Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 11:47 PM GMT

PDB ID	:	1YNF
Title	:	Crystal Structure of N-Succinylarginine Dihydrolase, AstB, bound to Substrate and Product, an Enzyme from the Arginine Catabolic Pathway of Escherichia coli
Authors	:	Tocilj, A.; Schrag, J.D.; Li, Y.; Schneider, B.L.; Reitzer, L.; Matte, A.; Cygler, M.
Deposited on	:	2005-01-24
Resolution	:	1.90 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:

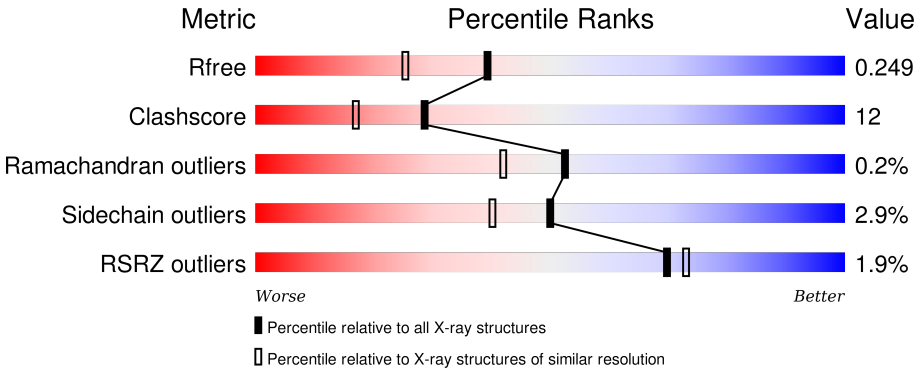
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 1.90 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}	91344	4755 (1.90-1.90)
Clashscore	102246	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (1.90-1.90)
RSRZ outliers	91569	4766 (1.90-1.90)

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	458	77% 16% • 6%
1	B	458	76% 16% • 6%
1	C	458	2% 73% 19% • 6%
1	D	458	4% 69% 24% • 6%
1	E	458	72% 21% • 6%

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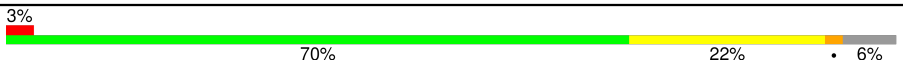
Mol	Chain	Length	Quality of chain
1	F	458	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 21526 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 Succinylarginine dihydrolase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	429	Total	C	N	O	S	Se	0	0	0
			3353	2102	612	627	3	9			
1	B	429	Total	C	N	O	S	Se	0	0	0
			3353	2102	612	627	3	9			
1	C	429	Total	C	N	O	S	Se	0	0	0
			3353	2102	612	627	3	9			
1	D	429	Total	C	N	O	S	Se	0	0	0
			3353	2102	612	627	3	9			
1	E	429	Total	C	N	O	S	Se	0	0	0
			3353	2102	612	627	3	9			
1	F	429	Total	C	N	O	S	Se	0	0	0
			3353	2102	612	627	3	9			

There are 126 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-10	MET	-	EXPRESSION TAG	UNP P76216
A	-9	GLY	-	EXPRESSION TAG	UNP P76216
A	-8	SER	-	EXPRESSION TAG	UNP P76216
A	-7	SER	-	EXPRESSION TAG	UNP P76216
A	-6	HIS	-	EXPRESSION TAG	UNP P76216
A	-5	HIS	-	EXPRESSION TAG	UNP P76216
A	-4	HIS	-	EXPRESSION TAG	UNP P76216
A	-3	HIS	-	EXPRESSION TAG	UNP P76216
A	-2	HIS	-	EXPRESSION TAG	UNP P76216
A	-1	HIS	-	EXPRESSION TAG	UNP P76216
A	0	GLY	-	EXPRESSION TAG	UNP P76216
A	1	SER	-	EXPRESSION TAG	UNP P76216
A	49	MSE	MET	MODIFIED RESIDUE	UNP P76216
A	106	MSE	MET	MODIFIED RESIDUE	UNP P76216
A	191	MSE	MET	MODIFIED RESIDUE	UNP P76216
A	285	MSE	MET	MODIFIED RESIDUE	UNP P76216
A	317	MSE	MET	MODIFIED RESIDUE	UNP P76216

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Chain	Residue	Modelled	Actual	Comment	Reference
A	318	MSE	MET	MODIFIED RESIDUE	UNP P76216
A	357	MSE	MET	MODIFIED RESIDUE	UNP P76216
A	385	MSE	MET	MODIFIED RESIDUE	UNP P76216
A	386	MSE	MET	MODIFIED RESIDUE	UNP P76216
B	-10	MET	-	EXPRESSION TAG	UNP P76216
B	-9	GLY	-	EXPRESSION TAG	UNP P76216
B	-8	SER	-	EXPRESSION TAG	UNP P76216
B	-7	SER	-	EXPRESSION TAG	UNP P76216
B	-6	HIS	-	EXPRESSION TAG	UNP P76216
B	-5	HIS	-	EXPRESSION TAG	UNP P76216
B	-4	HIS	-	EXPRESSION TAG	UNP P76216
B	-3	HIS	-	EXPRESSION TAG	UNP P76216
B	-2	HIS	-	EXPRESSION TAG	UNP P76216
B	-1	HIS	-	EXPRESSION TAG	UNP P76216
B	0	GLY	-	EXPRESSION TAG	UNP P76216
B	1	SER	-	EXPRESSION TAG	UNP P76216
B	49	MSE	MET	MODIFIED RESIDUE	UNP P76216
B	106	MSE	MET	MODIFIED RESIDUE	UNP P76216
B	191	MSE	MET	MODIFIED RESIDUE	UNP P76216
B	285	MSE	MET	MODIFIED RESIDUE	UNP P76216
B	317	MSE	MET	MODIFIED RESIDUE	UNP P76216
B	318	MSE	MET	MODIFIED RESIDUE	UNP P76216
B	357	MSE	MET	MODIFIED RESIDUE	UNP P76216
B	385	MSE	MET	MODIFIED RESIDUE	UNP P76216
B	386	MSE	MET	MODIFIED RESIDUE	UNP P76216
C	-10	MET	-	EXPRESSION TAG	UNP P76216
C	-9	GLY	-	EXPRESSION TAG	UNP P76216
C	-8	SER	-	EXPRESSION TAG	UNP P76216
C	-7	SER	-	EXPRESSION TAG	UNP P76216
C	-6	HIS	-	EXPRESSION TAG	UNP P76216
C	-5	HIS	-	EXPRESSION TAG	UNP P76216
C	-4	HIS	-	EXPRESSION TAG	UNP P76216
C	-3	HIS	-	EXPRESSION TAG	UNP P76216
C	-2	HIS	-	EXPRESSION TAG	UNP P76216
C	-1	HIS	-	EXPRESSION TAG	UNP P76216
C	0	GLY	-	EXPRESSION TAG	UNP P76216
C	1	SER	-	EXPRESSION TAG	UNP P76216
C	49	MSE	MET	MODIFIED RESIDUE	UNP P76216
C	106	MSE	MET	MODIFIED RESIDUE	UNP P76216
C	191	MSE	MET	MODIFIED RESIDUE	UNP P76216
C	285	MSE	MET	MODIFIED RESIDUE	UNP P76216
C	317	MSE	MET	MODIFIED RESIDUE	UNP P76216

