Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 08:47 AM GMT

PDB ID	:	3FZ3
Title	:	Crystal Structure of almond Pru1 protein
Authors	:	Jin, T.C.; Zhang, Y.Z.
Deposited on	:	2009-01-23
Resolution	:	2.40 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:

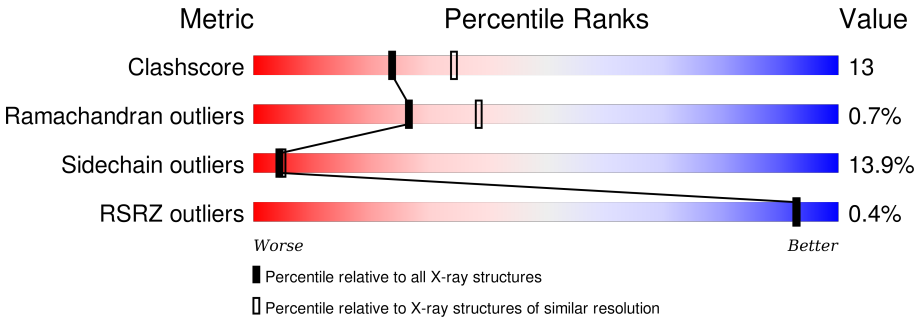
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.40 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	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (2.40-2.40)

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	531	48% 20% 5% 27%
1	B	531	% 51% 21% 5% 23%
1	C	531	% 53% 19% • 23%
1	D	531	52% 18% • 27%
1	E	531	50% 18% 5% 27%
1	F	531	52% 20% 5% 23%

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	CA	A	1	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 19957 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 Prunin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	388	Total	C	N	O	S	0	2	0
			3104	1926	583	591	4			
1	B	410	Total	C	N	O	S	0	1	0
			3296	2034	626	632	4			
1	C	410	Total	C	N	O	S	0	1	0
			3298	2035	628	631	4			
1	D	388	Total	C	N	O	S	0	1	0
			3102	1924	583	591	4			
1	E	388	Total	C	N	O	S	0	1	0
			3097	1922	580	591	4			
1	F	410	Total	C	N	O	S	0	2	0
			3302	2038	627	633	4			

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

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

- Molecule 4 is water.

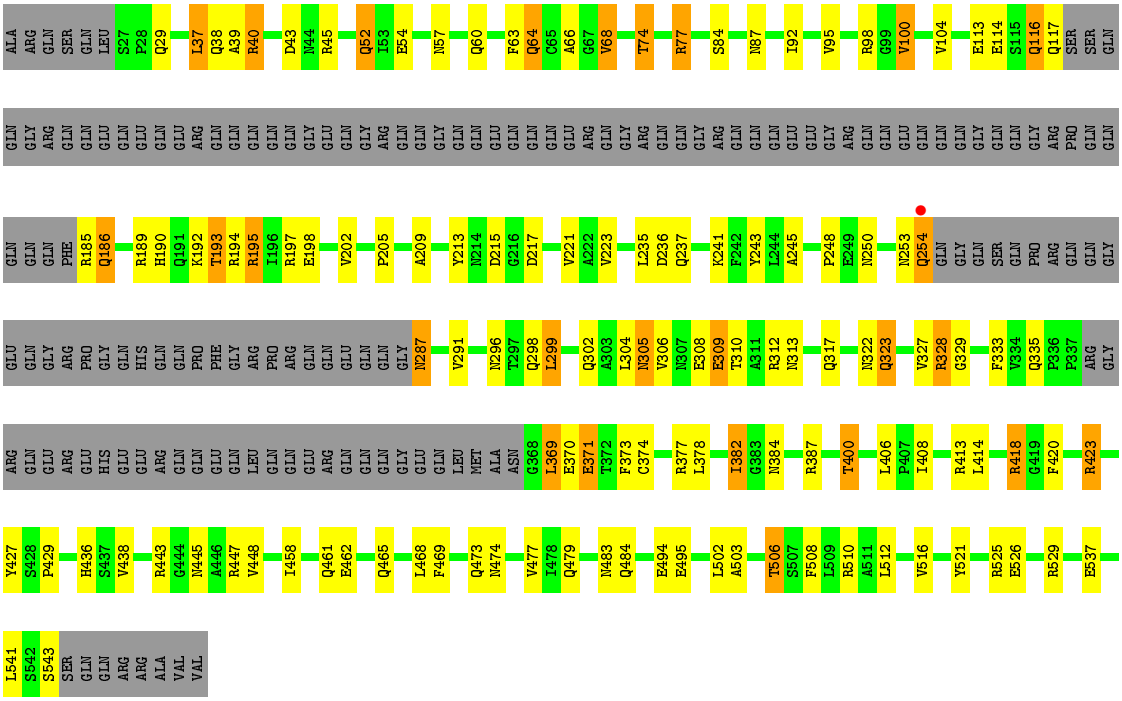
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	90	Total O 90 90	0	0
4	B	162	Total O 162 162	0	0
4	C	123	Total O 123 123	0	0
4	D	136	Total O 136 136	0	0
4	E	102	Total O 102 102	0	0
4	F	130	Total O 130 130	0	0

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.

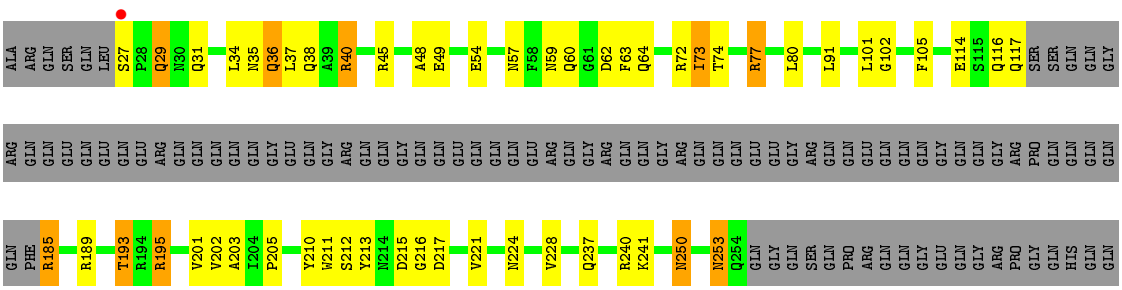
- Molecule 1: Prunin

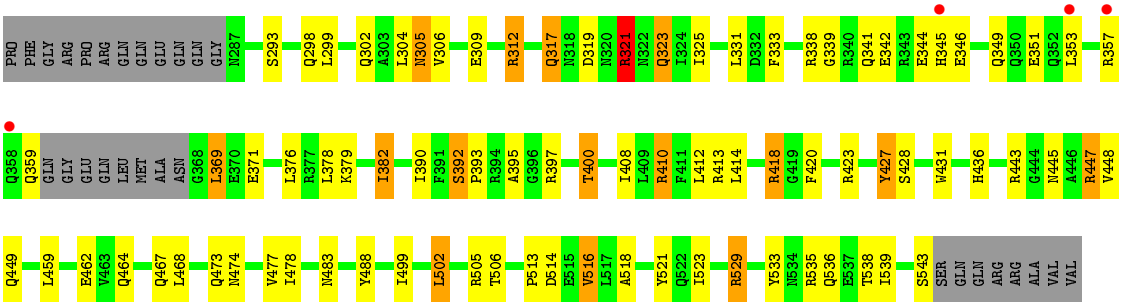
Chain A:

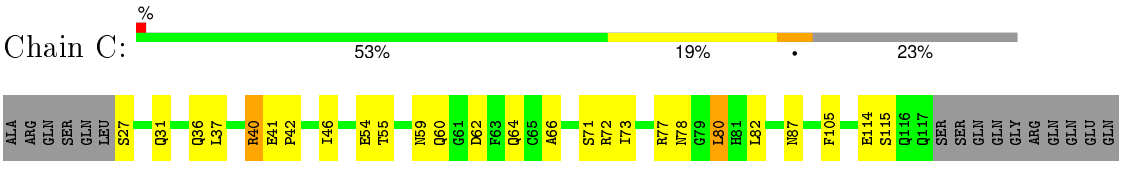


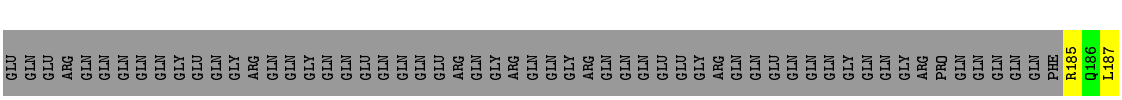
- Molecule 1: Prunin

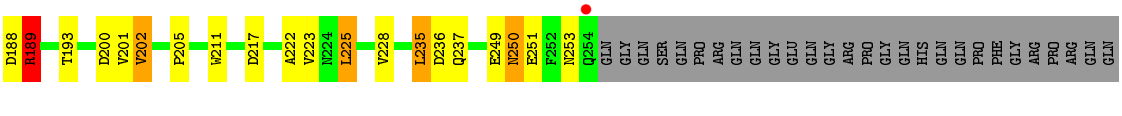
Chain B:

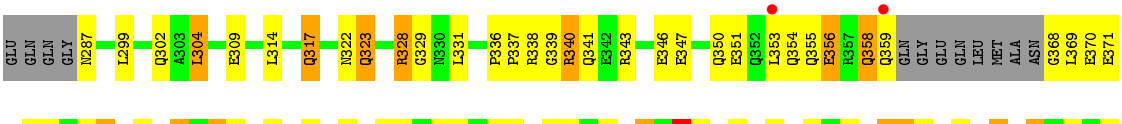


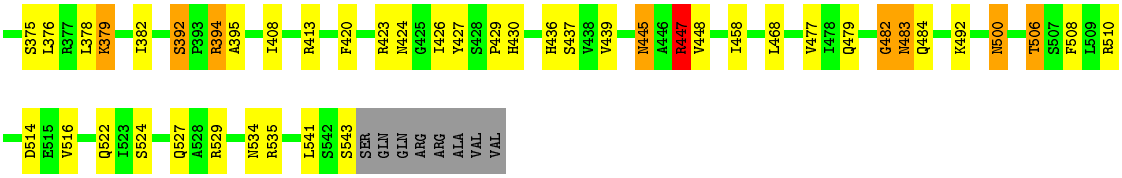










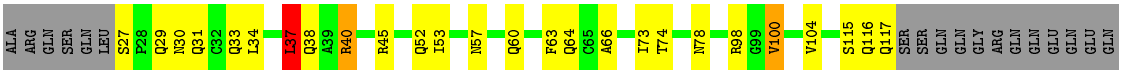


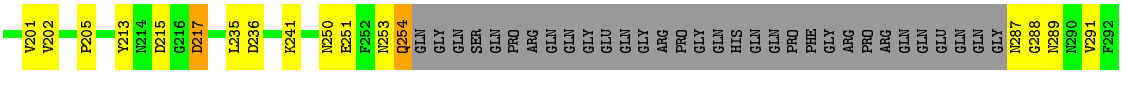
- Molecule 1: Prunin

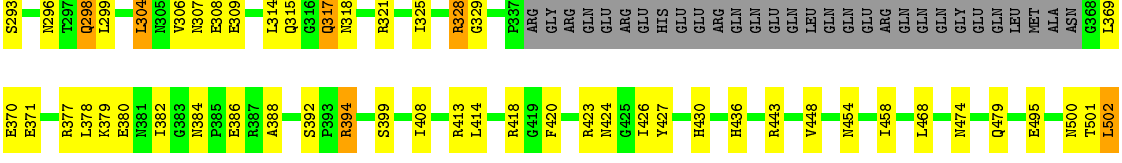
Chain C:

- Molecule 1: Prunin

Chain D:

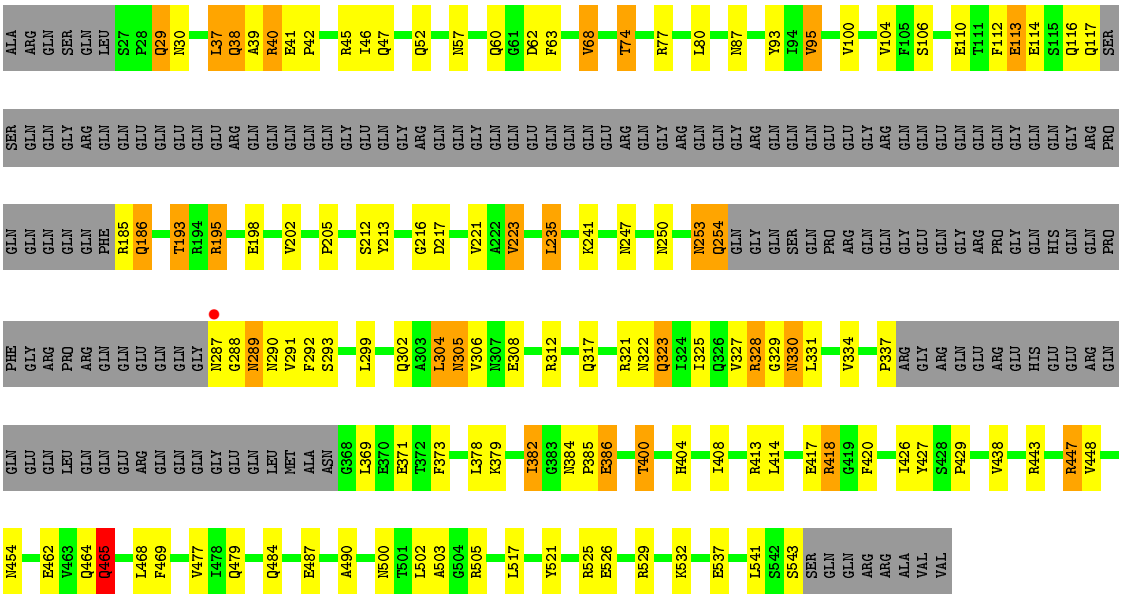






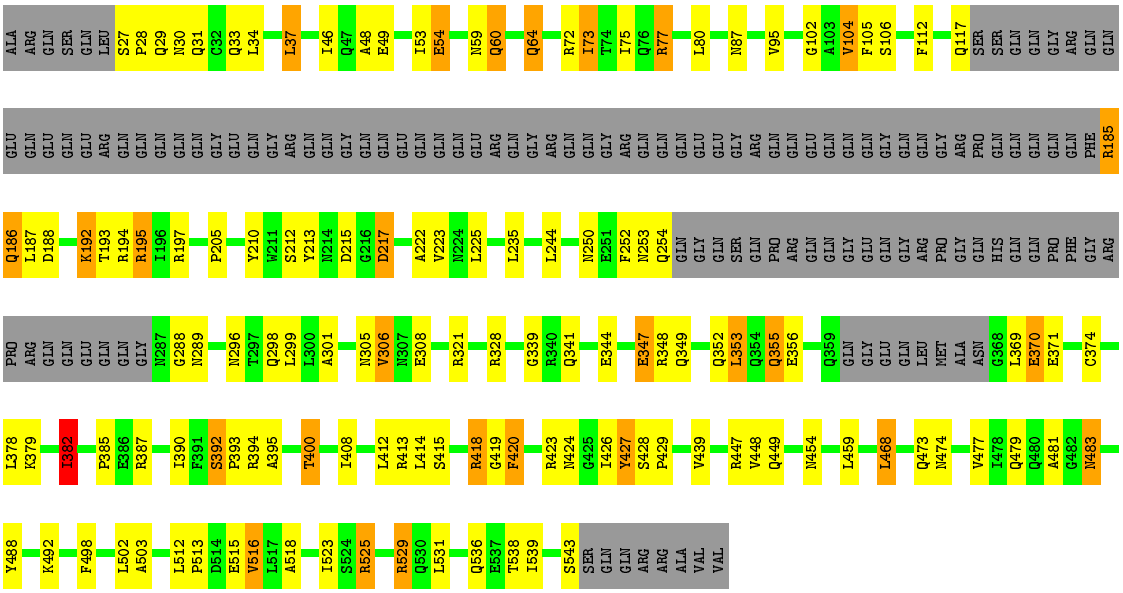
- Molecule 1: Prunin

Chain E:



- Molecule 1: Prunin

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, α, β, γ	151.02Å 151.02Å 165.37Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	36.08 – 2.40 36.09 – 2.40	Depositor EDS
% Data completeness (in resolution range)	88.7 (36.08-2.40) 88.0 (36.09-2.40)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.67 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.172 , 0.229 0.175 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	37.3	Xtriage
Anisotropy	0.575	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 38.1	EDS
Estimated twinning fraction	0.478 for h,-k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Outliers	1 of 142510 reflections (0.001%)	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	19957	wwPDB-VP
Average B, all atoms (Å^2)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.84% 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: NA, CA

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	0.69	0/3168	0.90	1/4291 (0.0%)
1	B	0.78	0/3358	1.01	6/4542 (0.1%)
1	C	0.74	0/3360	1.00	9/4544 (0.2%)
1	D	0.75	0/3163	0.98	3/4284 (0.1%)
1	E	0.72	0/3158	0.94	1/4278 (0.0%)
1	F	0.80	0/3367	1.02	3/4554 (0.1%)
All	All	0.75	0/19574	0.97	23/26493 (0.1%)

There are no bond length outliers.

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	321	ARG	NE-CZ-NH1	-7.18	116.71	120.30
1	D	195	ARG	NE-CZ-NH1	-6.43	117.09	120.30
1	C	189	ARG	NE-CZ-NH1	5.96	123.28	120.30
1	A	194	ARG	NE-CZ-NH1	5.93	123.27	120.30
1	C	236	ASP	CB-CG-OD2	5.87	123.58	118.30
1	C	514	ASP	CB-CG-OD1	5.82	123.53	118.30
1	F	468	LEU	CA-CB-CG	5.70	128.41	115.30
1	C	62	ASP	CB-CG-OD1	5.69	123.42	118.30
1	C	447	ARG	NE-CZ-NH1	5.55	123.08	120.30
1	E	80	LEU	CA-CB-CG	5.54	128.04	115.30
1	B	514	ASP	CB-CG-OD1	5.47	123.22	118.30
1	B	312	ARG	NE-CZ-NH1	-5.45	117.57	120.30
1	B	397	ARG	NE-CZ-NH1	-5.43	117.58	120.30
1	B	240	ARG	NE-CZ-NH1	-5.30	117.65	120.30
1	D	236	ASP	CB-CG-OD2	5.30	123.07	118.30
1	C	251	GLU	C-N-CA	5.20	134.69	121.70
1	D	37	LEU	CA-CB-CG	5.20	127.25	115.30
1	C	225	LEU	CA-CB-CG	5.14	127.11	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	382	ILE	CG1-CB-CG2	-5.13	100.11	111.40
1	C	200	ASP	CB-CG-OD1	5.12	122.91	118.30
1	C	331	LEU	CB-CG-CD2	-5.08	102.36	111.00
1	F	188	ASP	CB-CG-OD1	5.07	122.87	118.30
1	B	101	LEU	CA-C-N	5.00	126.20	116.20

