



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:52 AM 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 X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

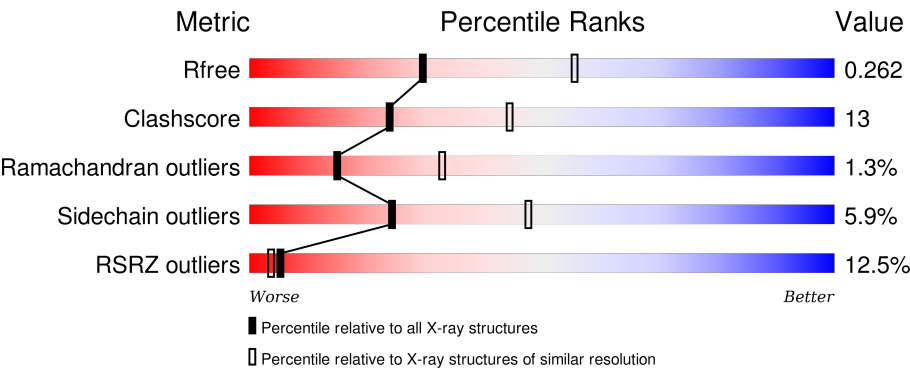
# 1 Overall quality at a glance i

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 <sub>free</sub>	91344	3152 (2.70-2.62)
Clashscore	102246	3524 (2.70-2.62)
Ramachandran outliers	100387	3469 (2.70-2.62)
Sidechain outliers	100360	3469 (2.70-2.62)
RSRZ outliers	91569	3161 (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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	
1	B	363	
1	C	363	
1	D	363	
1	E	363	

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Mol	Chain	Length	Quality of chain
1	F	363	<div><div></div><div>20%</div><div>72%</div><div>20%</div><div>• 5%</div></div>

## 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 (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

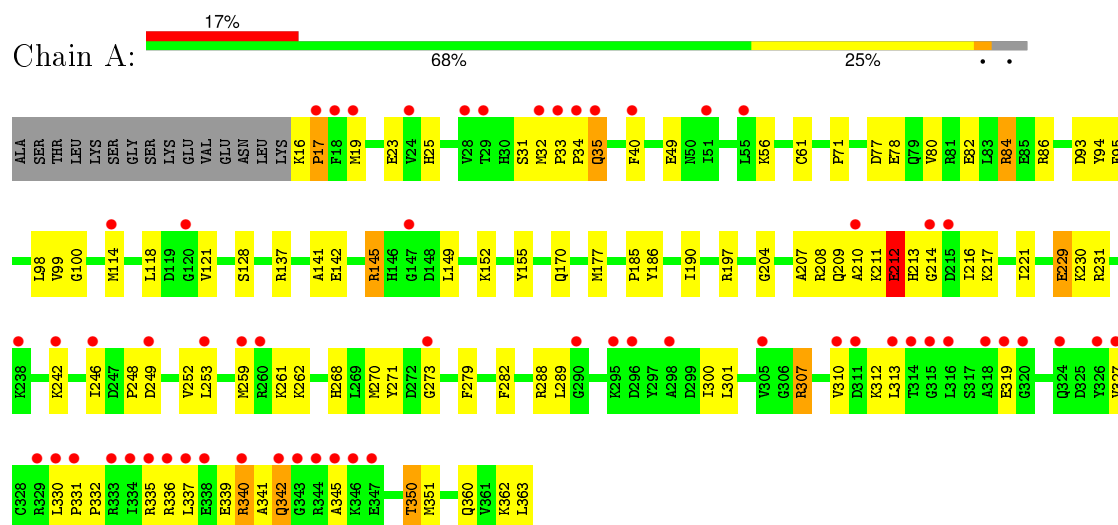
- Molecule 3 is water.