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Chain	Residue	Modelled	Actual	Comment	Reference
C	318	MSE	MET	MODIFIED RESIDUE	UNP P76216
C	357	MSE	MET	MODIFIED RESIDUE	UNP P76216
C	385	MSE	MET	MODIFIED RESIDUE	UNP P76216
C	386	MSE	MET	MODIFIED RESIDUE	UNP P76216
D	-10	MET	-	EXPRESSION TAG	UNP P76216
D	-9	GLY	-	EXPRESSION TAG	UNP P76216
D	-8	SER	-	EXPRESSION TAG	UNP P76216
D	-7	SER	-	EXPRESSION TAG	UNP P76216
D	-6	HIS	-	EXPRESSION TAG	UNP P76216
D	-5	HIS	-	EXPRESSION TAG	UNP P76216
D	-4	HIS	-	EXPRESSION TAG	UNP P76216
D	-3	HIS	-	EXPRESSION TAG	UNP P76216
D	-2	HIS	-	EXPRESSION TAG	UNP P76216
D	-1	HIS	-	EXPRESSION TAG	UNP P76216
D	0	GLY	-	EXPRESSION TAG	UNP P76216
D	1	SER	-	EXPRESSION TAG	UNP P76216
D	49	MSE	MET	MODIFIED RESIDUE	UNP P76216
D	106	MSE	MET	MODIFIED RESIDUE	UNP P76216
D	191	MSE	MET	MODIFIED RESIDUE	UNP P76216
D	285	MSE	MET	MODIFIED RESIDUE	UNP P76216
D	317	MSE	MET	MODIFIED RESIDUE	UNP P76216
D	318	MSE	MET	MODIFIED RESIDUE	UNP P76216
D	357	MSE	MET	MODIFIED RESIDUE	UNP P76216
D	385	MSE	MET	MODIFIED RESIDUE	UNP P76216
D	386	MSE	MET	MODIFIED RESIDUE	UNP P76216
E	-10	MET	-	EXPRESSION TAG	UNP P76216
E	-9	GLY	-	EXPRESSION TAG	UNP P76216
E	-8	SER	-	EXPRESSION TAG	UNP P76216
E	-7	SER	-	EXPRESSION TAG	UNP P76216
E	-6	HIS	-	EXPRESSION TAG	UNP P76216
E	-5	HIS	-	EXPRESSION TAG	UNP P76216
E	-4	HIS	-	EXPRESSION TAG	UNP P76216
E	-3	HIS	-	EXPRESSION TAG	UNP P76216
E	-2	HIS	-	EXPRESSION TAG	UNP P76216
E	-1	HIS	-	EXPRESSION TAG	UNP P76216
E	0	GLY	-	EXPRESSION TAG	UNP P76216
E	1	SER	-	EXPRESSION TAG	UNP P76216
E	49	MSE	MET	MODIFIED RESIDUE	UNP P76216
E	106	MSE	MET	MODIFIED RESIDUE	UNP P76216
E	191	MSE	MET	MODIFIED RESIDUE	UNP P76216
E	285	MSE	MET	MODIFIED RESIDUE	UNP P76216
E	317	MSE	MET	MODIFIED RESIDUE	UNP P76216

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Chain	Residue	Modelled	Actual	Comment	Reference
E	318	MSE	MET	MODIFIED RESIDUE	UNP P76216
E	357	MSE	MET	MODIFIED RESIDUE	UNP P76216
E	385	MSE	MET	MODIFIED RESIDUE	UNP P76216
E	386	MSE	MET	MODIFIED RESIDUE	UNP P76216
F	-10	MET	-	EXPRESSION TAG	UNP P76216
F	-9	GLY	-	EXPRESSION TAG	UNP P76216
F	-8	SER	-	EXPRESSION TAG	UNP P76216
F	-7	SER	-	EXPRESSION TAG	UNP P76216
F	-6	HIS	-	EXPRESSION TAG	UNP P76216
F	-5	HIS	-	EXPRESSION TAG	UNP P76216
F	-4	HIS	-	EXPRESSION TAG	UNP P76216
F	-3	HIS	-	EXPRESSION TAG	UNP P76216
F	-2	HIS	-	EXPRESSION TAG	UNP P76216
F	-1	HIS	-	EXPRESSION TAG	UNP P76216
F	0	GLY	-	EXPRESSION TAG	UNP P76216
F	1	SER	-	EXPRESSION TAG	UNP P76216
F	49	MSE	MET	MODIFIED RESIDUE	UNP P76216
F	106	MSE	MET	MODIFIED RESIDUE	UNP P76216
F	191	MSE	MET	MODIFIED RESIDUE	UNP P76216
F	285	MSE	MET	MODIFIED RESIDUE	UNP P76216
F	317	MSE	MET	MODIFIED RESIDUE	UNP P76216
F	318	MSE	MET	MODIFIED RESIDUE	UNP P76216
F	357	MSE	MET	MODIFIED RESIDUE	UNP P76216
F	385	MSE	MET	MODIFIED RESIDUE	UNP P76216
F	386	MSE	MET	MODIFIED RESIDUE	UNP P76216

- Molecule 2 is POTASSIUM ION (three-letter code: K) (formula: K).

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

- Molecule 3 is water.

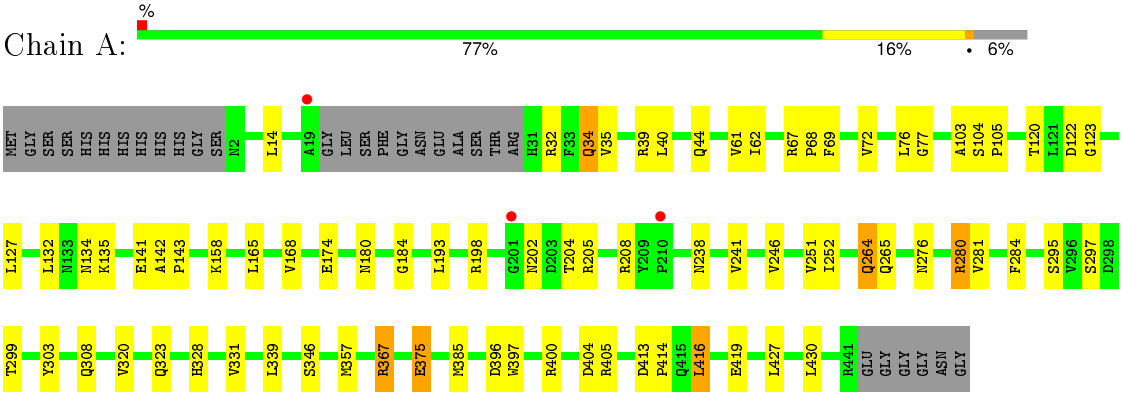
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	260	Total O 260 260	0	0
3	B	310	Total O 310 310	0	0
3	C	213	Total O 213 213	0	0
3	D	192	Total O 192 192	0	0
3	E	244	Total O 244 244	0	0
3	F	183	Total O 183 183	0	0

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.