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	3104	0	2974	95	0
1	B	3296	0	3143	97	0
1	C	3298	0	3148	88	0
1	D	3102	0	2972	66	0
1	E	3097	0	2963	97	0
1	F	3302	0	3151	111	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
3	A	2	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	2	0	0	0	0
3	F	2	0	0	0	0
4	A	90	0	0	7	0
4	B	162	0	0	11	0
4	C	123	0	0	5	0
4	D	136	0	0	4	0
4	E	102	0	0	5	0
4	F	130	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	19957	0	18351	494	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 (494) 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:B:250:ASN:HB3	1:B:253:ASN:ND2	1.43	1.30
1:B:250:ASN:CB	1:B:253:ASN:HD21	1.49	1.23
1:A:195:ARG:HH21	1:A:195:ARG:HG3	1.05	1.11
1:F:195:ARG:CG	1:F:195:ARG:HH21	1.67	1.08
1:F:195:ARG:NH2	1:F:195:ARG:HG3	1.53	1.05
1:E:195:ARG:CG	1:E:195:ARG:HH21	1.72	1.03
1:F:77:ARG:H	1:F:77:ARG:HD3	1.22	1.02
1:A:423:ARG:HH11	1:A:423:ARG:HB2	1.23	1.01
1:C:413:ARG:HD3	4:C:613:HOH:O	1.59	1.00
1:A:100:VAL:HG23	1:A:193:THR:HG23	1.42	0.98
1:B:390:ILE:HD13	1:B:539:ILE:HD12	1.44	0.97
1:E:327:VAL:HA	1:E:328:ARG:HB3	1.45	0.97
1:E:195:ARG:HG3	1:E:195:ARG:NH2	1.57	0.96
1:A:195:ARG:HH21	1:A:195:ARG:CG	1.79	0.94
1:E:195:ARG:HG3	1:E:195:ARG:HH21	0.79	0.94
1:E:331:LEU:HD12	1:F:515:GLU:HG2	1.51	0.93
1:C:447:ARG:HH11	1:C:447:ARG:HG2	1.33	0.92
1:C:340:ARG:H	1:C:341:GLN:CB	1.84	0.90
1:F:195:ARG:HH21	1:F:195:ARG:HG3	0.78	0.90
1:B:323:GLN:H	1:B:323:GLN:HE21	0.93	0.90
1:F:77:ARG:H	1:F:77:ARG:CD	1.86	0.88
1:A:195:ARG:NH2	1:A:195:ARG:HG3	1.77	0.88
1:D:53:ILE:HG12	1:D:73:ILE:HG13	1.56	0.87
1:A:423:ARG:HH11	1:A:423:ARG:CB	1.87	0.86
1:A:302:GLN:OE1	1:B:543:SER:HB2	1.75	0.85
1:F:34:LEU:HD13	1:F:37:LEU:HD21	1.57	0.85
1:E:328:ARG:HG3	1:E:328:ARG:O	1.75	0.84
1:D:287:ASN:HD22	1:D:317:GLN:HB3	1.41	0.84
1:F:339:GLY:HA2	4:F:752:HOH:O	1.76	0.84
1:A:100:VAL:CG2	1:A:193:THR:HG23	2.07	0.84
1:B:506:THR:HG22	4:B:941:HOH:O	1.78	0.83
1:D:30:ASN:HB3	1:D:33:GLN:HG3	1.60	0.83
1:F:77:ARG:N	1:F:77:ARG:HD3	1.94	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:323:GLN:H	1:B:323:GLN:NE2	1.74	0.82
1:C:339:GLY:HA2	1:C:340:ARG:HB3	1.61	0.81
1:A:37:LEU:HD22	1:A:458:ILE:HG13	1.60	0.81
1:F:390:ILE:CD1	1:F:539:ILE:HD12	2.11	0.81
1:B:323:GLN:N	1:B:323:GLN:HE21	1.77	0.81
1:B:529:ARG:HD2	4:B:1024:HOH:O	1.80	0.80
1:A:186:GLN:HA	4:B:1024:HOH:O	1.80	0.80
1:B:193:THR:HG23	4:B:952:HOH:O	1.81	0.79
1:E:331:LEU:CD1	1:F:515:GLU:HG2	2.12	0.79
1:A:423:ARG:HB2	1:A:423:ARG:NH1	1.97	0.79
1:E:447:ARG:NH1	1:E:462:GLU:HG2	1.98	0.79
1:E:323:GLN:H	1:E:323:GLN:HE21	1.30	0.79
1:D:454:ASN:O	1:F:289:ASN:HB2	1.81	0.79
1:B:445:ASN:HB2	1:B:462:GLU:OE1	1.85	0.77
1:E:185:ARG:HA	4:E:777:HOH:O	1.84	0.76
1:D:287:ASN:ND2	1:D:317:GLN:HB3	2.00	0.76
1:B:390:ILE:CD1	1:B:539:ILE:HD12	2.16	0.75
1:F:390:ILE:HD13	1:F:539:ILE:HD12	1.69	0.75
1:D:513:PRO:HD2	1:D:516:VAL:HG13	1.67	0.74
1:B:34:LEU:HD13	1:B:37:LEU:HD11	1.69	0.74
1:A:77:ARG:HD3	4:A:583:HOH:O	1.88	0.74
1:B:74:THR:HG23	1:B:221:VAL:HG22	1.70	0.74
1:B:185:ARG:O	1:C:529:ARG:HD2	1.88	0.73
1:A:377:ARG:HD3	4:A:1026:HOH:O	1.89	0.72
1:B:73:ILE:HG22	1:B:224:ASN:HD21	1.54	0.72
1:A:113:GLU:OE2	1:F:538:THR:HG23	1.90	0.71
1:E:328:ARG:CG	1:E:328:ARG:O	2.38	0.71
1:A:506:THR:HG22	4:A:577:HOH:O	1.91	0.71
1:A:423:ARG:HH11	1:A:423:ARG:CG	2.04	0.70
1:B:319:ASP:OD2	1:B:321:ARG:CD	2.39	0.70
1:A:382:ILE:HD13	1:A:418:ARG:HB2	1.73	0.70
1:A:309:GLU:HG2	1:A:312:ARG:HH22	1.56	0.70
1:C:448:VAL:HG22	1:C:479:GLN:HG2	1.74	0.70
1:E:250:ASN:HB3	1:E:253:ASN:OD1	1.92	0.69
1:C:185:ARG:HB2	1:C:189:ARG:HH21	1.57	0.69
1:E:186:GLN:HB2	1:F:529:ARG:NH1	2.07	0.69
1:B:412:LEU:O	1:B:413:ARG:HB2	1.93	0.69
1:C:250:ASN:HB3	1:C:253:ASN:HB2	1.75	0.69
1:C:340:ARG:N	1:C:341:GLN:CB	2.56	0.69
1:E:186:GLN:O	1:F:529:ARG:NH1	2.26	0.68
1:C:185:ARG:HB2	1:C:189:ARG:NH2	2.09	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:322:ASN:HB3	1:C:323:GLN:HE21	1.56	0.68
1:A:100:VAL:HG23	1:A:193:THR:CG2	2.20	0.67
1:C:338:ARG:HH11	1:C:343:ARG:HG3	1.59	0.67
1:D:304:LEU:HD13	1:E:503:ALA:HB2	1.77	0.67
1:E:77:ARG:CD	1:E:216:GLY:O	2.43	0.66
1:E:74:THR:HB	1:E:221:VAL:HG22	1.76	0.66
1:B:37:LEU:O	1:B:459:LEU:HD12	1.96	0.66
1:C:323:GLN:H	1:C:323:GLN:HE21	1.44	0.66
1:C:424:ASN:O	1:C:543:SER:HB3	1.95	0.66
1:C:340:ARG:HD3	1:C:343:ARG:HH21	1.61	0.66
1:F:513:PRO:HD2	1:F:516:VAL:HG13	1.76	0.66
1:E:447:ARG:HH12	1:E:462:GLU:HG2	1.60	0.66
1:E:77:ARG:HD2	1:E:216:GLY:O	1.95	0.66
1:A:308:GLU:HG2	1:A:312:ARG:NH1	2.11	0.65
1:F:412:LEU:O	1:F:413:ARG:HB2	1.96	0.65
1:D:534:ASN:HB3	1:F:305:ASN:HB3	1.79	0.65
1:B:250:ASN:HB3	1:B:253:ASN:HD21	0.60	0.65
1:C:77:ARG:HD2	1:C:217:ASP:O	1.97	0.65
1:D:195:ARG:NH1	1:D:215:ASP:OD1	2.27	0.65
1:E:323:GLN:H	1:E:323:GLN:NE2	1.93	0.65
1:A:461:GLN:HG2	1:A:462:GLU:H	1.60	0.65
1:B:319:ASP:OD2	1:B:321:ARG:HD2	1.95	0.65
1:C:185:ARG:CB	1:C:189:ARG:NH2	2.60	0.64
1:E:526:GLU:HB3	4:E:582:HOH:O	1.97	0.64
1:B:464:GLN:O	1:B:467:GLN:HG3	1.97	0.64
1:B:305:ASN:HB3	1:C:534:ASN:HB3	1.79	0.64
1:B:533:TYR:O	1:B:536:GLN:NE2	2.29	0.64
1:E:443[A]:ARG:HA	1:E:465:GLN:HG2	1.80	0.63
1:A:84:SER:OG	1:A:241:LYS:HE3	1.98	0.63
1:F:104:VAL:HG22	4:F:584:HOH:O	1.99	0.63
1:D:185:ARG:O	1:E:529:ARG:HD3	1.99	0.63
1:F:518:ALA:HA	1:F:523:ILE:HG13	1.80	0.63
1:A:448:VAL:HG22	1:A:479:GLN:HG2	1.80	0.63
1:F:390:ILE:HD11	1:F:539:ILE:HD12	1.80	0.63
1:A:461:GLN:HG2	1:A:462:GLU:N	2.13	0.63
1:B:77:ARG:HG2	1:B:216:GLY:O	1.99	0.62
1:A:185:ARG:HG2	4:B:1024:HOH:O	1.98	0.62
1:E:247:ASN:ND2	1:E:288:GLY:HA3	2.14	0.62
1:B:102:GLY:HA3	1:B:211:TRP:O	2.00	0.61
1:C:66:ALA:HA	1:C:436:HIS:CD2	2.35	0.61
