



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 08:55 PM GMT

PDB ID : 2J2F
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 validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

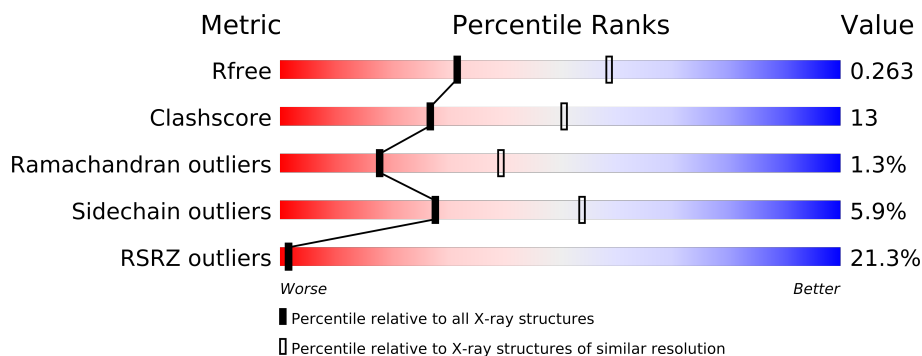
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

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}	66092	2232 (2.70-2.62)
Clashscore	79885	2700 (2.70-2.62)
Ramachandran outliers	78287	2657 (2.70-2.62)
Sidechain outliers	78261	2657 (2.70-2.62)
RSRZ outliers	66119	2234 (2.70-2.62)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	363	
1	B	363	
1	C	363	
1	D	363	
1	E	363	
1	F	363	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 17055 atoms, of which 0 are hydrogen and 0 are deuterium.

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 (three-letter code: FE) (formula: Fe).

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

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

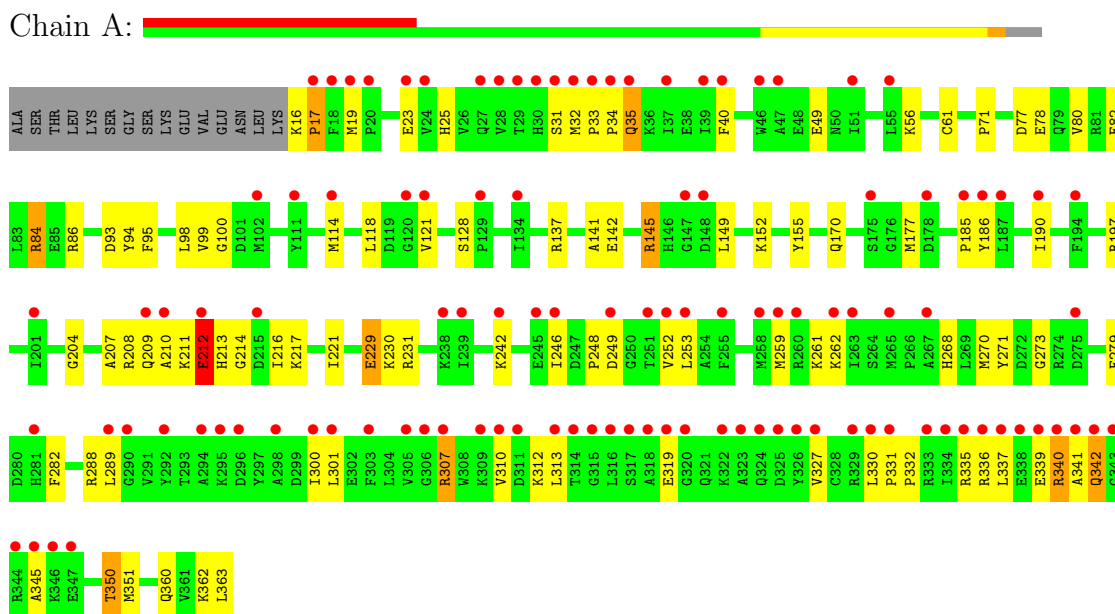
- Molecule 3 is water.

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

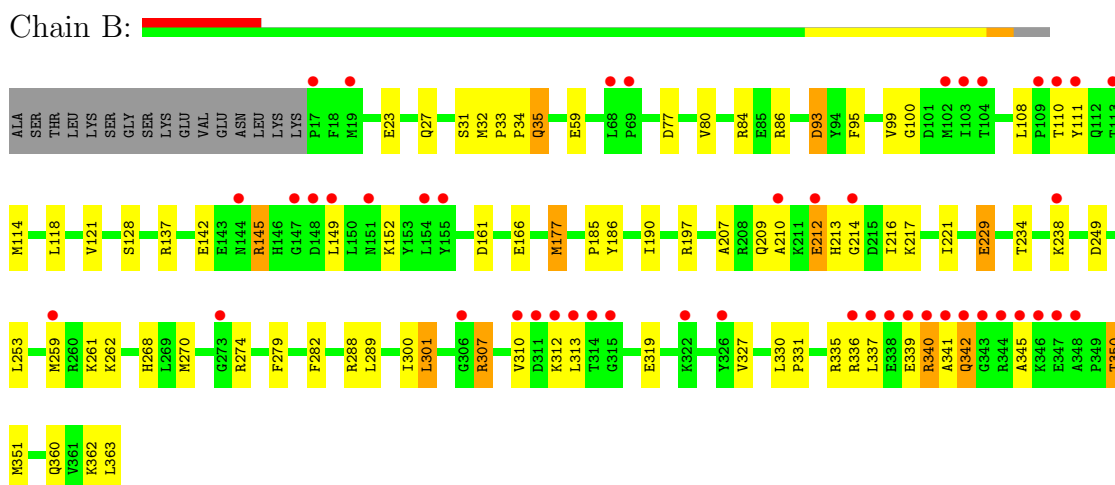
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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