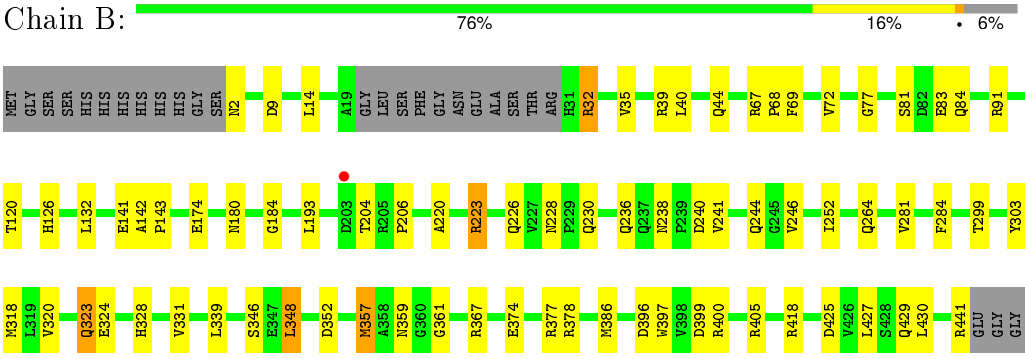
- Molecule 1: Succinylarginine dihydrolase

Chain A:



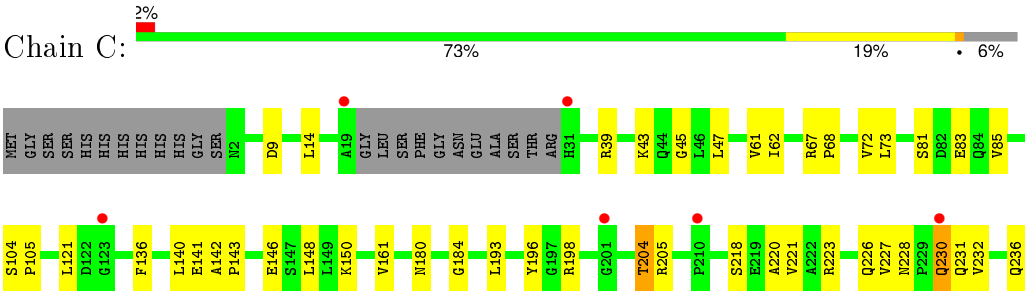
- Molecule 1: Succinylarginine dihydrolase

Chain B:

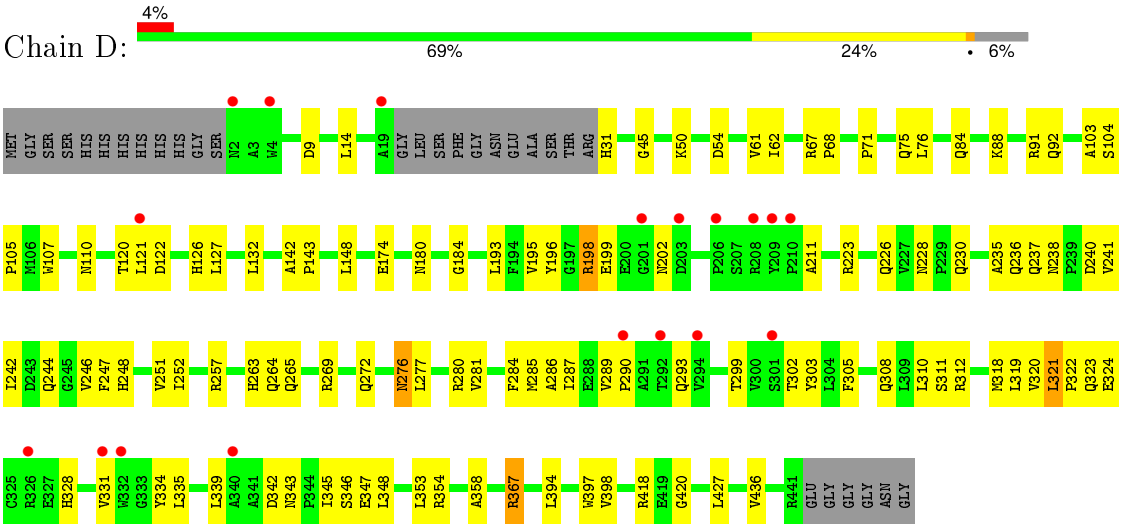


- Molecule 1: Succinylarginine dihydrolase

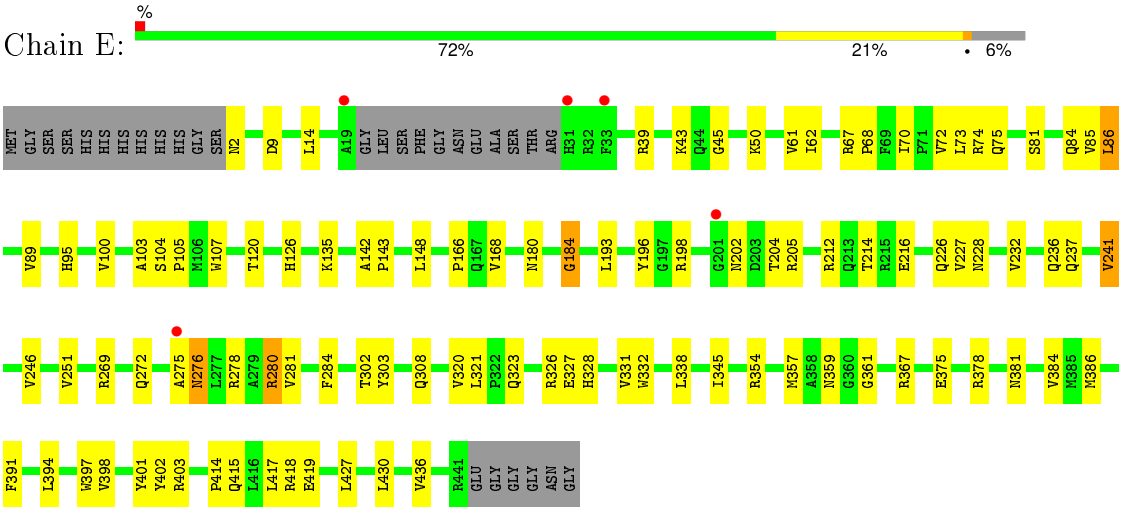
Chain C:



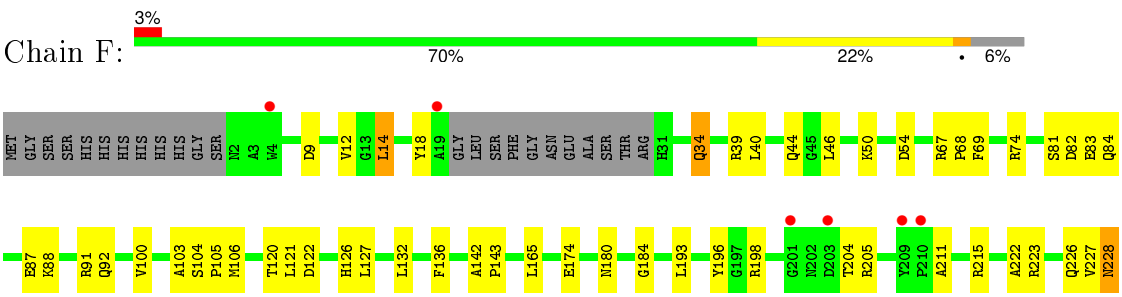
• Molecule 1: Succinylarginine dihydrolase

