



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 12:14 AM UTC

PDB ID : 1OQ7 / pdb_00001oq7
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 X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

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

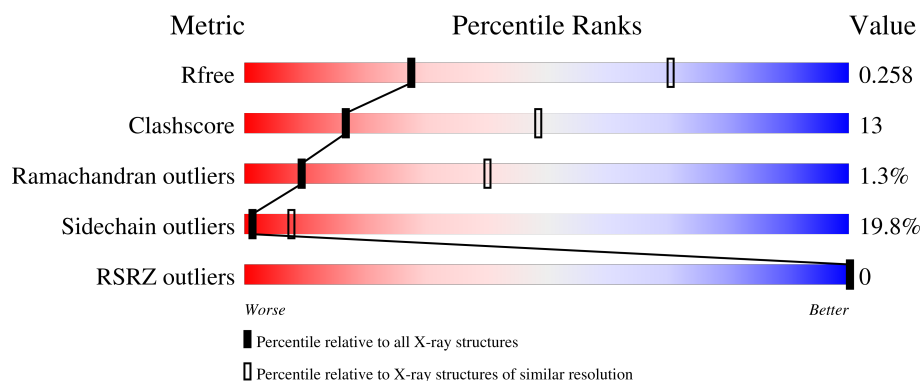
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

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))
R_{free}	180053	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	363	
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	57% 33% 5% 5%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 16848 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	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			

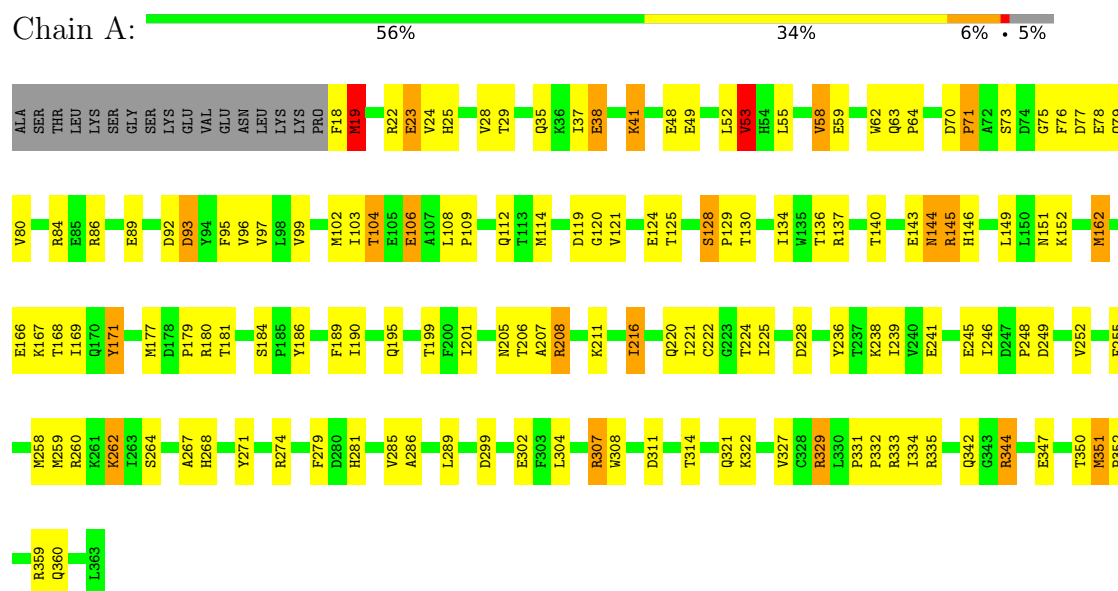
- Molecule 2 is STRONTIUM ION (CCD ID: SR) (formula: Sr).

