1:C:197:ARG:HG2	1:C:300:ILE:HG12	1.90	0.54
1:D:350:THR:CG2	1:D:360:GLN:HB3	2.38	0.54
1:E:288:ARG:NH1	1:E:362:LYS:O	2.39	0.54
1:F:341:ALA:HB1	1:F:345:ALA:HB2	1.89	0.54
1:A:94:TYR:HE1	1:A:98:LEU:HD22	1.72	0.54
1:C:23:GLU:OE2	1:C:268:HIS:HE1	1.90	0.54
1:F:186:TYR:O	1:F:190:ILE:HG12	2.08	0.54
1:F:259:MET:SD	1:F:301:LEU:HD21	2.47	0.54
1:C:341:ALA:O	1:C:345:ALA:HB3	2.08	0.54
1:B:100:GLY:HA3	1:B:282:PHE:CE1	2.43	0.53
1:A:145:ARG:HG3	1:A:145:ARG:HH11	1.72	0.53
1:B:114:MET:CE	1:B:177:MET:SD	2.97	0.53
1:A:229:GLU:OE1	1:A:229:GLU:CA	2.54	0.53
1:D:32:MET:HE2	1:D:186:TYR:HE1	1.74	0.53
1:F:78:GLU:OE1	3:F:2004:HOH:O	2.18	0.53
1:F:331:PRO:HB2	1:F:332:PRO:HD3	1.89	0.53
1:B:288:ARG:NH1	1:B:362:LYS:O	2.41	0.53
1:C:32:MET:HE3	1:C:186:TYR:HD1	1.74	0.53
1:A:341:ALA:HB1	1:A:345:ALA:HB2	1.90	0.53
1:B:152:LYS:NZ	1:C:151:ASN:OD1	2.39	0.53
1:D:248:PRO:O	1:D:252:VAL:HG23	2.09	0.53
1:F:152:LYS:HD2	3:F:2008:HOH:O	2.09	0.53
1:C:23:GLU:OE2	1:C:268:HIS:CE1	2.62	0.53
1:D:83:LEU:HD23	1:D:83:LEU:C	2.35	0.52
1:E:307:ARG:HD3	1:E:307:ARG:C	2.33	0.52
1:C:229:GLU:OE1	1:C:229:GLU:CA	2.55	0.52
1:C:248:PRO:O	1:C:252:VAL:HG23	2.09	0.52
1:B:229:GLU:OE1	1:B:229:GLU:CA	2.56	0.52
1:D:270:MET:HE1	1:D:282:PHE:HB3	1.91	0.52
1:E:259:MET:CE	1:E:327:VAL:HG13	2.38	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:27:GLN:HG3	1:C:125:THR:HG21	1.92	0.52
1:B:270:MET:HE2	1:B:279:PHE:CA	2.38	0.51
1:C:32:MET:HE2	1:C:186:TYR:CE1	2.45	0.51
1:F:32:MET:CE	1:F:185:PRO:HD2	2.40	0.51
1:F:35:GLN:H	1:F:35:GLN:HE21	1.57	0.51
1:F:307:ARG:O	1:F:307:ARG:HD3	2.10	0.51
1:C:307:ARG:O	1:C:307:ARG:HD3	2.11	0.51
1:A:270:MET:HE1	1:A:282:PHE:HB3	1.93	0.51
1:F:128:SER:O	1:F:137:ARG:NH2	2.44	0.51
1:B:80:VAL:O	1:B:84:ARG:HG3	2.10	0.51
1:D:32:MET:HE2	1:D:186:TYR:CE1	2.45	0.51
1:D:78:GLU:O	1:D:82:GLU:HG3	2.11	0.51
1:D:102:MET:HE3	1:D:151:ASN:HA	1.93	0.51
1:C:80:VAL:O	1:C:84:ARG:HG3	2.10	0.50
1:C:145:ARG:HH11	1:C:145:ARG:HG3	1.76	0.50
1:D:100:GLY:HA3	1:D:282:PHE:CE1	2.46	0.50
1:E:216:ILE:HG12	3:E:2019:HOH:O	2.10	0.50
1:B:32:MET:HE3	1:B:185:PRO:HD2	1.92	0.50
1:D:114:MET:HE2	1:D:177:MET:HB3	1.86	0.50
1:D:229:GLU:OE1	1:D:229:GLU:CA	2.59	0.50
1:F:270:MET:CE	1:F:279:PHE:HA	2.40	0.50
1:A:95:PHE:O	1:A:99:VAL:HG23	2.11	0.50
1:A:270:MET:HE2	1:A:279:PHE:CA	2.39	0.50
1:C:113:THR:O	1:C:117:THR:HG23	2.12	0.50
1:E:32:MET:HE3	1:E:186:TYR:HD1	1.76	0.50
1:E:259:MET:SD	1:E:301:LEU:HD11	2.52	0.50
1:B:32:MET:CE	1:B:185:PRO:HD2	2.41	0.50
1:C:142:GLU:CD	1:C:231:ARG:HH22	2.19	0.50
1:F:145:ARG:HG3	1:F:145:ARG:HH11	1.76	0.50
1:C:216:ILE:HG13	1:C:217:LYS:N	2.26	0.50
1:E:341:ALA:HB1	1:E:345:ALA:HB2	1.94	0.50
1:F:114:MET:HE1	1:F:177:MET:HB3	1.89	0.50
1:E:78:GLU:O	1:E:82:GLU:HG3	2.11	0.49
1:D:170:GLN:HG3	1:E:141:ALA:HB1	1.92	0.49
1:B:114:MET:HE2	1:B:177:MET:HB3	1.90	0.49
1:A:330:LEU:N	1:A:331:PRO:CD	2.75	0.49
1:E:229:GLU:OE1	1:E:229:GLU:CA	2.60	0.49
1:E:83:LEU:C	1:E:83:LEU:HD23	2.38	0.49
1:D:270:MET:HE2	1:D:279:PHE:CA	2.41	0.49
1:E:330:LEU:N	1:E:331:PRO:CD	2.76	0.49
1:F:32:MET:HE3	1:F:186:TYR:HD1	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:18:PHE:CD1	1:E:59:GLU:HG3	2.47	0.49
1:D:114:MET:CE	1:D:177:MET:SD	3.00	0.49
1:E:248:PRO:O	1:E:252:VAL:HG23	2.13	0.49
1:D:351:MET:HE2	1:D:352:PRO:HD2	1.95	0.48
1:A:248:PRO:O	1:A:252:VAL:HG23	2.13	0.48
1:D:288:ARG:NH1	1:D:362:LYS:O	2.46	0.48
1:C:78:GLU:O	1:C:82:GLU:HG3	2.14	0.48
1:C:95:PHE:O	1:C:99:VAL:HG23	2.13	0.48
1:C:209:GLN:HA	1:C:212:GLU:HG2	1.96	0.48
1:F:78:GLU:O	1:F:82:GLU:HG3	2.13	0.48
1:A:78:GLU:O	1:A:82:GLU:HG3	2.12	0.48
1:C:142:GLU:OE1	1:C:231:ARG:NH2	2.38	0.48
1:A:23:GLU:OE2	1:A:268:HIS:HE1	1.97	0.48
1:B:186:TYR:O	1:B:190:ILE:HG12	2.14	0.48
1:A:118:LEU:HB2	1:A:121:VAL:HG22	1.95	0.48
1:A:259:MET:CG	1:A:301:LEU:HD11	2.44	0.48
1:D:162:MET:O	1:D:166:GLU:HG3	2.14	0.47
1:F:341:ALA:O	1:F:345:ALA:HB3	2.14	0.47
1:B:207:ALA:O	1:B:210:ALA:HB3	2.15	0.47
1:E:310:VAL:HA	1:E:313:LEU:HD12	1.96	0.47
1:B:307:ARG:HD3	1:B:307:ARG:C	2.39	0.47
1:C:261:LYS:O	1:C:262:LYS:HB2	2.14	0.47
1:B:259:MET:HE2	1:B:301:LEU:HG	1.95	0.47
1:D:35:GLN:H	1:D:35:GLN:HE21	1.62	0.47
1:D:259:MET:CG	1:D:301:LEU:HD11	2.45	0.47
1:F:40:PHE:CZ	1:F:185:PRO:HB2	2.50	0.47
1:A:35:GLN:H	1:A:35:GLN:NE2	2.13	0.47
1:A:307:ARG:HD3	1:A:307:ARG:C	2.40	0.47
1:B:23:GLU:OE2	1:B:268:HIS:HE1	1.97	0.47
1:C:40:PHE:CZ	1:C:185:PRO:HB2	2.50	0.47
1:C:186:TYR:O	1:C:190:ILE:HG12	2.14	0.47