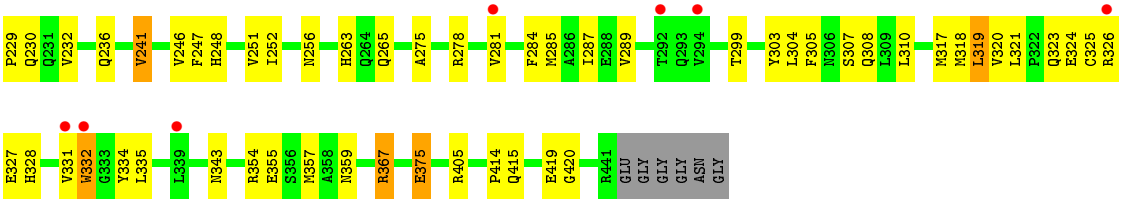


• Molecule 1: Succinylarginine dihydrolase



• Molecule 1: Succinylarginine dihydrolase




P229 Q230 Q231 V232 Q236 V241 V246 F247 H248 V251 I252 N256 H263 Q264 Q265 A275 R278 V281 F284 M285 A286 I287 E288 V289 T292 Q293 V294 T299 Y303 L304 F305 N306 S307 Q308 L309 L310 M317 M318 L319 V320 L321 P322 Q323 E324 C325 R326
E327 H328 V331 W332 G333 Y334 L335 L339 N343 R354 E355 S356 M357 A358 N359 R367 E375 R405 P414 Q415 E419 G420 R441 GLU GLY GLY GLY ASN GLY

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	55.83Å 94.17Å 139.66Å 75.41° 78.38° 89.74°	Depositor
Resolution (Å)	27.32 – 1.90 27.32 – 1.89	Depositor EDS
% Data completeness (in resolution range)	64.5 (27.32-1.90) 62.8 (27.32-1.89)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.04 (at 1.89Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.214 , 0.252 0.212 , 0.249	Depositor DCC
R_{free} test set	6944 reflections (5.08%)	DCC
Wilson B-factor (Å^2)	21.4	Xtriage
Anisotropy	0.502	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 25.3	EDS
Estimated twinning fraction	0.468 for h,-k,h-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 136811 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	21526	wwPDB-VP
Average B, all atoms (Å^2)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 22.16 % of the origin peak, indicating pseudo translational symmetry.The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 6.0306e-03.The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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: K

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	0.36	0/3415	0.58	0/4627
1	B	0.36	0/3415	0.58	0/4627
1	C	0.35	0/3415	0.59	0/4627
1	D	0.33	0/3415	0.57	0/4627
1	E	0.34	0/3415	0.58	0/4627
1	F	0.34	0/3415	0.57	0/4627
All	All	0.35	0/20490	0.58	0/27762

There are no bond length outliers.

There are no bond angle outliers.