1:A:310:THR:O	1:A:313:ASN:HB2	1.99	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:53:ILE:HG21	1:D:251:GLU:HG2	1.82	0.61
1:F:185:ARG:O	1:F:186:GLN:NE2	2.33	0.61
1:B:447:ARG:HD3	4:B:614:HOH:O	1.99	0.61
1:F:73:ILE:HD13	1:F:75:ILE:HG13	1.82	0.60
1:B:193:THR:CG2	4:B:952:HOH:O	2.43	0.60
1:E:443[B]:ARG:HA	1:E:465:GLN:HG2	1.83	0.60
1:E:448:VAL:HG22	1:E:479:GLN:HG2	1.82	0.60
1:A:197:ARG:NH1	4:A:582:HOH:O	2.34	0.60
1:A:100:VAL:CG2	1:A:193:THR:CG2	2.78	0.60
1:B:40[A]:ARG:NH1	1:B:62:ASP:OD1	2.35	0.60
1:F:387:ARG:HG3	1:F:387:ARG:O	2.01	0.60
1:E:68:VAL:HG21	1:E:438:VAL:HG21	1.83	0.60
1:B:319:ASP:OD2	1:B:321:ARG:HD3	2.01	0.59
1:C:370:GLU:OE2	1:D:506:THR:HG21	2.01	0.59
1:E:195:ARG:CG	1:E:195:ARG:NH2	2.42	0.59
1:A:400:THR:HG21	1:F:371:GLU:O	2.01	0.59
1:B:195:ARG:HH21	1:B:195:ARG:HB3	1.68	0.59
1:C:413:ARG:NH1	4:C:620:HOH:O	2.35	0.59
1:C:41:GLU:HB3	1:C:42:PRO:CD	2.32	0.59
1:E:418:ARG:NH1	1:E:487:GLU:HB3	2.18	0.59
1:D:287:ASN:N	1:D:288:GLY:HA2	2.17	0.58
1:D:40:ARG:HH11	1:D:60:GLN:HG3	1.67	0.58
1:B:73:ILE:CG2	1:B:224:ASN:HD21	2.16	0.58
1:E:186:GLN:HA	1:F:529:ARG:HD2	1.86	0.58
1:E:112:PHE:CD2	1:E:193:THR:HG22	2.38	0.58
1:D:66:ALA:HA	1:D:436:HIS:CD2	2.38	0.58
1:C:423:ARG:HD2	1:C:483:ASN:OD1	2.04	0.58
1:C:40:ARG:HH11	1:C:60:GLN:HG3	1.68	0.58
1:F:382:ILE:HD13	1:F:418:ARG:HB2	1.84	0.58
1:F:423:ARG:NH1	1:F:483:ASN:CG	2.56	0.57
1:F:448:VAL:HG12	1:F:459:LEU:HD23	1.85	0.57
1:E:57:ASN:O	1:E:60:GLN:HG3	2.04	0.57
1:F:423:ARG:NH1	1:F:483:ASN:OD1	2.37	0.57
4:B:615:HOH:O	1:E:400:THR:HG22	2.05	0.57
1:F:205:PRO:HG3	1:F:408:ILE:HD11	1.85	0.57
1:F:195:ARG:NH2	1:F:195:ARG:CG	2.40	0.57
1:C:249:GLU:H	1:C:323:GLN:HE22	1.53	0.57
1:A:296:ASN:HD22	1:A:299:LEU:H	1.51	0.57
1:E:57:ASN:HA	1:E:254:GLN:NE2	2.20	0.56
1:F:473:GLN:O	1:F:474:ASN:HB2	2.03	0.56
1:F:348:ARG:HG3	1:F:352:GLN:HE21	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:513:PRO:HD2	1:B:516:VAL:HG13	1.86	0.56
1:D:100:VAL:HG12	1:D:213:TYR:HB3	1.87	0.56
1:B:473:GLN:O	1:B:474:ASN:HB2	2.05	0.56
1:C:54:GLU:OE2	1:C:72:ARG:HD2	2.05	0.56
1:B:339:GLY:HA2	1:B:342:GLU:H	1.70	0.56
1:D:217:ASP:OD1	1:D:217:ASP:N	2.29	0.56
1:D:500:ASN:ND2	1:F:106:SER:HB2	2.21	0.56
1:A:529:ARG:HD3	1:C:185:ARG:O	2.06	0.56
1:B:102:GLY:O	1:B:210:TYR:HA	2.06	0.56
1:A:68:VAL:HG21	1:A:438:VAL:HG21	1.87	0.56
1:F:223:VAL:HG12	1:F:225:LEU:CD2	2.36	0.56
1:A:512:LEU:HD22	1:C:211:TRP:CD1	2.41	0.56
1:C:205:PRO:HG3	1:C:408:ILE:HD11	1.88	0.55
1:E:302:GLN:HE21	1:F:543:SER:HA	1.71	0.55
1:B:341:GLN:N	4:B:717:HOH:O	2.37	0.55
1:C:392:SER:HB3	1:C:395:ALA:HB3	1.88	0.55
1:D:474:ASN:ND2	1:F:87:ASN:HA	2.21	0.55
1:A:189:ARG:HH22	1:F:536:GLN:HE21	1.53	0.55
1:B:205:PRO:HG3	1:B:408:ILE:HD11	1.89	0.54
1:A:198:GLU:HB3	1:F:341:GLN:HE22	1.72	0.54
1:B:400:THR:HG21	1:E:371:GLU:O	2.08	0.54
1:E:38:GLN:NE2	1:E:40:ARG:HG2	2.22	0.54
1:E:327:VAL:HA	1:E:328:ARG:CB	2.28	0.54
1:C:115:SER:CB	1:D:394[A]:ARG:HB2	2.37	0.54
1:D:513:PRO:HD2	1:D:516:VAL:CG1	2.36	0.54
1:D:474:ASN:HD21	1:F:87:ASN:HA	1.70	0.54
1:E:327:VAL:CA	1:E:328:ARG:HB3	2.28	0.54
1:A:245:ALA:HB2	1:B:521:TYR:CE1	2.43	0.54
1:F:59:ASN:HA	1:F:64:GLN:NE2	2.23	0.54
1:C:522:GLN:HG2	4:C:612:HOH:O	2.07	0.54
1:D:31:GLN:NE2	4:D:11:HOH:O	2.41	0.54
1:E:464:GLN:O	1:E:465:GLN:C	2.46	0.53
1:A:195:ARG:CG	1:A:195:ARG:NH2	2.49	0.53
1:F:30:ASN:HB3	1:F:33:GLN:NE2	2.23	0.53
1:B:418:ARG:HD3	1:B:488:TYR:O	2.09	0.53
1:A:100:VAL:HG13	1:A:213:TYR:HB3	1.89	0.53
1:F:423:ARG:HH12	1:F:483:ASN:CG	2.11	0.53
1:D:53:ILE:CG1	1:D:73:ILE:HG13	2.34	0.53
1:A:117:GLN:HG2	4:F:577:HOH:O	2.07	0.53
1:E:39:ALA:HB2	1:E:469:PHE:HB3	1.90	0.53
1:A:443[B]:ARG:HA	1:A:465:GLN:HG3	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:213:TYR:CE2	1:F:215:ASP:HB3	2.44	0.53
1:D:426:ILE:HB	1:D:541:LEU:HB2	1.91	0.53
1:E:305:ASN:HD22	1:E:305:ASN:C	2.13	0.52
1:A:543:SER:HA	1:F:117:GLN:NE2	2.24	0.52
1:A:45:ARG:HD2	1:A:52:GLN:NE2	2.23	0.52
1:D:45:ARG:HD3	1:D:52:GLN:OE1	2.09	0.52
1:E:45:ARG:HH11	1:E:47:GLN:HB2	1.73	0.52
1:A:371:GLU:OE1	1:F:498:PHE:HB2	2.09	0.52
1:B:408:ILE:O	1:B:408:ILE:HG12	2.09	0.52
1:E:38:GLN:HG3	4:E:618:HOH:O	2.09	0.52
1:B:193:THR:HG21	1:B:333:PHE:HE2	1.74	0.52
1:A:60:GLN:O	1:A:64:GLN:HG2	2.10	0.52
1:F:355:GLN:HG3	1:F:356:GLU:N	2.25	0.52
1:A:377:ARG:NE	4:A:1026:HOH:O	2.42	0.52
1:F:393:PRO:C	1:F:394[B]:ARG:HD2	2.30	0.52
1:C:228:VAL:HG11	1:C:237:GLN:O	2.10	0.51
1:A:369:LEU:HD23	1:E:369:LEU:HD23	1.91	0.51
1:C:202:VAL:HB	1:C:379:LYS:HB3	1.91	0.51
1:E:305:ASN:O	1:E:305:ASN:ND2	2.40	0.51
1:C:350:GLN:HE22	1:C:353:LEU:HD23	1.76	0.51
1:D:289:ASN:HB3	1:E:454:ASN:O	2.11	0.51
1:F:418:ARG:HD3	1:F:488:TYR:O	2.10	0.51
1:C:37:LEU:HD22	1:C:458:ILE:HD12	1.93	0.51
1:C:77:ARG:CD	1:C:217:ASP:O	2.58	0.51
1:D:63:PHE:CZ	1:D:468:LEU:HD22	2.46	0.51
1:A:74:THR:HB	1:A:221:VAL:HG22	1.91	0.51
1:B:338:ARG:HA	1:E:386:GLU:OE1	2.11	0.51
1:F:296:ASN:OD1	1:F:298[B]:GLN:HB2	2.11	0.51
1:C:445:ASN:ND2	1:C:482:GLY:HA3	2.26	0.51
4:B:950:HOH:O	1:E:337:PRO:CG	2.58	0.51
1:E:205:PRO:HG3	1:E:408:ILE:HD11	1.93	0.50
1:C:447:ARG:NH1	1:C:447:ARG:HG2	2.11	0.50
1:C:114:GLU:HB2	1:C:187:LEU:HB3	1.94	0.50
1:B:73:ILE:HG22	1:B:224:ASN:ND2	2.25	0.50
1:A:537:GLU:OE1	1:A:541:LEU:HA	2.11	0.50
1:F:301:ALA:HB1	1:F:306:VAL:O	2.11	0.50
1:C:201:VAL:HG23	1:C:382:ILE:CG2	2.41	0.50
1:E:213:TYR:CD2	1:E:331:LEU:HD23	2.46	0.50
1:F:449:GLN:HA	1:F:459:LEU:O	2.10	0.50
1:B:447:ARG:HG3	1:B:448:VAL:N	2.25	0.50
1:E:77:ARG:HD3	1:E:216:GLY:O	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:502:LEU:HD11	1:F:244:LEU:HD22	1.94	0.50
1:B:448:VAL:HG12	1:B:459:LEU:HD23	1.93	0.50
1:D:501:THR:OG1	1:D:507:SER:HA	2.12	0.50
1:B:321:ARG:HB2	1:B:325:ILE:HG22	1.93	0.50
1:F:513:PRO:HD2	1:F:516:VAL:CG1	2.42	0.50
