



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 04:46 PM GMT

PDB ID : 1OQ7
Title : The crystal structure of the iron free (Apo-)form of Stearoyl Acyl Carrier Protein Desaturase from Ricinus Communis (Castor Bean).
Authors : Moche, M.; Shanklin, J.; Ghoshal, A.K.; Lindqvist, Y.
Deposited on : 2003-03-07
Resolution : 3.20 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>

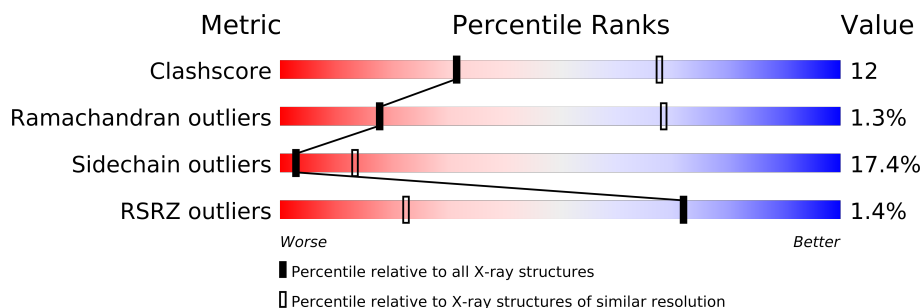
The following versions of software and data (see [references](#)) were used in the production of this report:

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 3.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	79885	1078 (3.26-3.14)
Ramachandran outliers	78287	1059 (3.26-3.14)
Sidechain outliers	78261	1058 (3.26-3.14)
RSRZ outliers	66119	1825 (3.30-3.10)

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	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	SR	C	364	-	X
2	SR	D	364	-	X

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 16848 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	346	Total	C	N	O	S	36	0	0
			2806	1780	487	525	14			
1	B	346	Total	C	N	O	S	36	0	0
			2806	1780	487	525	14			
1	C	346	Total	C	N	O	S	36	0	0
			2806	1780	487	525	14			
1	D	346	Total	C	N	O	S	36	0	0
			2806	1780	487	525	14			
1	E	346	Total	C	N	O	S	36	0	0
			2806	1780	487	525	14			
1	F	346	Total	C	N	O	S	36	0	0
			2806	1780	487	525	14			

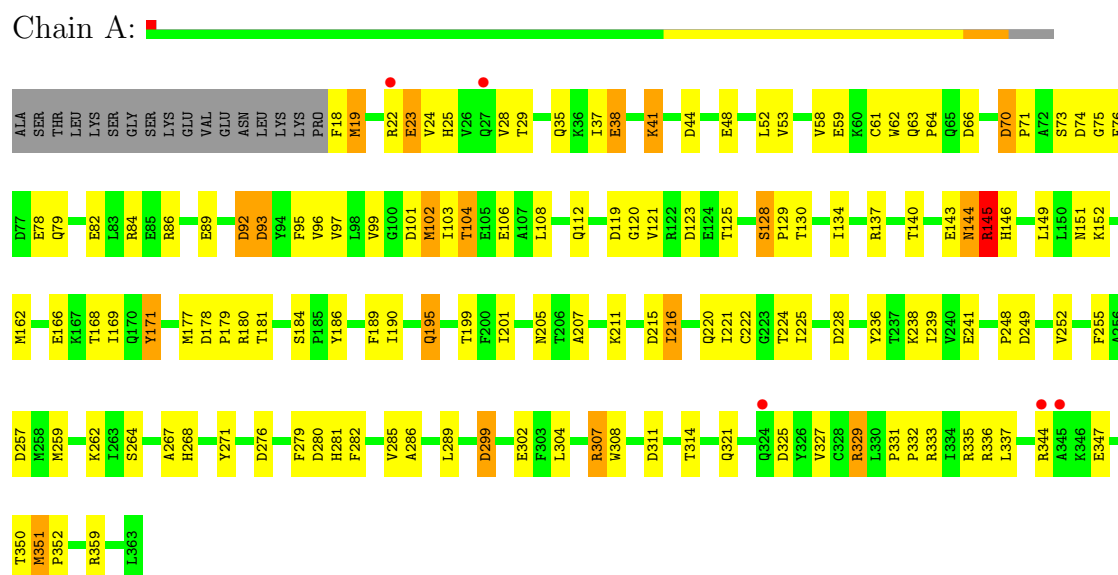
- Molecule 2 is STRONTIUM ION (three-letter code: SR) (formula: Sr).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	2	Total	Sr	0	0
			2	2		
2	E	2	Total	Sr	0	0
			2	2		
2	B	3	Total	Sr	0	0
			3	3		
2	C	2	Total	Sr	0	0
			2	2		
2	A	1	Total	Sr	0	0
			1	1		
2	F	2	Total	Sr	0	0
			2	2		

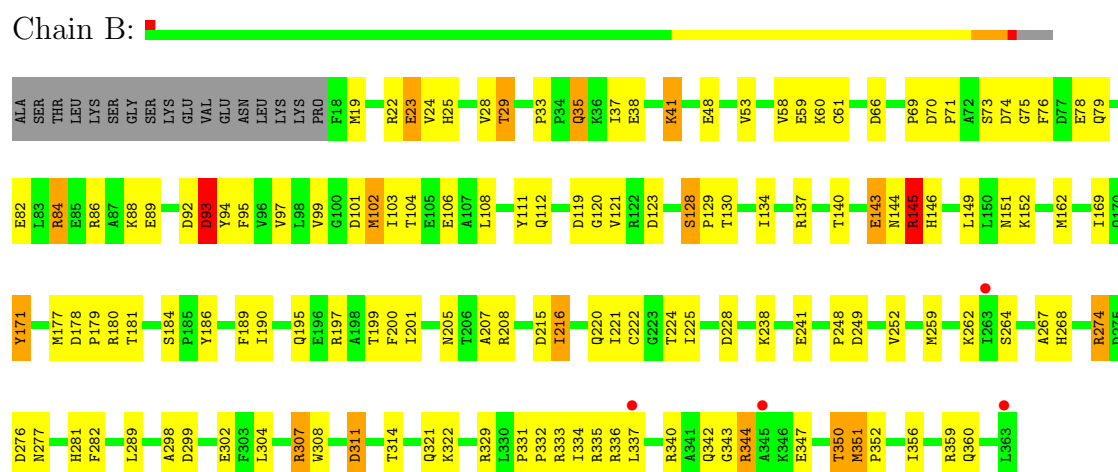
3 Residue-property plots

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

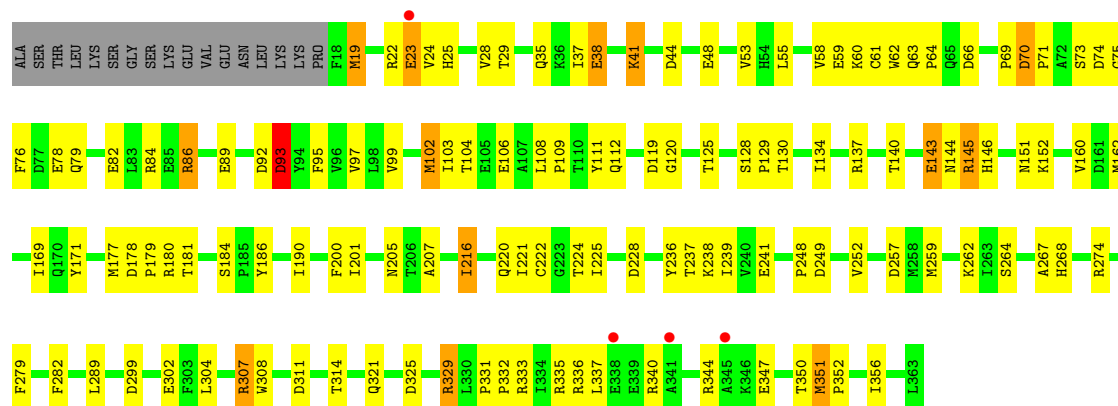


• Molecule 1: Acyl-[acyl-carrier protein] desaturase



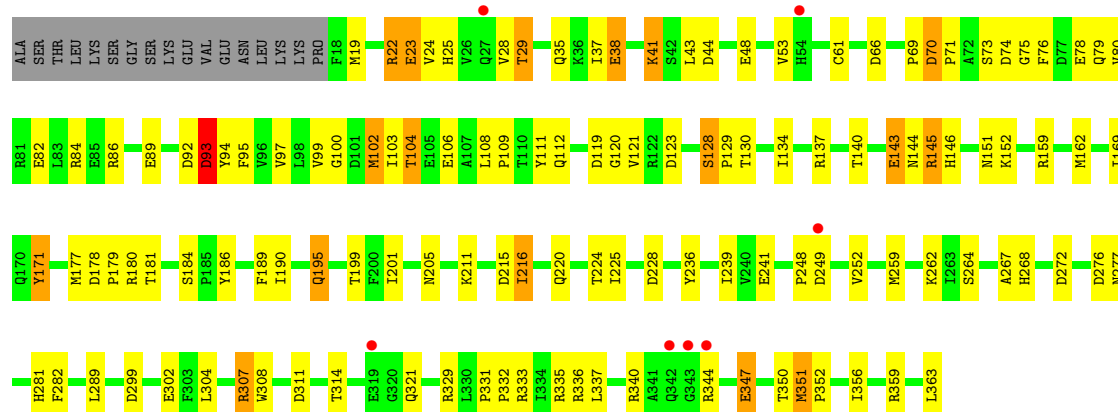
• Molecule 1: Acyl-[acyl-carrier protein] desaturase