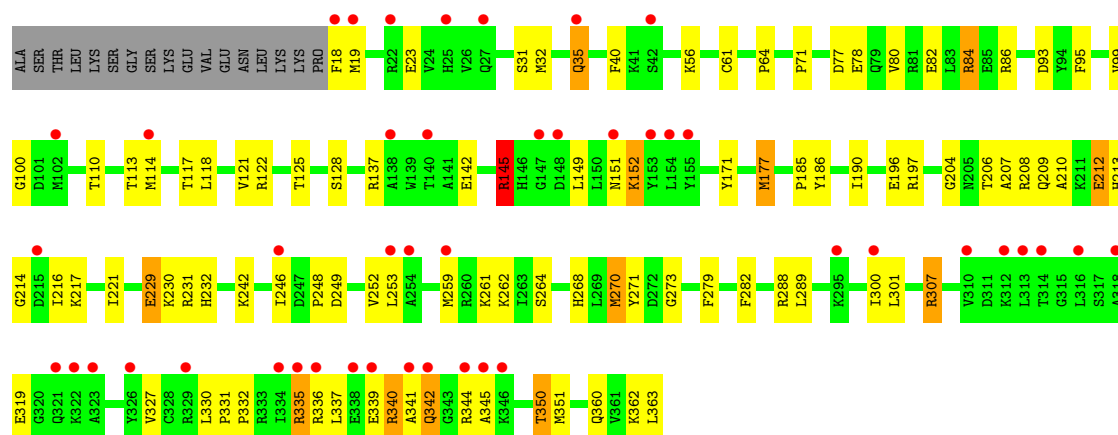


• Molecule 1: ACYL-[ACYL-CARRIER-PROTEIN]DESATURASE



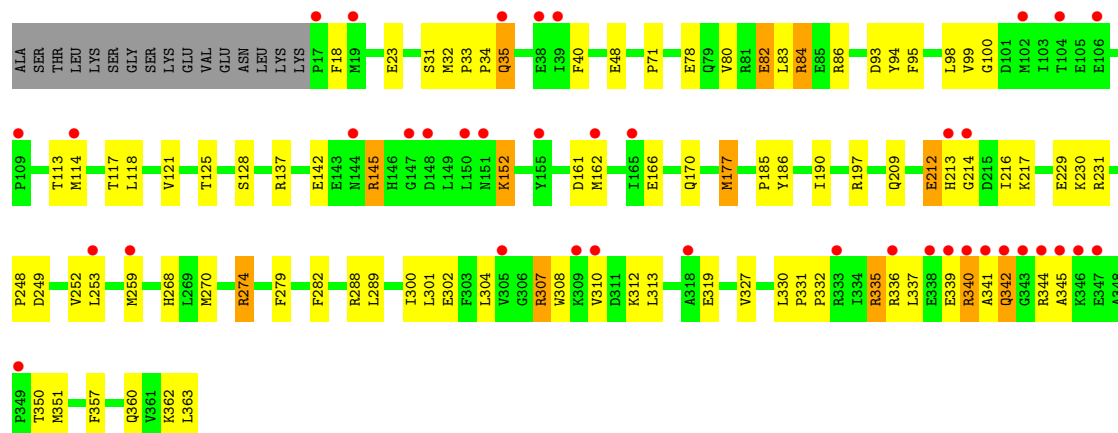
• Molecule 1: ACYL-[ACYL-CARRIER-PROTEIN]DESATURASE





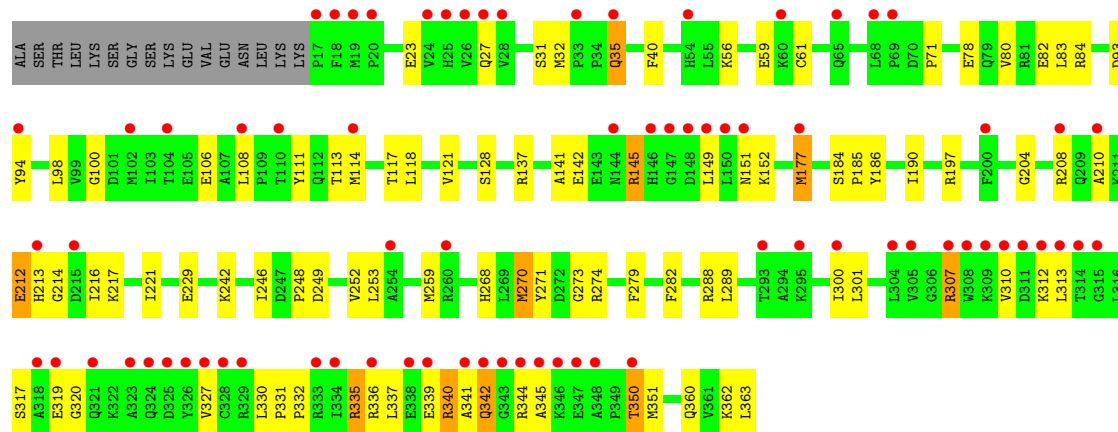
• Molecule 1: ACYL-[ACYL-CARRIER-PROTEIN]DESATURASE

Chain D:



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

Chain E:



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

Chain F:



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 33.67 – 2.65	Depositor EDS
% Data completeness (in resolution range)	98.4 (40.00-2.65) 97.9 (33.67-2.65)	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 0.233 , 0.263	Depositor DCC
R_{free} test set	3388 reflections (5.36%)	DCC
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 , 9.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	1 of 66623 reflections (0.002%)	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.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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	0.65	0/2893	0.69	4/3916 (0.1%)
1	B	0.80	0/2884	0.78	4/3904 (0.1%)
1	C	0.75	0/2876	0.75	5/3893 (0.1%)
1	D	0.79	1/2884 (0.0%)	0.77	2/3904 (0.1%)
1	E	0.71	0/2884	0.71	0/3904
1	F	0.69	0/2876	0.72	5/3893 (0.1%)
All	All	0.73	1/17297 (0.0%)	0.74	20/23414 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	82	GLU	CG-CD	5.80	1.60	1.51

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	86	ARG	NE-CZ-NH2	-9.38	115.61	120.30
1	C	86	ARG	NE-CZ-NH2	-9.13	115.73	120.30
1	B	86	ARG	NE-CZ-NH1	8.75	124.67	120.30
1	C	84	ARG	NE-CZ-NH2	-8.62	115.99	120.30
1	F	274	ARG	NE-CZ-NH1	7.90	124.25	120.30
1	C	86	ARG	NE-CZ-NH1	7.44	124.02	120.30
1	D	86	ARG	NE-CZ-NH2	-7.22	116.69	120.30
1	F	86	ARG	NE-CZ-NH2	-7.13	116.74	120.30
1	F	84	ARG	NE-CZ-NH2	-6.71	116.94	120.30
1	A	84	ARG	NE-CZ-NH2	-5.88	117.36	120.30
1	C	145	ARG	NE-CZ-NH1	5.70	123.15	120.30
1	F	74	ASP	CB-CG-OD1	5.63	123.36	118.30
1	B	77	ASP	CB-CG-OD1	5.53	123.28	118.30
1	A	86	ARG	NE-CZ-NH2	-5.51	117.55	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	77	ASP	CB-CG-OD1	5.40	123.16	118.30
1	D	84	ARG	NE-CZ-NH2	-5.38	117.61	120.30
1	B	145	ARG	NE-CZ-NH2	-5.20	117.70	120.30
1	A	77	ASP	CB-CG-OD1	5.04	122.84	118.30
1	F	274	ARG	NE-CZ-NH2	-5.00	117.80	120.30
1	A	86	ARG	NE-CZ-NH1	5.00	122.80	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2824	0	2765	83	2
1	B	2815	0	2753	70	1
1	C	2808	0	2745	80	0
1	D	2815	0	2753	74	0
1	E	2815	0	2753	79	0
1	F	2808	0	2745	71	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	3	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	439	3

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including

hydrogens) of the entry. The overall clashscore for this entry is 13.

All (439) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:16:LYS:HG2	1:A:19:MET:HE3	1.39	1.04
1:A:16:LYS:HG2	1:A:19:MET:CE	1.90	1.02
1:E:217:LYS:HE2	3:E:2018:HOH:O	1.67	0.95
1:D:114:MET:CE	1:D:177:MET:HB3	1.96	0.95
1:B:59:GLU:HG3	1:C:18:PHE:CD2	2.03	0.94
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:D:270:MET:HE1	1:D:279:PHE:HA	1.51	0.91
1:F:114:MET:CE	1:F:177:MET:HB3	2.02	0.90
1:B:270:MET:HE1	1:B:279:PHE:HA	1.57	0.86
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:HE21	1:D:342:GLN:HA	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:D:259:MET:SD	1:D:330:LEU:HD23	2.20	0.81
1:A:114:MET:CE	1:A:177:MET:HB3	2.09	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: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:A:270:MET:HE1	1:A:279:PHE:HA	1.65	0.77
1:F:342:GLN:HE21	1:F:342:GLN:HA	1.51	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:C:270:MET:HE1	1:C:279:PHE:HA	1.68	0.75
1:F:336:ARG:O	1:F:339:GLU:HB3	1.86	0.75
1:C:114:MET:HE2	1:C:177:MET:HB3	1.66	0.75
1:E:114:MET:HE2	1:E:177:MET:HB3	1.68	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: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:OE1	1:A:229:GLU:HA	1.88	0.72
1:E:270:MET:HE1	1:E:279:PHE:HA	1.72	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:HA	1:A:342:GLN:HE21	1.56	0.71