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	3353	0	3285	62	0
1	B	3353	0	3285	63	0
1	C	3353	0	3285	66	0
1	D	3353	0	3285	95	0
1	E	3353	0	3285	73	0
1	F	3353	0	3285	108	0
2	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	260	0	0	6	0
3	B	310	0	0	7	0
3	C	213	0	0	8	0
3	D	192	0	0	6	0
3	E	244	0	0	10	0
3	F	183	0	0	3	0
All	All	21526	0	19710	459	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 (459) 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:220:ALA:HA	1:B:223:ARG:HH12	0.99	1.15
1:B:220:ALA:HA	1:B:223:ARG:NH1	1.68	1.06
1:B:223:ARG:HB2	1:B:223:ARG:HH11	1.35	0.92
1:F:248:HIS:O	1:F:251:VAL:HG12	1.71	0.89
1:F:328:HIS:HB3	1:F:331:VAL:HG12	1.56	0.86
1:A:328:HIS:HD2	1:A:331:VAL:H	1.30	0.79
1:D:323:GLN:HE22	1:D:354:ARG:HH12	1.30	0.79
1:F:415:GLN:O	1:F:419:GLU:HG3	1.82	0.79
1:D:285:MSE:HE2	1:D:287:ILE:HG12	1.64	0.78
1:C:415:GLN:O	1:C:419:GLU:HG3	1.83	0.78
1:D:285:MSE:HE1	1:D:343:ASN:HB3	1.66	0.78
1:A:198:ARG:HD2	1:A:205:ARG:HH21	1.49	0.78
1:C:150:LYS:HD3	1:C:161:VAL:HB	1.66	0.77
1:E:415:GLN:O	1:E:419:GLU:HG3	1.84	0.77
1:F:246:VAL:HG13	1:F:251:VAL:CG1	2.15	0.76
1:B:357:MSE:HE3	1:B:361:GLY:C	2.07	0.75
1:A:158:LYS:NZ	1:A:375:GLU:HB3	2.02	0.75
1:D:312:ARG:HH22	1:D:347:GLU:CB	2.01	0.74
1:D:14:LEU:H	1:D:14:LEU:HD12	1.52	0.74
1:A:158:LYS:HZ1	1:A:375:GLU:HB3	1.52	0.74
1:D:198:ARG:HG2	1:D:211:ALA:HB3	1.69	0.74
1:F:285:MSE:HE2	1:F:287:ILE:HG12	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:238:ASN:O	1:D:241:VAL:HG12	1.88	0.73
1:B:220:ALA:CA	1:B:223:ARG:HH12	1.92	0.73
1:D:312:ARG:HH22	1:D:347:GLU:HB3	1.54	0.73
1:D:269:ARG:HD3	1:D:272:GLN:OE1	1.88	0.72
1:C:354:ARG:HG2	3:C:560:HOH:O	1.89	0.72
1:A:165:LEU:HD13	3:A:523:HOH:O	1.90	0.72
1:F:246:VAL:HG13	1:F:251:VAL:HG13	1.72	0.71
1:D:241:VAL:HG22	1:D:246:VAL:HG21	1.71	0.71
1:D:335:LEU:HB3	1:D:348:LEU:HD21	1.71	0.71
1:E:75:GLN:HG3	3:E:660:HOH:O	1.90	0.71
1:D:276:ASN:HD21	1:D:280:ARG:HE	1.38	0.71
1:F:18:TYR:HD2	1:F:359:ASN:HD21	1.39	0.70
1:F:241:VAL:HG13	1:F:246:VAL:HB	1.73	0.70
1:D:328:HIS:HD2	1:D:331:VAL:HG23	1.55	0.70
1:B:357:MSE:CE	1:B:357:MSE:HA	2.21	0.70
1:A:303:TYR:HB2	1:A:357:MSE:HE1	1.74	0.70
1:B:241:VAL:HG22	1:B:246:VAL:HG21	1.71	0.70
1:A:77:GLY:O	1:F:223:ARG:HG2	1.90	0.70
1:E:328:HIS:HD2	1:E:331:VAL:H	1.39	0.70
1:D:257:ARG:HD2	1:D:311:SER:OG	1.92	0.69
1:F:328:HIS:HA	3:F:539:HOH:O	1.92	0.69
1:F:69:PHE:HB3	1:F:100:VAL:CG2	2.22	0.69
1:B:223:ARG:CB	1:B:223:ARG:HH11	2.04	0.69
1:F:281:VAL:HB	1:F:284:PHE:HB2	1.75	0.68
1:F:328:HIS:CD2	1:F:331:VAL:H	2.10	0.68
1:D:328:HIS:CD2	1:D:331:VAL:HG23	2.28	0.68
1:C:380:VAL:HB	1:C:385:MSE:HE2	1.76	0.68
1:A:276:ASN:O	1:A:280:ARG:HG2	1.94	0.67
1:B:310:LEU:HD12	1:B:318:MSE:HE2	1.74	0.67
1:E:180:ASN:HB2	1:E:193:LEU:HB3	1.77	0.67
1:E:386:MSE:HE1	1:E:391:PHE:CD1	2.29	0.67
1:B:328:HIS:HD2	1:B:331:VAL:H	1.40	0.67
1:F:354:ARG:HG3	1:F:355:GLU:N	2.09	0.67
1:F:14:LEU:H	1:F:14:LEU:HD12	1.60	0.67
1:F:328:HIS:HB3	1:F:331:VAL:CG1	2.23	0.66
1:D:281:VAL:HB	1:D:284:PHE:HB2	1.78	0.66
1:F:328:HIS:HD2	1:F:331:VAL:H	1.42	0.66
1:F:285:MSE:HE1	1:F:343:ASN:HB3	1.78	0.66
1:F:275:ALA:HA	1:F:278:ARG:NH1	2.11	0.66
1:B:223:ARG:NH1	1:D:76:LEU:O	2.28	0.66
1:A:419:GLU:HG2	1:B:32:ARG:HB3	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:312:ARG:NH2	1:D:347:GLU:OE2	2.29	0.65
1:A:416:LEU:C	1:A:416:LEU:HD23	2.16	0.65
1:B:238:ASN:O	1:B:241:VAL:HG12	1.97	0.65
1:D:91:ARG:HH11	1:D:91:ARG:HG3	1.61	0.65
1:D:257:ARG:HD3	3:D:597:HOH:O	1.97	0.65
1:F:228:ASN:HD22	1:F:229:PRO:N	1.95	0.65
1:F:142:ALA:HB3	1:F:143:PRO:HD3	1.79	0.64
1:D:241:VAL:HG22	1:D:246:VAL:CG2	2.28	0.64
1:F:228:ASN:C	1:F:228:ASN:HD22	2.01	0.64
1:A:32:ARG:O	1:A:34:GLN:NE2	2.31	0.64
1:C:72:VAL:HG21	1:C:140:LEU:HD21	1.79	0.63
1:B:228:ASN:HD22	1:B:230:GLN:H	1.47	0.63
1:F:246:VAL:HA	1:F:251:VAL:HG11	1.80	0.63
1:C:354:ARG:HG3	3:C:616:HOH:O	1.98	0.63
1:E:126:HIS:CE1	1:E:226:GLN:HG3	2.34	0.62
1:A:14:LEU:HD12	1:A:14:LEU:H	1.64	0.62
1:E:328:HIS:CD2	1:E:331:VAL:HG23	2.34	0.62
1:D:121:LEU:HG	1:D:226:GLN:O	2.00	0.62
1:F:69:PHE:O	1:F:100:VAL:HG21	2.00	0.62
1:A:430:LEU:HD23	1:A:430:LEU:O	2.00	0.62
1:E:142:ALA:HB3	1:E:143:PRO:HD3	1.81	0.61
1:F:40:LEU:HD23	1:F:354:ARG:HH21	1.65	0.61
1:C:205:ARG:HD2	3:C:483:HOH:O	2.00	0.61
1:C:338:LEU:HD21	1:C:345:ILE:HD12	1.82	0.61
1:B:180:ASN:HB2	1:B:193:LEU:HB3	1.83	0.61
1:C:238:ASN:O	1:C:241:VAL:HG22	2.01	0.60
1:B:303:TYR:CE2	1:B:357:MSE:HE1	2.36	0.60