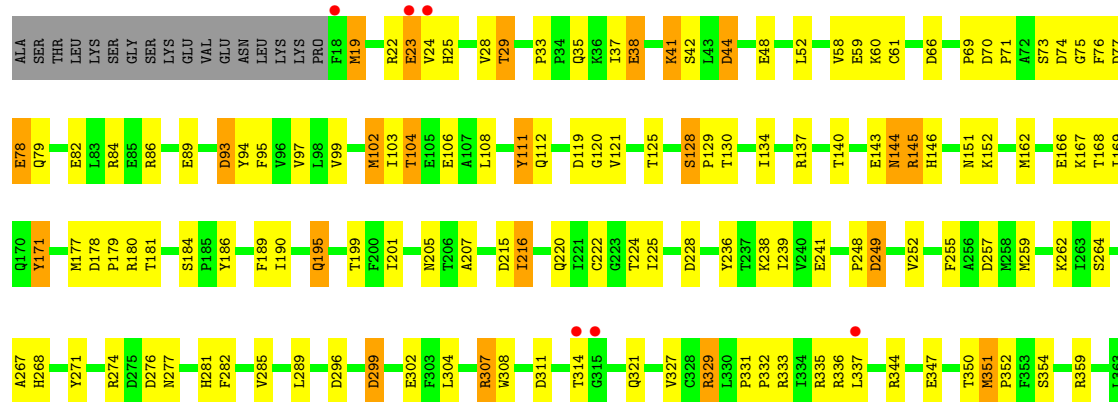
• Molecule 1: Acyl-[acyl-carrier protein] desaturase

Chain D:



• Molecule 1: Acyl-[acyl-carrier protein] desaturase

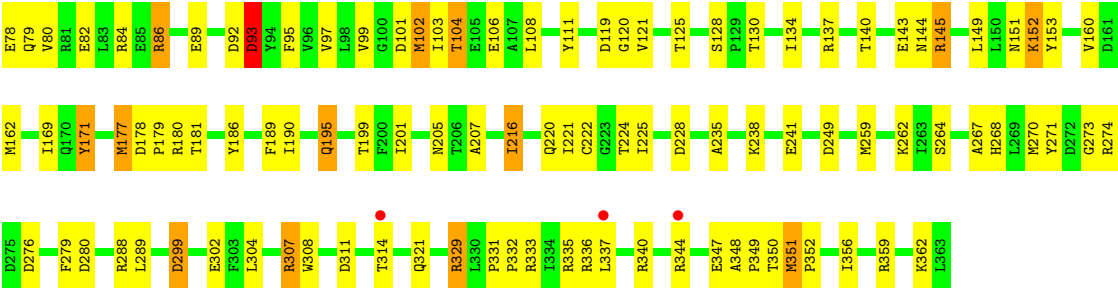
Chain E:



• Molecule 1: Acyl-[acyl-carrier protein] desaturase

Chain F:





4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α , β , γ	188.03Å 188.03Å 82.05Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.96 – 3.20 19.90 – 3.20	Depositor EDS
% Data completeness (in resolution range)	92.5 (19.96-3.20) 92.5 (19.90-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.25 (at 3.22Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.229 , 0.257 (Not available) , (Not available)	Depositor DCC
R_{free} test set	NotAvailable	DCC
Wilson B-factor (Å ²)	77.9	Xtriage
Anisotropy	0.010	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , -20.0	EDS
Estimated twinning fraction	0.069 for -h,-k,l 0.309 for h,-h-k,-l 0.069 for -k,-h,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Outliers	0 of 49227 reflections	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	16848	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.18% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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: SR

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	0.79	3/2874 (0.1%)	0.94	16/3892 (0.4%)
1	B	0.79	2/2874 (0.1%)	0.94	14/3892 (0.4%)
1	C	0.75	1/2874 (0.0%)	0.92	12/3892 (0.3%)
1	D	0.76	1/2874 (0.0%)	0.90	13/3892 (0.3%)
1	E	0.74	2/2874 (0.1%)	0.91	12/3892 (0.3%)
1	F	0.81	1/2874 (0.0%)	0.94	13/3892 (0.3%)
All	All	0.77	10/17244 (0.1%)	0.92	80/23352 (0.3%)

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	82	GLU	CG-CD	8.85	1.65	1.51
1	B	82	GLU	CG-CD	7.42	1.63	1.51
1	A	82	GLU	CG-CD	7.27	1.62	1.51
1	D	82	GLU	CG-CD	6.94	1.62	1.51
1	C	82	GLU	CG-CD	6.41	1.61	1.51
1	E	82	GLU	CG-CD	6.30	1.61	1.51
1	A	166	GLU	CD-OE2	6.26	1.32	1.25
1	B	82	GLU	CD-OE2	5.67	1.31	1.25
1	E	78	GLU	CD-OE1	5.25	1.31	1.25
1	A	61	CYS	CB-SG	-5.05	1.73	1.81