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
1:B:259:MET:HE3	1:B:327:VAL:HG13	1.74	0.69
1:A:118:LEU:HB2	1:A:121:VAL:CG2	2.23	0.69
1:E:336:ARG:O	1:E:339:GLU:HB3	1.92	0.69
1:B:229:GLU:OE1	1:B:229:GLU:HA	1.92	0.69
1:F:301:LEU:HD23	1:F:331:PRO:HG3	1.75	0.69
1:F:118:LEU:HB2	1:F:121:VAL:CG2	2.21	0.69
1:A:253:LEU:HD21	1:A:319:GLU:HG3	1.74	0.68
1:C:229:GLU:OE1	1:C:229:GLU:HA	1.92	0.68
1:E:217:LYS:HE3	3:E:2002:HOH:O	1.93	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:D:301:LEU:HD23	1:D:331:PRO:HG3	1.74	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: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:E:197:ARG:HG2	1:E:300:ILE:HG12	1.75	0.67
1:D:229:GLU:HA	1:D:229:GLU:OE1	1.93	0.67
1:E:307:ARG:O	1:E:307:ARG:HD3	1.95	0.67
1:F:212:GLU:O	1:F:214:GLY:N	2.27	0.67
1:A:155:TYR:CG	3:F:2008:HOH:O	2.46	0.67
1:A:259:MET:SD	1:A:330:LEU:HD23	2.34	0.67
1:F:114:MET:HE2	1:F:177:MET:HB3	1.76	0.66
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:A:259:MET:HE1	1:A:327:VAL:HG13	1.78	0.66
1:C:350:THR:HG23	1:C:360:GLN:HB3	1.78	0.65
1:F:229:GLU:HA	1:F:229:GLU:OE1	1.96	0.65
1:E:229:GLU:HA	1:E:229:GLU:OE1	1.97	0.65
1:B:128:SER:O	1:B:137:ARG:NH2	2.30	0.65
1:C:301:LEU:HD23	1:C:331:PRO:HG3	1.77	0.65
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
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:C:118:LEU:HB2	1:C:121:VAL:CG2	2.27	0.63