1:D:63:PHE:HZ	1:D:468:LEU:HD22	1.77	0.50
1:B:60:GLN:HB3	4:B:611:HOH:O	2.11	0.50
1:B:213:TYR:CE2	1:B:215:ASP:HB3	2.47	0.50
1:E:37:LEU:HD11	1:E:62:ASP:HB3	1.93	0.49
1:F:195:ARG:O	1:F:379:LYS:HE2	2.12	0.49
1:E:382:ILE:HD13	1:E:418:ARG:HB2	1.94	0.49
1:E:429:PRO:HA	1:E:477:VAL:O	2.11	0.49
1:C:355:GLN:HG3	1:C:356:GLU:N	2.26	0.49
1:F:250:ASN:ND2	1:F:253:ASN:OD1	2.46	0.49
1:B:228:VAL:HG11	1:B:237:GLN:O	2.13	0.49
1:A:287:ASN:HB3	4:A:1017:HOH:O	2.13	0.49
1:D:201:VAL:HG23	1:D:382:ILE:CG2	2.41	0.49
1:A:84:SER:O	1:A:209:ALA:HA	2.13	0.49
1:A:443[A]:ARG:HA	1:A:465:GLN:HG3	1.95	0.49
1:B:49:GLU:HB3	1:B:321:ARG:HB3	1.95	0.49
1:C:408:ILE:HG12	1:C:408:ILE:O	2.13	0.49
1:B:59:ASN:O	1:B:64:GLN:NE2	2.46	0.49
1:A:468:LEU:HD23	1:A:468:LEU:C	2.34	0.49
1:F:525:ARG:HB2	1:F:529:ARG:HH21	1.77	0.49
1:B:40[A]:ARG:HE	1:B:63:PHE:HE2	1.61	0.49
1:B:505:ARG:NH2	1:E:110:GLU:O	2.45	0.49
1:F:252:PHE:HE1	4:F:942:HOH:O	1.96	0.49
1:F:77:ARG:CG	1:F:217:ASP:O	2.61	0.48
1:F:53:ILE:HG12	1:F:73:ILE:HG12	1.96	0.48
1:D:27:SER:OG	1:D:29:GLN:NE2	2.46	0.48
1:A:52:GLN:HG2	1:A:74:THR:HG23	1.95	0.48
1:B:427:TYR:O	1:B:428:SER:C	2.51	0.48
1:A:370:GLU:HA	1:A:374:CYS:HB2	1.96	0.48
1:C:394[A]:ARG:HB2	1:D:115:SER:CB	2.43	0.48
1:C:524:SER:H	1:C:527:GLN:NE2	2.11	0.48
1:E:95:VAL:O	1:E:198:GLU:HG3	2.14	0.48
1:F:344:GLU:HA	1:F:347:GLU:HB2	1.94	0.48
1:A:423:ARG:NH1	1:A:423:ARG:CG	2.71	0.48
1:F:73:ILE:HG22	1:F:222:ALA:HB3	1.95	0.48
1:A:40:ARG:NH1	1:A:63:PHE:HE2	2.11	0.48
1:A:494:GLU:HG3	1:A:495:GLU:N	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:424:ASN:O	1:D:543:SER:HB3	2.14	0.48
1:F:427:TYR:O	1:F:428:SER:C	2.53	0.48
1:C:426:ILE:HB	1:C:541:LEU:HB2	1.96	0.48
1:E:304:LEU:HD13	1:F:503:ALA:HB2	1.96	0.47
1:B:392:SER:HB3	1:B:395:ALA:HB3	1.97	0.47
1:A:429:PRO:HA	1:A:477:VAL:O	2.14	0.47
1:B:185:ARG:HG2	1:B:189:ARG:HH12	1.79	0.47
1:A:377:ARG:CD	4:A:1026:HOH:O	2.53	0.47
1:B:431:TRP:HZ3	1:B:502:LEU:CD1	2.28	0.47
1:F:197:ARG:HH22	1:F:349:GLN:HE21	1.63	0.47
1:E:186:GLN:H	1:E:186:GLN:CD	2.18	0.47
1:F:423:ARG:HH12	1:F:483:ASN:ND2	2.12	0.47
1:B:357:ARG:HE	1:B:443:ARG:CD	2.27	0.47
1:D:296:ASN:OD1	1:D:298:GLN:HG2	2.14	0.47
1:D:29:GLN:H	1:D:29:GLN:CD	2.18	0.47
1:A:213:TYR:CE2	1:A:215:ASP:HB3	2.50	0.47
1:D:201:VAL:HG23	1:D:382:ILE:HG22	1.96	0.47
1:F:370:GLU:HA	1:F:374:CYS:HB2	1.97	0.47
1:C:41:GLU:HB3	1:C:42:PRO:HD2	1.95	0.46
1:F:185:ARG:C	1:F:186:GLN:NE2	2.68	0.46
1:E:63:PHE:HD1	1:E:68:VAL:O	1.98	0.46
1:D:205:PRO:HG3	1:D:408:ILE:HD11	1.96	0.46
1:F:48:ALA:O	1:F:49:GLU:C	2.52	0.46
1:E:413:ARG:HH11	1:E:413:ARG:HG2	1.80	0.46
1:F:353:LEU:HD12	1:F:385:PRO:HD3	1.96	0.46
1:E:321:ARG:CB	1:E:325:ILE:HG22	2.44	0.46
1:C:185:ARG:CB	1:C:189:ARG:HH22	2.29	0.46
1:D:34:LEU:HD13	1:D:37:LEU:HD11	1.97	0.46
1:E:289:ASN:HB3	1:F:454:ASN:O	2.16	0.46
1:F:429:PRO:HA	1:F:477:VAL:O	2.16	0.46
1:E:186:GLN:HB2	1:F:529:ARG:HH11	1.79	0.46
1:F:513:PRO:CD	1:F:516:VAL:HG13	2.44	0.46
1:D:448:VAL:HG22	1:D:479:GLN:HG2	1.97	0.46
1:A:309:GLU:HG2	1:A:312:ARG:NH2	2.25	0.46
1:E:331:LEU:HD12	1:F:515:GLU:CG	2.36	0.46
1:C:37:LEU:HD22	1:C:458:ILE:CD1	2.46	0.46
1:C:201:VAL:HG23	1:C:382:ILE:HG22	1.98	0.46
1:D:377:ARG:NH2	1:D:380:GLU:OE1	2.44	0.46
1:B:48:ALA:O	1:B:49:GLU:C	2.53	0.46
1:F:112:PHE:CE1	1:F:192:LYS:HB2	2.51	0.46
1:F:37:LEU:O	1:F:459:LEU:HD12	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:87:ASN:HB3	1:C:235:LEU:HD12	1.98	0.45
1:F:448:VAL:CG1	1:F:459:LEU:HD23	2.45	0.45
1:B:513:PRO:HD2	1:B:516:VAL:CG1	2.47	0.45
1:D:423:ARG:HG2	1:D:424:ASN:ND2	2.32	0.45
1:C:73:ILE:HG22	1:C:222:ALA:HB3	1.97	0.45
1:F:195:ARG:NH1	1:F:215:ASP:OD2	2.50	0.45
1:F:525:ARG:HB2	1:F:529:ARG:NH2	2.32	0.45
1:C:317:GLN:H	1:C:317:GLN:HG2	1.41	0.45
1:D:413:ARG:HA	1:D:495:GLU:HB2	1.97	0.45
1:C:114:GLU:HG3	1:C:188:ASP:N	2.31	0.45
1:F:448:VAL:HG22	1:F:479:GLN:HG2	1.98	0.45
1:B:102:GLY:HA2	1:B:211:TRP:CE2	2.51	0.45
1:A:84:SER:HG	1:A:241:LYS:HE3	1.81	0.45
1:D:321:ARG:HH12	1:D:325:ILE:HD13	1.82	0.45
1:E:195:ARG:O	1:E:379:LYS:HE2	2.17	0.45
1:C:413:ARG:CD	4:C:613:HOH:O	2.39	0.45
1:B:449:GLN:O	1:B:477:VAL:HA	2.16	0.45
1:B:357:ARG:HE	1:B:443:ARG:HD3	1.82	0.45
1:D:37:LEU:HD22	1:D:458:ILE:HG13	1.99	0.45
1:C:323:GLN:HE21	1:C:323:GLN:N	2.11	0.45
1:C:105:PHE:CZ	1:C:376:LEU:HD21	2.52	0.45
1:C:368:GLY:N	1:C:371:GLU:OE1	2.49	0.45
1:C:322:ASN:HB3	1:C:323:GLN:NE2	2.30	0.45
1:C:382:ILE:HD13	1:C:382:ILE:HG21	1.59	0.45
1:C:336:PRO:HA	1:C:337:PRO:HD2	1.70	0.45
1:C:358:GLN:HA	1:C:358:GLN:HE21	1.81	0.45
1:C:445:ASN:HD21	1:C:482:GLY:HA3	1.82	0.45
1:C:36:GLN:NE2	1:C:36:GLN:HA	2.31	0.45
1:D:293:SER:HA	1:D:315:GLN:HG2	1.99	0.45
1:C:223:VAL:HG12	1:C:225:LEU:CD2	2.48	0.44
1:B:345:HIS:O	1:B:349:GLN:HG2	2.17	0.44
1:E:418:ARG:HH12	1:E:487:GLU:HB3	1.83	0.44
1:F:392:SER:HB3	1:F:395:ALA:HB3	2.00	0.44
1:A:305:ASN:HD22	1:A:305:ASN:C	2.21	0.44
1:F:513:PRO:O	1:F:516:VAL:N	2.49	0.44
1:A:461:GLN:CG	1:A:462:GLU:H	2.28	0.44
1:E:329:GLY:CA	1:E:330:ASN:HB2	2.46	0.44
1:A:473:GLN:O	1:A:474:ASN:HB2	2.16	0.44
1:B:369:LEU:HD12	1:B:369:LEU:HA	1.74	0.44
1:D:525:ARG:HH11	1:D:525:ARG:HB2	1.82	0.44
1:F:288:GLY:O	1:F:289:ASN:HB3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:40:ARG:NH1	1:A:63:PHE:CE2	2.86	0.44
1:E:29:GLN:NE2	1:E:30:ASN:OD1	2.50	0.44
1:A:302:GLN:O	1:B:535:ARG:NH2	2.48	0.44
1:A:327:VAL:O	1:A:329:GLY:N	2.51	0.44
1:E:87:ASN:HA	1:F:474:ASN:HD21	1.82	0.44
1:C:31:GLN:NE2	4:C:874:HOH:O	2.51	0.44
1:D:328:ARG:HA	1:D:328:ARG:HD2	1.71	0.44
1:A:205:PRO:HG3	1:A:408:ILE:HD11	1.98	0.44
1:B:518:ALA:HA	1:B:523:ILE:HG13	2.00	0.44
1:B:54:GLU:CD	1:B:72:ARG:HH11	2.20	0.43
1:D:382:ILE:HD13	1:D:382:ILE:HG21	1.65	0.43
1:E:304:LEU:HD12	1:E:304:LEU:HA	1.85	0.43