All (80) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	74	ASP	CB-CG-OD2	8.91	126.32	118.30
1	B	74	ASP	CB-CG-OD2	8.04	125.53	118.30
1	F	92	ASP	CB-CG-OD2	7.74	125.27	118.30
1	C	92	ASP	CB-CG-OD2	7.59	125.13	118.30
1	B	84	ARG	NE-CZ-NH1	7.46	124.03	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	66	ASP	CB-CG-OD2	7.44	124.99	118.30
1	E	74	ASP	CB-CG-OD2	7.37	124.93	118.30
1	C	70	ASP	CB-CG-OD2	7.19	124.78	118.30
1	F	93	ASP	CB-CG-OD2	7.17	124.76	118.30
1	B	92	ASP	CB-CG-OD2	7.16	124.74	118.30
1	C	86	ARG	NE-CZ-NH1	7.11	123.85	120.30
1	F	86	ARG	NE-CZ-NH1	7.07	123.83	120.30
1	E	119	ASP	CB-CG-OD2	7.02	124.62	118.30
1	C	66	ASP	CB-CG-OD2	6.99	124.59	118.30
1	F	66	ASP	CB-CG-OD2	6.98	124.59	118.30
1	B	145	ARG	NE-CZ-NH1	6.79	123.69	120.30
1	D	74	ASP	CB-CG-OD2	6.74	124.36	118.30
1	A	66	ASP	CB-CG-OD2	6.52	124.17	118.30
1	A	92	ASP	CB-CG-OD2	6.49	124.14	118.30
1	F	74	ASP	CB-CG-OD2	6.38	124.04	118.30
1	D	92	ASP	CB-CG-OD2	6.37	124.03	118.30
1	E	178	ASP	CB-CG-OD2	6.36	124.03	118.30
1	D	272	ASP	CB-CG-OD2	6.36	124.02	118.30
1	F	178	ASP	CB-CG-OD2	6.31	123.98	118.30
1	A	276	ASP	CB-CG-OD2	6.19	123.87	118.30
1	A	215	ASP	CB-CG-OD2	6.17	123.86	118.30
1	B	123	ASP	CB-CG-OD2	6.17	123.86	118.30
1	F	82	GLU	OE1-CD-OE2	-6.13	115.95	123.30
1	B	274	ARG	NE-CZ-NH1	6.08	123.34	120.30
1	D	215	ASP	CB-CG-OD2	6.00	123.70	118.30
1	E	44	ASP	CB-CG-OD2	6.00	123.70	118.30
1	C	44	ASP	CB-CG-OD2	5.96	123.67	118.30
1	C	74	ASP	CB-CG-OD2	5.96	123.66	118.30
1	D	70	ASP	CB-CG-OD2	5.95	123.66	118.30
1	B	276	ASP	CB-CG-OD2	5.93	123.64	118.30
1	B	215	ASP	CB-CG-OD2	5.88	123.59	118.30
1	D	119	ASP	CB-CG-OD2	5.86	123.58	118.30
1	A	257	ASP	CB-CG-OD2	5.86	123.57	118.30
1	D	276	ASP	CB-CG-OD2	5.85	123.57	118.30
1	A	145	ARG	NE-CZ-NH1	5.76	123.18	120.30
1	C	119	ASP	CB-CG-OD2	5.71	123.44	118.30
1	A	178	ASP	CB-CG-OD2	5.70	123.43	118.30
1	F	299	ASP	CB-CG-OD2	5.67	123.40	118.30
1	D	123	ASP	CB-CG-OD2	5.66	123.39	118.30
1	E	77	ASP	CB-CG-OD2	5.61	123.35	118.30
1	B	178	ASP	CB-CG-OD2	5.60	123.34	118.30
1	B	119	ASP	CB-CG-OD2	5.58	123.33	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	215	ASP	CB-CG-OD2	5.58	123.32	118.30
1	B	66	ASP	CB-CG-OD2	5.57	123.32	118.30
1	D	66	ASP	CB-CG-OD2	5.57	123.31	118.30
1	E	257	ASP	CB-CG-OD2	5.57	123.31	118.30
1	A	119	ASP	CB-CG-OD2	5.57	123.31	118.30
1	D	178	ASP	CB-CG-OD2	5.57	123.31	118.30
1	C	93	ASP	CB-CG-OD2	5.56	123.30	118.30
1	A	44	ASP	CB-CG-OD2	5.55	123.30	118.30
1	F	276	ASP	CB-CG-OD2	5.55	123.30	118.30
1	E	249	ASP	CB-CG-OD2	5.47	123.23	118.30
1	C	274	ARG	NE-CZ-NH1	5.47	123.04	120.30
1	A	70	ASP	CB-CG-OD2	5.45	123.20	118.30
1	F	280	ASP	CB-CG-OD2	5.44	123.20	118.30
1	B	101	ASP	CB-CG-OD2	5.37	123.13	118.30
1	A	101	ASP	CB-CG-OD2	5.36	123.12	118.30
1	E	296	ASP	CB-CG-OD2	5.34	123.10	118.30
1	B	311	ASP	CB-CG-OD2	5.30	123.07	118.30
1	A	299	ASP	CB-CG-OD2	5.28	123.05	118.30
1	D	44	ASP	CB-CG-OD2	5.28	123.05	118.30
1	B	93	ASP	CB-CG-OD2	5.25	123.02	118.30
1	C	257	ASP	CB-CG-OD2	5.23	123.00	118.30
1	A	280	ASP	CB-CG-OD2	5.22	123.00	118.30
1	F	101	ASP	CB-CG-OD2	5.22	123.00	118.30
1	E	276	ASP	CB-CG-OD2	5.20	122.98	118.30
1	A	123	ASP	CB-CG-OD2	5.19	122.97	118.30
1	C	325	ASP	CB-CG-OD2	5.17	122.96	118.30
1	E	299	ASP	CB-CG-OD2	5.17	122.96	118.30
1	D	93	ASP	CB-CG-OD2	5.16	122.95	118.30
1	C	178	ASP	CB-CG-OD2	5.16	122.94	118.30
1	A	325	ASP	CB-CG-OD2	5.15	122.94	118.30
1	F	19	MET	CG-SD-CE	5.03	108.25	100.20
1	D	159	ARG	NE-CZ-NH1	-5.03	117.79	120.30
1	F	119	ASP	CB-CG-OD2	5.01	122.81	118.30

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	2806	0	2748	64	0
1	B	2806	0	2748	71	0
1	C	2806	0	2748	63	0
1	D	2806	0	2748	63	0
1	E	2806	0	2748	71	0
1	F	2806	0	2748	75	0
2	A	1	0	0	0	0
2	B	3	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
All	All	16848	0	16488	381	0

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 12.

All (381) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:307:ARG:HG2	1:C:307:ARG:HH11	1.11	1.11
1:A:307:ARG:HG2	1:A:307:ARG:HH11	1.12	1.09
1:D:307:ARG:HH11	1:D:307:ARG:HG2	1.15	1.09
1:E:307:ARG:HG2	1:E:307:ARG:HH11	1.12	1.07
1:F:307:ARG:HH11	1:F:307:ARG:HG2	1.17	1.04
1:B:307:ARG:HH11	1:B:307:ARG:HG2	1.19	1.04
1:B:95:PHE:O	1:B:99:VAL:HG23	1.73	0.88
1:F:23:GLU:OE1	1:F:25:HIS:ND1	2.08	0.85
1:B:102:MET:HE3	1:B:151:ASN:HB2	1.57	0.85
1:B:75:GLY:O	1:B:79:GLN:HG3	1.76	0.84
1:C:307:ARG:HH11	1:C:307:ARG:CG	1.91	0.82
1:A:95:PHE:O	1:A:99:VAL:HG23	1.80	0.82
1:E:307:ARG:CG	1:E:307:ARG:HH11	1.92	0.82
1:C:95:PHE:O	1:C:99:VAL:HG23	1.80	0.81
1:A:23:GLU:OE1	1:A:25:HIS:ND1	2.14	0.81
1:B:23:GLU:OE1	1:B:25:HIS:ND1	2.14	0.80
1:E:23:GLU:OE1	1:E:25:HIS:ND1	2.15	0.80
1:D:95:PHE:O	1:D:99:VAL:HG23	1.82	0.79
1:F:102:MET:HE2	1:F:106:GLU:HG3	1.66	0.77
1:E:95:PHE:O	1:E:99:VAL:HG23	1.85	0.77

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:307:ARG:CG	1:A:307:ARG:HH11	1.96	0.76
1:D:102:MET:HE3	1:D:151:ASN:HB2	1.68	0.76
1:A:102:MET:HE3	1:A:151:ASN:HD22	1.51	0.76
1:E:307:ARG:HG2	1:E:307:ARG:NH1	1.93	0.76
1:E:102:MET:HE3	1:E:151:ASN:HD22	1.51	0.76
1:A:307:ARG:NH1	1:A:307:ARG:HG2	1.93	0.75
1:F:307:ARG:CG	1:F:307:ARG:HH11	1.99	0.75
1:E:84:ARG:NH2	1:F:71:PRO:O	2.20	0.74
1:E:71:PRO:O	1:F:84:ARG:NH2	2.21	0.74
1:B:103:ILE:HG23	1:B:169:ILE:HG13	1.70	0.74
1:D:23:GLU:OE1	1:D:25:HIS:ND1	2.21	0.74
1:E:71:PRO:HA	1:E:76:PHE:CD1	2.24	0.73
1:A:103:ILE:HG23	1:A:169:ILE:HG13	1.71	0.72
1:C:23:GLU:OE1	1:C:25:HIS:ND1	2.22	0.72
1:C:102:MET:HE3	1:C:151:ASN:HB2	1.70	0.72
1:F:103:ILE:HG23	1:F:169:ILE:HG13	1.71	0.72
1:D:103:ILE:HG23	1:D:169:ILE:HG13	1.72	0.72
1:C:84:ARG:NH2	1:D:71:PRO:O	2.22	0.71
1:E:102:MET:HE3	1:E:151:ASN:HB2	1.71	0.71
1:D:75:GLY:O	1:D:79:GLN:HG3	1.90	0.71
1:A:104:THR:HG23	1:A:267:ALA:HB2	1.72	0.70
1:B:307:ARG:CG	1:B:307:ARG:HH11	2.00	0.70
1:D:93:ASP:N	1:D:93:ASP:OD1	2.24	0.70
1:D:104:THR:HG23	1:D:267:ALA:HB2	1.73	0.70
1:C:102:MET:HE2	1:C:106:GLU:CG	2.22	0.69
1:F:102:MET:HE3	1:F:151:ASN:HB2	1.73	0.69
1:F:102:MET:HE2	1:F:106:GLU:CG	2.22	0.69
1:F:102:MET:CE	1:F:106:GLU:HG3	2.23	0.69
1:E:103:ILE:HG23	1:E:169:ILE:HG13	1.74	0.69
1:E:75:GLY:O	1:E:79:GLN:HG3	1.92	0.68
1:D:307:ARG:HH11	1:D:307:ARG:CG	1.99	0.67
1:A:84:ARG:NH2	1:B:71:PRO:O	2.27	0.67
1:E:104:THR:HG23	1:E:267:ALA:HB2	1.76	0.66
1:C:71:PRO:O	1:D:84:ARG:NH2	2.28	0.66
1:A:207:ALA:HB2	1:A:222:CYS:HB2	1.77	0.66
1:B:104:THR:HG23	1:B:267:ALA:HB2	1.77	0.66
1:F:307:ARG:HG2	1:F:307:ARG:NH1	1.98	0.66
1:C:307:ARG:NH1	1:C:307:ARG:HG2	1.91	0.65
1:C:93:ASP:OD1	1:C:93:ASP:N	2.26	0.65
1:F:75:GLY:O	1:F:79:GLN:HG3	1.96	0.65
1:E:207:ALA:HB2	1:E:222:CYS:HB2	1.77	0.65
1:C:104:THR:HG23	1:C:267:ALA:HB2	1.79	0.65