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:HD3	1:D:307:ARG:O	1.98	0.63
1:A:350:THR:HG23	1:A:360:GLN:HB3	1.79	0.63
1:A:259:MET:CE	1:A:327:VAL:HG13	2.29	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: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:C:128:SER:O	1:C:137:ARG:NH2	2.34	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:A:155:TYR:CB	3:F:2008:HOH:O	2.48	0.61
1:D:114:MET:HE2	1:D:177:MET:HB3	1.83	0.61
1:E:114:MET:HE1	1:E:177:MET:SD	2.41	0.61
1:E:32:MET:HE3	1:E:186:TYR:HD1	1.65	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:331:PRO:HB2	1:E:332:PRO:HD3	1.83	0.60
1:E:80:VAL:O	1:E:84:ARG:HG3	2.02	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:212:GLU:C	1:B:214:GLY:H	2.05	0.60
1:B:118:LEU:HB2	1:B:121:VAL:CG2	2.32	0.60
1:E:32:MET:HE3	1:E:186:TYR:CD1	2.37	0.59
1:D:128:SER:O	1:D:137:ARG:NH2	2.34	0.59
1:A:71:PRO:O	1:F:84:ARG:NH2	2.31	0.59
1:F:152:LYS:CD	3:F:2008:HOH:O	2.50	0.59
1:A:197:ARG:HG2	1:A:300:ILE:HG12	1.85	0.59
1:B:114:MET:HE2	1:B:177:MET:HB3	1.84	0.59
1:C:271:TYR:CE2	1:C:273:GLY:HA2	2.38	0.59
1:D:71:PRO:O	1:E:84:ARG:NH2	2.33	0.59
1:A:307:ARG:HD3	1:A:307:ARG:O	2.02	0.59
1:B:270:MET:CE	1:B:279:PHE:HA	2.32	0.59
1:B:84:ARG:NH2	1:C:71:PRO:O	2.34	0.59
1:C:32:MET:HE3	1:C:186:TYR:HD1	1.69	0.58
1:B:341:ALA:HB1	1:B:345:ALA:HB2	1.84	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:D:341:ALA:HB1	1:D:345:ALA:HB2	1.86	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:16:LYS:CG	1:A:19:MET:HE3	2.23	0.57
1:C:100:GLY:HA3	1:C:282:PHE:CE1	2.39	0.57
1:C:32:MET:HE3	1:C:186:TYR:CD1	2.39	0.57
1:F:197:ARG:HG2	1:F:300:ILE:HG12	1.86	0.57
1:D:114:MET:HE1	1:D:177:MET:HB3	1.85	0.57
1:A:35:GLN:HE21	1:A:35:GLN:H	1.51	0.57
1:C:270:MET:CE	1:C:279:PHE:HA	2.35	0.57
1:E:35:GLN:HE21	1:E:35:GLN:H	1.52	0.56
1:F:259:MET:CE	1:F:327:VAL:HG13	2.35	0.56
1:E:301:LEU:HD23	1:E:331:PRO:HG3	1.86	0.56
1:B:161:ASP:OD2	1:D:78:GLU:OE2	2.23	0.56
1:F:32:MET:HE3	1:F:186:TYR:HD1	1.70	0.56
1:D:114:MET:HE2	1:D:177:MET:SD	2.45	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:186:TYR:O	1:A:190:ILE:HG12	2.05	0.56
1:A:128:SER:O	1:A:137:ARG:NH2	2.38	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:B:341:ALA:O	1:B:345:ALA:HB3	2.06	0.55
1:F:270:MET:HE1	1:F:279:PHE:HA	1.89	0.55
1:D:259:MET:CE	1:D:327:VAL:HG13	2.36	0.55
1:B:95:PHE:O	1:B:99:VAL:HG23	2.07	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: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:288:ARG:NH1	1:A:362:LYS:O	2.38	0.54
1:D:350:THR:CG2	1:D:360:GLN:HB3	2.38	0.54
1:C:35:GLN:HE21	1:C:35:GLN:H	1.55	0.54
1:C:197:ARG:HG2	1:C:300:ILE:HG12	1.90	0.54
1:B:32:MET:HE2	1:B:186:TYR:HE1	1.73	0.54
1:F:341:ALA:HB1	1:F:345:ALA:HB2	1.89	0.54
1:E:288:ARG:NH1	1:E:362:LYS:O	2.39	0.54
1:F:259:MET:SD	1:F:301:LEU:HD21	2.47	0.54
1:F:186:TYR:O	1:F:190:ILE:HG12	2.08	0.54
1:C:23:GLU:OE2	1:C:268:HIS:HE1	1.90	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:94:TYR:HE1	1:A:98:LEU:HD22	1.72	0.54
1:C:341:ALA:O	1:C:345:ALA:HB3	2.08	0.54
1:A:114:MET:HE2	1:A:177:MET:HB3	1.90	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:32:MET:HE3	1:A:186:TYR:HD1	1.72	0.53
1:A:229:GLU:CA	1:A:229:GLU:OE1	2.54	0.53
1:F:331:PRO:HB2	1:F:332:PRO:HD3	1.89	0.53
1:F:78:GLU:OE1	3:F:2004:HOH:O	2.18	0.53
1:D:32:MET:HE3	1:D:186:TYR:HD1	1.73	0.53
1:D:32:MET:HE3	1:D:186:TYR:CD1	2.43	0.53
1:B:288:ARG:NH1	1:B:362:LYS:O	2.41	0.53
1:F:152:LYS:HD2	3:F:2008:HOH:O	2.09	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:A:341:ALA:HB1	1:A:345:ALA:HB2	1.90	0.53
1:A:212:GLU:C	1:A:214:GLY:H	2.13	0.53
1:C:23:GLU:OE2	1:C:268:HIS:CE1	2.62	0.53
1:A:16:LYS:HG2	1:A:19:MET:HE1	1.89	0.52
1:C:229:GLU:CA	1:C:229:GLU:OE1	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:F:259:MET:HE1	1:F:327:VAL:HG13	1.92	0.52
1:D:259:MET:HE3	1:D:327:VAL:HG13	1.91	0.52
1:D:212:GLU:C	1:D:214:GLY:H	2.13	0.52
1:E:259:MET:CE	1:E:327:VAL:HG13	2.38	0.52
1:B:27:GLN:HG3	1:C:125:THR:HG21	1.92	0.52
1:F:270:MET:CE	1:F:279:PHE:HA	2.40	0.51
1:F:32:MET:CE	1:F:185:PRO:HD2	2.40	0.51
1:B:32:MET:HE2	1:B:186:TYR:CE1	2.45	0.51
1:B:32:MET:HE3	1:B:186:TYR:HD1	1.76	0.51
1:F:35:GLN:HE21	1:F:35:GLN:H	1.57	0.51
1:F:307:ARG:HD3	1:F:307:ARG:O	2.10	0.51
1:C:259:MET:HE1	1:C:327:VAL:HG13	1.91	0.51
1:C:307:ARG:HD3	1:C:307:ARG:O	2.11	0.51
1:B:114:MET:HE1	1:B:177:MET:HB3	1.89	0.51
1:F:212:GLU:C	1:F:214:GLY:H	2.13	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:78:GLU:O	1:D:82:GLU:HG3	2.11	0.51
1:C:145:ARG:HG3	1:C:145:ARG:HH11	1.76	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:216:ILE:HG12	3:E:2019:HOH:O	2.10	0.50
1:D:100:GLY:HA3	1:D:282:PHE:CE1	2.46	0.50
1:C:80:VAL:O	1:C:84:ARG:HG3	2.10	0.50
1:D:270:MET:CE	1:D:279:PHE:HA	2.32	0.50
1:A:114:MET:HE1	1:A:177:MET:SD	2.52	0.50
1:D:229:GLU:OE1	1:D:229:GLU:CA	2.59	0.50
1:E:259:MET:HE1	1:E:327:VAL:HG13	1.91	0.50
1:A:95:PHE:O	1:A:99:VAL:HG23	2.11	0.50
1:E:212:GLU:C	1:E:214:GLY:H	2.13	0.50
1:E:259:MET:SD	1:E:301:LEU:HD11	2.52	0.50
1:C:113:THR:O	1:C:117:THR:HG23	2.12	0.50
1:A:114:MET:CE	1:A:177:MET:SD	3.00	0.50
1:B:32:MET:CE	1:B:185:PRO:HD2	2.41	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:106:GLU:CD	3:E:2010:HOH:O	2.49	0.50
1:E:341:ALA:HB1	1:E:345:ALA:HB2	1.94	0.50
1:D:114:MET:CE	1:D:177:MET:SD	3.00	0.49
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:A:330:LEU:N	1:A:331:PRO:CD	2.75	0.49
1:E:229:GLU:CA	1:E:229:GLU:OE1	2.60	0.49
1:E:330:LEU:N	1:E:331:PRO:CD	2.76	0.49
1:D:18:PHE:CD1	1:E:59:GLU:HG3	2.47	0.49
1:B:114:MET:HE2	1:B:177:MET:SD	2.53	0.49
1:E:248:PRO:O	1:E:252:VAL:HG23	2.13	0.49
1:E:32:MET:HE2	1:E:186:TYR:HE1	1.78	0.48
1:A:32:MET:HE2	1:A:186:TYR:HE1	1.78	0.48
1:D:288:ARG:NH1	1:D:362:LYS:O	2.46	0.48
1:A:248:PRO:O	1:A:252:VAL:HG23	2.13	0.48
1:C:78:GLU:O	1:C:82:GLU:HG3	2.14	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:C:95:PHE:O	1:C:99:VAL:HG23	2.13	0.48
1:C:142:GLU:OE1	1:C:231:ARG:NH2	2.38	0.48
1:A:78:GLU:O	1:A:82:GLU:HG3	2.12	0.48
1:A:23:GLU:OE2	1:A:268:HIS:HE1	1.97	0.48
1:E:307:ARG:C	1:E:307:ARG:HD3	2.33	0.48
1:B:186:TYR:O	1:B:190:ILE:HG12	2.14	0.48
1:D:83:LEU:HD23	1:D:83:LEU:C	2.35	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:341:ALA:O	1:F:345:ALA:HB3	2.14	0.47
1:D:162:MET:O	1:D:166:GLU:HG3	2.14	0.47
1:A:32:MET:HE3	1:A:186:TYR:CD1	2.49	0.47
1:E:310:VAL:HA	1:E:313:LEU:HD12	1.96	0.47
1:B:207:ALA:O	1:B:210:ALA:HB3	2.15	0.47
1:C:261:LYS:O	1:C:262:LYS:HB2	2.14	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:D:35:GLN:HE21	1:D:35:GLN:H	1.62	0.47
1:C:331:PRO:HB2	1:C:332:PRO:HD3	1.96	0.47
1:C:186:TYR:O	1:C:190:ILE:HG12	2.14	0.47
1:C:40:PHE:CZ	1:C:185:PRO:HB2	2.50	0.47
1:A:35:GLN:NE2	1:A:35:GLN:H	2.13	0.47
1:D:161:ASP:OD2	1:F:78:GLU:OE2	2.33	0.47
1:B:23:GLU:OE2	1:B:268:HIS:HE1	1.97	0.47
1:F:259:MET:HE3	1:F:327:VAL:HG22	1.96	0.47
1:F:152:LYS:CE	3:F:2008:HOH:O	2.62	0.47
1:E:113:THR:O	1:E:117:THR:HG23	2.14	0.47