1:C:331:PRO:HB2	1:C:332:PRO:HD3	1.96	0.47
1:D:161:ASP:OD2	1:F:78:GLU:OE2	2.33	0.47
1:E:32:MET:HE1	1:E:40:PHE:CE2	2.50	0.47
1:E:113:THR:O	1:E:117:THR:HG23	2.14	0.47
1:F:152:LYS:CE	3:F:2008:HOH:O	2.62	0.47
1:F:271:TYR:CE2	1:F:273:GLY:HA2	2.50	0.47
1:C:212:GLU:C	1:C:214:GLY:H	2.23	0.47
1:C:259:MET:HE3	1:C:327:VAL:HG22	1.97	0.47
1:D:32:MET:HE3	1:D:186:TYR:HD1	1.79	0.47
1:D:113:THR:O	1:D:117:THR:HG23	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:32:MET:HE1	1:D:40:PHE:CE2	2.50	0.47
1:D:341:ALA:O	1:D:345:ALA:HB3	2.15	0.47
1:F:95:PHE:O	1:F:99:VAL:HG23	2.15	0.47
1:D:152:LYS:NZ	1:E:151:ASN:OD1	2.44	0.46
1:D:307:ARG:HD3	1:D:307:ARG:C	2.40	0.46
1:B:253:LEU:CD2	1:B:319:GLU:HG3	2.39	0.46
1:D:212:GLU:C	1:D:214:GLY:N	2.73	0.46
1:D:259:MET:HE2	1:D:301:LEU:HG	1.96	0.46
1:B:330:LEU:N	1:B:331:PRO:CD	2.77	0.46
1:A:341:ALA:O	1:A:345:ALA:HB3	2.15	0.46
1:B:270:MET:HE1	1:B:282:PHE:HB3	1.97	0.46
1:F:114:MET:CE	1:F:177:MET:SD	3.03	0.46
1:A:23:GLU:OE2	1:A:268:HIS:CE1	2.69	0.46
1:A:32:MET:HE1	1:A:40:PHE:CE2	2.51	0.46
1:C:330:LEU:N	1:C:331:PRO:CD	2.78	0.46
1:A:259:MET:SD	1:A:301:LEU:HD21	2.56	0.46
1:E:118:LEU:HB2	1:E:121:VAL:HG22	1.97	0.46
1:F:248:PRO:O	1:F:252:VAL:HG23	2.16	0.46
1:A:170:GLN:HG3	1:F:141:ALA:HB1	1.97	0.46
1:B:93:ASP:OD2	1:B:93:ASP:N	2.47	0.46
1:B:310:VAL:HA	1:B:313:LEU:HD12	1.98	0.46
1:C:259:MET:CE	1:C:327:VAL:HG13	2.46	0.46
1:D:118:LEU:HB2	1:D:121:VAL:HG22	1.98	0.46
1:C:351:MET:HE2	1:C:352:PRO:HD2	1.97	0.45
1:E:35:GLN:H	1:E:35:GLN:NE2	2.14	0.45
1:C:114:MET:CE	1:C:177:MET:SD	3.04	0.45
1:E:23:GLU:OE2	1:E:268:HIS:HE1	2.00	0.45
1:F:242:LYS:HE3	1:F:246:ILE:HD11	1.99	0.45
1:B:261:LYS:O	1:B:262:LYS:HB2	2.16	0.45
1:C:171:TYR:HB3	3:C:2021:HOH:O	2.16	0.45
1:A:32:MET:HE1	1:A:40:PHE:HE2	1.79	0.45
1:A:212:GLU:C	1:A:214:GLY:N	2.71	0.45
1:A:271:TYR:CE2	1:A:273:GLY:HA2	2.52	0.45
1:A:211:LYS:HE3	1:A:211:LYS:HB2	1.85	0.45
1:A:211:LYS:O	1:A:212:GLU:C	2.60	0.45
1:D:32:MET:HE1	1:D:40:PHE:HE2	1.80	0.45
1:F:229:GLU:OE1	1:F:229:GLU:CA	2.64	0.45
1:D:23:GLU:OE2	1:D:268:HIS:HE1	1.99	0.45
1:A:114:MET:HE2	1:A:177:MET:HB3	1.95	0.45
1:C:288:ARG:NH1	1:C:362:LYS:HB3	2.31	0.45
1:D:357:PHE:HA	3:F:2004:HOH:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:207:ALA:O	1:C:210:ALA:HB3	2.17	0.45
1:A:142:GLU:OE1	1:A:231:ARG:NH2	2.45	0.45
1:E:271:TYR:CE2	1:E:273:GLY:HA2	2.52	0.45
1:F:307:ARG:HD3	1:F:307:ARG:C	2.42	0.45
1:C:142:GLU:O	1:C:145:ARG:HG3	2.18	0.44
1:D:142:GLU:OE1	1:D:231:ARG:NH2	2.43	0.44
1:E:204:GLY:O	1:E:208:ARG:HG3	2.16	0.44
1:E:271:TYR:CZ	1:E:273:GLY:HA2	2.51	0.44
1:C:209:GLN:HA	1:C:212:GLU:CG	2.47	0.44
1:D:114:MET:HB3	3:D:2015:HOH:O	2.17	0.44
1:E:259:MET:CG	1:E:301:LEU:HD11	2.48	0.44
1:F:351:MET:HE2	1:F:352:PRO:HD2	2.00	0.44
1:A:142:GLU:O	1:A:145:ARG:HG3	2.18	0.44
1:C:32:MET:HE3	1:C:186:TYR:CD1	2.53	0.44
1:C:114:MET:HE1	1:C:177:MET:HB3	1.89	0.44
1:D:33:PRO:HA	1:D:34:PRO:HD3	1.84	0.44
1:E:270:MET:HE2	1:E:279:PHE:CA	2.47	0.44
1:E:270:MET:HE1	1:E:282:PHE:CB	2.47	0.44
1:A:310:VAL:HA	1:A:313:LEU:HD12	1.98	0.44
3:B:2028:HOH:O	1:C:152:LYS:NZ	2.47	0.44
1:D:330:LEU:N	1:D:331:PRO:CD	2.80	0.44
1:A:288:ARG:NH1	1:A:362:LYS:HB3	2.33	0.44
1:B:23:GLU:OE2	1:B:268:HIS:CE1	2.70	0.44
1:C:259:MET:HE1	1:C:327:VAL:HG13	1.99	0.44
1:C:317:SER:C	1:C:319:GLU:N	2.75	0.44
1:B:350:THR:CG2	1:B:360:GLN:HB3	2.45	0.44
1:F:209:GLN:HA	1:F:212:GLU:HG2	1.99	0.44
1:F:330:LEU:N	1:F:331:PRO:CD	2.81	0.44
1:C:149:LEU:HD21	1:C:221:ILE:HG23	2.00	0.44
1:F:152:LYS:HE3	3:F:2008:HOH:O	2.18	0.44
1:C:56:LYS:HB3	1:C:61:CYS:SG	2.58	0.44
1:E:94:TYR:HE1	1:E:98:LEU:HD22	1.83	0.44
1:F:304:LEU:HB3	1:F:308:TRP:CZ3	2.53	0.44
1:A:141:ALA:HB1	1:F:170:GLN:HG3	2.00	0.43
1:D:342:GLN:HA	1:D:342:GLN:NE2	2.24	0.43
1:E:212:GLU:C	1:E:214:GLY:N	2.73	0.43
1:F:100:GLY:HA3	1:F:282:PHE:CE1	2.53	0.43
1:E:56:LYS:HB3	1:E:61:CYS:SG	2.58	0.43
1:E:149:LEU:HD21	1:E:221:ILE:HG23	2.00	0.43
1:B:342:GLN:HE21	1:B:342:GLN:CA	2.25	0.43
1:C:242:LYS:HE3	1:C:246:ILE:HD11	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:259:MET:CG	1:F:301:LEU:HD11	2.49	0.43
1:A:209:GLN:HA	1:A:212:GLU:CG	2.48	0.43
1:D:125:THR:HG21	1:E:27:GLN:HG3	2.00	0.43
1:D:142:GLU:O	1:D:145:ARG:HG3	2.19	0.43
1:E:142:GLU:O	1:E:145:ARG:HG3	2.18	0.43
1:E:341:ALA:O	1:E:345:ALA:HB3	2.18	0.43
1:F:83:LEU:C	1:F:83:LEU:HD23	2.44	0.43
1:A:40:PHE:CZ	1:A:185:PRO:HB2	2.53	0.43
1:A:100:GLY:HA3	1:A:282:PHE:CE1	2.54	0.43
1:C:32:MET:HE1	1:C:40:PHE:CE2	2.54	0.43