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

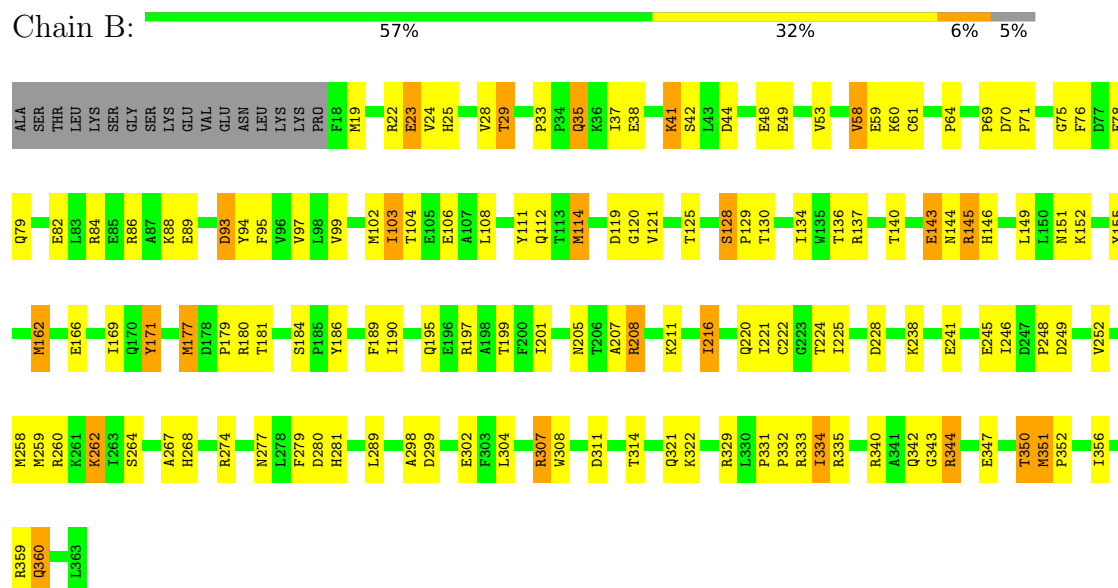
3 Residue-property plots

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

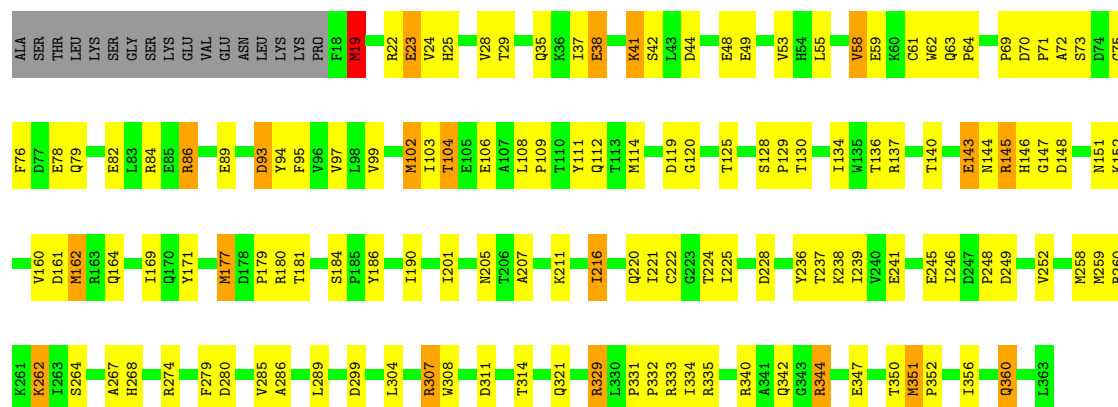


• Molecule 1: Acyl-[acyl-carrier protein] desaturase



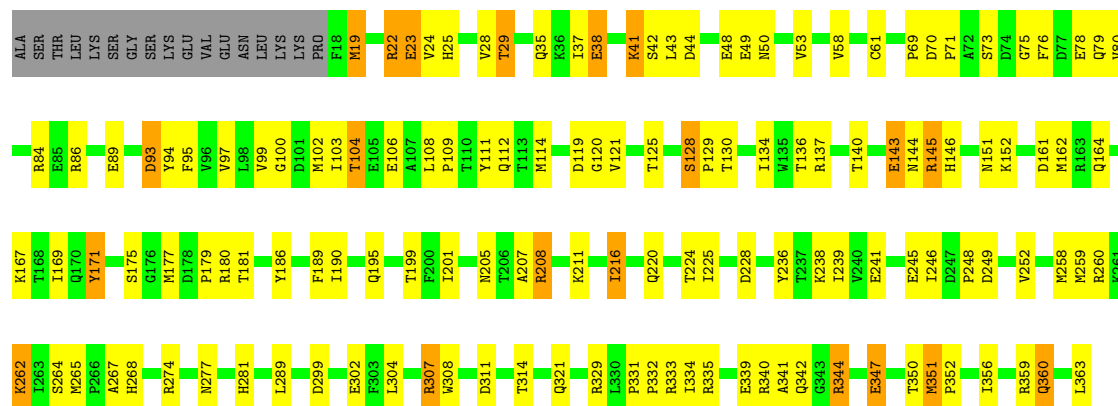
• Molecule 1: Acyl-[acyl-carrier protein] desaturase

Chain C:  58% 32% 5% 5%



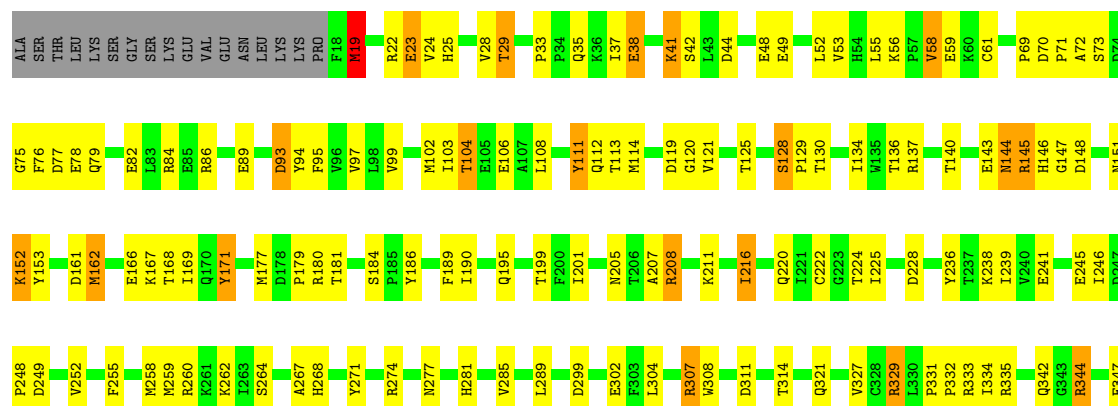
• Molecule 1: Acyl-[acyl-carrier protein] desaturase

Chain D:  57% 33% 6% 5%



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

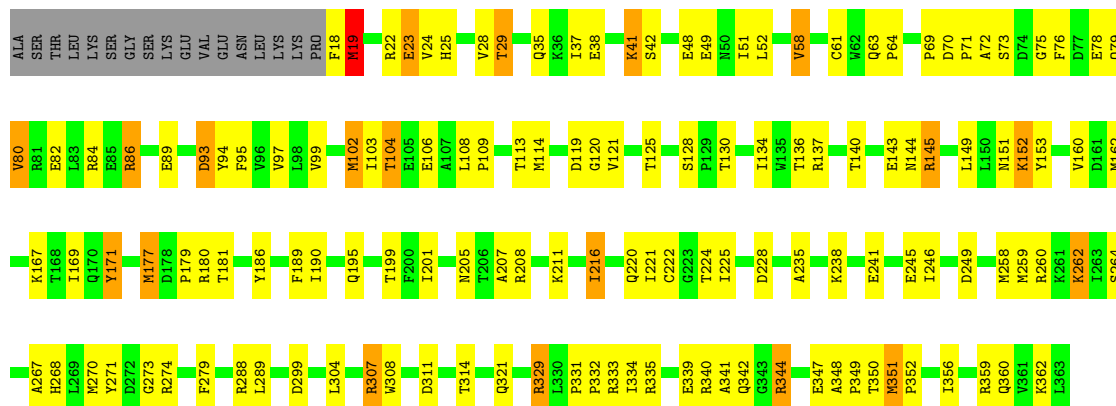
Chain E:  55% 34% 6% 5%





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

Chain F: 57% 33% 5% 5%



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 19.96 – 3.20	Depositor EDS
% Data completeness (in resolution range)	92.5 (19.96-3.20) 92.5 (19.96-3.20)	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) , 0.258	Depositor DCC
R_{free} test set	1543 reflections (3.13%)	wwPDB-VP
Wilson B-factor (Å ²)	77.9	Xtriage
Anisotropy	0.010	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 33.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.069 for -h,-k,l 0.309 for h,-h-k,-l 0.069 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.95	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.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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	0.96	6/2874 (0.2%)	1.13	2/3892 (0.1%)
1	B	0.94	3/2874 (0.1%)	1.12	4/3892 (0.1%)
1	C	0.94	3/2874 (0.1%)	1.11	4/3892 (0.1%)
1	D	0.93	2/2874 (0.1%)	1.09	4/3892 (0.1%)
1	E	0.90	3/2874 (0.1%)	1.10	5/3892 (0.1%)
1	F	0.99	5/2874 (0.2%)	1.14	3/3892 (0.1%)
All	All	0.94	22/17244 (0.1%)	1.11	22/23352 (0.1%)