1:B:54:GLU:OE2	1:B:72:ARG:HD2	2.17	0.43
1:C:468:LEU:C	1:C:468:LEU:HD23	2.39	0.43
1:F:525:ARG:H	1:F:525:ARG:NH2	2.17	0.43
1:F:387:ARG:CG	1:F:387:ARG:O	2.67	0.43
1:C:114:GLU:HG3	1:C:188:ASP:H	1.84	0.43
1:A:406:LEU:HG	1:A:408:ILE:HG22	2.00	0.43
1:A:521:TYR:CD1	1:C:314:LEU:HA	2.53	0.43
1:E:290:ASN:OD1	1:E:292:PHE:HB2	2.18	0.43
1:D:529:ARG:HD2	1:F:186:GLN:HB3	1.99	0.43
1:B:57:ASN:O	1:B:60:GLN:HG3	2.18	0.43
1:C:80:LEU:HD13	1:C:82:LEU:HD23	2.00	0.43
1:E:308:GLU:HG2	1:E:312:ARG:HH11	1.84	0.43
1:E:321:ARG:HB3	1:E:325:ILE:HG22	2.00	0.43
1:F:28:PRO:O	1:F:31:GLN:HG2	2.19	0.43
1:C:437:SER:OG	1:C:492:LYS:HE2	2.18	0.43
1:A:87:ASN:HA	1:B:474:ASN:ND2	2.33	0.43
1:C:439:VAL:O	1:C:468:LEU:HA	2.19	0.43
1:A:186:GLN:O	1:B:529:ARG:NH2	2.52	0.43
1:F:49:GLU:OE2	1:F:321:ARG:HD2	2.19	0.43
1:A:236:ASP:HB2	1:B:29:GLN:O	2.18	0.43
1:A:92:ILE:HD12	1:A:202:VAL:HG13	2.00	0.43
1:A:243:TYR:HB2	1:A:248:PRO:HG3	2.01	0.43
1:F:419:GLY:HA3	1:F:488:TYR:CZ	2.54	0.43
1:B:371:GLU:O	1:E:400:THR:HG21	2.18	0.43
1:A:299:LEU:HD13	1:B:478:ILE:HG12	2.01	0.43
1:C:115:SER:OG	1:D:394[A]:ARG:HB2	2.19	0.43
1:C:375:SER:HB3	4:D:939:HOH:O	2.19	0.43
1:B:538:THR:HG23	1:E:113:GLU:OE2	2.18	0.43
1:D:321:ARG:NH1	1:D:325:ILE:HD13	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:388:ALA:HA	1:D:399:SER:OG	2.19	0.43
1:C:328:ARG:HD2	1:C:328:ARG:HA	1.77	0.43
1:A:39:ALA:HB2	1:A:469:PHE:HB3	2.01	0.43
1:B:36:GLN:O	1:B:37:LEU:HD12	2.19	0.43
1:E:87:ASN:HA	1:F:474:ASN:ND2	2.33	0.43
1:E:369:LEU:HD12	4:E:588:HOH:O	2.19	0.43
1:E:114:GLU:HG3	1:E:334:VAL:HG22	2.00	0.43
1:F:223:VAL:HG12	1:F:225:LEU:HD22	2.00	0.42
1:C:328:ARG:CZ	1:C:329:GLY:H	2.32	0.42
1:D:78:ASN:ND2	1:D:329:GLY:O	2.52	0.42
1:A:461:GLN:CG	1:A:462:GLU:N	2.81	0.42
1:D:304:LEU:CD1	1:E:503:ALA:HB2	2.48	0.42
1:D:430:HIS:HB2	1:D:500:ASN:O	2.19	0.42
1:A:371:GLU:O	1:F:400:THR:HG21	2.19	0.42
1:B:201:VAL:CG2	1:B:382:ILE:HG21	2.50	0.42
1:B:392:SER:HA	1:B:393:PRO:HD3	1.89	0.42
1:E:41:GLU:HB3	1:E:42:PRO:HD2	2.01	0.42
1:A:308:GLU:O	1:A:308:GLU:HG3	2.19	0.42
1:E:417:GLU:HB3	1:E:490:ALA:HB3	2.02	0.42
1:F:185:ARG:HH21	1:F:185:ARG:HG2	1.85	0.42
1:A:190:HIS:ND1	1:B:513:PRO:HG3	2.35	0.42
1:A:189:ARG:HH22	1:F:536:GLN:NE2	2.16	0.42
1:F:105:PHE:HE1	1:F:194:ARG:NH1	2.18	0.42
1:E:404:HIS:HE1	4:E:601:HOH:O	2.02	0.42
1:E:517:LEU:HD11	1:E:532:LYS:HE3	2.02	0.42
1:B:105:PHE:CZ	1:B:376:LEU:HD21	2.54	0.42
1:F:420:PHE:C	1:F:420:PHE:CD1	2.93	0.42
1:A:503:ALA:HB2	1:C:304:LEU:HD13	2.02	0.42
1:C:287:ASN:CB	1:C:317:GLN:HE21	2.33	0.42
1:D:314:LEU:HA	1:E:521:TYR:CD1	2.54	0.42
1:F:102:GLY:O	1:F:210:TYR:HA	2.20	0.42
1:E:235:LEU:HD23	1:E:235:LEU:HA	1.73	0.42
1:A:235:LEU:HD23	1:B:436:HIS:HE1	1.85	0.42
1:A:510:ARG:HE	1:A:510:ARG:HB3	1.63	0.42
1:D:116:GLN:O	1:D:117:GLN:HB3	2.19	0.42
1:D:307:ASN:OD1	1:D:309:GLU:HB3	2.20	0.42
1:A:66:ALA:HA	1:A:436:HIS:CD2	2.55	0.42
1:A:423:ARG:HG3	1:A:423:ARG:HH11	1.81	0.41
1:A:333:PHE:CD2	1:A:335:GLN:HB2	2.55	0.41
1:C:506:THR:HG21	1:D:370:GLU:OE2	2.20	0.41
1:E:112:PHE:CE2	1:E:193:THR:HG22	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:505:ARG:HB2	1:B:538:THR:HG22	2.03	0.41
1:B:423:ARG:HD3	1:B:483:ASN:HD22	1.85	0.41
1:F:439:VAL:O	1:F:468:LEU:HA	2.20	0.41
1:B:323:GLN:N	1:B:323:GLN:NE2	2.51	0.41
1:E:322:ASN:HB3	1:E:323:GLN:NE2	2.36	0.41
1:C:535:ARG:HA	1:C:535:ARG:HD3	1.76	0.41
1:C:429:PRO:HA	1:C:477:VAL:O	2.20	0.41
1:A:193:THR:HG21	1:A:333:PHE:CE2	2.55	0.41
1:B:410:ARG:C	1:B:410:ARG:HD3	2.41	0.41
1:B:331:LEU:HD21	1:C:516:VAL:HG12	2.02	0.41
1:A:116:GLN:H	1:A:116:GLN:HG3	1.66	0.41
1:D:384:ASN:HB2	4:D:757:HOH:O	2.20	0.41
1:D:298:GLN:HB3	1:D:308:GLU:OE1	2.21	0.41
1:C:59:ASN:HA	1:C:64:GLN:NE2	2.35	0.41
1:E:93:TYR:HB3	1:E:223:VAL:HG23	2.02	0.41
1:D:535:ARG:HD3	1:D:535:ARG:HA	1.66	0.41
1:F:60:GLN:H	1:F:60:GLN:HG2	1.56	0.41
1:B:35:ASN:HA	1:B:35:ASN:HD22	1.56	0.41
1:F:77:ARG:HG3	1:F:217:ASP:O	2.21	0.41
1:E:186:GLN:N	1:E:186:GLN:CD	2.74	0.41
1:F:424:ASN:HA	1:F:481:ALA:O	2.21	0.41
1:F:449:GLN:O	1:F:477:VAL:HA	2.21	0.41
1:B:193:THR:HG21	1:B:333:PHE:CE2	2.53	0.41
1:B:449:GLN:HA	1:B:459:LEU:O	2.21	0.41
1:B:513:PRO:CD	1:B:516:VAL:HG13	2.50	0.41
1:E:39:ALA:HA	1:E:468:LEU:O	2.21	0.41
1:C:78:ASN:ND2	1:C:329:GLY:O	2.53	0.41
1:D:57:ASN:HD21	1:D:254:GLN:HB2	1.86	0.41
1:A:57:ASN:HA	1:A:254:GLN:NE2	2.35	0.41
1:E:384:ASN:HA	1:E:385:PRO:HD2	1.96	0.41
1:F:531:LEU:HA	1:F:531:LEU:HD23	1.87	0.41
1:C:338:ARG:NH1	1:C:343:ARG:HG3	2.30	0.41
1:E:112:PHE:CE2	1:E:193:THR:CG2	3.04	0.41
1:F:423:ARG:NH1	1:F:483:ASN:ND2	2.68	0.41
1:A:373:PHE:CZ	1:E:373:PHE:CE1	3.09	0.40
1:E:426:ILE:HB	1:E:541:LEU:HB2	2.02	0.40
1:E:100:VAL:CG2	1:E:193:THR:OG1	2.69	0.40
1:A:384:ASN:O	1:A:387:ARG:HB3	2.20	0.40
1:F:54:GLU:CD	1:F:72:ARG:HH11	2.24	0.40
1:B:91:LEU:HD23	1:B:203:ALA:HA	2.03	0.40
1:E:505:ARG:HG3	1:E:537:GLU:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:410:ARG:O	1:B:413:ARG:NH1	2.54	0.40
1:F:426:ILE:HG22	1:F:427:TYR:N	2.36	0.40
1:C:55:THR:HG22	1:C:71:SER:HB2	2.03	0.40
1:A:322:ASN:HB3	1:A:323:GLN:H	1.75	0.40
1:C:340:ARG:HB2	1:C:343:ARG:HE	1.87	0.40
1:C:430:HIS:HB2	1:C:500:ASN:O	2.21	0.40
1:D:443:ARG:HD3	4:D:933:HOH:O	2.20	0.40
1:B:317:GLN:HE21	1:B:317:GLN:HB3	1.75	0.40
1:B:312:ARG:HG3	1:B:317:GLN:OE1	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	382/531 (72%)	342 (90%)	36 (9%)	4 (1%)	19 28
1	B	403/531 (76%)	371 (92%)	32 (8%)	0	100 100
1	C	403/531 (76%)	375 (93%)	24 (6%)	4 (1%)	19 28
1	D	381/531 (72%)	356 (93%)	23 (6%)	2 (0%)	34 48
1	E	381/531 (72%)	354 (93%)	22 (6%)	5 (1%)	15 21
1	F	404/531 (76%)	372 (92%)	30 (7%)	2 (0%)	34 48
All	All	2354/3186 (74%)	2170 (92%)	167 (7%)	17 (1%)	26 38