1:C:206:THR:O	1:C:210:ALA:HB2	2.18	0.43
1:C:259:MET:CG	1:C:301:LEU:HD11	2.48	0.43
1:D:212:GLU:H	1:D:212:GLU:HG2	1.67	0.43
1:E:32:MET:HE1	1:E:40:PHE:HE2	1.81	0.43
1:F:32:MET:HE1	1:F:40:PHE:CE2	2.53	0.43
1:F:32:MET:HE2	1:F:186:TYR:HE1	1.83	0.43
1:B:94:TYR:CD1	1:B:94:TYR:C	2.96	0.43
1:B:234:THR:O	1:B:238:LYS:HG2	2.18	0.43
1:C:78:GLU:HG2	3:C:2004:HOH:O	2.19	0.43
1:C:350:THR:CG2	1:C:360:GLN:HB3	2.45	0.43
1:A:271:TYR:CZ	1:A:273:GLY:HA2	2.53	0.43
1:D:317:SER:C	1:D:319:GLU:N	2.76	0.43
1:B:166:GLU:OE2	1:C:64:PRO:HB2	2.19	0.43
1:E:149:LEU:CD2	1:E:221:ILE:HG23	2.49	0.43
1:F:261:LYS:O	1:F:262:LYS:HB2	2.18	0.43
1:C:307:ARG:HD3	1:C:307:ARG:C	2.44	0.42
1:A:114:MET:CE	1:A:177:MET:SD	3.00	0.42
1:A:149:LEU:HD21	1:A:221:ILE:HG23	2.01	0.42
1:E:317:SER:O	1:E:320:GLY:N	2.52	0.42
1:F:23:GLU:OE2	1:F:268:HIS:CE1	2.72	0.42
1:F:270:MET:HE2	1:F:279:PHE:CA	2.47	0.42
1:A:204:GLY:O	1:A:208:ARG:HG3	2.19	0.42
1:A:335:ARG:O	1:A:336:ARG:C	2.62	0.42
1:A:56:LYS:HB3	1:A:61:CYS:SG	2.59	0.42
1:C:253:LEU:CD2	1:C:319:GLU:HG3	2.44	0.42
1:C:270:MET:HE1	1:C:282:PHE:HB3	2.01	0.42
1:D:114:MET:HE3	1:D:177:MET:HB3	1.95	0.42
1:F:288:ARG:NH1	1:F:362:LYS:O	2.48	0.42
1:E:335:ARG:O	1:E:336:ARG:C	2.63	0.42
1:F:32:MET:HE2	1:F:186:TYR:CE1	2.54	0.42
1:F:212:GLU:C	1:F:214:GLY:N	2.75	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:271:TYR:CZ	1:F:273:GLY:HA2	2.55	0.42
1:A:33:PRO:HA	1:A:34:PRO:HD3	1.81	0.42
1:B:33:PRO:HA	1:B:34:PRO:HD3	1.80	0.42
1:B:110:THR:HG22	1:B:114:MET:HE3	2.01	0.42
1:B:149:LEU:HD21	1:B:221:ILE:HG23	2.02	0.42
1:D:337:LEU:C	1:D:339:GLU:H	2.27	0.42
1:A:242:LYS:HE3	1:A:246:ILE:HD11	2.02	0.42
1:C:204:GLY:O	1:C:208:ARG:HG3	2.19	0.42
1:D:40:PHE:CZ	1:D:185:PRO:HB2	2.55	0.42
1:A:155:TYR:HB2	3:F:2008:HOH:O	2.18	0.42
1:A:317:SER:C	1:A:319:GLU:N	2.77	0.42
1:B:209:GLN:HA	1:B:212:GLU:CG	2.49	0.42
1:E:108:LEU:HA	1:E:111:TYR:CD2	2.55	0.42
1:E:335:ARG:O	1:E:339:GLU:HB2	2.19	0.42
1:D:32:MET:CE	1:D:185:PRO:HD2	2.50	0.42
1:E:242:LYS:HE3	1:E:246:ILE:HD11	2.02	0.42
1:D:209:GLN:HA	1:D:212:GLU:CG	2.49	0.41
1:E:253:LEU:CD2	1:E:319:GLU:HG3	2.48	0.41
1:C:32:MET:HE1	1:C:40:PHE:HE2	1.84	0.41
1:C:35:GLN:H	1:C:35:GLN:NE2	2.16	0.41
1:C:208:ARG:HB3	1:C:208:ARG:HH11	1.86	0.41
1:C:32:MET:CE	1:C:185:PRO:HD2	2.50	0.41
1:E:145:ARG:HG3	1:E:145:ARG:NH1	2.32	0.41
1:E:317:SER:C	1:E:319:GLU:N	2.78	0.41
1:B:142:GLU:O	1:B:145:ARG:HG3	2.20	0.41
1:A:78:GLU:HG2	3:A:2005:HOH:O	2.20	0.41
1:A:207:ALA:O	1:A:210:ALA:HB3	2.20	0.41
1:B:108:LEU:HA	1:B:111:TYR:CD2	2.56	0.41
1:D:230:LYS:HA	1:D:230:LYS:HD2	1.86	0.41
1:F:310:VAL:HA	1:F:313:LEU:HD12	2.02	0.41
1:B:209:GLN:HA	1:B:212:GLU:HG2	2.02	0.41
1:E:32:MET:CE	1:E:186:TYR:CD1	3.03	0.41
1:A:83:LEU:C	1:A:83:LEU:HD23	2.45	0.41
1:A:94:TYR:CD1	1:A:94:TYR:C	2.99	0.41
1:B:32:MET:HE1	1:B:40:PHE:CE2	2.56	0.41
1:B:216:ILE:HG13	1:B:217:LYS:N	2.36	0.41
1:D:304:LEU:HB3	1:D:308:TRP:CZ3	2.56	0.41
1:F:209:GLN:HA	1:F:212:GLU:CG	2.50	0.41
1:D:63:GLN:O	1:D:64:PRO:C	2.61	0.41
1:D:310:VAL:HA	1:D:313:LEU:HD12	2.03	0.41
1:C:196:GLU:OE1	1:C:232:HIS:HB2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:216:ILE:HG13	1:D:217:LYS:N	2.37	0.40
1:F:35:GLN:H	1:F:35:GLN:NE2	2.20	0.40
1:A:216:ILE:HG13	1:A:217:LYS:N	2.37	0.40
1:A:261:LYS:O	1:A:262:LYS:HB2	2.21	0.40
1:B:149:LEU:CD2	1:B:221:ILE:HG23	2.52	0.40
1:C:335:ARG:O	1:C:339:GLU:HB2	2.20	0.40
1:E:94:TYR:OH	1:E:210:ALA:HB2	2.21	0.40
1:E:351:MET:HE2	1:E:352:PRO:HD2	2.02	0.40
1:F:33:PRO:HA	1:F:34:PRO:HD3	1.83	0.40
1:F:110:THR:HG22	1:F:114:MET:HE3	2.02	0.40
1:A:32:MET:HE3	1:A:186:TYR:HD1	1.87	0.40
1:A:230:LYS:HD2	1:A:230:LYS:HA	1.87	0.40
1:B:259:MET:HG2	1:B:301:LEU:HD11	2.04	0.40
1:C:106:GLU:CD	3:C:2008:HOH:O	2.64	0.40
1:C:230:LYS:HD2	1:C:230:LYS:HA	1.90	0.40
1:D:48:GLU:O	1:D:48:GLU:HG2	2.22	0.40
1:E:40:PHE:CZ	1:E:185:PRO:HB2	2.56	0.40
1:F:259:MET:HE3	1:F:327:VAL:HG22	2.03	0.40
1:B:83:LEU:C	1:B:83:LEU:HD23	2.46	0.40
1:F:23:GLU:OE2	1:F:268:HIS:HE1	2.03	0.40
1:F:211:LYS:HE3	1:F:211:LYS:HB2	1.94	0.40
1:B:32:MET:HE2	1:B:186:TYR:CD1	2.56	0.40
1:C:270:MET:HE2	1:C:279:PHE:CA	2.48	0.40
1:D:302:GLU:OE1	1:D:335:ARG:NH2	2.54	0.40
1:F:108:LEU:HA	1:F:111:TYR:CD2	2.57	0.40
1:F:270:MET:HE1	1:F:282:PHE:HB3	2.02	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:25:HIS:CD2	1:A:49:GLU:OE2[4_555]	2.15	0.05
1:A:25:HIS:CD2	1:A:49:GLU:OE1[4_555]	2.18	0.02
1:B:339:GLU:OE1	1:F:35:GLN:OE1[4_555]	2.19	0.01