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

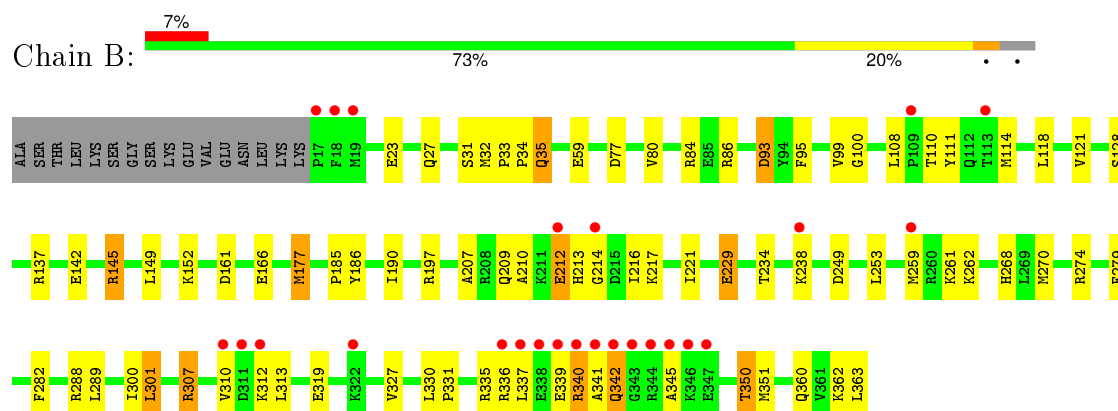
### 3 Residue-property plots

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.

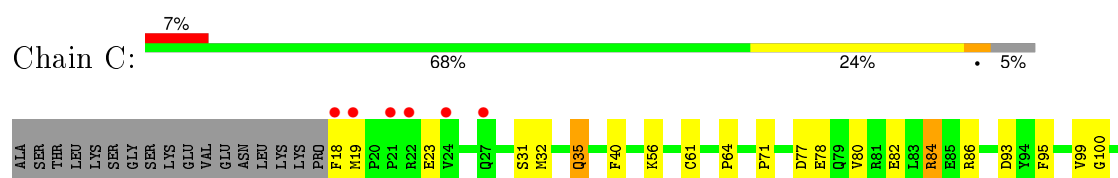
#### • Molecule 1: ACYL-[ACYL-CARRIER-PROTEIN] DESATURASE

