Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 09:24 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 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

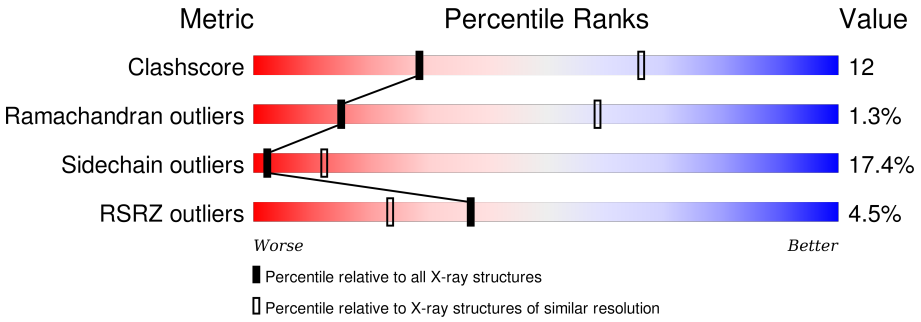
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 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	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)
RSRZ outliers	91569	1129 (3.24-3.16)

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. 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 <=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	5% 57% 33% 5% 5%
1	B	363	4% 58% 33% • • 5%
1	C	363	3% 60% 31% • 5%
1	D	363	4% 60% 30% 5% 5%
1	E	363	4% 58% 31% 6% 5%
1	F	363	4% 59% 31% • • 5%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

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

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 (three-letter code: SR) (formula: Sr).

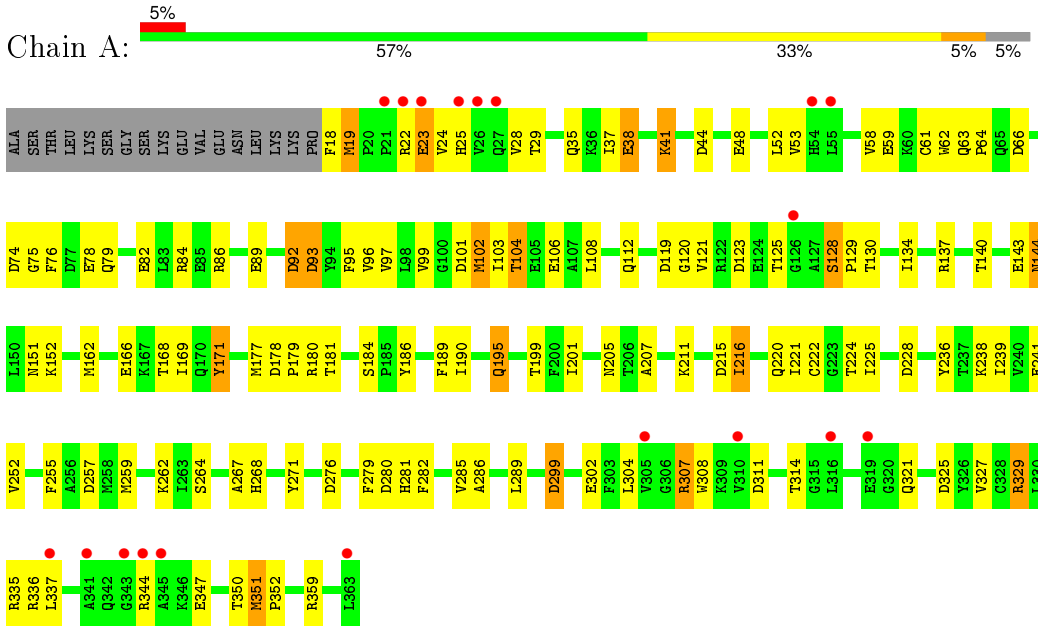
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	2	Total	Sr	0	0
			2	2		
2	E	2	Total	Sr	0	0
			2	2		
2	B	3	Total	Sr	0	0
			3	3		
2	C	2	Total	Sr	0	0
			2	2		
2	A	1	Total	Sr	0	0
			1	1		
2	F	2	Total	Sr	0	0
			2	2		

3 Residue-property plots (i)

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.