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	346/363 (95%)	317 (92%)	23 (7%)	6 (2%)	7	12
1	B	345/363 (95%)	324 (94%)	17 (5%)	4 (1%)	10	17
1	C	344/363 (95%)	321 (93%)	19 (6%)	4 (1%)	10	17
1	D	345/363 (95%)	316 (92%)	25 (7%)	4 (1%)	10	17
1	E	345/363 (95%)	317 (92%)	24 (7%)	4 (1%)	10	17
1	F	344/363 (95%)	317 (92%)	22 (6%)	5 (2%)	8	13
All	All	2069/2178 (95%)	1912 (92%)	130 (6%)	27 (1%)	9	16

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	17	PRO
1	A	213	HIS
1	A	340	ARG
1	B	213	HIS
1	B	340	ARG
1	C	340	ARG
1	D	340	ARG
1	E	213	HIS
1	E	340	ARG
1	F	213	HIS
1	F	340	ARG
1	B	335	ARG
1	C	213	HIS
1	D	213	HIS
1	A	212	GLU
1	A	335	ARG
1	B	337	LEU
1	C	335	ARG
1	C	337	LEU
1	D	335	ARG

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Mol	Chain	Res	Type
1	D	337	LEU
1	E	335	ARG
1	F	335	ARG
1	F	337	LEU
1	A	337	LEU
1	E	337	LEU
1	F	212	GLU