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	265	MET	SD-CE	8.51	2.00	1.79
1	F	19	MET	SD-CE	7.35	1.98	1.79
1	D	19	MET	SD-CE	7.00	1.97	1.79
1	A	19	MET	SD-CE	6.82	1.96	1.79
1	A	71	PRO	C-O	-6.40	1.15	1.24
1	A	162	MET	SD-CE	6.36	1.95	1.79
1	E	19	MET	SD-CE	6.19	1.95	1.79
1	C	72	ALA	CA-CB	-6.13	1.44	1.53
1	C	19	MET	SD-CE	6.04	1.94	1.79
1	A	53	VAL	CA-CB	5.99	1.62	1.54
1	E	72	ALA	CA-CB	-5.92	1.45	1.53
1	C	86	ARG	NE-CZ	5.81	1.39	1.33
1	B	162	MET	SD-CE	5.54	1.93	1.79
1	A	80	VAL	CA-CB	-5.53	1.48	1.54
1	F	72	ALA	CA-CB	-5.51	1.45	1.53
1	B	114	MET	SD-CE	5.31	1.92	1.79
1	B	155	TYR	C-O	-5.31	1.18	1.24
1	F	82	GLU	CG-CD	5.27	1.65	1.52
1	F	80	VAL	CA-CB	-5.25	1.48	1.54
1	E	162	MET	SD-CE	5.22	1.92	1.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	86	ARG	NE-CZ	5.19	1.38	1.33
1	A	77	ASP	C-O	-5.07	1.18	1.24

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	119	ASP	N-CA-C	8.64	120.38	110.97
1	B	119	ASP	N-CA-C	8.31	120.02	110.97
1	D	119	ASP	N-CA-C	6.77	118.34	110.97
1	D	360	GLN	N-CA-C	6.66	119.68	108.02
1	A	360	GLN	N-CA-C	6.57	119.51	108.02
1	C	119	ASP	N-CA-C	6.49	118.04	110.97
1	E	119	ASP	N-CA-C	6.43	118.87	111.02
1	A	119	ASP	N-CA-C	6.28	118.68	111.02
1	C	360	GLN	N-CA-C	6.20	119.05	108.02
1	F	360	GLN	N-CA-C	6.15	118.78	108.02
1	B	360	GLN	N-CA-C	6.11	118.72	108.02
1	E	56	LYS	N-CA-C	-6.00	102.10	109.65
1	D	164	GLN	N-CA-C	-5.97	104.85	111.36
1	E	360	GLN	N-CA-C	5.95	118.44	108.02
1	C	164	GLN	N-CA-C	-5.93	104.90	111.36
1	B	103	ILE	N-CA-C	-5.68	105.19	110.53
1	B	82	GLU	N-CA-C	-5.66	105.11	111.28
1	E	82	GLU	N-CA-C	-5.60	105.25	111.36
1	D	50	ASN	N-CA-C	5.57	121.10	113.97
1	F	82	GLU	N-CA-C	-5.35	105.53	111.36
1	C	82	GLU	N-CA-C	-5.25	105.56	111.28
1	E	77	ASP	N-CA-C	5.16	116.59	111.07

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	2806	0	2748	74	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2806	0	2748	76	0
1	C	2806	0	2748	73	0
1	D	2806	0	2748	70	0
1	E	2806	0	2748	79	0
1	F	2806	0	2748	83	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	420	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 13.