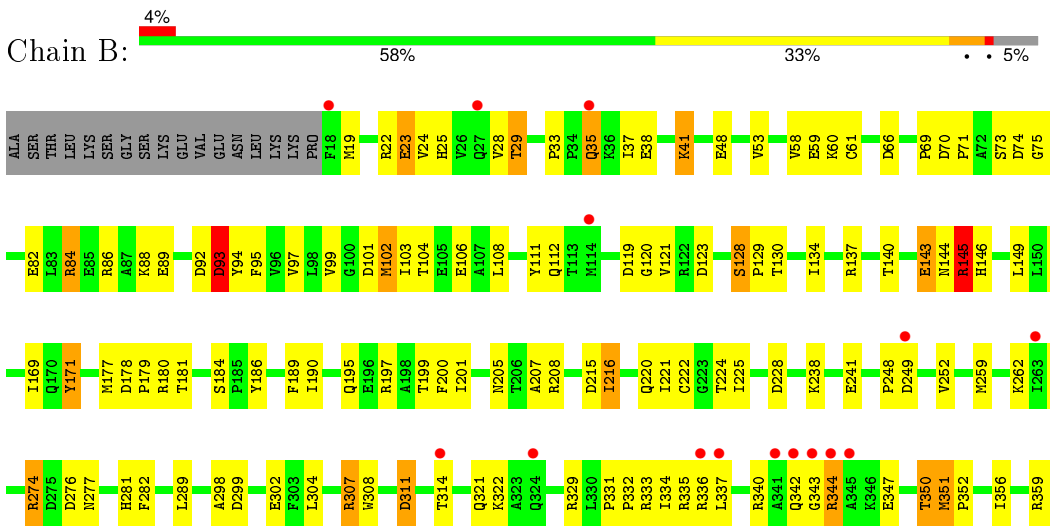
- Molecule 1: Acyl-[acyl-carrier protein] desaturase

Chain A:



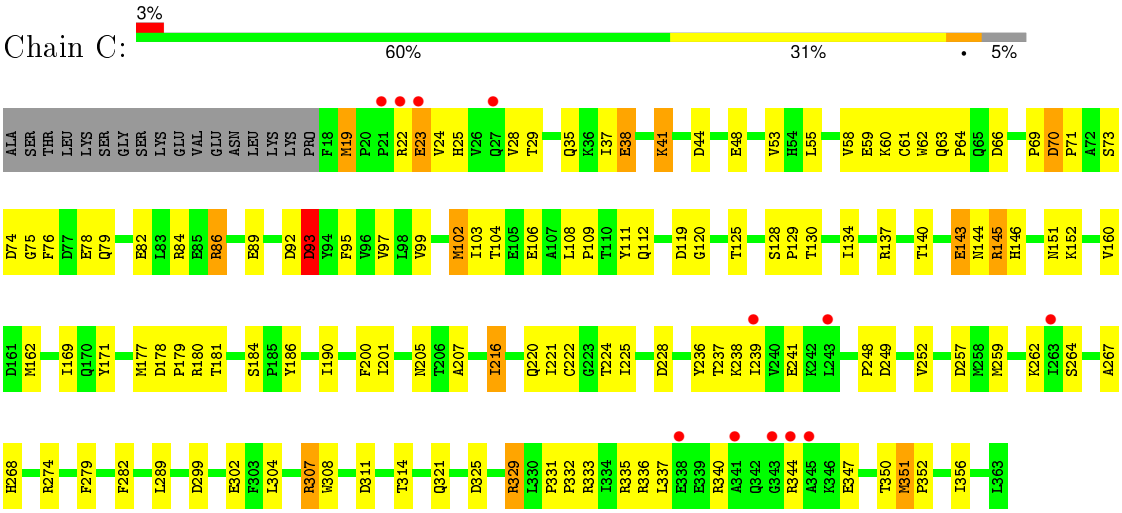
- Molecule 1: Acyl-[acyl-carrier protein] desaturase

Chain B:



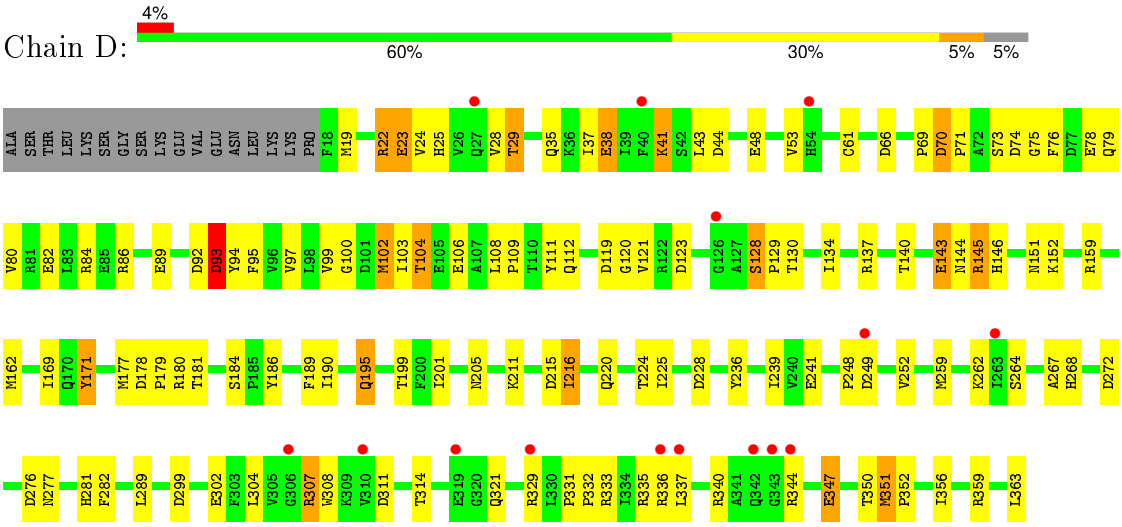
- Molecule 1: Acyl-[acyl-carrier protein] desaturase

Chain C:



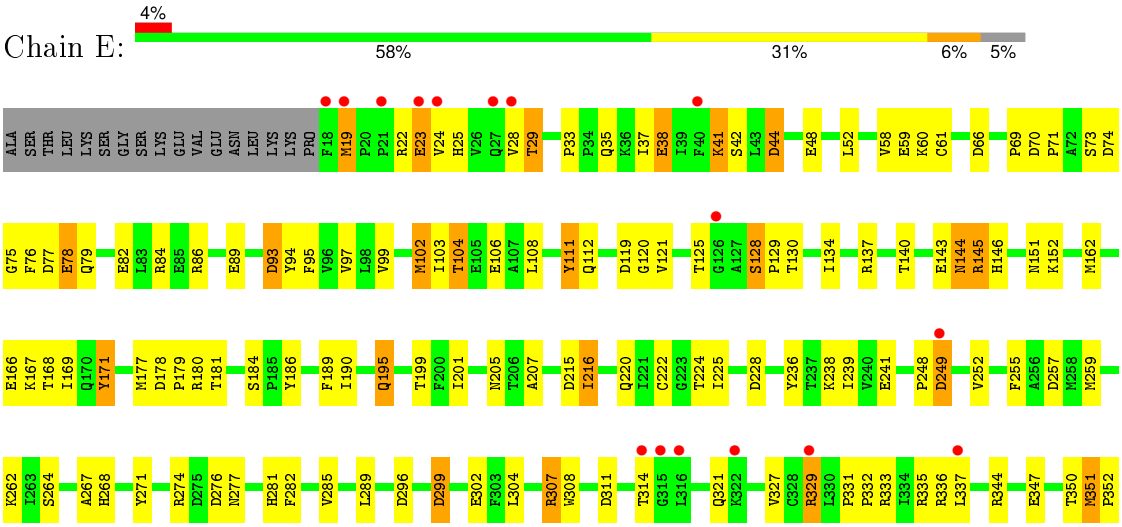
- Molecule 1: Acyl-[acyl-carrier protein] desaturase

Chain D:



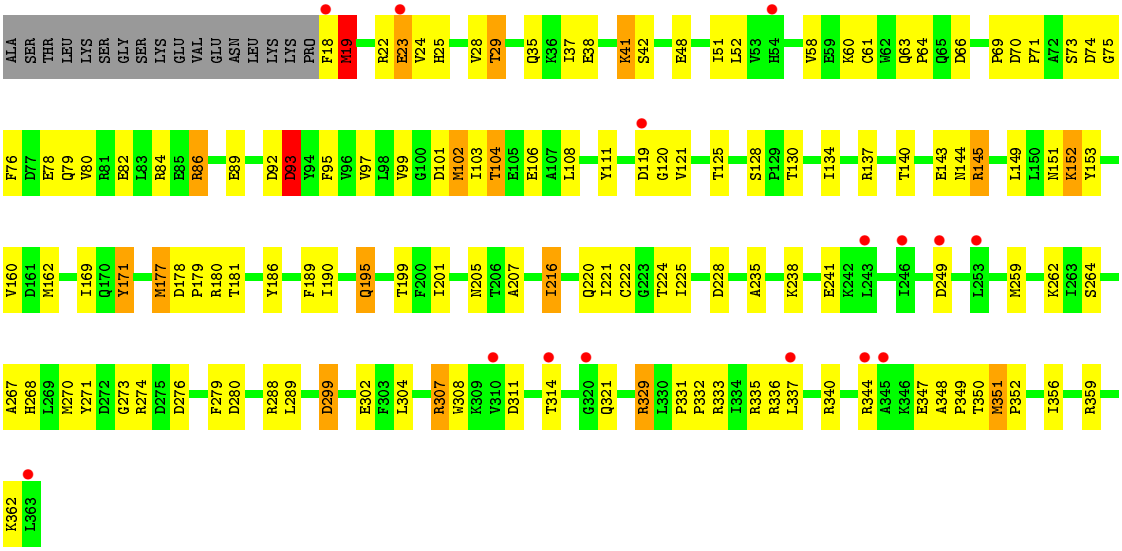
- Molecule 1: Acyl-[acyl-carrier protein] desaturase

Chain E:



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

Chain F:



4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [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)	0.28 , 34.4	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[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.26$	Xtriage
Outliers	0 of 49227 reflections	Xtriage
F_o,F_c correlation	0.91	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	0.79	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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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 Too-close contacts (i)

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	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

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 12.

All (381) 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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:95:PHE:O	1:E:99:VAL:HG23	1.85	0.77
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

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

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

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

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

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

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

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

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

5.3.1 Protein backbone (i)

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%)	16	60
1	B	344/363 (95%)	307 (89%)	31 (9%)	6 (2%)	11	52
1	C	344/363 (95%)	311 (90%)	30 (9%)	3 (1%)	21	67
1	D	344/363 (95%)	307 (89%)	32 (9%)	5 (2%)	13	55
1	E	344/363 (95%)	309 (90%)	31 (9%)	4 (1%)	16	60
1	F	344/363 (95%)	305 (89%)	34 (10%)	5 (2%)	13	55
All	All	2064/2178 (95%)	1849 (90%)	188 (9%)	27 (1%)	15	59

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

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Mol	Chain	Res	Type
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%)	2	12
1	B	300/315 (95%)	247 (82%)	53 (18%)	2	11
1	C	300/315 (95%)	249 (83%)	51 (17%)	2	12
1	D	300/315 (95%)	248 (83%)	52 (17%)	2	12
1	E	300/315 (95%)	244 (81%)	56 (19%)	2	10
1	F	300/315 (95%)	250 (83%)	50 (17%)	3	13
All	All	1800/1890 (95%)	1486 (83%)	314 (17%)	2	12

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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 molecules 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.

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

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^{th} 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%)	0.35	19 (5%)	29	16	29, 38, 44, 47	8 (2%)
1	B	346/363 (95%)	0.24	16 (4%)	36	23	29, 38, 44, 47	8 (2%)
1	C	346/363 (95%)	0.26	12 (3%)	48	32	29, 38, 44, 47	8 (2%)
1	D	346/363 (95%)	0.29	15 (4%)	39	25	29, 38, 44, 47	8 (2%)
1	E	346/363 (95%)	0.32	16 (4%)	36	23	29, 38, 44, 47	8 (2%)
1	F	346/363 (95%)	0.37	15 (4%)	39	25	29, 38, 44, 47	8 (2%)
All	All	2076/2178 (95%)	0.30	93 (4%)	37	23	29, 38, 44, 47	48 (2%)