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	302/315 (96%)	284 (94%)	18 (6%)	17	30
1	B	301/315 (96%)	284 (94%)	17 (6%)	19	32
1	C	300/315 (95%)	282 (94%)	18 (6%)	17	30
1	D	301/315 (96%)	283 (94%)	18 (6%)	17	30
1	E	301/315 (96%)	284 (94%)	17 (6%)	19	32
1	F	300/315 (95%)	282 (94%)	18 (6%)	17	30
All	All	1805/1890 (96%)	1699 (94%)	106 (6%)	18	30

All (106) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	SER
1	A	35	GLN
1	A	93	ASP
1	A	145	ARG
1	A	152	LYS
1	A	212	GLU
1	A	229	GLU
1	A	249	ASP
1	A	264	SER
1	A	270	MET
1	A	289	LEU

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Mol	Chain	Res	Type
1	A	301	LEU
1	A	312	LYS
1	A	340	ARG
1	A	342	GLN
1	A	350	THR
1	A	351	MET
1	A	363	LEU
1	B	31	SER
1	B	35	GLN
1	B	93	ASP
1	B	145	ARG
1	B	152	LYS
1	B	177	MET
1	B	212	GLU
1	B	229	GLU
1	B	249	ASP
1	B	289	LEU
1	B	301	LEU
1	B	312	LYS
1	B	340	ARG
1	B	342	GLN
1	B	350	THR
1	B	351	MET
1	B	363	LEU
1	C	19	MET
1	C	35	GLN
1	C	145	ARG
1	C	152	LYS
1	C	177	MET
1	C	212	GLU
1	C	229	GLU
1	C	249	ASP
1	C	264	SER
1	C	270	MET
1	C	289	LEU
1	C	301	LEU
1	C	312	LYS
1	C	340	ARG
1	C	342	GLN
1	C	350	THR
1	C	351	MET
1	C	363	LEU