All (420) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:307:ARG:HH11	1:C:307:ARG:HG2	1.11	1.11
1:A:307:ARG:HH11	1:A:307:ARG:HG2	1.12	1.09
1:D:307:ARG:HG2	1:D:307:ARG:HH11	1.15	1.09
1:E:307:ARG:HG2	1:E:307:ARG:HH11	1.12	1.07
1:F:307:ARG:HG2	1:F:307:ARG:HH11	1.17	1.04
1:B:307:ARG:HG2	1:B:307:ARG:HH11	1.19	1.04
1:E:102:MET:HE3	1:E:151:ASN:HB2	1.53	0.91
1:B:102:MET:HE3	1:B:151:ASN:HB2	1.54	0.90
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: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:HH11	1:E:307:ARG:CG	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:F:351:MET:HE3	1:F:352:PRO:O	1.79	0.81
1:F:102:MET:HE2	1:F:106:GLU:HG3	1.64	0.80
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:E:95:PHE:O	1:E:99:VAL:HG23	1.85	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:307:ARG:HH11	1:A:307:ARG:CG	1.96	0.76
1:D:102:MET:HE3	1:D:151:ASN:HB2	1.68	0.76
1:E:307:ARG:HG2	1:E:307:ARG:NH1	1.93	0.76
1:A:307:ARG:HG2	1:A:307:ARG:NH1	1.93	0.75
1:A:102:MET:HE3	1:A:151:ASN:HB2	1.68	0.75
1:F:307:ARG:HH11	1:F:307:ARG:CG	1.99	0.75
1:E:84:ARG:NH2	1:F:71:PRO:O	2.20	0.74
1:C:351:MET:HE3	1:C:352:PRO:O	1.88	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:B:351:MET:HE3	1:B:352:PRO:O	1.89	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:E:351:MET:HE3	1:E:352:PRO:O	1.89	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:F:102:MET:HE3	1:F:151:ASN:HB2	1.72	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:HH11	1:B:307:ARG:CG	2.00	0.70
1:D:93:ASP:N	1:D:93:ASP:OD1	2.24	0.70
1:F:102:MET:HE2	1:F:106:GLU:CG	2.21	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	2.23	0.69
1:A:351:MET:HE3	1:A:352:PRO:O	1.93	0.69
1:E:103:ILE:HG23	1:E:169:ILE:HG13	1.74	0.69
1:F:102:MET:CE	1:F:106:GLU:HG3	2.23	0.69
1:B:102:MET:HE2	1:B:106:GLU:HG3	1.76	0.68
1:E:75:GLY:O	1:E:79:GLN:HG3	1.92	0.68
1:B:102:MET:HE2	1:B:106:GLU:CG	2.23	0.68
1:D:351:MET:HE3	1:D:352:PRO:O	1.94	0.68
1:E:102:MET:HE2	1:E:106:GLU:CG	2.23	0.67
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:93:ASP:OD1	1:C:93:ASP:N	2.26	0.65
1:C:307:ARG:HG2	1:C:307:ARG:NH1	1.91	0.65
1:E:207:ALA:HB2	1:E:222:CYS:HB2	1.77	0.65
1:F:75:GLY:O	1:F:79:GLN:HG3	1.96	0.65
1:E:102:MET:HE2	1:E:106:GLU:HG3	1.77	0.65
1:C:104:THR:HG23	1:C:267:ALA:HB2	1.79	0.65
1:B:93:ASP:OD1	1:B:93:ASP:N	2.24	0.65
1:F:95:PHE:O	1:F:99:VAL:HG23	1.97	0.65
1:A:149:LEU:HD21	1:A:221:ILE:HG23	1.79	0.64
1:D:71:PRO:HA	1:D:76:PHE:CD1	2.32	0.64
1:A:70:ASP:OD1	1:A:70:ASP:C	2.38	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:A:71:PRO:HA	1:A:76:PHE:CD1	2.33	0.64
1:E:93:ASP:OD1	1:E:93:ASP:N	2.30	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: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:D:102:MET:HE2	1:D:106:GLU:HG3	1.82	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:A:179:PRO:HG2	1:A:181:THR:HG23	1.84	0.60
1:A:102:MET:HE2	1:A:106:GLU:CG	2.32	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:B:38:GLU:HB2	1:F:38:GLU:CD	2.26	0.60
1:A:23:GLU:HG3	1:A:268:HIS:NE2	2.17	0.59
1:C:114:MET:HE1	1:D:125:THR:O	2.02	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: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:OD1	1:A:93:ASP:N	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:102:MET:HE2	1:A:106:GLU:HG3	1.85	0.58
1:C:331:PRO:HB2	1:C:332:PRO:HD3	1.85	0.58
1:E:125:THR:O	1:F:114:MET:HE1	2.04	0.58
1:B:61:CYS:HB3	1:B:145:ARG:NH2	2.19	0.58
1:B:38:GLU:CB	1:F:38:GLU:CD	2.77	0.58
1:A:114:MET:HE1	1:B:125:THR:O	2.04	0.57
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:C:125:THR:O	1:D:114:MET:HE1	2.05	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:A:186:TYR:O	1:A:190:ILE:HG13	2.04	0.56
1:F:93:ASP:OD1	1:F:93:ASP:N	2.27	0.56
1:C:186:TYR:O	1:C:190:ILE:HG13	2.05	0.56
1:C:299:ASP:OD1	1:C:335:ARG:NH2	2.38	0.56
1:E:102:MET:CE	1:E:106:GLU:HG3	2.36	0.56
1:D:299:ASP:OD1	1:D:335:ARG:NH2	2.38	0.55
1:B:108:LEU:HD21	1:B:140:THR:HG23	1.89	0.55
1:C:108:LEU:HD21	1:C:140:THR:HG23	1.89	0.55
1:D:331:PRO:HB2	1:D:332:PRO:HD3	1.87	0.55
1:C:70:ASP:OD1	1:C:70:ASP:C	2.48	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: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:128:SER:O	1:E:137:ARG:NH2	2.42	0.53
1:B:299:ASP:OD1	1:B:335:ARG:NH2	2.42	0.53
1:D:61:CYS:HB3	1:D:145:ARG:HH21	1.74	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:70:ASP:OD1	1:F:70:ASP:C	2.52	0.52
1:A:125:THR:O	1:B:114:MET:HE1	2.09	0.52
1:D:179:PRO:HG2	1:D:181:THR:HG23	1.91	0.52
1:F:128:SER:O	1:F:137:ARG:NH2	2.42	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:D:102:MET:CE	1:D:106:GLU:HG3	2.41	0.51
1:E:102:MET:CE	1:E:151:ASN:HD22	2.24	0.51
1:A:37:ILE:HG23	1:A:120:GLY:HA2	1.92	0.51
1:D:236:TYR:HA	1:D:239:ILE:HD12	1.92	0.51
1:E:201:ILE:O	1:E:205:ASN:ND2	2.44	0.51
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: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:149:LEU:HD21	1:B:221:ILE:HG23	1.94	0.49
1:B:207:ALA:HB2	1:B:222:CYS:HB2	1.94	0.49
1:B:352:PRO:HA	1:B:359:ARG:O	2.12	0.49