1:F:271:TYR:CE2	1:F:273:GLY:HA2	2.50	0.47
1:E:114:MET:HE2	1:E:177:MET:SD	2.54	0.47
1:D:113:THR:O	1:D:117:THR:HG23	2.14	0.47
1:F:114:MET:CE	1:F:177:MET:SD	3.03	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:B:253:LEU:CD2	1:B:319:GLU:HG3	2.39	0.46
1:D:259:MET:HE3	1:D:327:VAL:HG22	1.98	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:C:330:LEU:N	1:C:331:PRO:CD	2.78	0.46
1:A:23:GLU:OE2	1:A:268:HIS:CE1	2.69	0.46
1:E:118:LEU:HB2	1:E:121:VAL:HG22	1.97	0.46
1:A:259:MET:SD	1:A:301:LEU:HD21	2.56	0.46
1:F:248:PRO:O	1:F:252:VAL:HG23	2.16	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:A:170:GLN:HG3	1:F:141:ALA:HB1	1.97	0.46
1:B:93:ASP:N	1:B:93:ASP:OD2	2.47	0.46
1:B:310:VAL:HA	1:B:313:LEU:HD12	1.98	0.46
1:E:35:GLN:NE2	1:E:35:GLN:H	2.14	0.45
1:B:32:MET:HE1	1:B:185:PRO:HD2	1.99	0.45
1:C:114:MET:CE	1:C:177:MET:SD	3.04	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:270:MET:HE2	1:F:270:MET:HB3	1.82	0.45
1:F:242:LYS:HE3	1:F:246:ILE:HD11	1.99	0.45
1:E:23:GLU:OE2	1:E:268:HIS:HE1	2.00	0.45
1:C:142:GLU:CD	1:C:231:ARG:HH22	2.19	0.45
1:B:261:LYS:O	1:B:262:LYS:HB2	2.16	0.45
1:F:32:MET:HE3	1:F:186:TYR:CD1	2.49	0.45
1:C:171:TYR:HB3	3:C:2021:HOH:O	2.16	0.45
1:A:271:TYR:CE2	1:A:273:GLY:HA2	2.52	0.45
1:A:211:LYS:HB2	1:A:211:LYS:HE3	1.85	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: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
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:C:142:GLU:O	1:C:145:ARG:HG3	2.18	0.44
1:E:271:TYR:CZ	1:E:273:GLY:HA2	2.51	0.44
1:E:204:GLY:O	1:E:208:ARG:HG3	2.16	0.44
1:D:142:GLU:OE1	1:D:231:ARG:NH2	2.43	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:E:83:LEU:HD23	1:E:83:LEU:C	2.38	0.44
1:A:142:GLU:O	1:A:145:ARG:HG3	2.18	0.44
1:D:33:PRO:HA	1:D:34:PRO:HD3	1.84	0.44
1:D:330:LEU:N	1:D:331:PRO:CD	2.80	0.44
3:B:2028:HOH:O	1:C:152:LYS:NZ	2.47	0.44
1:A:310:VAL:HA	1:A:313:LEU:HD12	1.98	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:F:330:LEU:N	1:F:331:PRO:CD	2.81	0.44
1:F:209:GLN:HA	1:F:212:GLU:HG2	1.99	0.44
1:B:350:THR:CG2	1:B:360:GLN:HB3	2.45	0.44
1:F:152:LYS:HE3	3:F:2008:HOH:O	2.18	0.44
1:D:32:MET:HE1	1:D:185:PRO:HD2	1.99	0.44
1:C:149:LEU:HD21	1:C:221:ILE:HG23	2.00	0.44
1:B:270:MET:HB3	1:B:270:MET:HE2	1.78	0.44
1:B:114:MET:HE1	1:B:177:MET:SD	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:C:56:LYS:HB3	1:C:61:CYS:SG	2.58	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:342:GLN:NE2	1:D:342:GLN:HA	2.24	0.43
1:A:141:ALA:HB1	1:F:170:GLN:HG3	2.00	0.43
1:F:100:GLY:HA3	1:F:282:PHE:CE1	2.53	0.43
1:E:259:MET:HE3	1:E:327:VAL:HG22	2.00	0.43
1:E:149:LEU:HD21	1:E:221:ILE:HG23	2.00	0.43
1:E:56:LYS:HB3	1:E:61:CYS:SG	2.58	0.43
1:B:342:GLN:HE21	1:B:342:GLN:CA	2.25	0.43
1:F:259:MET:CG	1:F:301:LEU:HD11	2.49	0.43
1:C:242:LYS:HE3	1:C:246:ILE:HD11	1.99	0.43
1:A:209:GLN:HA	1:A:212:GLU:CG	2.48	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:D:142:GLU:O	1:D:145:ARG:HG3	2.19	0.43
1:D:125:THR:HG21	1:E:27:GLN:HG3	2.00	0.43
1:C:259:MET:CG	1:C:301:LEU:HD11	2.48	0.43
1:D:212:GLU:HG2	1:D:212:GLU:H	1.67	0.43
1:C:206:THR:O	1:C:210:ALA:HB2	2.18	0.43
1:A:100:GLY:HA3	1:A:282:PHE:CE1	2.54	0.43
1:A:40:PHE:CZ	1:A:185:PRO:HB2	2.53	0.43
1:B:234:THR:O	1:B:238:LYS:HG2	2.18	0.43
1:C:350:THR:CG2	1:C:360:GLN:HB3	2.45	0.43
1:A:32:MET:HE2	1:A:186:TYR:CE1	2.54	0.43
1:C:78:GLU:HG2	3:C:2004:HOH:O	2.19	0.43
1:A:270:MET:HB3	1:A:270:MET:HE2	1.77	0.43
1:A:271:TYR:CZ	1:A:273:GLY:HA2	2.53	0.43
1:F:114:MET:HE1	1:F:177:MET:HB3	1.94	0.43
1:A:259:MET:HE3	1:A:327:VAL:HG22	2.01	0.43
1:E:149:LEU:CD2	1:E:221:ILE:HG23	2.49	0.43
1:B:166:GLU:OE2	1:C:64:PRO:HB2	2.19	0.43
1:F:261:LYS:O	1:F:262:LYS:HB2	2.18	0.43
1:C:114:MET:HE2	1:C:177:MET:SD	2.59	0.42
1:E:317:SER:O	1:E:320:GLY:N	2.52	0.42
1:A:149:LEU:HD21	1:A:221:ILE:HG23	2.01	0.42
1:F:23:GLU:OE2	1:F:268:HIS:CE1	2.72	0.42
1:A:114:MET:HE1	1:A:177:MET:HB3	1.94	0.42
1:A:204:GLY:O	1:A:208:ARG:HG3	2.19	0.42
1:B:307:ARG:C	1:B:307:ARG:HD3	2.39	0.42
1:C:253:LEU:CD2	1:C:319:GLU:HG3	2.44	0.42
1:F:270:MET:HE3	1:F:278:LEU:HG	2.00	0.42
1:A:56:LYS:HB3	1:A:61:CYS:SG	2.59	0.42
1:F:288:ARG:NH1	1:F:362:LYS:O	2.48	0.42
1:E:270:MET:HB3	1:E:270:MET:HE2	1.85	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:271:TYR:CZ	1:F:273:GLY:HA2	2.55	0.42
1:C:212:GLU:C	1:C:214:GLY:H	2.23	0.42
1:C:32:MET:HE2	1:C:186:TYR:HE1	1.85	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:149:LEU:HD21	1:B:221:ILE:HG23	2.02	0.42
1:D:40:PHE:CZ	1:D:185:PRO:HB2	2.55	0.42
1:C:204:GLY:O	1:C:208:ARG:HG3	2.19	0.42
1:A:242:LYS:HE3	1:A:246:ILE:HD11	2.02	0.42
1:B:209:GLN:HA	1:B:212:GLU:CG	2.49	0.42
1:E:335:ARG:O	1:E:339:GLU:HB2	2.19	0.42
1:A:155:TYR:HB2	3:F:2008:HOH:O	2.18	0.42
1:D:307:ARG:C	1:D:307:ARG:HD3	2.40	0.42
1:E:108:LEU:HA	1:E:111:TYR:CD2	2.55	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:F:114:MET:HE2	1:F:177:MET:SD	2.60	0.41
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:35:GLN:NE2	1:C:35:GLN:H	2.16	0.41
1:C:208:ARG:HH11	1:C:208:ARG:HB3	1.86	0.41
1:E:145:ARG:NH1	1:E:145:ARG:HG3	2.32	0.41
1:C:32:MET:CE	1:C:185:PRO:HD2	2.50	0.41
1:D:270:MET:HB3	1:D:270:MET:HE2	1.72	0.41
1:E:270:MET:HE1	1:E:282:PHE:HB3	2.02	0.41
1:B:142:GLU:O	1:B:145:ARG:HG3	2.20	0.41
1:A:307:ARG:HD3	1:A:307:ARG:C	2.40	0.41
1:A:78:GLU:HG2	3:A:2005:HOH:O	2.20	0.41
1:F:310:VAL:HA	1:F:313:LEU:HD12	2.02	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:HD2	1:D:230:LYS:HA	1.86	0.41
1:B:209:GLN:HA	1:B:212:GLU:HG2	2.02	0.41
1:B:259:MET:HE3	1:B:327:VAL:HG22	2.03	0.41
1:E:32:MET:CE	1:E:186:TYR:CD1	3.03	0.41
1:C:110:THR:HG22	1:C:114:MET:HE3	2.02	0.41
1:F:209:GLN:HA	1:F:212:GLU:CG	2.50	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:D:310:VAL:HA	1:D:313:LEU:HD12	2.03	0.41
1:E:212:GLU:C	1:E:214:GLY:N	2.73	0.40
1:F:35:GLN:NE2	1:F:35:GLN:H	2.20	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:216:ILE:HG13	1:D:217:LYS:N	2.37	0.40
1:C:196:GLU:OE1	1:C:232:HIS:HB2	2.21	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:B:149:LEU:CD2	1:B:221:ILE:HG23	2.52	0.40
1:A:216:ILE:HG13	1:A:217:LYS:N	2.37	0.40
1:F:33:PRO:HA	1:F:34:PRO:HD3	1.83	0.40
1:A:261:LYS:O	1:A:262:LYS:HB2	2.21	0.40
1:B:259:MET:HG2	1:B:301:LEU:HD11	2.04	0.40
1:A:211:LYS:O	1:A:212:GLU:C	2.60	0.40
1:D:48:GLU:O	1:D:48:GLU:HG2	2.22	0.40
1:A:230:LYS:HD2	1:A:230:LYS:HA	1.87	0.40
1:C:230:LYS:HA	1:C:230:LYS:HD2	1.90	0.40
1:E:40:PHE:CZ	1:E:185:PRO:HB2	2.56	0.40
1:B:32:MET:HE3	1:B:186:TYR:CD1	2.55	0.40
1:F:23:GLU:OE2	1:F:268:HIS:HE1	2.03	0.40
1:F:211:LYS:HB2	1:F:211:LYS:HE3	1.94	0.40
1:F:110:THR:HG22	1:F:114:MET:HE3	2.04	0.40
1:B:110:THR:HG22	1:B:114:MET:HE3	2.03	0.40
1:F:108:LEU:HA	1:F:111:TYR:CD2	2.57	0.40
1:D:302:GLU:OE1	1:D:335:ARG:NH2	2.54	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	Distance(Å)	Clash(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%)	14 30