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:93:ASP:N	1:B:93:ASP:OD1	2.24	0.65
1:F:95:PHE:O	1:F:99:VAL:HG23	1.97	0.65
1:D:71:PRO:HA	1:D:76:PHE:CD1	2.32	0.64
1:A:149:LEU:HD21	1:A:221:ILE:HG23	1.79	0.64
1:F:71:PRO:HA	1:F:76:PHE:CD1	2.33	0.64
1:C:103:ILE:HG23	1:C:169:ILE:HG13	1.79	0.64
1:F:104:THR:HG23	1:F:267:ALA:HB2	1.78	0.64
1:E:93:ASP:N	1:E:93:ASP:OD1	2.30	0.64
1:A:71:PRO:HA	1:A:76:PHE:CD1	2.33	0.64
1:B:102:MET:HE2	1:B:106:GLU:CG	2.27	0.64
1:C:71:PRO:HA	1:C:76:PHE:CD1	2.33	0.63
1:D:102:MET:HE2	1:D:106:GLU:CG	2.28	0.63
1:A:71:PRO:O	1:B:84:ARG:NH2	2.32	0.62
1:D:102:MET:HE2	1:D:106:GLU:HG3	1.82	0.62
1:D:307:ARG:HG2	1:D:307:ARG:NH1	1.95	0.62
1:E:186:TYR:O	1:E:190:ILE:HG13	2.00	0.62
1:C:102:MET:HE2	1:C:106:GLU:HG3	1.81	0.62
1:B:307:ARG:HG2	1:B:307:ARG:NH1	1.99	0.61
1:E:299:ASP:OD1	1:E:335:ARG:NH2	2.34	0.60
1:B:102:MET:HE2	1:B:106:GLU:HG3	1.82	0.60
1:A:179:PRO:HG2	1:A:181:THR:HG23	1.84	0.60
1:B:61:CYS:HB3	1:B:145:ARG:HH21	1.66	0.60
1:D:23:GLU:HG3	1:D:268:HIS:NE2	2.15	0.60
1:A:23:GLU:HG3	1:A:268:HIS:NE2	2.17	0.59
1:B:102:MET:CE	1:B:106:GLU:HG3	2.32	0.59
1:E:23:GLU:HG3	1:E:268:HIS:NE2	2.17	0.59
1:A:70:ASP:C	1:A:70:ASP:OD1	2.38	0.59
1:A:299:ASP:OD1	1:A:335:ARG:NH2	2.35	0.59
1:F:207:ALA:HB2	1:F:222:CYS:HB2	1.85	0.59
1:A:93:ASP:N	1:A:93:ASP:OD1	2.34	0.59
1:A:128:SER:O	1:A:137:ARG:NH2	2.36	0.59
1:B:71:PRO:HA	1:B:76:PHE:CD1	2.38	0.59
1:C:331:PRO:HB2	1:C:332:PRO:HD3	1.85	0.58
1:B:61:CYS:HB3	1:B:145:ARG:NH2	2.19	0.58
1:C:102:MET:CE	1:C:106:GLU:HG3	2.34	0.57
1:B:23:GLU:HG3	1:B:268:HIS:NE2	2.19	0.57
1:D:128:SER:O	1:D:137:ARG:NH2	2.38	0.57
1:C:23:GLU:HG3	1:C:268:HIS:NE2	2.20	0.57
1:F:299:ASP:OD1	1:F:335:ARG:NH2	2.38	0.57
1:F:93:ASP:N	1:F:93:ASP:OD1	2.27	0.56
1:A:186:TYR:O	1:A:190:ILE:HG13	2.04	0.56
1:C:186:TYR:O	1:C:190:ILE:HG13	2.05	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:102:MET:CE	1:E:106:GLU:HG3	2.36	0.56
1:C:299:ASP:OD1	1:C:335:ARG:NH2	2.38	0.56
1:D:299:ASP:OD1	1:D:335:ARG:NH2	2.38	0.55
1:D:331:PRO:HB2	1:D:332:PRO:HD3	1.87	0.55
1:C:108:LEU:HD21	1:C:140:THR:HG23	1.89	0.55
1:B:108:LEU:HD21	1:B:140:THR:HG23	1.89	0.55
1:B:38:GLU:HB2	1:F:38:GLU:CD	2.26	0.55
1:C:128:SER:O	1:C:137:ARG:NH2	2.40	0.55
1:B:186:TYR:O	1:B:190:ILE:HG13	2.07	0.55
1:D:112:GLN:HG3	1:D:140:THR:OG1	2.07	0.55
1:E:307:ARG:CG	1:E:307:ARG:NH1	2.60	0.54
1:A:75:GLY:O	1:A:79:GLN:HG3	2.08	0.53
1:C:99:VAL:O	1:C:103:ILE:HG13	2.08	0.53
1:F:23:GLU:HG3	1:F:268:HIS:NE2	2.24	0.53
1:B:38:GLU:CB	1:F:38:GLU:CD	2.77	0.53
1:B:145:ARG:NH1	1:B:228:ASP:OD2	2.41	0.53
1:B:201:ILE:O	1:B:205:ASN:ND2	2.42	0.53
1:E:179:PRO:HG2	1:E:181:THR:HG23	1.90	0.53
1:E:102:MET:HE3	1:E:151:ASN:ND2	2.22	0.53
1:E:128:SER:O	1:E:137:ARG:NH2	2.42	0.53
1:D:61:CYS:HB3	1:D:145:ARG:HH21	1.74	0.53
1:B:299:ASP:OD1	1:B:335:ARG:NH2	2.42	0.53
1:F:351:MET:HE2	1:F:352:PRO:O	2.09	0.53
1:C:97:VAL:HG21	1:C:289:LEU:HD12	1.91	0.52
1:D:186:TYR:O	1:D:190:ILE:HG13	2.08	0.52
1:F:331:PRO:HB2	1:F:332:PRO:HD3	1.89	0.52
1:A:112:GLN:HG3	1:A:140:THR:OG1	2.10	0.52
1:A:58:VAL:HB	1:B:171:TYR:CE1	2.44	0.52
1:C:61:CYS:HB3	1:C:145:ARG:NH2	2.25	0.52
1:F:128:SER:O	1:F:137:ARG:NH2	2.42	0.52
1:D:179:PRO:HG2	1:D:181:THR:HG23	1.91	0.52
1:E:102:MET:HE2	1:E:106:GLU:CG	2.40	0.52
1:A:195:GLN:O	1:A:199:THR:HG23	2.09	0.52
1:D:143:GLU:OE1	1:D:146:HIS:ND1	2.43	0.52
1:A:99:VAL:O	1:A:103:ILE:HG13	2.10	0.52
1:F:221:ILE:O	1:F:225:ILE:HG13	2.10	0.52
1:B:38:GLU:HA	1:B:41:LYS:HB2	1.92	0.51
1:C:160:VAL:HG12	1:C:356:ILE:HG22	1.90	0.51
1:F:149:LEU:HD21	1:F:221:ILE:HG23	1.92	0.51
1:A:37:ILE:HG23	1:A:120:GLY:HA2	1.92	0.51
1:F:351:MET:CE	1:F:352:PRO:O	2.58	0.51
1:E:201:ILE:O	1:E:205:ASN:ND2	2.44	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:236:TYR:HA	1:D:239:ILE:HD12	1.92	0.51
1:C:70:ASP:OD1	1:C:70:ASP:C	2.48	0.50
1:A:149:LEU:CD2	1:A:221:ILE:HG23	2.42	0.50
1:C:61:CYS:HB3	1:C:145:ARG:HH21	1.77	0.50
1:E:61:CYS:HB3	1:E:145:ARG:HH21	1.77	0.50
1:D:102:MET:CE	1:D:106:GLU:HG3	2.41	0.50
1:A:59:GLU:HG2	1:B:171:TYR:OH	2.12	0.50
1:A:352:PRO:HA	1:A:359:ARG:O	2.12	0.50
1:B:352:PRO:HA	1:B:359:ARG:O	2.12	0.49
1:B:207:ALA:HB2	1:B:222:CYS:HB2	1.94	0.49
1:B:149:LEU:HD21	1:B:221:ILE:HG23	1.94	0.49
1:E:195:GLN:O	1:E:199:THR:HG23	2.12	0.49
1:B:102:MET:HE3	1:B:151:ASN:HD22	1.77	0.49
1:A:331:PRO:HB2	1:A:332:PRO:HD3	1.94	0.49
1:B:277:ASN:HB2	1:B:281:HIS:CE1	2.48	0.49
1:C:125:THR:HG23	1:D:29:THR:HG22	1.93	0.49
1:C:307:ARG:NH1	1:C:307:ARG:CG	2.60	0.49
1:A:102:MET:HE3	1:A:151:ASN:ND2	2.24	0.49
1:C:207:ALA:HB2	1:C:222:CYS:HB2	1.94	0.49
1:E:69:PRO:HA	1:E:79:GLN:OE1	2.13	0.48
1:B:143:GLU:OE1	1:B:146:HIS:ND1	2.46	0.48
1:E:93:ASP:HB2	1:E:289:LEU:HD11	1.95	0.48
1:D:351:MET:HG2	1:D:363:LEU:HD13	1.94	0.48