1:B:14:LEU:HD12	1:B:14:LEU:H	1.67	0.60
1:D:285:MSE:HE1	1:D:343:ASN:CB	2.30	0.60
1:B:35:VAL:CG1	1:B:405:ARG:HG3	2.32	0.60
1:B:357:MSE:HE2	1:B:357:MSE:HA	1.83	0.60
1:F:198:ARG:HD3	1:F:211:ALA:HB3	1.83	0.60
1:D:104:SER:N	1:D:105:PRO:HD2	2.16	0.60
1:E:386:MSE:HE1	1:E:391:PHE:HD1	1.67	0.60
1:C:238:ASN:HD22	1:C:241:VAL:HG13	1.66	0.60
1:E:86:LEU:HD12	1:E:417:LEU:HD22	1.83	0.59
1:B:105:PRO:HG3	1:B:141:GLU:HG2	1.84	0.59
1:A:328:HIS:CD2	1:A:331:VAL:H	2.18	0.59
1:A:400:ARG:O	1:B:32:ARG:HG3	2.02	0.59
1:B:120:THR:HG21	1:B:126:HIS:HD2	1.66	0.59
1:C:142:ALA:HB3	1:C:143:PRO:HD3	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:323:GLN:NE2	1:D:354:ARG:HH12	1.99	0.59
1:A:105:PRO:HG3	1:A:141:GLU:HG2	1.85	0.59
1:A:241:VAL:HG22	1:A:246:VAL:HG21	1.84	0.59
1:F:104:SER:N	1:F:105:PRO:HD2	2.18	0.58
1:C:273:LEU:O	1:C:277:LEU:HD13	2.03	0.58
1:C:121:LEU:HD13	1:C:226:GLN:O	2.04	0.58
1:A:142:ALA:HB3	1:A:143:PRO:HD3	1.86	0.58
1:C:378:ARG:HB3	1:C:378:ARG:NH1	2.18	0.58
1:D:285:MSE:HE2	1:D:287:ILE:CG1	2.33	0.58
1:D:14:LEU:N	1:D:14:LEU:HD12	2.18	0.58
1:E:104:SER:N	1:E:105:PRO:HD2	2.19	0.58
1:D:328:HIS:CD2	1:D:331:VAL:H	2.21	0.58
1:B:2:ASN:HB2	3:B:686:HOH:O	2.03	0.58
1:F:69:PHE:HB3	1:F:100:VAL:HG22	1.85	0.57
1:F:14:LEU:N	1:F:14:LEU:HD12	2.18	0.57
1:D:312:ARG:NH2	1:D:347:GLU:HB3	2.20	0.56
1:F:34:GLN:HA	1:F:34:GLN:HE21	1.71	0.56
1:E:14:LEU:HD11	1:E:402:TYR:HA	1.86	0.56
1:D:312:ARG:NH1	3:D:614:HOH:O	2.39	0.56
1:F:278:ARG:HG2	1:F:284:PHE:HD1	1.70	0.56
1:C:43:LYS:O	1:C:47:LEU:HG	2.05	0.56
1:C:39:ARG:HD3	3:C:600:HOH:O	2.04	0.56
1:E:281:VAL:HB	1:E:284:PHE:HB2	1.87	0.56
1:E:81:SER:O	1:E:85:VAL:HG23	2.06	0.56
1:F:228:ASN:ND2	1:F:230:GLN:H	2.03	0.56
1:A:180:ASN:HB2	1:A:193:LEU:HB3	1.86	0.55
1:F:40:LEU:O	1:F:44:GLN:HG3	2.06	0.55
1:D:290:PRO:HG2	1:D:293:GLN:HG3	1.88	0.55
1:E:354:ARG:HG2	3:E:585:HOH:O	2.06	0.55
1:F:325:CYS:O	1:F:331:VAL:HG13	2.07	0.55
1:E:81:SER:OG	1:E:84:GLN:HG3	2.06	0.55
1:B:339:LEU:HD13	1:B:348:LEU:HD13	1.87	0.55
1:F:14:LEU:HD22	1:F:420:GLY:HA2	1.89	0.55
1:C:198:ARG:HD2	1:C:205:ARG:NH2	2.21	0.55
1:A:238:ASN:O	1:A:241:VAL:HG12	2.07	0.55
1:E:276:ASN:HD21	1:E:280:ARG:HD2	1.71	0.55
1:C:308:GLN:HB2	1:C:320:VAL:HB	1.88	0.55
1:C:105:PRO:HG3	1:C:141:GLU:HG2	1.88	0.55
1:C:238:ASN:HB3	1:C:241:VAL:HG22	1.89	0.55
1:E:338:LEU:HD21	1:E:345:ILE:HD12	1.89	0.54
1:C:150:LYS:HD3	1:C:161:VAL:CB	2.36	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:241:VAL:HG22	1:B:246:VAL:CG2	2.36	0.54
1:F:252:ILE:HD12	1:F:299:THR:HG21	1.89	0.54
1:B:441:ARG:NH2	3:B:583:HOH:O	2.35	0.54
1:A:252:ILE:CD1	1:A:299:THR:HG21	2.38	0.54
1:E:95:HIS:CD2	1:E:95:HIS:H	2.25	0.54
1:C:220:ALA:HA	1:C:223:ARG:NH1	2.23	0.54
1:C:148:LEU:HD23	1:C:436:VAL:HG21	1.90	0.54
1:D:142:ALA:HB3	1:D:143:PRO:HD3	1.88	0.54
1:B:69:PHE:O	1:B:72:VAL:HG12	2.08	0.54
1:B:228:ASN:ND2	1:B:230:GLN:H	2.06	0.54
1:F:69:PHE:H	1:F:100:VAL:HG22	1.73	0.54
1:F:14:LEU:CD1	1:F:14:LEU:H	2.21	0.54
1:E:2:ASN:N	3:E:653:HOH:O	2.41	0.54
1:B:328:HIS:CD2	1:B:331:VAL:H	2.23	0.53
1:E:414:PRO:O	1:E:418:ARG:HG3	2.09	0.53
1:C:81:SER:O	1:C:85:VAL:HG23	2.09	0.53
1:D:289:VAL:HG22	1:D:334:TYR:CZ	2.44	0.53
1:C:180:ASN:HB2	1:C:193:LEU:HB3	1.91	0.53
1:D:122:ASP:HB3	1:D:226:GLN:HE22	1.73	0.53
1:D:14:LEU:H	1:D:14:LEU:CD1	2.20	0.53
1:E:184:GLY:HA2	3:E:553:HOH:O	2.09	0.53
1:E:415:GLN:HA	1:E:418:ARG:NH1	2.24	0.53
1:D:199:GLU:HG2	1:D:202:ASN:HB3	1.90	0.53
1:D:91:ARG:NH1	1:D:91:ARG:HG3	2.24	0.53
1:B:323:GLN:NE2	1:B:352:ASP:HB2	2.24	0.52
1:F:256:ASN:HD22	1:F:317:MSE:SE	2.43	0.52
1:C:281:VAL:HB	1:C:284:PHE:HB2	1.91	0.52
1:E:403:ARG:HG3	3:E:623:HOH:O	2.09	0.52
1:E:148:LEU:HD23	1:E:436:VAL:HG21	1.91	0.52
1:E:394:LEU:O	1:E:398:VAL:HG23	2.10	0.52
1:D:312:ARG:HH22	1:D:347:GLU:HB2	1.74	0.52
1:C:14:LEU:HD12	1:C:420:GLY:HA2	1.92	0.52
1:F:332:TRP:HA	1:F:332:TRP:CE3	2.44	0.52
1:B:126:HIS:CE1	1:B:226:GLN:HG3	2.45	0.52
1:D:264:GLN:HG3	1:D:265:GLN:HG3	1.92	0.52
1:D:240:ASP:O	1:D:244:GLN:HG3	2.09	0.52
1:B:281:VAL:HB	1:B:284:PHE:HB2	1.92	0.52
1:A:39:ARG:HD3	1:A:404:ASP:OD2	2.10	0.52
1:B:396:ASP:O	1:B:400:ARG:HG3	2.10	0.52
1:E:326:ARG:HD2	1:E:332:TRP:CD2	2.44	0.52
1:D:303:TYR:HA	3:D:578:HOH:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:103:ALA:C	1:D:105:PRO:HD2	2.30	0.51
1:B:328:HIS:CD2	1:B:331:VAL:HG23	2.45	0.51
1:F:289:VAL:HG22	1:F:334:TYR:CZ	2.46	0.51
1:B:120:THR:HG21	1:B:126:HIS:CD2	2.44	0.51
1:F:328:HIS:CB	1:F:331:VAL:HG12	2.36	0.51