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	345/363 (95%)	324 (94%)	17 (5%)	4 (1%)	19	42
1	C	344/363 (95%)	321 (93%)	19 (6%)	4 (1%)	19	42
1	D	345/363 (95%)	316 (92%)	25 (7%)	4 (1%)	19	42
1	E	345/363 (95%)	317 (92%)	24 (7%)	4 (1%)	19	42
1	F	344/363 (95%)	317 (92%)	22 (6%)	5 (2%)	15	34
All	All	2069/2178 (95%)	1912 (92%)	130 (6%)	27 (1%)	18	39

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
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%)	286 (95%)	16 (5%)	32	60
1	B	301/315 (96%)	284 (94%)	17 (6%)	30	56
1	C	300/315 (95%)	279 (93%)	21 (7%)	21	44
1	D	301/315 (96%)	284 (94%)	17 (6%)	30	56
1	E	301/315 (96%)	281 (93%)	20 (7%)	24	47
1	F	300/315 (95%)	284 (95%)	16 (5%)	32	60
All	All	1805/1890 (96%)	1698 (94%)	107 (6%)	28	54

All (107) 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	289	LEU
1	A	307	ARG
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	177	MET
1	B	212	GLU
1	B	229	GLU
1	B	249	ASP

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Mol	Chain	Res	Type
1	B	274	ARG
1	B	289	LEU
1	B	301	LEU
1	B	307	ARG
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	31	SER
1	C	35	GLN
1	C	93	ASP
1	C	122	ARG
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	307	ARG
1	C	340	ARG
1	C	342	GLN
1	C	344	ARG
1	C	350	THR
1	C	351	MET
1	C	363	LEU
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	274	ARG
1	D	289	LEU
1	D	307	ARG

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Mol	Chain	Res	Type
1	D	312	LYS
1	D	340	ARG
1	D	342	GLN
1	D	344	ARG
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	152	LYS
1	E	177	MET
1	E	184	SER
1	E	212	GLU
1	E	249	ASP
1	E	270	MET
1	E	274	ARG
1	E	289	LEU
1	E	307	ARG
1	E	312	LYS
1	E	340	ARG
1	E	342	GLN
1	E	344	ARG
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	249	ASP
1	F	270	MET
1	F	274	ARG
1	F	289	LEU
1	F	307	ARG
1	F	340	ARG
1	F	342	GLN
1	F	350	THR
1	F	351	MET
1	F	363	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) 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	50	ASN
1	B	268	HIS
1	B	342	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	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 ⓘ

There are no RNA chains in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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%)	1.52	110 (31%) 1 1	31, 33, 34, 50	0
1	B	347/363 (95%)	0.94	46 (13%) 4 3	31, 33, 34, 48	0
1	C	346/363 (95%)	0.98	45 (13%) 4 3	22, 33, 34, 36	0
1	D	347/363 (95%)	0.91	39 (11%) 6 5	31, 33, 34, 44	0
1	E	347/363 (95%)	1.18	75 (21%) 1 1	31, 33, 34, 50	0
1	F	346/363 (95%)	1.78	130 (37%) 1 1	31, 33, 34, 45	0
All	All	2081/2178 (95%)	1.22	445 (21%) 1 1	22, 33, 34, 50	0

All (445) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	345	ALA	11.6
1	B	345	ALA	9.2
1	D	344	ARG	9.0
1	F	341	ALA	8.9
1	E	345	ALA	8.9
1	F	310	VAL	8.4
1	B	342	GLN	8.0
1	F	344	ARG	7.6
1	A	338	GLU	7.5
1	F	345	ALA	7.2
1	C	338	GLU	7.1
1	E	344	ARG	6.8
1	B	341	ALA	6.6
1	B	343	GLY	6.5
1	C	18	PHE	6.3
1	F	244	PHE	6.3
1	F	35	GLN	6.3
1	A	19	MET	6.3
1	C	342	GLN	6.1