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Mol	Chain	Res	Type
1	D	31	SER
1	D	35	GLN
1	D	93	ASP
1	D	145	ARG
1	D	152	LYS
1	D	177	MET
1	D	212	GLU
1	D	249	ASP
1	D	270	MET
1	D	274	ARG
1	D	289	LEU
1	D	301	LEU
1	D	312	LYS
1	D	340	ARG
1	D	342	GLN
1	D	350	THR
1	D	351	MET
1	D	363	LEU
1	E	31	SER
1	E	35	GLN
1	E	93	ASP
1	E	145	ARG
1	E	177	MET
1	E	212	GLU
1	E	249	ASP
1	E	270	MET
1	E	274	ARG
1	E	289	LEU
1	E	301	LEU
1	E	312	LYS
1	E	340	ARG
1	E	342	GLN
1	E	350	THR
1	E	351	MET
1	E	363	LEU
1	F	35	GLN
1	F	93	ASP
1	F	145	ARG
1	F	152	LYS
1	F	177	MET
1	F	212	GLU
1	F	229	GLU

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Mol	Chain	Res	Type
1	F	249	ASP
1	F	270	MET
1	F	274	ARG
1	F	289	LEU
1	F	301	LEU
1	F	312	LYS
1	F	340	ARG
1	F	342	GLN
1	F	350	THR
1	F	351	MET
1	F	363	LEU

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	35	GLN
1	A	268	HIS
1	A	342	GLN
1	B	35	GLN
1	B	268	HIS
1	B	342	GLN
1	C	27	GLN
1	C	35	GLN
1	C	50	ASN
1	C	268	HIS
1	C	342	GLN
1	D	35	GLN
1	D	50	ASN
1	D	268	HIS
1	D	342	GLN
1	E	27	GLN
1	E	35	GLN
1	E	50	ASN
1	E	268	HIS
1	E	342	GLN
1	F	35	GLN
1	F	50	ASN
1	F	268	HIS
1	F	342	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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

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	348/363 (95%)	1.82	131 (37%) 1 0	31, 33, 34, 50	0
1	B	347/363 (95%)	0.70	18 (5%) 33 25	31, 33, 34, 48	0
1	C	346/363 (95%)	0.96	41 (11%) 9 7	22, 33, 34, 36	0
1	D	347/363 (95%)	0.80	29 (8%) 17 12	31, 33, 34, 44	0
1	E	347/363 (95%)	1.01	44 (12%) 8 6	31, 33, 34, 50	0
1	F	346/363 (95%)	2.01	148 (42%) 0 0	31, 33, 34, 45	0
All	All	2081/2178 (95%)	1.22	411 (19%) 3 2	22, 33, 34, 50	0

All (411) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	74	ASP	7.0
1	D	345	ALA	6.2
1	D	344	ARG	6.2
1	C	18	PHE	6.1
1	B	345	ALA	5.6
1	E	345	ALA	5.6
1	A	120	GLY	5.5
1	F	155	TYR	5.3
1	F	76	PHE	5.3
1	F	83	LEU	5.3
1	F	160	VAL	5.2
1	F	193	SER	5.1
1	F	345	ALA	5.0
1	F	40	PHE	5.0
1	F	153	TYR	4.9
1	A	24	VAL	4.9
1	F	310	VAL	4.9
1	A	71	PRO	4.8
1	F	77	ASP	4.8

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Mol	Chain	Res	Type	RSRZ
1	A	129	PRO	4.7
1	A	19	MET	4.7
1	A	72	ALA	4.7
1	F	72	ALA	4.7
1	C	338	GLU	4.6
1	F	125	THR	4.6
1	E	344	ARG	4.6
1	A	75	GLY	4.6
1	F	251	THR	4.6
1	F	156	LEU	4.6
1	F	71	PRO	4.5
1	A	155	TYR	4.5
1	A	79	GLN	4.4
1	E	338	GLU	4.4
1	F	344	ARG	4.3
1	A	148	ASP	4.3
1	F	74	ASP	4.3
1	A	114	MET	4.2
1	B	259	MET	4.2
1	F	158	GLY	4.2
1	A	78	GLU	4.2
1	F	88	LYS	4.2
1	A	69	PRO	4.2
1	B	341	ALA	4.2
1	B	342	GLN	4.1
1	F	120	GLY	4.1
1	F	328	CYS	4.0
1	A	188	GLY	4.0
1	F	301	LEU	4.0
1	A	260	ARG	4.0
1	F	73	SER	4.0
1	A	68	LEU	4.0
1	F	186	TYR	3.9
1	A	338	GLU	3.9
1	F	69	PRO	3.8
1	F	35	GLN	3.8
1	D	346	LYS	3.8
1	A	156	LEU	3.8
1	F	75	GLY	3.8
1	A	81	ARG	3.8
1	A	253	LEU	3.8
1	A	259	MET	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	65	GLN	3.8
1	F	253	LEU	3.8
1	F	154	LEU	3.8
1	F	300	ILE	3.8
1	A	70	ASP	3.7
1	A	76	PHE	3.7
1	C	344	ARG	3.7
1	D	259	MET	3.7
1	F	90	ILE	3.7
1	A	210	ALA	3.7
1	D	341	ALA	3.7
1	C	259	MET	3.7
1	B	338	GLU	3.7
1	F	92	ASP	3.6
1	A	77	ASP	3.6
1	A	158	GLY	3.6
1	A	64	PRO	3.6
1	F	78	GLU	3.6
1	F	80	VAL	3.6
1	F	164	GLN	3.6
1	A	73	SER	3.6
1	A	242	LYS	3.6
1	F	216	ILE	3.5
1	A	60	LYS	3.5
1	D	318	ALA	3.5
1	F	157	SER	3.5
1	F	341	ALA	3.5
1	B	310	VAL	3.5
1	F	94	TYR	3.5
1	F	190	ILE	3.5
1	C	158	GLY	3.5
1	E	310	VAL	3.5
1	F	96	VAL	3.5
1	F	81	ARG	3.5
1	F	84	ARG	3.5
1	C	155	TYR	3.4
1	F	314	THR	3.4
1	F	259	MET	3.4
1	F	87	ALA	3.4
1	F	304	LEU	3.4
1	B	344	ARG	3.4
1	F	338	GLU	3.4