1:A:125:THR:HG23	1:B:29:THR:HG22	1.95	0.48
1:A:18:PHE:CD2	1:B:59:GLU:HG3	2.48	0.48
1:C:58:VAL:HB	1:D:171:TYR:CE1	2.48	0.48
1:A:145:ARG:NH1	1:A:228:ASP:OD2	2.47	0.48
1:F:80:VAL:O	1:F:84:ARG:HG3	2.13	0.48
1:F:186:TYR:O	1:F:190:ILE:HG13	2.13	0.48
1:B:179:PRO:HG2	1:B:181:THR:HG23	1.96	0.48
1:A:146:HIS:ND1	1:A:225:ILE:HG23	2.29	0.48
1:C:112:GLN:HG3	1:C:140:THR:OG1	2.14	0.48
1:E:37:ILE:HG23	1:E:120:GLY:HA2	1.95	0.48
1:F:201:ILE:O	1:F:205:ASN:ND2	2.47	0.48
1:F:177:MET:HG2	1:F:179:PRO:HD3	1.95	0.48
1:C:221:ILE:O	1:C:225:ILE:HG13	2.14	0.47
1:D:108:LEU:HD21	1:D:140:THR:HG23	1.96	0.47
1:A:304:LEU:HB3	1:A:308:TRP:CZ3	2.49	0.47
1:D:248:PRO:O	1:D:252:VAL:HG23	2.14	0.47
1:E:97:VAL:HG21	1:E:289:LEU:HD12	1.96	0.47
1:F:70:ASP:C	1:F:70:ASP:OD1	2.52	0.47
1:A:236:TYR:HA	1:A:239:ILE:HD12	1.95	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:171:TYR:CE1	1:B:58:VAL:HB	2.50	0.47
1:D:356:ILE:HD12	1:D:359:ARG:HB2	1.95	0.47
1:F:160:VAL:HG12	1:F:356:ILE:HG22	1.96	0.47
1:B:69:PRO:HA	1:B:79:GLN:OE1	2.15	0.47
1:B:216:ILE:H	1:B:216:ILE:HG13	1.49	0.47
1:D:38:GLU:HA	1:D:41:LYS:HB2	1.97	0.47
1:C:304:LEU:HB3	1:C:308:TRP:CZ3	2.50	0.47
1:F:304:LEU:HB3	1:F:308:TRP:CZ3	2.50	0.47
1:E:59:GLU:HG3	1:F:18:PHE:CD2	2.49	0.47
1:D:351:MET:CE	1:D:352:PRO:O	2.62	0.47
1:A:102:MET:HE3	1:A:151:ASN:HB2	1.96	0.47
1:B:350:THR:HG22	1:B:360:GLN:OE1	2.15	0.47
1:B:331:PRO:HB2	1:B:332:PRO:HD3	1.96	0.47
1:D:61:CYS:HB3	1:D:145:ARG:NH2	2.30	0.46
1:D:216:ILE:HG13	1:D:216:ILE:H	1.47	0.46
1:C:75:GLY:O	1:C:79:GLN:HG3	2.15	0.46
1:B:146:HIS:ND1	1:B:225:ILE:HG23	2.30	0.46
1:D:304:LEU:HB3	1:D:308:TRP:CZ3	2.51	0.46
1:B:69:PRO:HB3	1:B:79:GLN:HB2	1.98	0.46
1:C:145:ARG:NH1	1:C:228:ASP:OD2	2.48	0.46
1:E:102:MET:CE	1:E:151:ASN:HD22	2.24	0.46
1:F:63:GLN:HB3	1:F:64:PRO:CD	2.46	0.46
1:C:59:GLU:HG2	1:D:171:TYR:OH	2.16	0.46
1:E:61:CYS:HB3	1:E:145:ARG:NH2	2.30	0.46
1:A:41:LYS:HD3	1:A:41:LYS:HA	1.50	0.46
1:C:38:GLU:HA	1:C:41:LYS:HB2	1.97	0.46
1:E:236:TYR:HA	1:E:239:ILE:HD12	1.97	0.46
1:E:216:ILE:H	1:E:216:ILE:HG13	1.49	0.46
1:E:38:GLU:HA	1:E:41:LYS:HB2	1.98	0.46
1:B:128:SER:O	1:B:137:ARG:NH2	2.49	0.46
1:C:102:MET:CE	1:C:151:ASN:HD22	2.28	0.45
1:F:102:MET:CE	1:F:151:ASN:HD22	2.29	0.45
1:A:93:ASP:HB2	1:A:289:LEU:HD11	1.98	0.45
1:F:41:LYS:HA	1:F:41:LYS:HD3	1.49	0.45
1:D:37:ILE:HG23	1:D:120:GLY:HA2	1.98	0.45
1:F:19:MET:HG2	1:F:19:MET:H	1.47	0.45
1:D:145:ARG:NH1	1:D:228:ASP:OD2	2.49	0.45
1:F:288:ARG:NH1	1:F:362:LYS:O	2.50	0.45
1:E:29:THR:HG22	1:F:125:THR:HG23	1.98	0.45
1:E:331:PRO:HB2	1:E:332:PRO:HD3	1.97	0.45
1:D:195:GLN:O	1:D:199:THR:HG23	2.15	0.45
1:C:143:GLU:OE1	1:C:146:HIS:ND1	2.50	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:121:VAL:HG21	1:E:189:PHE:CZ	2.51	0.45
1:F:38:GLU:HA	1:F:41:LYS:HB2	1.99	0.45
1:F:61:CYS:HB3	1:F:145:ARG:NH2	2.32	0.45
1:A:108:LEU:HD21	1:A:140:THR:HG23	2.00	0.44
1:E:166:GLU:OE1	1:F:64:PRO:HD2	2.17	0.44
1:B:128:SER:HA	1:B:129:PRO:HD3	1.87	0.44
1:E:248:PRO:O	1:E:252:VAL:HG23	2.17	0.44
1:B:342:GLN:C	1:B:344:ARG:H	2.21	0.44
1:E:352:PRO:HA	1:E:359:ARG:O	2.17	0.44
1:E:171:TYR:CE1	1:F:58:VAL:HB	2.52	0.44
1:E:277:ASN:HB2	1:E:281:HIS:CE1	2.52	0.44
1:A:19:MET:HG2	1:A:19:MET:H	1.42	0.44
1:E:102:MET:HE3	1:E:151:ASN:CB	2.45	0.44
1:F:93:ASP:HB2	1:F:289:LEU:HD11	1.99	0.44
1:C:351:MET:HE2	1:C:352:PRO:O	2.18	0.44
1:B:88:LYS:HE3	1:B:88:LYS:HB3	1.81	0.44
1:F:348:ALA:HB1	1:F:349:PRO:HD2	1.98	0.44
1:E:42:SER:C	1:E:44:ASP:H	2.21	0.44
1:A:38:GLU:HA	1:A:41:LYS:HB2	1.99	0.44
1:C:329:ARG:HB2	1:C:329:ARG:HE	1.59	0.44
1:A:255:PHE:CE2	1:A:327:VAL:HG11	2.53	0.44
1:D:93:ASP:HB2	1:D:289:LEU:HD11	2.00	0.44
1:B:112:GLN:HG3	1:B:140:THR:OG1	2.18	0.44
1:F:179:PRO:HG2	1:F:181:THR:HG23	1.99	0.44
1:B:304:LEU:HB3	1:B:308:TRP:CZ3	2.53	0.44
1:A:248:PRO:O	1:A:252:VAL:HG23	2.18	0.44
1:B:248:PRO:O	1:B:252:VAL:HG23	2.17	0.44
1:A:281:HIS:O	1:A:285:VAL:HG23	2.17	0.44
1:C:201:ILE:O	1:C:205:ASN:ND2	2.51	0.44
1:F:121:VAL:HG21	1:F:189:PHE:CZ	2.52	0.44
1:F:75:GLY:O	1:F:76:PHE:C	2.56	0.44
1:C:69:PRO:HA	1:C:79:GLN:OE1	2.17	0.44
1:E:58:VAL:HB	1:F:171:TYR:CE1	2.53	0.44
1:B:197:ARG:O	1:B:201:ILE:HG13	2.18	0.43
1:F:99:VAL:O	1:F:103:ILE:HG13	2.19	0.43
1:C:146:HIS:ND1	1:C:225:ILE:HG23	2.33	0.43
1:F:271:TYR:CZ	1:F:273:GLY:HA2	2.53	0.43
1:C:128:SER:HA	1:C:129:PRO:HD3	1.85	0.43
1:F:64:PRO:HB3	1:F:149:LEU:HB2	2.00	0.43
1:B:195:GLN:O	1:B:199:THR:HG23	2.18	0.43
1:D:94:TYR:C	1:D:94:TYR:CD1	2.92	0.43
1:A:75:GLY:O	1:A:76:PHE:C	2.56	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:108:LEU:O	1:D:109:PRO:C	2.55	0.43
1:B:37:ILE:HG23	1:B:120:GLY:HA2	2.00	0.43
1:A:201:ILE:O	1:A:205:ASN:ND2	2.52	0.43
1:C:37:ILE:HG23	1:C:120:GLY:HA2	1.99	0.43