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	328[A]	ARG
1	A	328[B]	ARG
1	C	340	ARG

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Mol	Chain	Res	Type
1	E	328	ARG
1	E	330	ASN
1	F	37	LEU
1	A	237	GLN
1	D	235	LEU
1	E	235	LEU
1	E	465	GLN
1	A	192	LYS
1	C	250	ASN
1	D	318	ASN
1	E	106	SER
1	C	235	LEU
1	F	235	LEU
1	C	482	GLY

5.3.2 Protein sidechains (i)

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	330/452 (73%)	272 (82%)	58 (18%)	2 2
1	B	349/452 (77%)	293 (84%)	56 (16%)	3 3
1	C	349/452 (77%)	312 (89%)	37 (11%)	8 12
1	D	330/452 (73%)	289 (88%)	41 (12%)	6 7
1	E	329/452 (73%)	281 (85%)	48 (15%)	4 4
1	F	350/452 (77%)	304 (87%)	46 (13%)	5 6
All	All	2037/2712 (75%)	1751 (86%)	286 (14%)	4 5

All (286) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	GLN
1	A	37	LEU
1	A	38	GLN
1	A	40	ARG

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Mol	Chain	Res	Type
1	A	43	ASP
1	A	52	GLN
1	A	54	GLU
1	A	64	GLN
1	A	68	VAL
1	A	74	THR
1	A	77	ARG
1	A	95	VAL
1	A	98	ARG
1	A	100	VAL
1	A	104	VAL
1	A	114	GLU
1	A	116	GLN
1	A	186	GLN
1	A	193	THR
1	A	195	ARG
1	A	217	ASP
1	A	223	VAL
1	A	250	ASN
1	A	253	ASN
1	A	254	GLN
1	A	287	ASN
1	A	291	VAL
1	A	298	GLN
1	A	299	LEU
1	A	304	LEU
1	A	305	ASN
1	A	306	VAL
1	A	309	GLU
1	A	317	GLN
1	A	323	GLN
1	A	328[A]	ARG
1	A	328[B]	ARG
1	A	369	LEU
1	A	371	GLU
1	A	378	LEU
1	A	382	ILE
1	A	400	THR
1	A	413	ARG
1	A	414	LEU
1	A	418	ARG
1	A	420	PHE

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Mol	Chain	Res	Type
1	A	423	ARG
1	A	427	TYR
1	A	445	ASN
1	A	447	ARG
1	A	483	ASN
1	A	484	GLN
1	A	502	LEU
1	A	506	THR
1	A	508	PHE
1	A	516	VAL
1	A	525	ARG
1	A	526	GLU
1	B	27	SER
1	B	29	GLN
1	B	31	GLN
1	B	36	GLN
1	B	38	GLN
1	B	40[A]	ARG
1	B	40[B]	ARG
1	B	45	ARG
1	B	73	ILE
1	B	77	ARG
1	B	80	LEU
1	B	114	GLU
1	B	116	GLN
1	B	117	GLN
1	B	185	ARG
1	B	193	THR
1	B	195	ARG
1	B	202	VAL
1	B	212	SER
1	B	217	ASP
1	B	241	LYS
1	B	250	ASN
1	B	253	ASN
1	B	293	SER
1	B	298	GLN
1	B	299	LEU
1	B	302	GLN
1	B	304	LEU
1	B	305	ASN
1	B	306	VAL