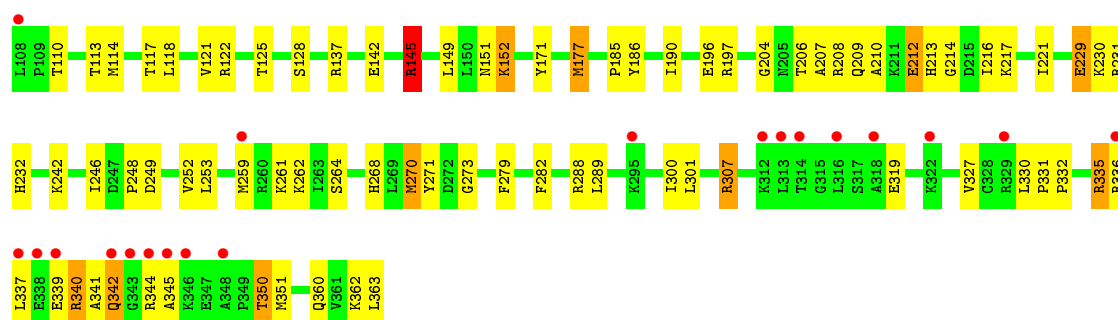


#### • Molecule 1: ACYL-[ACYL-CARRIER-PROTEIN] DESATURASE

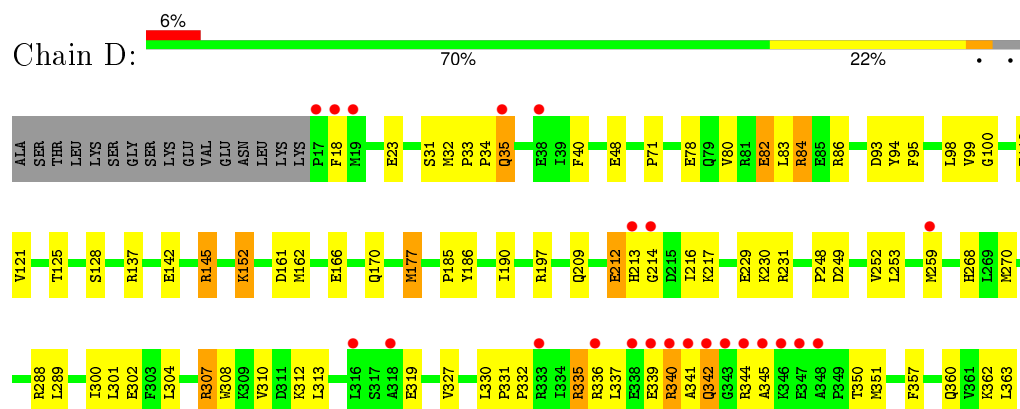


#### • Molecule 1: ACYL-[ACYL-CARRIER-PROTEIN] DESATURASE

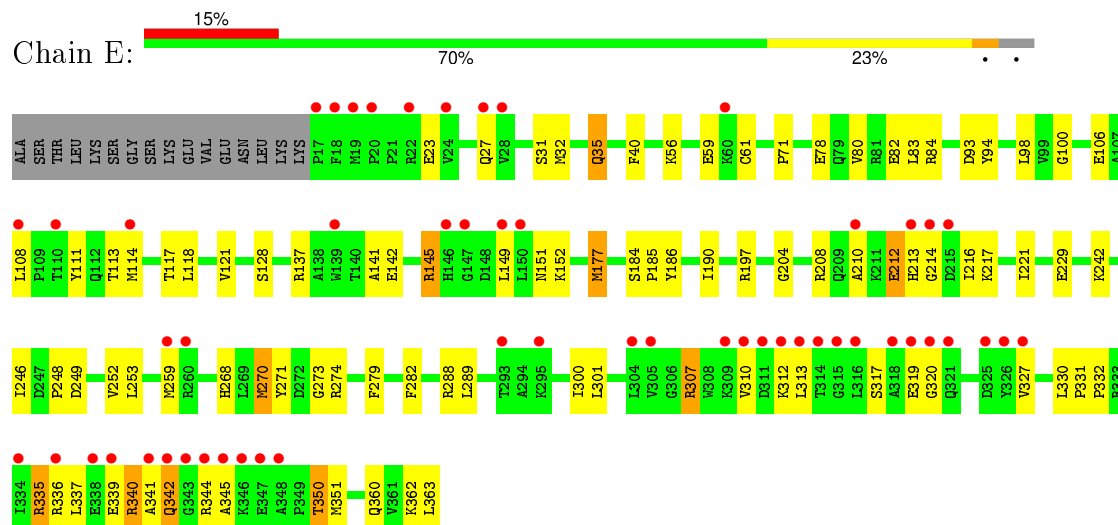




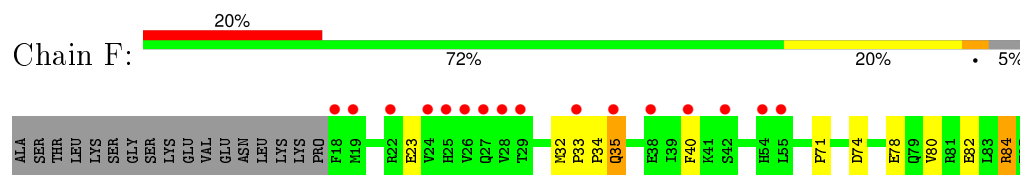
• Molecule 1: ACYL-[ACYL-CARRIER-PROTEIN] DESATURASE

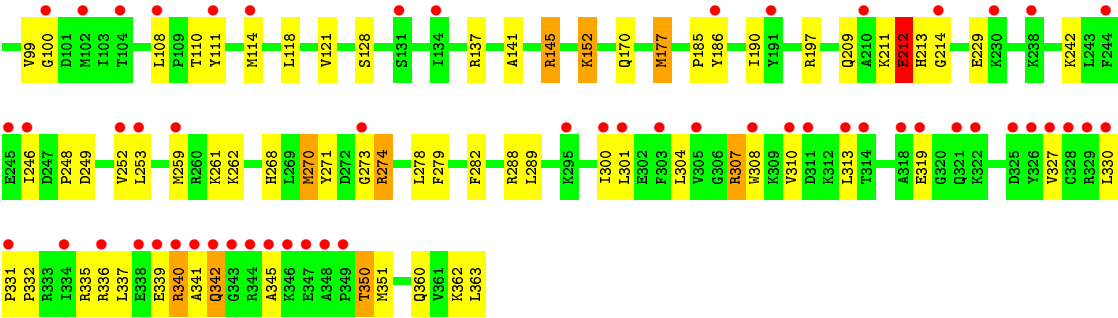


• Molecule 1: ACYL-[ACYL-CARRIER-PROTEIN] DESATURASE



• 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, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	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 (5.36%)	DCC
Wilson B-factor (Å <sup>2</sup> )	43.2	Xtriage
Anisotropy	0.476	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 66.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	1 of 66623 reflections (0.002%)	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	17055	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	0.65	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 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	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

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 13.