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Mol	Chain	Res	Type	RSRZ
1	C	74	ASP	3.4
1	A	80	VAL	3.4
1	F	355	TRP	3.4
1	F	152	LYS	3.4
1	A	86	ARG	3.4
1	F	161	ASP	3.4
1	A	292	TYR	3.3
1	A	313	LEU	3.3
1	A	40	PHE	3.3
1	F	255	PHE	3.3
1	A	112	GLN	3.3
1	A	258	MET	3.3
1	F	162	MET	3.3
1	A	334	ILE	3.3
1	F	163	ARG	3.3
1	E	18	PHE	3.3
1	F	308	TRP	3.3
1	B	343	GLY	3.3
1	F	356	ILE	3.3
1	F	79	GLN	3.2
1	F	244	PHE	3.2
1	F	245	GLU	3.2
1	E	341	ALA	3.2
1	F	28	VAL	3.2
1	D	253	LEU	3.2
1	E	17	PRO	3.2
1	F	360	GLN	3.2
1	B	214	GLY	3.2
1	A	152	LYS	3.2
1	F	191	TYR	3.2
1	C	339	GLU	3.1
1	D	342	GLN	3.1
1	F	65	GLN	3.1
1	E	343	GLY	3.1
1	F	132	TRP	3.1
1	A	57	PRO	3.1
1	A	305	VAL	3.1
1	E	74	ASP	3.1
1	E	172	LEU	3.1
1	F	82	GLU	3.1
1	F	353	PHE	3.1
1	A	326	TYR	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	83	LEU	3.1
1	F	215	ASP	3.1
1	F	252	VAL	3.1
1	A	154	LEU	3.0
1	F	99	VAL	3.0
1	A	344	ARG	3.0
1	F	210	ALA	3.0
1	F	327	VAL	3.0
1	F	150	LEU	3.0
1	A	61	CYS	3.0
1	E	94	TYR	3.0
1	F	181	THR	3.0
1	F	290	GLY	3.0
1	E	313	LEU	2.9
1	F	346	LYS	2.9
1	F	42	SER	2.9
1	D	74	ASP	2.9
1	F	318	ALA	2.9
1	F	361	VAL	2.9
1	A	187	LEU	2.9
1	F	91	PRO	2.9
1	C	27	GLN	2.9
1	F	131	SER	2.9
1	A	328	CYS	2.9
1	A	107	ALA	2.9
1	A	194	PHE	2.9
1	D	349	PRO	2.9
1	F	147	GLY	2.9
1	A	215	ASP	2.8
1	C	152	LYS	2.8
1	F	167	LYS	2.8
1	C	114	MET	2.8
1	A	263	ILE	2.8
1	F	151	ASN	2.8
1	E	215	ASP	2.8
1	F	66	ASP	2.8
1	F	118	LEU	2.8
1	F	149	LEU	2.8
1	F	305	VAL	2.8
1	A	52	LEU	2.8
1	E	273	GLY	2.8
1	F	243	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	323	ALA	2.8
1	D	338	GLU	2.8
1	F	89	GLU	2.8
1	A	51	ILE	2.8
1	F	68	LEU	2.8
1	C	19	MET	2.8
1	F	18	PHE	2.8
1	F	33	PRO	2.7
1	F	349	PRO	2.7
1	A	85	GLU	2.7
1	A	298	ALA	2.7
1	B	339	GLU	2.7
1	C	70	ASP	2.7
1	C	345	ALA	2.7
1	F	86	ARG	2.7
1	F	359	ARG	2.7
1	C	71	PRO	2.7
1	A	289	LEU	2.7
1	A	59	GLU	2.7
1	A	160	VAL	2.7
1	A	291	VAL	2.7
1	F	274	ARG	2.7
1	A	157	SER	2.7
1	E	339	GLU	2.7
1	A	87	ALA	2.7
1	E	254	ALA	2.7
1	F	53	VAL	2.7
1	F	121	VAL	2.7
1	C	342	GLN	2.6
1	D	79	GLN	2.6
1	F	246	ILE	2.6
1	F	115	LEU	2.6
1	A	335	ARG	2.6
1	A	346	LYS	2.6
1	F	26	VAL	2.6
1	C	69	PRO	2.6
1	A	123	ASP	2.6
1	E	170	GLN	2.6
1	F	342	GLN	2.6
1	F	98	LEU	2.6
1	D	343	GLY	2.6
1	F	144	ASN	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	62	TRP	2.6
1	F	64	PRO	2.6
1	A	63	GLN	2.6
1	C	294	ALA	2.6
1	A	251	THR	2.6
1	D	73	SER	2.6
1	D	114	MET	2.6
1	F	165	ILE	2.6
1	C	154	LEU	2.6
1	E	155	TYR	2.6
1	A	82	GLU	2.6
1	F	302	GLU	2.6
1	A	185	PRO	2.6
1	A	310	VAL	2.6
1	B	311	ASP	2.5
1	A	95	PHE	2.5
1	B	18	PHE	2.5
1	C	341	ALA	2.5
1	E	19	MET	2.5
1	F	218	LEU	2.5
1	F	363	LEU	2.5
1	F	54	HIS	2.5
1	C	326	TYR	2.5
1	C	160	VAL	2.5
1	A	303	PHE	2.5
1	F	357	PHE	2.5
1	E	169	ILE	2.5
1	F	119	ASP	2.5
1	F	311	ASP	2.5
1	B	17	PRO	2.5
1	A	267	ALA	2.5
1	A	340	ARG	2.5
1	F	203	HIS	2.5
1	E	126	GLY	2.5
1	F	114	MET	2.5
1	F	179	PRO	2.5
1	F	303	PHE	2.5
1	F	50	ASN	2.4
1	A	264	SER	2.4
1	A	147	GLY	2.4
1	A	127	ALA	2.4
1	A	84	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	150	LEU	2.4
1	F	358	ASP	2.4
1	F	85	GLU	2.4
1	A	109	PRO	2.4
1	D	310	VAL	2.4
1	E	305	VAL	2.4
1	D	340	ARG	2.4
1	F	29	THR	2.4
1	F	51	ILE	2.4
1	A	124	GLU	2.4
1	A	35	GLN	2.4
1	F	27	GLN	2.4
1	C	83	LEU	2.4
1	F	225	ILE	2.4
1	A	23	GLU	2.4
1	A	245	GLU	2.4
1	F	339	GLU	2.4
1	E	308	TRP	2.4
1	D	305	VAL	2.4
1	A	341	ALA	2.4
1	A	153	TYR	2.3
1	C	253	LEU	2.3
1	E	314	THR	2.3
1	B	19	MET	2.3
1	A	255	PHE	2.3
1	F	227	ALA	2.3
1	A	134	ILE	2.3
1	A	190	ILE	2.3
1	A	162	MET	2.3
1	F	38	GLU	2.3
1	A	178	ASP	2.3
1	C	73	SER	2.3
1	A	176	GLY	2.3
1	A	198	ALA	2.3
1	F	103	ILE	2.3
1	A	94	TYR	2.3
1	A	347	GLU	2.3
1	A	66	ASP	2.3
1	D	17	PRO	2.3
1	F	70	ASP	2.3
1	A	218	LEU	2.3
1	A	301	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	165	ILE	2.3
1	A	239	ILE	2.3
1	E	110	THR	2.3
1	C	156	LEU	2.3
1	F	201	ILE	2.2
1	A	314	THR	2.2
1	A	131	SER	2.2
1	E	75	GLY	2.2
1	F	250	GLY	2.2
1	A	327	VAL	2.2
1	E	68	LEU	2.2
1	E	304	LEU	2.2
1	E	327	VAL	2.2
1	E	282	PHE	2.2
1	F	95	PHE	2.2
1	A	32	MET	2.2
1	F	329	ARG	2.2
1	E	27	GLN	2.2
1	D	218	LEU	2.2
1	A	121	VAL	2.2
1	A	139	TRP	2.2
1	F	291	VAL	2.2
1	A	141	ALA	2.2
1	A	125	THR	2.2
1	E	293	THR	2.2
1	F	185	PRO	2.2
1	A	56	LYS	2.2
1	C	68	LEU	2.2
1	E	120	GLY	2.2
1	F	36	LYS	2.2
1	A	26	VAL	2.2
1	A	265	MET	2.2
1	C	308	TRP	2.2
1	F	39	ILE	2.2
1	F	116	ASN	2.2
1	F	170	GLN	2.2
1	E	330	LEU	2.2
1	F	100	GLY	2.2
1	A	18	PHE	2.2
1	D	76	PHE	2.2
1	B	210	ALA	2.1
1	D	107	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	294	ALA	2.1
1	A	91	PRO	2.1
1	D	71	PRO	2.1
1	A	144	ASN	2.1
1	A	324	GLN	2.1
1	C	60	LYS	2.1
1	D	19	MET	2.1
1	A	290	GLY	2.1
1	B	315	GLY	2.1
1	D	120	GLY	2.1
1	C	77	ASP	2.1
1	C	157	SER	2.1
1	D	69	PRO	2.1
1	F	352	PRO	2.1
1	A	191	TYR	2.1
1	B	337	LEU	2.1
1	E	156	LEU	2.1
1	E	171	TYR	2.1
1	E	271	TYR	2.1
1	C	121	VAL	2.1
1	F	325	ASP	2.1
1	F	309	LYS	2.1
1	E	65	GLN	2.1
1	E	114	MET	2.1
1	B	273	GLY	2.1
1	C	153	TYR	2.1
1	C	273	GLY	2.1
1	D	326	TYR	2.1
1	A	221	ILE	2.1
1	A	49	GLU	2.1
1	E	210	ALA	2.1
1	F	219	ALA	2.1
1	C	65	GLN	2.1
1	A	269	LEU	2.1
1	C	120	GLY	2.1
1	C	81	ARG	2.0
1	C	329	ARG	2.0
1	F	159	ARG	2.0
1	A	115	LEU	2.0
1	A	304	LEU	2.0
1	A	216	ILE	2.0
1	D	216	ILE	2.0