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Mol	Chain	Res	Type
1	B	309	GLU
1	B	317	GLN
1	B	321	ARG
1	B	323	GLN
1	B	344	GLU
1	B	346	GLU
1	B	351	GLU
1	B	353	LEU
1	B	359	GLN
1	B	369	LEU
1	B	378	LEU
1	B	379	LYS
1	B	382	ILE
1	B	392	SER
1	B	400	THR
1	B	410	ARG
1	B	414	LEU
1	B	418	ARG
1	B	420	PHE
1	B	427	TYR
1	B	447	ARG
1	B	468	LEU
1	B	499	ILE
1	B	502	LEU
1	B	516	VAL
1	B	529	ARG
1	C	27	SER
1	C	40	ARG
1	C	46	ILE
1	C	80	LEU
1	C	189	ARG
1	C	193	THR
1	C	202	VAL
1	C	299	LEU
1	C	302	GLN
1	C	304	LEU
1	C	309	GLU
1	C	317	GLN
1	C	323	GLN
1	C	328	ARG
1	C	346	GLU
1	C	347	GLU

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Mol	Chain	Res	Type
1	C	351	GLU
1	C	354	GLN
1	C	356	GLU
1	C	358	GLN
1	C	359	GLN
1	C	369	LEU
1	C	378	LEU
1	C	379	LYS
1	C	392	SER
1	C	394[A]	ARG
1	C	394[B]	ARG
1	C	420	PHE
1	C	427	TYR
1	C	445	ASN
1	C	447	ARG
1	C	483	ASN
1	C	484	GLN
1	C	500	ASN
1	C	506	THR
1	C	508	PHE
1	C	510	ARG
1	D	37	LEU
1	D	38	GLN
1	D	40	ARG
1	D	64	GLN
1	D	74	THR
1	D	98	ARG
1	D	100	VAL
1	D	104	VAL
1	D	193	THR
1	D	195	ARG
1	D	202	VAL
1	D	217	ASP
1	D	241	LYS
1	D	250	ASN
1	D	253	ASN
1	D	254	GLN
1	D	291	VAL
1	D	298	GLN
1	D	299	LEU
1	D	304	LEU
1	D	306	VAL

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Mol	Chain	Res	Type
1	D	317	GLN
1	D	328	ARG
1	D	369	LEU
1	D	371	GLU
1	D	378	LEU
1	D	379	LYS
1	D	386	GLU
1	D	392	SER
1	D	394[A]	ARG
1	D	394[B]	ARG
1	D	414	LEU
1	D	418	ARG
1	D	420	PHE
1	D	427	TYR
1	D	502	LEU
1	D	506	THR
1	D	508	PHE
1	D	510	ARG
1	D	525	ARG
1	D	536	GLN
1	E	29	GLN
1	E	37	LEU
1	E	38	GLN
1	E	40	ARG
1	E	46	ILE
1	E	52	GLN
1	E	68	VAL
1	E	74	THR
1	E	95	VAL
1	E	104	VAL
1	E	113	GLU
1	E	116	GLN
1	E	117	GLN
1	E	186	GLN
1	E	193	THR
1	E	195	ARG
1	E	202	VAL
1	E	212	SER
1	E	217	ASP
1	E	223	VAL
1	E	241	LYS
1	E	253	ASN

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Mol	Chain	Res	Type
1	E	254	GLN
1	E	287	ASN
1	E	289	ASN
1	E	291	VAL
1	E	293	SER
1	E	299	LEU
1	E	304	LEU
1	E	305	ASN
1	E	306	VAL
1	E	317	GLN
1	E	323	GLN
1	E	378	LEU
1	E	382	ILE
1	E	386	GLU
1	E	400	THR
1	E	414	LEU
1	E	418	ARG
1	E	420	PHE
1	E	427	TYR
1	E	447	ARG
1	E	465	GLN
1	E	484	GLN
1	E	500	ASN
1	E	502	LEU
1	E	525	ARG
1	E	543	SER
1	F	27	SER
1	F	29	GLN
1	F	46	ILE
1	F	54	GLU
1	F	60	GLN
1	F	64	GLN
1	F	73	ILE
1	F	77	ARG
1	F	80	LEU
1	F	95	VAL
1	F	104	VAL
1	F	185	ARG
1	F	186	GLN
1	F	187	LEU
1	F	192	LYS
1	F	193	THR

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Mol	Chain	Res	Type
1	F	195	ARG
1	F	212	SER
1	F	217	ASP
1	F	254	GLN
1	F	299	LEU
1	F	306	VAL
1	F	308	GLU
1	F	328	ARG
1	F	347	GLU
1	F	353	LEU
1	F	355	GLN
1	F	369	LEU
1	F	370	GLU
1	F	378	LEU
1	F	382	ILE
1	F	392	SER
1	F	400	THR
1	F	414	LEU
1	F	415	SER
1	F	418	ARG
1	F	420	PHE
1	F	427	TYR
1	F	447	ARG
1	F	483	ASN
1	F	492	LYS
1	F	502	LEU
1	F	512	LEU
1	F	516	VAL
1	F	525	ARG
1	F	529	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (89) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	29	GLN
1	A	47	GLN
1	A	52	GLN
1	A	57	ASN
1	A	59	ASN
1	A	76	GLN
1	A	90	GLN
1	A	238	ASN

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Mol	Chain	Res	Type
1	A	247	ASN
1	A	254	GLN
1	A	289	ASN
1	A	296	ASN
1	A	315	GLN
1	A	317	GLN
1	A	323	GLN
1	A	445	ASN
1	A	527	GLN
1	B	30	ASN
1	B	35	ASN
1	B	36	GLN
1	B	64	GLN
1	B	218	GLN
1	B	224	ASN
1	B	253	ASN
1	B	289	ASN
1	B	323	GLN
1	B	341	GLN
1	B	474	ASN
1	B	483	ASN
1	B	500	ASN
1	C	30	ASN
1	C	31	GLN
1	C	36	GLN
1	C	47	GLN
1	C	78	ASN
1	C	218	GLN
1	C	224	ASN
1	C	238	ASN
1	C	317	GLN
1	C	323	GLN
1	C	350	GLN
1	C	358	GLN
1	C	359	GLN
1	C	445	ASN
1	C	527	GLN
1	D	29	GLN
1	D	30	ASN
1	D	31	GLN
1	D	57	ASN
1	D	78	ASN

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Mol	Chain	Res	Type
1	D	253	ASN
1	D	287	ASN
1	D	305	ASN
1	D	335	GLN
1	D	424	ASN
1	D	454	ASN
1	D	474	ASN
1	D	480	GLN
1	D	500	ASN
1	D	530	GLN
1	D	536	GLN
1	E	38	GLN
1	E	44	ASN
1	E	52	GLN
1	E	117	GLN
1	E	247	ASN
1	E	254	GLN
1	E	302	GLN
1	E	323	GLN
1	E	424	ASN
1	E	465	GLN
1	E	522	GLN
1	F	29	GLN
1	F	33	GLN
1	F	64	GLN
1	F	76	GLN
1	F	81	HIS
1	F	117	GLN
1	F	186	GLN
1	F	218	GLN
1	F	224	ASN
1	F	250	ASN
1	F	302	GLN
1	F	341	GLN
1	F	359	GLN
1	F	474	ASN
1	F	500	ASN
1	F	522	GLN
1	F	536	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 15 ligands modelled in this entry, 15 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	388/531 (73%)	-0.01	1 (0%) 94 94	27, 45, 66, 84	0
1	B	410/531 (77%)	0.01	5 (1%) 81 81	21, 39, 81, 96	0
1	C	410/531 (77%)	-0.04	3 (0%) 89 88	22, 38, 80, 103	0
1	D	388/531 (73%)	-0.06	0 100 100	21, 37, 61, 87	0
1	E	388/531 (73%)	-0.01	1 (0%) 94 94	26, 45, 67, 80	0
1	F	410/531 (77%)	-0.06	0 100 100	21, 38, 75, 86	0
All	All	2394/3186 (75%)	-0.03	10 (0%) 93 93	21, 41, 68, 103	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	359	GLN	5.2
1	B	27	SER	3.1
1	B	357	ARG	2.9
1	C	353	LEU	2.8
1	B	353	LEU	2.6
1	E	287	ASN	2.5
1	A	254	GLN	2.4
1	C	254	GLN	2.3
1	B	358	GLN	2.2
1	B	345	HIS	2.1

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 (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{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	CA	A	1	1/1	0.92	0.21	2.97	52,52,52,52	0
2	CA	E	5	1/1	0.99	0.18	1.28	51,51,51,51	0
3	NA	F	7	1/1	0.97	0.22	1.23	53,53,53,53	0
2	CA	C	3	1/1	0.99	0.18	0.28	45,45,45,45	0
2	CA	D	4	1/1	0.99	0.17	0.26	45,45,45,45	0
2	CA	B	2	1/1	0.97	0.15	-0.95	53,53,53,53	0
3	NA	C	552	1/1	0.96	0.31	-	51,51,51,51	0
3	NA	F	552	1/1	0.97	0.23	-	43,43,43,43	0
3	NA	E	552	1/1	0.94	0.25	-	67,67,67,67	0
3	NA	A	552	1/1	0.96	0.26	-	53,53,53,53	0
3	NA	D	552	1/1	0.94	0.35	-	58,58,58,58	0
3	NA	B	552	1/1	0.99	0.29	-	40,40,40,40	0
2	CA	F	6	1/1	0.98	0.14	-	51,51,51,51	0
3	NA	A	9	1/1	0.98	0.18	-	50,50,50,50	0
3	NA	E	8	1/1	0.99	0.20	-	44,44,44,44	0

6.5 Other polymers (i)

There are no such residues in this entry.