1:E:195:GLN:O	1:E:199:THR:HG23	2.12	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:E:114:MET:HE1	1:F:125:THR:O	2.12	0.49
1:B:342:GLN:C	1:B:344:ARG:H	2.21	0.49
1:C:307:ARG:CG	1:C:307:ARG:NH1	2.60	0.49
1:C:207:ALA:HB2	1:C:222:CYS:HB2	1.94	0.49
1:B:143:GLU:OE1	1:B:146:HIS:ND1	2.46	0.48
1:E:69:PRO:HA	1:E:79:GLN:OE1	2.13	0.48
1:D:351:MET:HG2	1:D:363:LEU:HD13	1.94	0.48
1:E:93:ASP:HB2	1:E:289:LEU:HD11	1.95	0.48
1:A:18:PHE:CD2	1:B:59:GLU:HG3	2.48	0.48
1:A:125:THR:HG23	1:B:29:THR:HG22	1.95	0.48
1:A:145:ARG:NH1	1:A:228:ASP:OD2	2.47	0.48
1:C:58:VAL:HB	1:D:171:TYR:CE1	2.48	0.48
1:F:75:GLY:O	1:F:76:PHE:C	2.56	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:80:VAL:O	1:F:84:ARG:HG3	2.13	0.48
1:D:94:TYR:CD1	1:D:94:TYR:C	2.92	0.48
1:F:186:TYR:O	1:F:190:ILE:HG13	2.13	0.48
1:A:75:GLY:O	1:A:76:PHE:C	2.56	0.48
1:A:146:HIS:ND1	1:A:225:ILE:HG23	2.29	0.48
1:B:179:PRO:HG2	1:B:181:THR:HG23	1.96	0.48
1:E:70:ASP:OD1	1:E:70:ASP:C	2.56	0.48
1:C:112:GLN:HG3	1:C:140:THR:OG1	2.14	0.48
1:C:177:MET:HE2	1:C:179:PRO:HG3	1.96	0.48
1:E:37:ILE:HG23	1:E:120:GLY:HA2	1.95	0.48
1:E:42:SER:C	1:E:44:ASP:H	2.21	0.48
1:F:177:MET:HG2	1:F:179:PRO:HD3	1.95	0.48
1:F:201:ILE:O	1:F:205:ASN:ND2	2.47	0.48
1:C:221:ILE:O	1:C:225:ILE:HG13	2.14	0.47
1:A:304:LEU:HB3	1:A:308:TRP:CZ3	2.49	0.47
1:D:108:LEU:HD21	1:D:140:THR:HG23	1.96	0.47
1:D:248:PRO:O	1:D:252:VAL:HG23	2.14	0.47
1:A:236:TYR:HA	1:A:239:ILE:HD12	1.95	0.47
1:E:97:VAL:HG21	1:E:289:LEU:HD12	1.96	0.47
1:A:171:TYR:CE1	1:B:58:VAL:HB	2.50	0.47
1:F:177:MET:HE2	1:F:179:PRO:HG3	1.97	0.47
1:D:356:ILE:HD12	1:D:359:ARG:HB2	1.95	0.47
1:E:94:TYR:CD1	1:E:94:TYR:C	2.91	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:C:304:LEU:HB3	1:C:308:TRP:CZ3	2.50	0.47
1:D:38:GLU:HA	1:D:41:LYS:HB2	1.97	0.47
1:D:108:LEU:O	1:D:109:PRO:C	2.55	0.47
1:E:59:GLU:HG3	1:F:18:PHE:CD2	2.49	0.47
1:F:304:LEU:HB3	1:F:308:TRP:CZ3	2.50	0.47
1:B:331:PRO:HB2	1:B:332:PRO:HD3	1.96	0.47
1:B:350:THR:HG22	1:B:360:GLN:OE1	2.15	0.47
1:D:61:CYS:HB3	1:D:145:ARG:NH2	2.30	0.46
1:D:216:ILE:H	1:D:216:ILE:HG13	1.47	0.46
1:C:53:VAL:C	1:C:55:LEU:H	2.23	0.46
1:B:146:HIS:ND1	1:B:225:ILE:HG23	2.30	0.46
1:C:75:GLY:O	1:C:79:GLN:HG3	2.15	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:102:MET:CE	1:A:151:ASN:HD22	2.28	0.46
1:C:59:GLU:HG2	1:D:171:TYR:OH	2.16	0.46
1:E:75:GLY:O	1:E:76:PHE:C	2.57	0.46
1:F:63:GLN:HB3	1:F:64:PRO:CD	2.46	0.46
1:A:41:LYS:HA	1:A:41:LYS:HD3	1.50	0.46
1:C:38:GLU:HA	1:C:41:LYS:HB2	1.97	0.46
1:E:61:CYS:HB3	1:E:145:ARG:NH2	2.30	0.46
1:C:75:GLY:O	1:C:76:PHE:C	2.58	0.46
1:E:38:GLU:HA	1:E:41:LYS:HB2	1.98	0.46
1:E:216:ILE:H	1:E:216:ILE:HG13	1.49	0.46
1:E:236:TYR:HA	1:E:239:ILE:HD12	1.97	0.46
1:B:128:SER:O	1:B:137:ARG:NH2	2.49	0.46
1:B:70:ASP:C	1:B:70:ASP:OD1	2.58	0.45
1:C:102:MET:CE	1:C:151:ASN:HD22	2.28	0.45
1:A:93:ASP:HB2	1:A:289:LEU:HD11	1.98	0.45
1:C:108:LEU:O	1:C:109:PRO:C	2.59	0.45
1:D:37:ILE:HG23	1:D:120:GLY:HA2	1.98	0.45
1:D:351:MET:CE	1:D:352:PRO:O	2.62	0.45
1:F:19:MET:H	1:F:19:MET:HG2	1.47	0.45
1:F:41:LYS:HA	1:F:41:LYS:HD3	1.49	0.45
1:F:102:MET:CE	1:F:151:ASN:HD22	2.29	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:B:94:TYR:CD1	1:B:94:TYR:C	2.95	0.45
1:D:195:GLN:O	1:D:199:THR:HG23	2.15	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:A:285:VAL:O	1:A:286:ALA:C	2.59	0.45
1:C:143:GLU:OE1	1:C:146:HIS:ND1	2.50	0.45
1:B:207:ALA:O	1:B:208:ARG:C	2.59	0.45
1:D:99:VAL:O	1:D:100:GLY:C	2.59	0.45
1:E:121:VAL:HG21	1:E:189:PHE:CZ	2.51	0.45
1:E:151:ASN:O	1:E:152:LYS:C	2.59	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:A:166:GLU:CD	1:B:64:PRO:HD2	2.43	0.44
1:B:128:SER:HA	1:B:129:PRO:HD3	1.87	0.44
1:B:177:MET:HE2	1:B:179:PRO:HG3	1.99	0.44
1:E:166:GLU:OE1	1:F:64:PRO:HD2	2.17	0.44
1:E:248:PRO:O	1:E:252:VAL:HG23	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:94:TYR:CD1	1:F:94:TYR:C	2.95	0.44
1:D:70:ASP:C	1:D:70:ASP:OD1	2.58	0.44
1:D:75:GLY:O	1:D:76:PHE:C	2.58	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:E:352:PRO:HA	1:E:359:ARG:O	2.17	0.44
1:A:19:MET:H	1:A:19:MET:HG2	1.42	0.44
1:A:207:ALA:O	1:A:208:ARG:C	2.59	0.44
1:B:88:LYS:HB3	1:B:88:LYS:HE3	1.81	0.44
1:F:93:ASP:HB2	1:F:289:LEU:HD11	1.99	0.44
1:F:348:ALA:HB1	1:F:349:PRO:HD2	1.98	0.44
1:A:38:GLU:HA	1:A:41:LYS:HB2	1.99	0.44
1:A:255:PHE:CE2	1:A:327:VAL:HG11	2.53	0.44
1:C:329:ARG:HE	1:C:329:ARG:HB2	1.59	0.44
1:E:207:ALA:O	1:E:208:ARG:C	2.61	0.44
1:A:248:PRO:O	1:A:252:VAL:HG23	2.18	0.44
1:A:342:GLN:C	1:A:344:ARG:H	2.26	0.44
1:B:112:GLN:HG3	1:B:140:THR:OG1	2.18	0.44
1:B:248:PRO:O	1:B:252:VAL:HG23	2.17	0.44
1:B:304:LEU:HB3	1:B:308:TRP:CZ3	2.53	0.44
1:D:93:ASP:HB2	1:D:289:LEU:HD11	2.00	0.44
1:D:161:ASP:OD1	1:D:161:ASP:C	2.61	0.44
1:F:179:PRO:HG2	1:F:181:THR:HG23	1.99	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:C:69:PRO:HA	1:C:79:GLN:OE1	2.17	0.44
1:C:161:ASP:C	1:C:161:ASP:OD1	2.60	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:C:146:HIS:ND1	1:C:225:ILE:HG23	2.33	0.43
1:F:99:VAL:O	1:F:103:ILE:HG13	2.19	0.43
1:F:108:LEU:O	1:F:109:PRO:C	2.60	0.43