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Mol	Chain	Res	Type	RSRZ
1	E	165	ILE	2.0
1	F	273	GLY	2.0
1	D	329	ARG	2.0
1	F	282	PHE	2.0
1	A	88	LYS	2.0
1	A	138	ALA	2.0
1	A	217	LYS	2.0
1	C	138	ALA	2.0
1	C	249	ASP	2.0
1	C	254	ALA	2.0
1	E	286	ALA	2.0
1	E	168	THR	2.0
1	A	330	LEU	2.0
1	F	221	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](#)

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	FE	A	370	1/1	0.87	0.07	48,48,48,48	0
2	FE	F	370	1/1	0.90	0.05	48,48,48,48	0
2	FE	B	371	1/1	0.95	0.08	49,49,49,49	0
2	FE	A	371	1/1	0.95	0.06	50,50,50,50	0
2	FE	C	370	1/1	0.96	0.09	48,48,48,48	0
2	FE	C	371	1/1	0.97	0.12	50,50,50,50	0
2	FE	D	370	1/1	0.97	0.05	48,48,48,48	0
2	FE	B	370	1/1	0.97	0.07	48,48,48,48	0
2	FE	F	371	1/1	0.97	0.13	49,49,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	FE	D	371	1/1	0.98	0.08	50,50,50,50	0
2	FE	E	370	1/1	0.98	0.04	48,48,48,48	0
2	FE	E	371	1/1	0.99	0.09	49,49,49,49	0

6.5 Other polymers [i](#)

There are no such residues in this entry.