All (439) 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	1.39	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
1:B:336:ARG:O	1:B:339:GLU:HB3	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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	Interatomic distance (Å)	Clash overlap (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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:341:ALA:HB1	1:D:345:ALA:HB2	1.86	0.58
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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	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%)	11	25
1	B	345/363 (95%)	324 (94%)	17 (5%)	4 (1%)	16	35
1	C	344/363 (95%)	321 (93%)	19 (6%)	4 (1%)	16	35
1	D	345/363 (95%)	316 (92%)	25 (7%)	4 (1%)	16	35
1	E	345/363 (95%)	317 (92%)	24 (7%)	4 (1%)	16	35
1	F	344/363 (95%)	317 (92%)	22 (6%)	5 (2%)	13	28
All	All	2069/2178 (95%)	1912 (92%)	130 (6%)	27 (1%)	15	33

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%)	286 (95%)	16 (5%)	28	54
1	B	301/315 (96%)	284 (94%)	17 (6%)	26	50
1	C	300/315 (95%)	279 (93%)	21 (7%)	19	38
1	D	301/315 (96%)	284 (94%)	17 (6%)	26	50
1	E	301/315 (96%)	281 (93%)	20 (7%)	21	42
1	F	300/315 (95%)	284 (95%)	16 (5%)	28	54
All	All	1805/1890 (96%)	1698 (94%)	107 (6%)	24	48

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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 [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 carbohydrates 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	348/363 (95%)	0.88	60 (17%) <b>2</b> <b>1</b>	31, 33, 34, 50	0
1	B	347/363 (95%)	0.36	25 (7%) <b>18</b> <b>16</b>	31, 33, 34, 48	0
1	C	346/363 (95%)	0.40	26 (7%) <b>17</b> <b>14</b>	22, 33, 34, 36	0
1	D	347/363 (95%)	0.29	23 (6%) <b>22</b> <b>19</b>	31, 33, 34, 44	0
1	E	347/363 (95%)	0.84	54 (15%) <b>3</b> <b>2</b>	31, 33, 34, 50	0
1	F	346/363 (95%)	1.13	72 (20%) <b>1</b> <b>1</b>	31, 33, 34, 45	0
All	All	2081/2178 (95%)	0.65	260 (12%) <b>5</b> <b>4</b>	22, 33, 34, 50	0

All (260) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	345	ALA	11.7
1	E	345	ALA	10.1
1	E	338	GLU	9.0
1	B	345	ALA	9.0
1	E	344	ARG	8.6
1	D	344	ARG	8.3
1	F	345	ALA	8.1
1	F	344	ARG	7.9
1	B	341	ALA	7.6
1	C	338	GLU	7.6
1	A	338	GLU	7.3
1	C	18	PHE	7.1
1	F	341	ALA	7.1
1	B	342	GLN	6.7
1	F	35	GLN	6.7
1	D	346	LYS	6.5
1	B	343	GLY	6.3
1	F	338	GLU	6.3
1	F	310	VAL	6.3

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Mol	Chain	Res	Type	RSRZ
1	E	346	LYS	6.1
1	F	329	ARG	6.0
1	A	19	MET	6.0
1	F	24	VAL	5.9
1	C	19	MET	5.9
1	D	341	ALA	5.7
1	E	18	PHE	5.6
1	F	18	PHE	5.6
1	A	260	ARG	5.5
1	E	313	LEU	5.4
1	D	347	GLU	5.3
1	B	344	ARG	5.1
1	A	344	ARG	5.1
1	E	24	VAL	5.0
1	C	344	ARG	5.0
1	A	253	LEU	4.9
1	F	26	VAL	4.9
1	C	342	GLN	4.8
1	C	339	GLU	4.7
1	D	17	PRO	4.7
1	B	19	MET	4.7
1	F	252	VAL	4.7
1	F	27	GLN	4.6
1	A	35	GLN	4.6
1	E	305	VAL	4.5
1	A	334	ILE	4.5
1	D	339	GLU	4.4
1	A	345	ALA	4.4
1	E	347	GLU	4.4
1	F	343	GLY	4.4
1	F	339	GLU	4.3
1	F	322	LYS	4.2
1	E	339	GLU	4.2
1	E	341	ALA	4.2
1	A	305	VAL	4.1
1	E	343	GLY	4.1
1	C	322	LYS	4.1
1	D	342	GLN	4.1
1	F	330	LEU	4.1
1	E	342	GLN	4.1
1	F	25	HIS	4.1
1	E	314	THR	4.1