1:A:252:ILE:HD12	1:A:299:THR:HG21	1.92	0.51
1:A:281:VAL:HB	1:A:284:PHE:HB2	1.93	0.51
1:E:14:LEU:CD1	1:E:402:TYR:HA	2.41	0.51
1:D:247:PHE:CD1	1:D:248:HIS:ND1	2.79	0.51
1:E:166:PRO:HA	3:E:625:HOH:O	2.10	0.51
1:C:136:PHE:HD2	1:E:168:VAL:HG21	1.75	0.51
1:F:328:HIS:HD2	1:F:331:VAL:N	2.09	0.51
1:C:146:GLU:O	1:C:150:LYS:HG2	2.11	0.51
1:E:198:ARG:HE	1:E:214:THR:HG22	1.76	0.51
1:D:247:PHE:HD1	1:D:248:HIS:ND1	2.09	0.50
1:F:44:GLN:HE22	1:F:354:ARG:HG2	1.76	0.50
1:C:136:PHE:CD2	1:E:168:VAL:HG21	2.46	0.50
1:E:328:HIS:CD2	1:E:331:VAL:H	2.23	0.50
1:F:88:LYS:O	1:F:92:GLN:HG3	2.11	0.50
1:C:103:ALA:C	1:C:105:PRO:HD2	2.32	0.50
1:F:120:THR:HG21	1:F:126:HIS:HD2	1.76	0.50
1:F:74:ARG:NH2	1:F:82:ASP:OD1	2.45	0.50
1:C:328:HIS:HB2	3:C:551:HOH:O	2.12	0.50
1:B:397:TRP:CH2	1:B:427:LEU:HD22	2.46	0.50
1:C:230:GLN:H	1:C:230:GLN:HE21	1.58	0.50
1:D:196:TYR:CE1	1:D:236:GLN:HB2	2.47	0.50
1:F:122:ASP:HB3	1:F:226:GLN:HE22	1.77	0.49
1:D:228:ASN:OD1	1:D:230:GLN:HG2	2.13	0.49
1:F:285:MSE:HE1	1:F:343:ASN:CB	2.42	0.49
1:D:251:VAL:O	1:D:251:VAL:HG12	2.13	0.49
1:A:297:SER:HB2	3:A:660:HOH:O	2.11	0.49
1:C:228:ASN:OD1	1:C:230:GLN:NE2	2.44	0.49
1:F:122:ASP:CB	1:F:226:GLN:HE22	2.26	0.49
1:E:196:TYR:CE1	1:E:236:GLN:HB2	2.47	0.49
1:F:180:ASN:HB2	1:F:193:LEU:HB3	1.93	0.49
1:A:35:VAL:CG1	1:A:405:ARG:HG3	2.43	0.49
1:D:312:ARG:HG3	3:D:614:HOH:O	2.12	0.48
1:B:357:MSE:HE3	1:B:361:GLY:O	2.13	0.48
1:E:50:LYS:HD3	1:E:391:PHE:CG	2.48	0.48
1:C:230:GLN:H	1:C:230:GLN:NE2	2.11	0.48
1:E:397:TRP:CH2	1:E:427:LEU:HD22	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:418:ARG:NH1	1:D:418:ARG:HG3	2.28	0.48
1:B:83:GLU:OE2	1:B:418:ARG:NH2	2.46	0.48
1:B:240:ASP:O	1:B:244:GLN:HG3	2.13	0.48
1:F:241:VAL:HG13	1:F:246:VAL:CB	2.43	0.48
1:A:120:THR:HG22	1:A:123:GLY:N	2.28	0.48
1:E:72:VAL:HG11	1:E:100:VAL:HG12	1.95	0.48
1:F:83:GLU:O	1:F:87:GLU:HG3	2.12	0.48
1:F:310:LEU:HD12	1:F:318:MSE:HE2	1.94	0.48
1:F:228:ASN:HD22	1:F:229:PRO:CD	2.25	0.48
1:C:104:SER:N	1:C:105:PRO:CD	2.77	0.48
1:A:127:LEU:HD12	1:A:127:LEU:N	2.29	0.48
1:D:50:LYS:HE2	1:D:54:ASP:OD1	2.13	0.48
1:A:396:ASP:O	1:A:400:ARG:HG3	2.13	0.48
1:D:180:ASN:HB2	1:D:193:LEU:HB3	1.95	0.48
1:E:276:ASN:ND2	1:E:280:ARG:HD2	2.28	0.48
1:A:69:PHE:O	1:A:72:VAL:HG12	2.14	0.48
1:D:14:LEU:HD22	1:D:420:GLY:HA2	1.95	0.48
1:D:328:HIS:HD2	1:D:331:VAL:H	1.61	0.48
1:C:385:MSE:O	1:C:390:LEU:HD12	2.13	0.48
1:C:196:TYR:CE1	1:C:236:GLN:HB2	2.48	0.48
1:D:263:HIS:ND1	1:D:264:GLN:N	2.62	0.48
1:E:251:VAL:O	1:E:251:VAL:HG12	2.14	0.47
1:D:122:ASP:CB	1:D:226:GLN:HE22	2.27	0.47
1:E:269:ARG:NE	1:E:272:GLN:OE1	2.47	0.47
1:B:83:GLU:HB2	3:B:585:HOH:O	2.14	0.47
1:B:77:GLY:HA3	1:D:223:ARG:HB3	1.96	0.47
1:C:252:ILE:HD12	1:C:299:THR:HG21	1.97	0.47
1:D:61:VAL:HG22	1:D:62:ILE:N	2.29	0.47
1:F:251:VAL:HG22	1:F:251:VAL:O	2.14	0.47
1:D:284:PHE:CZ	1:D:286:ALA:HB2	2.49	0.47
1:A:158:LYS:HZ1	1:A:375:GLU:CD	2.17	0.47
1:E:415:GLN:HA	1:E:418:ARG:HH11	1.79	0.47
1:C:390:LEU:HD22	1:C:394:LEU:CD1	2.44	0.47
1:E:323:GLN:O	1:E:327:GLU:HG2	2.14	0.47
1:F:227:VAL:HG11	1:F:232:VAL:CG1	2.44	0.47
1:C:400:ARG:HD2	1:C:401:TYR:CE1	2.50	0.47
1:A:416:LEU:O	1:A:416:LEU:HD23	2.14	0.47
3:C:558:HOH:O	1:F:122:ASP:HA	2.15	0.47
1:C:45:GLY:HA3	3:C:568:HOH:O	2.15	0.47
1:F:12:VAL:HG22	1:F:106:MSE:HE3	1.96	0.47
1:D:110:ASN:HB3	1:D:132:LEU:HD21	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:121:LEU:HG	1:F:226:GLN:O	2.15	0.47
1:D:120:THR:HG21	1:D:126:HIS:HD2	1.80	0.46
1:F:222:ALA:O	1:F:227:VAL:HG23	2.14	0.46
1:F:263:HIS:CE1	1:F:265:GLN:HG3	2.50	0.46
1:F:100:VAL:O	1:F:100:VAL:HG22	2.15	0.46
1:C:228:ASN:HB3	1:C:231:GLN:HG3	1.97	0.46
1:D:418:ARG:HG3	1:D:418:ARG:HH11	1.79	0.46
1:A:397:TRP:CH2	1:A:427:LEU:HD22	2.50	0.46
1:D:342:ASP:OD1	1:D:342:ASP:O	2.34	0.46
1:F:198:ARG:HB2	1:F:205:ARG:HH21	1.81	0.46
1:C:14:LEU:CD1	1:C:420:GLY:HA2	2.46	0.46
1:A:339:LEU:HD11	1:A:346:SER:C	2.36	0.46
1:F:323:GLN:HE22	1:F:326:ARG:HD3	1.81	0.46
1:C:227:VAL:HG11	1:C:232:VAL:HG22	1.97	0.46
1:F:307:SER:HB2	1:F:319:LEU:HD23	1.98	0.46
1:E:328:HIS:HD2	1:E:331:VAL:N	2.09	0.46
1:E:202:ASN:OD1	1:E:204:THR:HB	2.15	0.46
1:C:251:VAL:HG12	1:C:251:VAL:O	2.16	0.46
1:C:397:TRP:CH2	1:C:427:LEU:HD22	2.50	0.46
1:D:67:ARG:HA	1:D:68:PRO:C	2.35	0.46
1:E:381:ASN:O	1:E:384:VAL:HG22	2.15	0.46
1:F:247:PHE:CD1	1:F:248:HIS:ND1	2.84	0.46
1:B:425:ASP:O	1:B:429:GLN:HG3	2.16	0.46
1:F:67:ARG:HA	1:F:68:PRO:C	2.36	0.46
1:A:134:ASN:OD1	1:A:135:LYS:HE2	2.15	0.46