1:F:271:TYR:CZ	1:F:273:GLY:HA2	2.53	0.43
1:B:195:GLN:O	1:B:199:THR:HG23	2.18	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:A:201:ILE:O	1:A:205:ASN:ND2	2.52	0.43
1:B:37:ILE:HG23	1:B:120:GLY:HA2	2.00	0.43
1:C:37:ILE:HG23	1:C:120:GLY:HA2	1.99	0.43
1:C:42:SER:C	1:C:44:ASP:H	2.26	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:147:GLY:O	1:E:148:ASP:C	2.62	0.43
1:E:166:GLU:CD	1:F:64:PRO:HD2	2.43	0.43
1:D:347:GLU:H	1:D:347:GLU:HG3	1.64	0.43
1:E:41:LYS:HA	1:E:41:LYS:HD3	1.49	0.43
1:A:97:VAL:HG21	1:A:289:LEU:HD12	2.00	0.43
1:B:42:SER:C	1:B:44:ASP:H	2.26	0.43
1:C:216:ILE:H	1:C:216:ILE:HG13	1.50	0.43
1:D:42:SER:C	1:D:44:ASP:H	2.26	0.43
1:E:304:LEU:HB3	1:E:308:TRP:CZ3	2.53	0.43
1:F:331:PRO:HB2	1:F:332:PRO:CD	2.49	0.43
1:B:102:MET:CE	1:B:151:ASN:HD22	2.31	0.43
1:D:22:ARG:H	1:D:22:ARG:HG2	1.73	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:A:108:LEU:O	1:A:109:PRO:C	2.61	0.43
1:C:62:TRP:CH2	1:C:145:ARG:HG3	2.53	0.43
1:C:179:PRO:HG2	1:C:181:THR:HG23	2.00	0.43
1:E:53:VAL:C	1:E:55:LEU:H	2.25	0.43
1:F:51:ILE:HG23	1:F:235:ALA:HB1	1.99	0.43
1:F:152:LYS:O	1:F:153:TYR:C	2.58	0.43
1:F:329:ARG:HE	1:F:329:ARG:HB2	1.62	0.43
1:A:53:VAL:C	1:A:55:LEU:H	2.26	0.42
1:B:41:LYS:HA	1:B:41:LYS:HD3	1.48	0.42
1:D:146:HIS:ND1	1:D:225:ILE:HG23	2.34	0.42
1:A:64:PRO:HD2	1:B:166:GLU:CD	2.43	0.42
1:F:108:LEU:HD21	1:F:140:THR:HG23	2.01	0.42
1:F:195:GLN:O	1:F:199:THR:HG23	2.19	0.42
1:E:125:THR:HG23	1:F:29:THR:HG22	2.00	0.42
1:F:69:PRO:HA	1:F:79:GLN:OE1	2.19	0.42
1:F:339:GLU:C	1:F:341:ALA:H	2.28	0.42
1:B:38:GLU:HB2	1:F:38:GLU:OE1	2.19	0.42
1:B:298:ALA:HB2	1:B:334:ILE:HG22	2.00	0.42
1:D:277:ASN:HB2	1:D:281:HIS:CE1	2.55	0.42
1:D:339:GLU:C	1:D:341:ALA:H	2.28	0.42
1:F:61:CYS:HB3	1:F:145:ARG:HH21	1.85	0.42
1:F:342:GLN:C	1:F:344:ARG:H	2.27	0.42
1:A:121:VAL:HG21	1:A:189:PHE:CZ	2.55	0.42
1:B:279:PHE:O	1:B:280:ASP:C	2.62	0.42
1:D:342:GLN:C	1:D:344:ARG:H	2.27	0.42
1:F:351:MET:CE	1:F:352:PRO:O	2.58	0.42
1:D:351:MET:O	1:D:351:MET:HG3	2.16	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:145:ARG:NH1	1:E:228:ASP:OD2	2.52	0.42
1:E:255:PHE:CE2	1:E:327:VAL:HG11	2.53	0.42
1:E:281:HIS:O	1:E:285:VAL:HG23	2.19	0.42
1:C:285:VAL:O	1:C:286:ALA:C	2.62	0.42
1:D:143:GLU:OE1	1:D:146:HIS:CE1	2.72	0.42
1:E:19:MET:H	1:E:19:MET:HG2	1.56	0.42
1:E:99:VAL:O	1:E:103:ILE:HG13	2.19	0.42
1:E:153:TYR:CD2	1:E:153:TYR:C	2.98	0.42
1:C:147:GLY:O	1:C:148:ASP:C	2.63	0.42
1:D:41:LYS:HD3	1:D:41:LYS:HA	1.50	0.42
1:A:205:ASN:O	1:A:206:THR:C	2.61	0.42
1:A:329:ARG:HE	1:A:329:ARG:HB2	1.63	0.42
1:C:41:LYS:HA	1:C:41:LYS:HD3	1.45	0.42
1:D:207:ALA:O	1:D:208:ARG:C	2.61	0.42
1:F:352:PRO:HA	1:F:359:ARG:O	2.19	0.42
1:B:38:GLU:HB2	1:F:38:GLU:CG	2.50	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:C:342:GLN:C	1:C:344:ARG:H	2.28	0.42
1:A:168:THR:HA	1:A:271:TYR:O	2.20	0.41
1:C:236:TYR:HA	1:C:239:ILE:HD12	2.01	0.41
1:D:102:MET:CE	1:D:151:ASN:HD22	2.32	0.41
1:E:108:LEU:HD22	1:E:144:ASN:HB2	2.01	0.41
1:A:268:HIS:HA	1:A:279:PHE:CD1	2.54	0.41
1:B:356:ILE:HD12	1:B:359:ARG:HB2	2.02	0.41
1:C:63:GLN:HB3	1:C:64:PRO:CD	2.50	0.41
1:E:108:LEU:HD21	1:E:140:THR:HG23	2.03	0.41
1:F:268:HIS:HA	1:F:279:PHE:CG	2.55	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:B:38:GLU:CB	1:F:38:GLU:CG	2.98	0.41
1:C:161:ASP:O	1:C:162:MET:C	2.63	0.41
1:D:121:VAL:HG21	1:D:189:PHE:CZ	2.55	0.41
1:D:128:SER:HA	1:D:129:PRO:HD3	1.84	0.41
1:D:307:ARG:CG	1:D:307:ARG:NH1	2.66	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:E:102:MET:HE1	1:E:151:ASN:HD22	1.85	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:GLN:HB3	1:A:64:PRO:CD	2.50	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:E:128:SER:HA	1:E:129:PRO:HD3	1.82	0.41
1:E:168:THR:HA	1:E:271:TYR:O	2.20	0.41
1:E:207:ALA:HB2	1:E:222:CYS:CB	2.46	0.41
1:F:37:ILE:HG23	1:F:120:GLY:HA2	2.01	0.41
1:F:216:ILE:H	1:F:216:ILE:HG13	1.49	0.41
1:A:108:LEU:HD22	1:A:144:ASN:HB2	2.03	0.41
1:A:128:SER:HA	1:A:129:PRO:HD3	1.85	0.41
1:C:19:MET:H	1:C:19:MET:HG2	1.44	0.41
1:C:268:HIS:HA	1:C:279:PHE:CG	2.56	0.41
1:E:106:GLU:C	1:E:108:LEU:H	2.29	0.41
1:E:161:ASP:OD1	1:E:161:ASP:C	2.64	0.41
1:E:342:GLN:C	1:E:344:ARG:H	2.29	0.41
1:A:216:ILE:H	1:A:216:ILE:HG13	1.54	0.40
1:B:93:ASP:HB2	1:B:289:LEU:HD11	2.04	0.40
1:C:94:TYR:CD1	1:C:94:TYR:C	2.99	0.40
1:E:329:ARG:HE	1:E:329:ARG:HB2	1.62	0.40
1:F:106:GLU:C	1:F:108:LEU:H	2.30	0.40
1:F:307:ARG:CG	1:F:307:ARG:NH1	2.67	0.40
1:A:102:MET:HE3	1:A:151:ASN:HD22	1.86	0.40
1:B:121:VAL:HG21	1:B:189:PHE:CZ	2.56	0.40
1:C:279:PHE:O	1:C:280:ASP:C	2.63	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: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: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%)	10	42
1	B	344/363 (95%)	307 (89%)	31 (9%)	6 (2%)	7	35
1	C	344/363 (95%)	311 (90%)	30 (9%)	3 (1%)	14	47
1	D	344/363 (95%)	307 (89%)	32 (9%)	5 (2%)	8	37
1	E	344/363 (95%)	309 (90%)	31 (9%)	4 (1%)	10	42
1	F	344/363 (95%)	305 (89%)	34 (10%)	5 (2%)	8	37
All	All	2064/2178 (95%)	1849 (90%)	188 (9%)	27 (1%)	9	40