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Mol	Chain	Res	Type	RSRZ
1	F	252	VAL	6.1
1	B	344	ARG	5.9
1	E	338	GLU	5.9
1	F	328	CYS	5.9
1	F	19	MET	5.9
1	F	318	ALA	5.8
1	E	343	GLY	5.7
1	D	346	LYS	5.7
1	A	32	MET	5.6
1	F	253	LEU	5.6
1	A	260	ARG	5.5
1	F	342	GLN	5.4
1	E	346	LYS	5.4
1	B	19	MET	5.3
1	A	24	VAL	5.3
1	F	338	GLU	5.2
1	C	344	ARG	5.2
1	F	301	LEU	5.2
1	F	329	ARG	5.2
1	A	120	GLY	5.1
1	F	28	VAL	5.0
1	F	40	PHE	5.0
1	A	253	LEU	5.0
1	F	304	LEU	5.0
1	F	343	GLY	5.0
1	D	342	GLN	4.9
1	A	340	ARG	4.9
1	F	18	PHE	4.9
1	A	344	ARG	4.9
1	F	186	TYR	4.9
1	C	19	MET	4.8
1	E	313	LEU	4.8
1	E	339	GLU	4.8
1	A	313	LEU	4.7
1	A	334	ILE	4.7
1	F	325	ASP	4.7
1	F	314	THR	4.6
1	D	340	ARG	4.6
1	F	27	GLN	4.6
1	F	245	GLU	4.6
1	A	114	MET	4.5
1	F	120	GLY	4.5

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Mol	Chain	Res	Type	RSRZ
1	F	26	VAL	4.5
1	C	318	ALA	4.5
1	F	311	ASP	4.4
1	F	308	TRP	4.4
1	D	347	GLU	4.4
1	A	259	MET	4.4
1	D	341	ALA	4.3
1	B	338	GLU	4.3
1	F	38	GLU	4.3
1	E	318	ALA	4.3
1	F	327	VAL	4.3
1	A	329	ARG	4.3
1	A	318	ALA	4.3
1	A	35	GLN	4.3
1	E	295	LYS	4.3
1	E	341	ALA	4.2
1	A	305	VAL	4.2
1	C	313	LEU	4.2
1	F	303	PHE	4.1
1	E	310	VAL	4.1
1	A	40	PHE	4.1
1	D	338	GLU	4.1
1	C	339	GLU	4.1
1	C	322	LYS	4.1
1	A	194	PHE	4.1
1	B	337	LEU	4.1
1	F	24	VAL	4.0
1	F	243	LEU	4.0
1	A	337	LEU	4.0
1	F	259	MET	4.0
1	D	343	GLY	4.0
1	E	347	GLU	4.0
1	A	315	GLY	3.9
1	F	322	LYS	3.9
1	E	27	GLN	3.9
1	E	342	GLN	3.9
1	F	313	LEU	3.9
1	F	315	GLY	3.8
1	E	18	PHE	3.8
1	A	324	GLN	3.8
1	F	54	HIS	3.8
1	B	312	LYS	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	314	THR	3.8
1	D	17	PRO	3.8
1	A	335	ARG	3.8
1	A	346	LYS	3.7
1	F	255	PHE	3.7
1	C	329	ARG	3.7
1	E	147	GLY	3.7
1	F	22	ARG	3.6
1	A	242	LYS	3.6
1	F	336	ARG	3.6
1	F	300	ILE	3.6
1	F	191	TYR	3.6
1	D	318	ALA	3.6
1	E	309	LYS	3.6
1	E	312	LYS	3.5
1	D	339	GLU	3.5
1	A	33	PRO	3.5
1	F	305	VAL	3.5
1	E	325	ASP	3.5
1	F	32	MET	3.5
1	F	25	HIS	3.4
1	B	259	MET	3.4
1	F	337	LEU	3.4
1	A	333	ARG	3.4
1	B	346	LYS	3.4
1	B	109	PRO	3.4
1	B	214	GLY	3.4
1	A	326	TYR	3.4
1	F	326	TYR	3.4
1	F	250	GLY	3.4
1	F	33	PRO	3.4
1	F	246	ILE	3.4
1	F	295	LYS	3.4
1	F	316	LEU	3.4
1	D	259	MET	3.4
1	B	315	GLY	3.4
1	F	346	LYS	3.4
1	F	31	SER	3.4
1	F	334	ILE	3.3
1	F	42	SER	3.3
1	F	131	SER	3.3
1	E	260	ARG	3.3