1:A:308:GLN:HB2	1:A:320:VAL:HB	1.98	0.45
1:E:107:TRP:HH2	1:E:359:ASN:HB3	1.81	0.45
1:E:39:ARG:O	1:E:43:LYS:HG2	2.16	0.45
1:E:103:ALA:C	1:E:105:PRO:HD2	2.37	0.45
1:D:88:LYS:HB3	1:D:92:GLN:NE2	2.31	0.45
1:D:339:LEU:HD22	1:D:348:LEU:HD13	1.98	0.45
1:B:206:PRO:HD2	3:B:588:HOH:O	2.16	0.45
1:A:120:THR:HG21	1:A:122:ASP:OD1	2.16	0.45
1:A:120:THR:CG2	1:A:122:ASP:H	2.28	0.45
1:C:299:THR:HG23	1:C:305:PHE:HD1	1.81	0.45
1:C:95:HIS:H	1:C:95:HIS:CD2	2.35	0.45
1:F:103:ALA:C	1:F:105:PRO:HD2	2.37	0.45
1:D:148:LEU:HD23	1:D:436:VAL:HG21	1.99	0.45
1:D:339:LEU:HD11	1:D:346:SER:C	2.36	0.45
1:E:120:THR:HG21	1:E:126:HIS:HD2	1.81	0.45
1:D:84:GLN:O	1:D:88:LYS:HG3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:308:GLN:HB2	1:B:320:VAL:HB	1.99	0.45
1:C:238:ASN:O	1:C:241:VAL:CG2	2.65	0.45
1:E:14:LEU:HB2	3:E:662:HOH:O	2.17	0.45
1:F:120:THR:HG21	1:F:126:HIS:CD2	2.52	0.45
1:E:67:ARG:HA	1:E:68:PRO:C	2.37	0.45
1:A:367:ARG:HD2	1:A:367:ARG:C	2.37	0.45
1:D:331:VAL:O	1:D:335:LEU:HD23	2.17	0.45
1:F:354:ARG:HG3	1:F:355:GLU:H	1.78	0.45
1:F:204:THR:HG22	1:F:236:GLN:HE22	1.82	0.45
1:F:132:LEU:HD23	1:F:174:GLU:HA	1.98	0.45
1:A:168:VAL:HG21	1:F:136:PHE:HD2	1.82	0.45
1:C:326:ARG:HD2	1:C:332:TRP:CD2	2.52	0.45
1:D:71:PRO:O	1:D:75:GLN:HG3	2.17	0.45
1:D:328:HIS:HD2	1:D:331:VAL:CG2	2.29	0.44
1:C:378:ARG:CB	1:C:378:ARG:HH11	2.30	0.44
1:B:339:LEU:HD11	1:B:346:SER:C	2.37	0.44
1:D:289:VAL:HG22	1:D:334:TYR:OH	2.17	0.44
1:D:310:LEU:HD12	1:D:318:MSE:HE2	1.98	0.44
1:B:40:LEU:O	1:B:44:GLN:HG3	2.17	0.44
1:F:247:PHE:HD1	1:F:248:HIS:ND1	2.15	0.44
1:D:211:ALA:HA	3:D:547:HOH:O	2.17	0.44
1:A:104:SER:N	1:A:105:PRO:CD	2.80	0.44
1:E:39:ARG:HD2	3:E:656:HOH:O	2.18	0.44
1:A:40:LEU:O	1:A:44:GLN:HG3	2.17	0.44
1:D:237:GLN:HB3	1:D:242:ILE:HD11	1.98	0.44
1:B:357:MSE:HE3	1:B:357:MSE:HA	1.99	0.44
1:D:104:SER:HA	1:D:107:TRP:CZ3	2.53	0.44
1:F:375:GLU:HB2	3:F:547:HOH:O	2.16	0.44
1:B:378:ARG:HD2	3:B:704:HOH:O	2.16	0.44
1:D:127:LEU:N	1:D:127:LEU:HD12	2.32	0.44
1:C:205:ARG:HB3	3:C:483:HOH:O	2.18	0.44
1:A:67:ARG:HA	1:A:68:PRO:C	2.39	0.44
1:F:230:GLN:NE2	3:F:561:HOH:O	2.50	0.44
1:B:142:ALA:HB3	1:B:143:PRO:HD3	1.98	0.44
1:B:223:ARG:CG	1:B:223:ARG:HH11	2.30	0.44
1:B:104:SER:N	1:B:105:PRO:CD	2.81	0.44
1:B:324:GLU:CD	1:B:324:GLU:H	2.20	0.44
1:A:264:GLN:HE21	1:A:264:GLN:HB2	1.63	0.44
1:A:72:VAL:O	1:A:76:LEU:HG	2.18	0.43
1:C:285:MSE:HE1	1:C:344:PRO:HD3	1.99	0.43
1:C:73:LEU:HD13	1:C:89:VAL:HG21	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:122:ASP:CG	1:F:226:GLN:HE22	2.21	0.43
1:E:107:TRP:NE1	1:E:361:GLY:HA3	2.34	0.43
1:E:73:LEU:HD13	1:E:89:VAL:HG21	1.99	0.43
1:F:304:LEU:HD11	1:F:335:LEU:HD21	2.00	0.43
1:F:278:ARG:HG2	1:F:284:PHE:CD1	2.51	0.43
1:E:14:LEU:HD11	1:E:401:TYR:O	2.18	0.43
1:F:289:VAL:HG22	1:F:334:TYR:OH	2.18	0.43
1:F:91:ARG:HG3	1:F:92:GLN:N	2.34	0.43
1:F:196:TYR:CE2	1:F:215:ARG:HD2	2.53	0.43
1:F:127:LEU:N	1:F:127:LEU:HD12	2.32	0.43
1:C:14:LEU:CD2	1:C:402:TYR:HA	2.47	0.43
1:F:50:LYS:HZ3	1:F:54:ASP:CG	2.22	0.43
1:D:241:VAL:CG2	1:D:246:VAL:HG21	2.43	0.43
1:C:241:VAL:HG11	1:C:265:GLN:O	2.18	0.43
1:E:308:GLN:HB2	1:E:320:VAL:HB	1.99	0.43
1:C:61:VAL:HG22	1:C:62:ILE:N	2.34	0.43
1:F:88:LYS:HG2	1:F:91:ARG:NH2	2.33	0.43
1:A:132:LEU:HD23	1:A:174:GLU:HA	1.99	0.43
1:C:247:PHE:CD1	1:C:248:HIS:ND1	2.86	0.43
1:A:413:ASP:HA	1:A:414:PRO:HD3	1.87	0.43
1:D:252:ILE:HD12	1:D:299:THR:HG21	2.00	0.43
1:D:312:ARG:NH2	1:D:347:GLU:CB	2.77	0.43
1:B:299:THR:HG23	3:B:465:HOH:O	2.18	0.43
1:A:295:SER:HB2	3:A:582:HOH:O	2.17	0.43
1:B:67:ARG:HA	1:B:68:PRO:C	2.39	0.43
1:E:338:LEU:HD21	1:E:345:ILE:CD1	2.49	0.43
1:D:132:LEU:HD23	1:D:174:GLU:HA	2.01	0.43
1:F:323:GLN:HG3	1:F:327:GLU:OE2	2.18	0.43
1:A:120:THR:HG22	1:A:123:GLY:H	1.83	0.43
1:D:324:GLU:N	1:D:324:GLU:OE1	2.47	0.43
1:F:332:TRP:HA	1:F:332:TRP:HE3	1.84	0.42
1:D:299:THR:HG23	1:D:305:PHE:HD1	1.84	0.42
1:E:227:VAL:HG11	1:E:232:VAL:HG22	2.01	0.42
1:C:381:ASN:O	1:C:384:VAL:HG22	2.19	0.42
1:D:246:VAL:HG13	1:D:251:VAL:HB	2.01	0.42
1:B:323:GLN:HE22	1:B:352:ASP:HB2	1.84	0.42
1:F:69:PHE:CB	1:F:100:VAL:HG22	2.48	0.42
1:F:40:LEU:HD23	1:F:354:ARG:NH2	2.34	0.42
1:D:308:GLN:HB2	1:D:320:VAL:HB	2.01	0.42
1:E:228:ASN:N	3:E:612:HOH:O	2.52	0.42
1:B:252:ILE:CD1	1:B:299:THR:HG21	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:308:GLN:NE2	1:F:367:ARG:HG2	2.34	0.42
1:F:331:VAL:HG13	1:F:332:TRP:N	2.34	0.42
1:F:228:ASN:ND2	1:F:228:ASN:C	2.71	0.42
1:E:275:