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Mol	Chain	Res	Type	RSRZ
1	A	340	ARG	4.0
1	B	340	ARG	4.0
1	B	346	LYS	4.0
1	A	329	ARG	3.9
1	A	335	ARG	3.9
1	D	340	ARG	3.9
1	F	19	MET	3.9
1	F	342	GLN	3.9
1	E	310	VAL	3.9
1	F	28	VAL	3.9
1	F	318	ALA	3.9
1	F	245	GLU	3.8
1	F	253	LEU	3.8
1	F	301	LEU	3.8
1	E	27	GLN	3.8
1	A	318	ALA	3.8
1	A	313	LEU	3.8
1	F	325	ASP	3.8
1	E	17	PRO	3.8
1	D	343	GLY	3.8
1	D	338	GLU	3.7
1	F	328	CYS	3.7
1	A	34	PRO	3.7
1	A	18	PHE	3.7
1	C	24	VAL	3.7
1	A	259	MET	3.7
1	A	40	PHE	3.7
1	B	347	GLU	3.7
1	A	24	VAL	3.6
1	A	120	GLY	3.6
1	F	244	PHE	3.6
1	B	339	GLU	3.6
1	F	186	TYR	3.6
1	F	311	ASP	3.6
1	B	338	GLU	3.6
1	E	348	ALA	3.5
1	A	347	GLU	3.5
1	B	214	GLY	3.5
1	F	336	ARG	3.4
1	B	17	PRO	3.4
1	E	295	LYS	3.4
1	A	326	TYR	3.4

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Mol	Chain	Res	Type	RSRZ
1	F	214	GLY	3.4
1	A	210	ALA	3.4
1	C	329	ARG	3.4
1	F	346	LYS	3.4
1	E	319	GLU	3.4
1	F	38	GLU	3.4
1	D	18	PHE	3.4
1	A	290	GLY	3.4
1	B	337	LEU	3.3
1	F	22	ARG	3.3
1	C	318	ALA	3.3
1	A	337	LEU	3.3
1	A	336	ARG	3.3
1	A	319	GLU	3.3
1	A	114	MET	3.3
1	A	346	LYS	3.2
1	A	320	GLY	3.2
1	C	346	LYS	3.2
1	E	304	LEU	3.2
1	F	327	VAL	3.2
1	F	40	PHE	3.2
1	F	314	THR	3.2
1	C	27	GLN	3.2
1	D	259	MET	3.1
1	C	312	LYS	3.1
1	D	19	MET	3.1
1	A	51	ILE	3.0
1	F	295	LYS	3.0
1	E	19	MET	3.0
1	E	312	LYS	3.0
1	A	333	ARG	3.0
1	C	336	ARG	3.0
1	F	259	MET	3.0
1	F	42	SER	3.0
1	C	316	LEU	3.0
1	B	259	MET	3.0
1	D	213	HIS	3.0
1	E	213	HIS	3.0
1	F	313	LEU	3.0
1	E	260	ARG	3.0
1	F	340	ARG	3.0
1	F	131	SER	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	330	LEU	2.9
1	A	246	ILE	2.9
1	E	327	VAL	2.9
1	B	311	ASP	2.9
1	E	318	ALA	2.9
1	F	331	PRO	2.9
1	E	293	THR	2.9
1	D	318	ALA	2.9
1	D	336	ARG	2.8
1	A	314	THR	2.8
1	F	104	THR	2.8
1	B	109	PRO	2.8
1	A	215	ASP	2.8
1	F	114	MET	2.8
1	E	326	TYR	2.8
1	E	325	ASP	2.8
1	B	312	LYS	2.7
1	F	334	ILE	2.7
1	A	33	PRO	2.7
1	C	314	THR	2.7
1	D	214	GLY	2.7
1	B	336	ARG	2.7
1	E	22	ARG	2.7
1	E	149	LEU	2.7
1	C	345	ALA	2.6
1	E	316	LEU	2.6
1	A	17	PRO	2.6
1	A	249	ASP	2.6
1	F	319	GLU	2.6
1	E	147	GLY	2.6
1	F	54	HIS	2.6
1	F	300	ILE	2.6
1	F	326	TYR	2.5
1	E	214	GLY	2.5
1	F	29	THR	2.5
1	E	311	ASP	2.5
1	E	259	MET	2.5
1	C	259	MET	2.5
1	C	295	LYS	2.5
1	A	55	LEU	2.5
1	A	32	MET	2.5
1	E	336	ARG	2.5