1:E:102:MET:HE2	1:E:106:GLU:HG3	1.99	0.43
1:E:351:MET:HE2	1:E:352:PRO:O	2.19	0.43
1:D:347:GLU:H	1:D:347:GLU:HG3	1.64	0.43
1:E:41:LYS:HD3	1:E:41:LYS:HA	1.49	0.43
1:E:70:ASP:C	1:E:70:ASP:OD1	2.56	0.43
1:A:97:VAL:HG21	1:A:289:LEU:HD12	2.00	0.43
1:F:331:PRO:HB2	1:F:332:PRO:CD	2.49	0.43
1:D:351:MET:HE2	1:D:352:PRO:O	2.19	0.43
1:E:304:LEU:HB3	1:E:308:TRP:CZ3	2.53	0.43
1:C:216:ILE:HG13	1:C:216:ILE:H	1.50	0.43
1:B:102:MET:CE	1:B:151:ASN:HD22	2.31	0.43
1:D:97:VAL:HG21	1:D:289:LEU:HD12	2.00	0.43
1:E:146:HIS:ND1	1:E:225:ILE:HG23	2.33	0.43
1:D:22:ARG:H	1:D:22:ARG:HG2	1.73	0.43
1:C:62:TRP:CH2	1:C:145:ARG:HG3	2.53	0.43
1:F:51:ILE:HG23	1:F:235:ALA:HB1	1.99	0.43
1:C:179:PRO:HG2	1:C:181:THR:HG23	2.00	0.43
1:F:329:ARG:HB2	1:F:329:ARG:HE	1.62	0.43
1:B:41:LYS:HD3	1:B:41:LYS:HA	1.48	0.42
1:D:146:HIS:ND1	1:D:225:ILE:HG23	2.34	0.42
1:C:351:MET:CE	1:C:352:PRO:O	2.67	0.42
1:E:94:TYR:C	1:E:94:TYR:CD1	2.91	0.42
1:F:195:GLN:O	1:F:199:THR:HG23	2.19	0.42
1:F:108:LEU:HD21	1:F:140:THR:HG23	2.01	0.42
1:F:69:PRO:HA	1:F:79:GLN:OE1	2.19	0.42
1:E:125:THR:HG23	1:F:29:THR:HG22	2.00	0.42
1:B:102:MET:HE3	1:B:151:ASN:CB	2.41	0.42
1:B:38:GLU:HB2	1:F:38:GLU:OE1	2.19	0.42
1:F:61:CYS:HB3	1:F:145:ARG:HH21	1.85	0.42
1:D:277:ASN:HB2	1:D:281:HIS:CE1	2.55	0.42
1:B:298:ALA:HB2	1:B:334:ILE:HG22	2.00	0.42
1:A:121:VAL:HG21	1:A:189:PHE:CZ	2.55	0.42
1:E:145:ARG:NH1	1:E:228:ASP:OD2	2.52	0.42
1:D:351:MET:O	1:D:351:MET:HG3	2.16	0.42
1:E:281:HIS:O	1:E:285:VAL:HG23	2.19	0.42
1:E:255:PHE:CE2	1:E:327:VAL:HG11	2.53	0.42
1:E:99:VAL:O	1:E:103:ILE:HG13	2.19	0.42
1:D:143:GLU:OE1	1:D:146:HIS:CE1	2.72	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:19:MET:H	1:E:19:MET:HG2	1.56	0.42
1:B:351:MET:CE	1:B:352:PRO:O	2.67	0.42
1:D:41:LYS:HD3	1:D:41:LYS:HA	1.50	0.42
1:F:102:MET:HE3	1:F:151:ASN:HD22	1.85	0.42
1:A:102:MET:CE	1:A:151:ASN:HD22	2.28	0.42
1:F:352:PRO:HA	1:F:359:ARG:O	2.19	0.42
1:C:41:LYS:HA	1:C:41:LYS:HD3	1.45	0.42
1:A:329:ARG:HE	1:A:329:ARG:HB2	1.63	0.42
1:D:75:GLY:O	1:D:76:PHE:C	2.58	0.42
1:B:97:VAL:HG21	1:B:289:LEU:HD12	2.02	0.42
1:C:331:PRO:HB2	1:C:332:PRO:CD	2.50	0.42
1:B:38:GLU:HB2	1:F:38:GLU:CG	2.50	0.42
1:D:102:MET:CE	1:D:151:ASN:HD22	2.32	0.41
1:C:236:TYR:HA	1:C:239:ILE:HD12	2.01	0.41
1:A:168:THR:HA	1:A:271:TYR:O	2.20	0.41
1:E:108:LEU:HD22	1:E:144:ASN:HB2	2.01	0.41
1:C:53:VAL:C	1:C:55:LEU:H	2.23	0.41
1:A:268:HIS:HA	1:A:279:PHE:CD1	2.54	0.41
1:F:268:HIS:HA	1:F:279:PHE:CG	2.55	0.41
1:A:351:MET:HE2	1:A:352:PRO:O	2.21	0.41
1:B:356:ILE:HD12	1:B:359:ARG:HB2	2.02	0.41
1:E:108:LEU:HD21	1:E:140:THR:HG23	2.03	0.41
1:C:63:GLN:HB3	1:C:64:PRO:CD	2.50	0.41
1:C:237:THR:HB	1:C:307:ARG:HE	1.85	0.41
1:D:80:VAL:O	1:D:84:ARG:HG3	2.19	0.41
1:D:307:ARG:CG	1:D:307:ARG:NH1	2.66	0.41
1:E:75:GLY:O	1:E:76:PHE:C	2.57	0.41
1:D:128:SER:HA	1:D:129:PRO:HD3	1.84	0.41
1:B:38:GLU:CB	1:F:38:GLU:CG	2.98	0.41
1:D:121:VAL:HG21	1:D:189:PHE:CZ	2.55	0.41
1:A:62:TRP:CH2	1:A:145:ARG:HG3	2.56	0.41
1:C:248:PRO:O	1:C:252:VAL:HG23	2.20	0.41
1:C:75:GLY:O	1:C:76:PHE:C	2.58	0.41
1:A:92:ASP:O	1:A:96:VAL:HG23	2.20	0.41
1:C:93:ASP:HB2	1:C:289:LEU:HD11	2.03	0.41
1:F:97:VAL:HG21	1:F:289:LEU:HD12	2.03	0.41
1:E:207:ALA:HB2	1:E:222:CYS:CB	2.46	0.41
1:C:108:LEU:O	1:C:109:PRO:C	2.59	0.41
1:E:128:SER:HA	1:E:129:PRO:HD3	1.82	0.41
1:A:63:GLN:HB3	1:A:64:PRO:CD	2.50	0.41
1:E:168:THR:HA	1:E:271:TYR:O	2.20	0.41
1:B:70:ASP:OD1	1:B:70:ASP:C	2.58	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:216:ILE:HG13	1:F:216:ILE:H	1.49	0.41
1:B:35:GLN:OE1	1:F:42:SER:HA	2.21	0.41
1:D:201:ILE:O	1:D:205:ASN:ND2	2.54	0.41
1:F:37:ILE:HG23	1:F:120:GLY:HA2	2.01	0.41
1:C:268:HIS:HA	1:C:279:PHE:CG	2.56	0.41
1:A:128:SER:HA	1:A:129:PRO:HD3	1.85	0.41
1:A:108:LEU:HD22	1:A:144:ASN:HB2	2.03	0.41
1:C:19:MET:HG2	1:C:19:MET:H	1.44	0.41
1:F:307:ARG:CG	1:F:307:ARG:NH1	2.67	0.40
1:B:93:ASP:HB2	1:B:289:LEU:HD11	2.04	0.40
1:A:216:ILE:HG13	1:A:216:ILE:H	1.54	0.40
1:B:94:TYR:C	1:B:94:TYR:CD1	2.95	0.40
1:E:329:ARG:HB2	1:E:329:ARG:HE	1.62	0.40
1:E:351:MET:CE	1:E:352:PRO:O	2.68	0.40
1:B:121:VAL:HG21	1:B:189:PHE:CZ	2.56	0.40
1:E:104:THR:O	1:E:111:TYR:OH	2.25	0.40
1:F:145:ARG:NH1	1:F:228:ASP:OD2	2.54	0.40
1:A:285:VAL:O	1:A:286:ALA:C	2.59	0.40
1:D:70:ASP:OD1	1:D:70:ASP:C	2.58	0.40
1:F:152:LYS:O	1:F:153:TYR:C	2.58	0.40
1:A:102:MET:CE	1:A:106:GLU:HG3	2.52	0.40
1:D:69:PRO:HA	1:D:79:GLN:OE1	2.22	0.40
1:D:99:VAL:O	1:D:100:GLY:C	2.59	0.40
1:B:207:ALA:O	1:B:208:ARG:C	2.59	0.40
1:E:112:GLN:HG3	1:E:140:THR:OG1	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	344/363 (95%)	310 (90%)	30 (9%)	4 (1%)	19	70
1	B	344/363 (95%)	307 (89%)	31 (9%)	6 (2%)	14	62
1	C	344/363 (95%)	311 (90%)	30 (9%)	3 (1%)	25	76