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%)	238 (79%)	62 (21%)	1	7
1	B	300/315 (95%)	242 (81%)	58 (19%)	1	8
1	C	300/315 (95%)	242 (81%)	58 (19%)	1	8
1	D	300/315 (95%)	239 (80%)	61 (20%)	1	7
1	E	300/315 (95%)	240 (80%)	60 (20%)	1	7
1	F	300/315 (95%)	243 (81%)	57 (19%)	1	9
All	All	1800/1890 (95%)	1444 (80%)	356 (20%)	1	8

All (356) 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	49	GLU
1	A	58	VAL
1	A	73	SER
1	A	78	GLU
1	A	86	ARG
1	A	89	GLU
1	A	93	ASP
1	A	104	THR
1	A	106	GLU
1	A	124	GLU
1	A	128	SER
1	A	130	THR
1	A	134	ILE

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Mol	Chain	Res	Type
1	A	136	THR
1	A	143	GLU
1	A	144	ASN
1	A	145	ARG
1	A	152	LYS
1	A	162	MET
1	A	167	LYS
1	A	171	TYR
1	A	177	MET
1	A	180	ARG
1	A	184	SER
1	A	208	ARG
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	245	GLU
1	A	246	ILE
1	A	249	ASP
1	A	258	MET
1	A	259	MET
1	A	260	ARG
1	A	262	LYS
1	A	264	SER
1	A	274	ARG
1	A	302	GLU
1	A	307	ARG
1	A	311	ASP
1	A	314	THR
1	A	321	GLN
1	A	322	LYS
1	A	329	ARG
1	A	333	ARG
1	A	334	ILE
1	A	344	ARG
1	A	347	GLU
1	A	350	THR
1	A	351	MET
1	B	19	MET
1	B	22	ARG

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Mol	Chain	Res	Type
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	49	GLU
1	B	58	VAL
1	B	60	LYS
1	B	78	GLU
1	B	86	ARG
1	B	89	GLU
1	B	93	ASP
1	B	111	TYR
1	B	128	SER
1	B	130	THR
1	B	134	ILE
1	B	136	THR
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	208	ARG
1	B	211	LYS
1	B	216	ILE
1	B	220	GLN
1	B	224	THR
1	B	238	LYS
1	B	241	GLU
1	B	245	GLU
1	B	246	ILE
1	B	249	ASP
1	B	258	MET
1	B	259	MET
1	B	260	ARG
1	B	262	LYS
1	B	264	SER