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Mol	Chain	Res	Type	RSRZ
1	F	214	GLY	3.3
1	F	339	GLU	3.3
1	F	330	LEU	3.3
1	A	342	GLN	3.3
1	F	125	THR	3.3
1	B	347	GLU	3.3
1	E	314	THR	3.3
1	D	213	HIS	3.3
1	E	328	CYS	3.2
1	E	19	MET	3.2
1	F	323	ALA	3.2
1	A	29	THR	3.2
1	E	326	TYR	3.2
1	C	345	ALA	3.2
1	D	19	MET	3.2
1	E	311	ASP	3.2
1	F	256	ALA	3.2
1	F	190	ILE	3.2
1	B	340	ARG	3.2
1	A	345	ALA	3.2
1	B	310	VAL	3.2
1	A	249	ASP	3.2
1	A	341	ALA	3.1
1	A	311	ASP	3.1
1	A	187	LEU	3.1
1	F	29	THR	3.1
1	C	42	SER	3.1
1	C	114	MET	3.1
1	A	238	LYS	3.1
1	F	132	TRP	3.1
1	A	290	GLY	3.1
1	C	346	LYS	3.1
1	E	114	MET	3.1
1	F	114	MET	3.1
1	C	326	TYR	3.1
1	E	26	VAL	3.1
1	A	301	LEU	3.1
1	D	214	GLY	3.1
1	E	149	LEU	3.1
1	D	102	MET	3.1
1	F	312	LYS	3.0
1	E	304	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
1	F	251	THR	3.0
1	C	312	LYS	3.0
1	B	17	PRO	3.0
1	F	331	PRO	3.0
1	A	215	ASP	3.0
1	B	148	ASP	3.0
1	F	55	LEU	3.0
1	F	102	MET	3.0
1	E	94	TYR	3.0
1	A	147	GLY	3.0
1	C	259	MET	3.0
1	C	314	THR	3.0
1	E	323	ALA	3.0
1	A	51	ILE	3.0
1	A	289	LEU	3.0
1	F	118	LEU	3.0
1	A	27	GLN	3.0
1	B	311	ASP	3.0
1	E	148	ASP	3.0
1	F	47	ALA	3.0
1	A	245	GLU	2.9
1	D	336	ARG	2.9
1	A	306	GLY	2.9
1	A	347	GLU	2.9
1	E	329	ARG	2.9
1	C	27	GLN	2.9
1	F	104	THR	2.9
1	A	265	MET	2.9
1	E	305	VAL	2.9
1	F	321	GLN	2.9
1	A	186	TYR	2.9
1	D	148	ASP	2.9
1	F	119	ASP	2.9
1	A	134	ILE	2.8
1	E	150	LEU	2.8
1	F	37	ILE	2.8
1	F	34	PRO	2.8
1	A	310	VAL	2.8
1	A	31	SER	2.8
1	F	347	GLU	2.8
1	B	144	ASN	2.8
1	F	36	LYS	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	330	LEU	2.8
1	D	310	VAL	2.8
1	C	316	LEU	2.8
1	C	334	ILE	2.8
1	A	298	ALA	2.8
1	C	148	ASP	2.8
1	B	339	GLU	2.8
1	D	39	ILE	2.8
1	E	348	ALA	2.8
1	F	193	SER	2.8
1	F	319	GLU	2.8
1	A	258	MET	2.8
1	A	319	GLU	2.7
1	E	308	TRP	2.7
1	C	295	LYS	2.7
1	F	260	ARG	2.7
1	A	275	ASP	2.7
1	E	24	VAL	2.7
1	F	53	VAL	2.7
1	F	100	GLY	2.7
1	F	340	ARG	2.7
1	D	349	PRO	2.7
1	C	147	GLY	2.7
1	C	155	TYR	2.7
1	D	162	MET	2.7
1	E	151	ASN	2.7
1	E	334	ILE	2.7
1	B	113	THR	2.7
1	A	323	ALA	2.7
1	A	295	LYS	2.7
1	A	34	PRO	2.7
1	F	265	MET	2.7
1	F	46	TRP	2.7
1	A	327	VAL	2.7
1	A	322	LYS	2.7
1	B	322	LYS	2.7
1	B	69	PRO	2.6
1	A	246	ILE	2.6
1	E	213	HIS	2.6
1	E	321	GLN	2.6
1	A	336	ARG	2.6
1	A	129	PRO	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	343	GLY	2.6
1	C	246	ILE	2.6
1	D	35	GLN	2.6
1	F	216	ILE	2.6
1	B	314	THR	2.6
1	A	252	VAL	2.6
1	E	324	GLN	2.6
1	A	18	PHE	2.6
1	F	21	PRO	2.6
1	F	51	ILE	2.6
1	E	65	GLN	2.6
1	F	147	GLY	2.6
1	F	332	PRO	2.6
1	A	210	ALA	2.6
1	A	296	ASP	2.5
1	D	151	ASN	2.5
1	D	309	LYS	2.5
1	F	363	LEU	2.5
1	B	238	LYS	2.5
1	B	336	ARG	2.5
1	E	28	VAL	2.5
1	B	151	ASN	2.5
1	B	154	LEU	2.5
1	D	333	ARG	2.5
1	E	307	ARG	2.5
1	A	148	ASP	2.5
1	F	151	ASN	2.5
1	A	255	PHE	2.5
1	E	146	HIS	2.5
1	F	94	TYR	2.5
1	F	155	TYR	2.5
1	A	316	LEU	2.5
1	C	25	HIS	2.5
1	E	17	PRO	2.5
1	A	325	ASP	2.5
1	E	254	ALA	2.5
1	E	54	HIS	2.5
1	A	294	ALA	2.5
1	A	28	VAL	2.5
1	A	320	GLY	2.4
1	F	215	ASP	2.4
1	A	300	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	336	ARG	2.4
1	D	109	PRO	2.4
1	A	251	THR	2.4
1	B	104	THR	2.4
1	D	165	ILE	2.4
1	B	111	TYR	2.4
1	B	102	MET	2.4
1	E	20	PRO	2.4
1	D	144	ASN	2.4
1	A	30	HIS	2.4
1	C	321	GLN	2.4
1	E	333	ARG	2.4
1	E	215	ASP	2.4
1	E	319	GLU	2.3
1	F	101	ASP	2.3
1	C	140	THR	2.3
1	C	253	LEU	2.3
1	E	108	LEU	2.3
1	E	210	ALA	2.3
1	F	361	VAL	2.3
1	C	151	ASN	2.3
1	C	35	GLN	2.3
1	D	253	LEU	2.3
1	F	181	THR	2.3
1	A	239	ILE	2.3
1	F	150	LEU	2.3
1	E	327	VAL	2.3
1	A	303	PHE	2.3
1	E	60	LYS	2.3
1	A	55	LEU	2.3
1	E	293	THR	2.3
1	C	323	ALA	2.3
1	F	210	ALA	2.3
1	A	17	PRO	2.3
1	B	147	GLY	2.3
1	B	313	LEU	2.3
1	A	190	ILE	2.3
1	A	292	TYR	2.3
1	B	306	GLY	2.3
1	E	315	GLY	2.3
1	C	310	VAL	2.3
1	E	69	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	46	TRP	2.3
1	C	335	ARG	2.3
1	C	154	LEU	2.3
1	F	148	ASP	2.2
1	F	302	GLU	2.2
1	E	25	HIS	2.2
1	F	99	VAL	2.2
1	E	33	PRO	2.2
1	F	230	LYS	2.2
1	A	317	SER	2.2
1	B	212	GLU	2.2
1	E	35	GLN	2.2
1	A	339	GLU	2.2
1	B	149	LEU	2.2
1	B	155	TYR	2.2
1	B	110	THR	2.2
1	B	103	ILE	2.2
1	B	68	LEU	2.2
1	E	350	THR	2.2
1	F	189	PHE	2.2
1	F	324	GLN	2.2
1	F	249	ASP	2.2
1	E	177	MET	2.2
1	A	281	HIS	2.2
1	F	50	ASN	2.2
1	D	305	VAL	2.2
1	A	209	GLN	2.2
1	F	238	LYS	2.2
1	C	254	ALA	2.2
1	F	109	PRO	2.2
1	E	200	PHE	2.2
1	D	150	LEU	2.2
1	F	110	THR	2.1
1	A	121	VAL	2.1
1	F	121	VAL	2.1
1	F	129	PRO	2.1
1	F	201	ILE	2.1
1	C	153	TYR	2.1
1	C	341	ALA	2.1
1	F	103	ILE	2.1
1	C	215	ASP	2.1
1	F	108	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	144	ASN	2.1
1	E	336	ARG	2.1
1	B	273	GLY	2.1
1	A	23	GLU	2.1
1	A	307	ARG	2.1
1	C	138	ALA	2.1
1	F	180	ARG	2.1
1	F	149	LEU	2.1
1	E	110	THR	2.1
1	A	47	ALA	2.1
1	A	331	PRO	2.1
1	B	326	TYR	2.1
1	D	155	TYR	2.1
1	F	194	PHE	2.1
1	A	212	GLU	2.1
1	D	104	THR	2.1
1	E	102	MET	2.1
1	A	111	TYR	2.1
1	D	147	GLY	2.1
1	F	144	ASN	2.1
1	B	348	ALA	2.1
1	A	39	ILE	2.1
1	C	300	ILE	2.1
1	E	300	ILE	2.1
1	C	22	ARG	2.1
1	F	122	ARG	2.1
1	E	68	LEU	2.1
1	E	104	THR	2.0
1	A	178	ASP	2.0
1	A	102	MET	2.0
1	D	114	MET	2.0
1	E	208	ARG	2.0
1	A	201	ILE	2.0
1	A	263	ILE	2.0
1	A	267	ALA	2.0
1	B	210	ALA	2.0
1	D	106	GLU	2.0
1	C	102	MET	2.0
1	A	262	LYS	2.0
1	F	273	GLY	2.0
1	F	154	LEU	2.0
1	D	38	GLU	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	309	LYS	2.0
1	A	37	ILE	2.0
1	A	175	SER	2.0
1	A	20	PRO	2.0
1	A	185	PRO	2.0
1	F	254	ALA	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	FE	D	370	1/1	0.13	-1.76	48,48,48,48	0
2	FE	E	370	1/1	0.13	-2.02	48,48,48,48	0
2	FE	B	370	1/1	0.12	-2.65	48,48,48,48	0
2	FE	C	371	1/1	0.06	-2.79	50,50,50,50	0
2	FE	D	371	1/1	0.06	-3.26	50,50,50,50	0
2	FE	B	371	1/1	0.11	-3.40	49,49,49,49	0
2	FE	C	370	1/1	0.07	-3.95	48,48,48,48	0
2	FE	F	370	1/1	0.06	-4.03	48,48,48,48	0
2	FE	E	371	1/1	0.02	-4.04	49,49,49,49	0
2	FE	A	370	1/1	0.07	-4.07	48,48,48,48	0
2	FE	A	371	1/1	0.05	-4.13	50,50,50,50	0
2	FE	F	371	1/1	0.04	-5.28	49,49,49,49	0

6.5 Other polymers ⓘ

There are no such residues in this entry.