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	342	GLN	2.5
1	A	29	THR	2.5
1	A	242	LYS	2.5
1	F	321	GLN	2.4
1	F	238	LYS	2.4
1	A	310	VAL	2.4
1	F	134	ILE	2.4
1	F	305	VAL	2.4
1	C	343	GLY	2.4
1	A	296	ASP	2.4
1	F	33	PRO	2.4
1	F	303	PHE	2.4
1	B	113	THR	2.4
1	D	333	ARG	2.4
1	A	315	GLY	2.4
1	B	322	LYS	2.4
1	E	215	ASP	2.4
1	D	316	LEU	2.3
1	B	310	VAL	2.3
1	F	55	LEU	2.3
1	F	348	ALA	2.3
1	A	327	VAL	2.3
1	B	212	GLU	2.3
1	E	60	LYS	2.3
1	E	108	LEU	2.3
1	E	150	LEU	2.3
1	D	348	ALA	2.3
1	F	246	ILE	2.3
1	A	147	GLY	2.3
1	F	273	GLY	2.3
1	A	295	LYS	2.3
1	F	108	LEU	2.3
1	E	114	MET	2.3
1	A	316	LEU	2.2
1	E	20	PRO	2.2
1	A	298	ALA	2.2
1	A	28	VAL	2.2
1	A	238	LYS	2.2
1	C	313	LEU	2.2
1	D	38	GLU	2.2
1	E	28	VAL	2.2
1	E	321	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	214	GLY	2.1
1	F	347	GLU	2.1
1	F	349	PRO	2.1
1	C	22	ARG	2.1
1	B	238	LYS	2.1
1	F	100	GLY	2.1
1	E	146	HIS	2.1
1	F	308	TRP	2.1
1	E	320	GLY	2.1
1	E	334	ILE	2.1
1	D	35	GLN	2.1
1	C	337	LEU	2.1
1	E	315	GLY	2.1
1	A	311	ASP	2.1
1	A	343	GLY	2.1
1	A	324	GLN	2.1
1	F	102	MET	2.1
1	F	210	ALA	2.1
1	C	108	LEU	2.0
1	E	210	ALA	2.0
1	C	21	PRO	2.0
1	E	139	TRP	2.0
1	E	309	LYS	2.0
1	E	110	THR	2.0
1	A	331	PRO	2.0
1	B	18	PHE	2.0
1	A	273	GLY	2.0
1	F	230	LYS	2.0
1	C	348	ALA	2.0
1	F	111	TYR	2.0
1	F	191	TYR	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 [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. 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, 95<sup>th</sup> 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	FE	A	371	1/1	0.93	0.07	-2.46	50,50,50,50	0
2	FE	E	371	1/1	0.99	0.05	-2.54	49,49,49,49	0
2	FE	E	370	1/1	0.96	0.06	-2.74	48,48,48,48	0
2	FE	A	370	1/1	0.94	0.07	-2.83	48,48,48,48	0
2	FE	F	371	1/1	0.90	0.08	-3.28	49,49,49,49	0
2	FE	B	370	1/1	0.92	0.06	-4.00	48,48,48,48	0
2	FE	C	371	1/1	0.97	0.03	-4.42	50,50,50,50	0
2	FE	C	370	1/1	0.95	0.04	-4.50	48,48,48,48	0
2	FE	D	371	1/1	0.97	0.03	-4.86	50,50,50,50	0
2	FE	B	371	1/1	0.98	0.06	-4.93	49,49,49,49	0
2	FE	F	370	1/1	0.96	0.04	-5.34	48,48,48,48	0
2	FE	D	370	1/1	0.94	0.04	-5.44	48,48,48,48	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.