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Mol	Chain	Res	Type
1	B	274	ARG
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	334	ILE
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
1	C	41	LYS
1	C	48	GLU
1	C	49	GLU
1	C	58	VAL
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	104	THR
1	C	111	TYR
1	C	130	THR
1	C	134	ILE
1	C	136	THR
1	C	143	GLU
1	C	144	ASN
1	C	145	ARG
1	C	152	LYS
1	C	162	MET
1	C	171	TYR

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Mol	Chain	Res	Type
1	C	177	MET
1	C	180	ARG
1	C	184	SER
1	C	211	LYS
1	C	216	ILE
1	C	220	GLN
1	C	224	THR
1	C	238	LYS
1	C	241	GLU
1	C	245	GLU
1	C	246	ILE
1	C	249	ASP
1	C	258	MET
1	C	259	MET
1	C	260	ARG
1	C	262	LYS
1	C	264	SER
1	C	274	ARG
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	334	ILE
1	C	344	ARG
1	C	347	GLU
1	C	350	THR
1	C	351	MET
1	C	360	GLN
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	49	GLU
1	D	58	VAL
1	D	73	SER

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Mol	Chain	Res	Type
1	D	78	GLU
1	D	86	ARG
1	D	89	GLU
1	D	93	ASP
1	D	104	THR
1	D	111	TYR
1	D	128	SER
1	D	130	THR
1	D	134	ILE
1	D	136	THR
1	D	143	GLU
1	D	144	ASN
1	D	145	ARG
1	D	152	LYS
1	D	162	MET
1	D	167	LYS
1	D	171	TYR
1	D	175	SER
1	D	177	MET
1	D	180	ARG
1	D	208	ARG
1	D	211	LYS
1	D	216	ILE
1	D	220	GLN
1	D	224	THR
1	D	238	LYS
1	D	241	GLU
1	D	245	GLU
1	D	246	ILE
1	D	249	ASP
1	D	258	MET
1	D	259	MET
1	D	260	ARG
1	D	262	LYS
1	D	264	SER
1	D	274	ARG
1	D	302	GLU
1	D	307	ARG
1	D	311	ASP
1	D	314	THR
1	D	321	GLN
1	D	329	ARG

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Mol	Chain	Res	Type
1	D	333	ARG
1	D	334	ILE
1	D	344	ARG
1	D	347	GLU
1	D	350	THR
1	D	351	MET
1	D	360	GLN
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	49	GLU
1	E	58	VAL
1	E	73	SER
1	E	78	GLU
1	E	86	ARG
1	E	89	GLU
1	E	93	ASP
1	E	104	THR
1	E	111	TYR
1	E	113	THR
1	E	128	SER
1	E	130	THR
1	E	134	ILE
1	E	136	THR
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
1	E	184	SER
1	E	208	ARG
1	E	211	LYS

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Mol	Chain	Res	Type
1	E	216	ILE
1	E	220	GLN
1	E	224	THR
1	E	238	LYS
1	E	241	GLU
1	E	245	GLU
1	E	246	ILE
1	E	249	ASP
1	E	258	MET
1	E	259	MET
1	E	260	ARG
1	E	264	SER
1	E	274	ARG
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	334	ILE
1	E	344	ARG
1	E	347	GLU
1	E	350	THR
1	E	351	MET
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	49	GLU
1	F	58	VAL
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	113	THR
1	F	130	THR
1	F	134	ILE
1	F	136	THR
1	F	143	GLU
1	F	144	ASN
1	F	145	ARG
1	F	152	LYS
1	F	162	MET
1	F	167	LYS
1	F	171	TYR
1	F	177	MET
1	F	180	ARG
1	F	208	ARG
1	F	211	LYS
1	F	216	ILE
1	F	220	GLN
1	F	224	THR
1	F	238	LYS
1	F	241	GLU
1	F	245	GLU
1	F	246	ILE
1	F	249	ASP
1	F	258	MET
1	F	259	MET
1	F	260	ARG
1	F	262	LYS
1	F	264	SER
1	F	274	ARG
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	334	ILE
1	F	344	ARG
1	F	347	GLU
1	F	350	THR
1	F	351	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	HIS
1	A	151	ASN
1	A	277	ASN
1	A	321	GLN
1	B	27	GLN
1	B	30	HIS
1	B	277	ASN
1	B	281	HIS
1	B	321	GLN
1	C	30	HIS
1	C	50	ASN
1	C	151	ASN
1	C	321	GLN
1	D	30	HIS
1	D	151	ASN
1	D	321	GLN
1	E	151	ASN
1	E	321	GLN
1	F	27	GLN
1	F	30	HIS
1	F	321	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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%)	-1.39	0 100 100	16, 38, 44, 47	8 (2%)
1	B	346/363 (95%)	-1.37	0 100 100	16, 38, 44, 47	8 (2%)
1	C	346/363 (95%)	-1.37	0 100 100	16, 38, 44, 47	8 (2%)
1	D	346/363 (95%)	-1.38	0 100 100	16, 38, 44, 47	8 (2%)
1	E	346/363 (95%)	-1.40	0 100 100	16, 38, 44, 47	8 (2%)
1	F	346/363 (95%)	-1.39	0 100 100	16, 38, 44, 47	8 (2%)
All	All	2076/2178 (95%)	-1.38	0 100 100	16, 38, 44, 47	48 (2%)

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	SR	B	366	1/1	0.98	0.14	128,128,128,128	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SR	E	365	1/1	0.98	0.13	153,153,153,153	0
2	SR	B	365	1/1	0.99	0.15	144,144,144,144	0
2	SR	A	364	1/1	0.99	0.09	142,142,142,142	0
2	SR	C	365	1/1	0.99	0.07	171,171,171,171	0
2	SR	D	364	1/1	0.99	0.05	130,130,130,130	0
2	SR	E	364	1/1	0.99	0.04	119,119,119,119	0
2	SR	B	364	1/1	0.99	0.05	118,118,118,118	0
2	SR	F	365	1/1	0.99	0.10	126,126,126,126	0
2	SR	D	365	1/1	1.00	0.04	159,159,159,159	0
2	SR	F	364	1/1	1.00	0.06	127,127,127,127	0
2	SR	C	364	1/1	1.00	0.12	151,151,151,151	0

6.5 Other polymers [i](#)

There are no such residues in this entry.