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	344/363 (95%)	307 (89%)	32 (9%)	5 (2%)	15	64
1	E	344/363 (95%)	309 (90%)	31 (9%)	4 (1%)	19	70
1	F	344/363 (95%)	305 (89%)	34 (10%)	5 (2%)	15	64
All	All	2064/2178 (95%)	1849 (90%)	188 (9%)	27 (1%)	18	68

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	29	THR
1	B	29	THR
1	C	29	THR
1	D	29	THR
1	E	29	THR
1	F	29	THR
1	C	340	ARG
1	D	340	ARG
1	F	340	ARG
1	A	262	LYS
1	B	340	ARG
1	C	262	LYS
1	D	262	LYS
1	E	262	LYS
1	F	262	LYS
1	B	262	LYS
1	A	52	LEU
1	D	43	LEU
1	E	52	LEU
1	F	52	LEU
1	F	270	MET
1	D	53	VAL
1	A	53	VAL
1	B	343	GLY
1	B	33	PRO
1	B	53	VAL
1	E	33	PRO

5.3.2 Protein sidechains ⓘ

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

conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	300/315 (95%)	248 (83%)	52 (17%)	3	13
1	B	300/315 (95%)	247 (82%)	53 (18%)	3	13
1	C	300/315 (95%)	249 (83%)	51 (17%)	3	14
1	D	300/315 (95%)	248 (83%)	52 (17%)	3	13
1	E	300/315 (95%)	244 (81%)	56 (19%)	2	11
1	F	300/315 (95%)	250 (83%)	50 (17%)	3	14
All	All	1800/1890 (95%)	1486 (83%)	314 (17%)	3	13

All (314) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	MET
1	A	22	ARG
1	A	23	GLU
1	A	24	VAL
1	A	28	VAL
1	A	35	GLN
1	A	38	GLU
1	A	41	LYS
1	A	48	GLU
1	A	73	SER
1	A	78	GLU
1	A	86	ARG
1	A	89	GLU
1	A	93	ASP
1	A	102	MET
1	A	104	THR
1	A	128	SER
1	A	130	THR
1	A	134	ILE
1	A	143	GLU
1	A	144	ASN
1	A	145	ARG
1	A	152	LYS
1	A	162	MET
1	A	171	TYR
1	A	177	MET
1	A	180	ARG
1	A	184	SER

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Mol	Chain	Res	Type
1	A	195	GLN
1	A	211	LYS
1	A	216	ILE
1	A	220	GLN
1	A	224	THR
1	A	238	LYS
1	A	241	GLU
1	A	249	ASP
1	A	259	MET
1	A	264	SER
1	A	282	PHE
1	A	302	GLU
1	A	307	ARG
1	A	311	ASP
1	A	314	THR
1	A	321	GLN
1	A	329	ARG
1	A	333	ARG
1	A	336	ARG
1	A	337	LEU
1	A	344	ARG
1	A	347	GLU
1	A	350	THR
1	A	351	MET
1	B	19	MET
1	B	22	ARG
1	B	23	GLU
1	B	24	VAL
1	B	28	VAL
1	B	35	GLN
1	B	41	LYS
1	B	48	GLU
1	B	60	LYS
1	B	73	SER
1	B	78	GLU
1	B	86	ARG
1	B	89	GLU
1	B	93	ASP
1	B	102	MET
1	B	111	TYR
1	B	128	SER
1	B	130	THR

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Mol	Chain	Res	Type
1	B	134	ILE
1	B	143	GLU
1	B	144	ASN
1	B	145	ARG
1	B	152	LYS
1	B	162	MET
1	B	171	TYR
1	B	177	MET
1	B	180	ARG
1	B	184	SER
1	B	200	PHE
1	B	216	ILE
1	B	220	GLN
1	B	224	THR
1	B	238	LYS
1	B	241	GLU
1	B	249	ASP
1	B	259	MET
1	B	264	SER
1	B	274	ARG
1	B	282	PHE
1	B	302	GLU
1	B	307	ARG
1	B	311	ASP
1	B	314	THR
1	B	321	GLN
1	B	322	LYS
1	B	329	ARG
1	B	333	ARG
1	B	336	ARG
1	B	337	LEU
1	B	344	ARG
1	B	347	GLU
1	B	350	THR
1	B	351	MET
1	C	19	MET
1	C	22	ARG
1	C	23	GLU
1	C	24	VAL
1	C	28	VAL
1	C	35	GLN
1	C	38	GLU