All (93) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	343	GLY	6.0
1	E	314	THR	5.8
1	C	341	ALA	5.5
1	F	314	THR	4.8
1	A	22	ARG	4.7
1	E	24	VAL	4.7
1	C	345	ALA	4.6
1	E	23	GLU	4.4
1	F	337	LEU	4.3
1	D	344	ARG	4.2
1	B	18	PHE	4.2
1	B	337	LEU	4.1
1	E	126	GLY	4.1
1	F	18	PHE	4.1
1	F	243	LEU	4.1
1	F	345	ALA	3.9
1	B	344	ARG	3.9
1	A	27	GLN	3.8
1	D	249	ASP	3.8

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Mol	Chain	Res	Type	RSRZ
1	D	329	ARG	3.7
1	E	18	PHE	3.6
1	D	54	HIS	3.6
1	A	344	ARG	3.5
1	E	316	LEU	3.5
1	E	315	GLY	3.5
1	A	26	VAL	3.5
1	F	246	ILE	3.5
1	A	21	PRO	3.4
1	F	344	ARG	3.4
1	C	23	GLU	3.3
1	C	344	ARG	3.3
1	D	337	LEU	3.2
1	A	337	LEU	3.2
1	E	19	MET	3.2
1	A	319	GLU	3.1
1	D	343	GLY	3.1
1	B	263	ILE	3.0
1	A	25	HIS	2.9
1	A	343	GLY	2.9
1	A	23	GLU	2.7
1	B	27	GLN	2.7
1	B	249	ASP	2.7
1	B	363	LEU	2.7
1	F	249	ASP	2.7
1	E	249	ASP	2.7
1	C	338	GLU	2.7
1	C	243	LEU	2.7
1	C	343	GLY	2.7
1	D	319	GLU	2.6
1	D	27	GLN	2.6
1	C	27	GLN	2.5
1	F	119	ASP	2.5
1	C	22	ARG	2.5
1	B	35	GLN	2.5
1	E	21	PRO	2.4
1	D	126	GLY	2.4
1	E	337	LEU	2.4
1	D	40	PHE	2.4
1	F	310	VAL	2.4
1	A	341	ALA	2.4
1	A	126	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	305	VAL	2.4
1	B	336	ARG	2.3
1	A	54	HIS	2.3
1	B	114	MET	2.3
1	E	322	LYS	2.3
1	C	263	ILE	2.3
1	F	363	LEU	2.3
1	C	239	ILE	2.3
1	F	54	HIS	2.3
1	A	55	LEU	2.2
1	A	363	LEU	2.2
1	B	345	ALA	2.2
1	D	342	GLN	2.1
1	E	40	PHE	2.1
1	B	324	GLN	2.1
1	E	27	GLN	2.1
1	F	23	GLU	2.1
1	D	336	ARG	2.1
1	D	263	ILE	2.1
1	E	329	ARG	2.1
1	B	341	ALA	2.1
1	A	345	ALA	2.1
1	D	306	GLY	2.1
1	B	342	GLN	2.1
1	D	310	VAL	2.1
1	F	320	GLY	2.1
1	A	310	VAL	2.1
1	F	253	LEU	2.1
1	C	21	PRO	2.0
1	E	28	VAL	2.0
1	A	316	LEU	2.0
1	B	314	THR	2.0

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

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

6.3 Carbohydrates (i)

There are no 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, 95^{th} 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^2)	Q<0.9
2	SR	C	364	1/1	0.82	0.33	4.11	151,151,151,151	0
2	SR	D	364	1/1	0.63	0.20	0.28	130,130,130,130	0
2	SR	B	364	1/1	0.97	0.21	-0.43	118,118,118,118	0
2	SR	B	366	1/1	0.87	0.22	-0.64	128,128,128,128	0
2	SR	A	364	1/1	0.81	0.18	-1.32	142,142,142,142	0
2	SR	E	364	1/1	0.90	0.17	-1.76	119,119,119,119	0
2	SR	C	365	1/1	0.69	0.18	-1.89	171,171,171,171	0
2	SR	B	365	1/1	0.95	0.19	-2.20	144,144,144,144	0
2	SR	E	365	1/1	0.84	0.16	-2.40	153,153,153,153	0
2	SR	F	364	1/1	0.94	0.11	-5.09	127,127,127,127	0
2	SR	D	365	1/1	0.92	0.08	-5.18	159,159,159,159	0
2	SR	F	365	1/1	0.83	0.11	-9.31	126,126,126,126	0

6.5 Other polymers

There are no such residues in this entry.