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Mol	Chain	Res	Type
1	C	41	LYS
1	C	48	GLU
1	C	60	LYS
1	C	73	SER
1	C	78	GLU
1	C	86	ARG
1	C	89	GLU
1	C	93	ASP
1	C	102	MET
1	C	111	TYR
1	C	130	THR
1	C	134	ILE
1	C	143	GLU
1	C	144	ASN
1	C	145	ARG
1	C	152	LYS
1	C	162	MET
1	C	171	TYR
1	C	177	MET
1	C	180	ARG
1	C	184	SER
1	C	200	PHE
1	C	216	ILE
1	C	220	GLN
1	C	224	THR
1	C	238	LYS
1	C	241	GLU
1	C	249	ASP
1	C	259	MET
1	C	264	SER
1	C	282	PHE
1	C	302	GLU
1	C	307	ARG
1	C	311	ASP
1	C	314	THR
1	C	321	GLN
1	C	329	ARG
1	C	333	ARG
1	C	336	ARG
1	C	337	LEU
1	C	344	ARG
1	C	347	GLU

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Mol	Chain	Res	Type
1	C	350	THR
1	C	351	MET
1	D	19	MET
1	D	22	ARG
1	D	23	GLU
1	D	24	VAL
1	D	28	VAL
1	D	35	GLN
1	D	38	GLU
1	D	41	LYS
1	D	48	GLU
1	D	73	SER
1	D	78	GLU
1	D	86	ARG
1	D	89	GLU
1	D	93	ASP
1	D	102	MET
1	D	104	THR
1	D	111	TYR
1	D	128	SER
1	D	130	THR
1	D	134	ILE
1	D	143	GLU
1	D	144	ASN
1	D	145	ARG
1	D	152	LYS
1	D	162	MET
1	D	171	TYR
1	D	177	MET
1	D	180	ARG
1	D	184	SER
1	D	195	GLN
1	D	211	LYS
1	D	216	ILE
1	D	220	GLN
1	D	224	THR
1	D	241	GLU
1	D	249	ASP
1	D	259	MET
1	D	264	SER
1	D	282	PHE
1	D	302	GLU

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Mol	Chain	Res	Type
1	D	307	ARG
1	D	311	ASP
1	D	314	THR
1	D	321	GLN
1	D	329	ARG
1	D	333	ARG
1	D	336	ARG
1	D	337	LEU
1	D	344	ARG
1	D	347	GLU
1	D	350	THR
1	D	351	MET
1	E	19	MET
1	E	22	ARG
1	E	23	GLU
1	E	24	VAL
1	E	28	VAL
1	E	35	GLN
1	E	38	GLU
1	E	41	LYS
1	E	48	GLU
1	E	60	LYS
1	E	73	SER
1	E	78	GLU
1	E	86	ARG
1	E	89	GLU
1	E	93	ASP
1	E	102	MET
1	E	104	THR
1	E	111	TYR
1	E	128	SER
1	E	130	THR
1	E	134	ILE
1	E	143	GLU
1	E	144	ASN
1	E	145	ARG
1	E	152	LYS
1	E	162	MET
1	E	167	LYS
1	E	171	TYR
1	E	177	MET
1	E	180	ARG

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Mol	Chain	Res	Type
1	E	184	SER
1	E	195	GLN
1	E	216	ILE
1	E	220	GLN
1	E	224	THR
1	E	238	LYS
1	E	241	GLU
1	E	249	ASP
1	E	259	MET
1	E	264	SER
1	E	274	ARG
1	E	282	PHE
1	E	302	GLU
1	E	307	ARG
1	E	311	ASP
1	E	314	THR
1	E	321	GLN
1	E	329	ARG
1	E	333	ARG
1	E	336	ARG
1	E	337	LEU
1	E	344	ARG
1	E	347	GLU
1	E	350	THR
1	E	351	MET
1	E	354	SER
1	F	19	MET
1	F	22	ARG
1	F	23	GLU
1	F	24	VAL
1	F	28	VAL
1	F	35	GLN
1	F	41	LYS
1	F	48	GLU
1	F	60	LYS
1	F	73	SER
1	F	78	GLU
1	F	86	ARG
1	F	89	GLU
1	F	93	ASP
1	F	102	MET
1	F	104	THR

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Mol	Chain	Res	Type
1	F	111	TYR
1	F	130	THR
1	F	134	ILE
1	F	143	GLU
1	F	144	ASN
1	F	145	ARG
1	F	152	LYS
1	F	162	MET
1	F	171	TYR
1	F	177	MET
1	F	180	ARG
1	F	195	GLN
1	F	216	ILE
1	F	220	GLN
1	F	224	THR
1	F	238	LYS
1	F	241	GLU
1	F	249	ASP
1	F	259	MET
1	F	264	SER
1	F	274	ARG
1	F	302	GLU
1	F	307	ARG
1	F	311	ASP
1	F	314	THR
1	F	321	GLN
1	F	329	ARG
1	F	333	ARG
1	F	336	ARG
1	F	337	LEU
1	F	344	ARG
1	F	347	GLU
1	F	350	THR
1	F	351	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	151	ASN
1	A	321	GLN
1	B	27	GLN
1	B	151	ASN

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Mol	Chain	Res	Type
1	B	321	GLN
1	C	27	GLN
1	C	151	ASN
1	C	321	GLN
1	D	27	GLN
1	D	151	ASN
1	D	195	GLN
1	D	321	GLN
1	E	151	ASN
1	E	321	GLN
1	F	27	GLN
1	F	151	ASN
1	F	195	GLN
1	F	321	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	346/363 (95%)	0.32	5 (1%)	72 22	29, 38, 44, 47	8 (2%)
1	B	346/363 (95%)	0.28	4 (1%)	75 26	29, 38, 44, 47	8 (2%)
1	C	346/363 (95%)	0.30	4 (1%)	75 26	29, 38, 44, 47	8 (2%)
1	D	346/363 (95%)	0.33	7 (2%)	62 17	29, 38, 44, 47	8 (2%)
1	E	346/363 (95%)	0.31	6 (1%)	67 19	29, 38, 44, 47	8 (2%)
1	F	346/363 (95%)	0.28	4 (1%)	75 26	29, 38, 44, 47	8 (2%)
All	All	2076/2178 (95%)	0.30	30 (1%)	72 22	29, 38, 44, 47	48 (2%)

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	23	GLU	3.7
1	D	343	GLY	3.2
1	D	344	ARG	3.1
1	C	341	ALA	3.0
1	F	337	LEU	2.9
1	A	345	ALA	2.9
1	A	344	ARG	2.8
1	D	27	GLN	2.8
1	C	345	ALA	2.7
1	B	345	ALA	2.6
1	F	314	THR	2.6
1	B	337	LEU	2.6
1	A	324	GLN	2.4
1	B	263	ILE	2.4
1	E	314	THR	2.3
1	F	18	PHE	2.3
1	E	315	GLY	2.3
1	C	338	GLU	2.2
1	F	344	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	54	HIS	2.2
1	D	319	GLU	2.2
1	A	27	GLN	2.1
1	B	363	LEU	2.1
1	D	249	ASP	2.1
1	E	24	VAL	2.1
1	E	337	LEU	2.1
1	A	22	ARG	2.1
1	E	18	PHE	2.1
1	C	23	GLU	2.0
1	D	342	GLN	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	SR	C	364	1/1	0.47	6.97	151,151,151,151	0
2	SR	D	364	1/1	0.34	2.38	130,130,130,130	0
2	SR	E	364	1/1	0.32	1.72	119,119,119,119	0
2	SR	B	364	1/1	0.30	1.18	118,118,118,118	0
2	SR	B	365	1/1	0.29	-0.44	144,144,144,144	0
2	SR	B	366	1/1	0.23	-2.07	128,128,128,128	0
2	SR	C	365	1/1	0.21	-2.18	171,171,171,171	0
2	SR	A	364	1/1	0.20	-2.40	142,142,142,142	0
2	SR	E	365	1/1	0.19	-2.57	153,153,153,153	0
2	SR	D	365	1/1	0.17	-2.68	159,159,159,159	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	SR	F	364	1/1	0.15	-2.71	127,127,127,127	0
2	SR	F	365	1/1	0.20	-2.82	126,126,126,126	0

6.5 Other polymers ⓘ

There are no such residues in this entry.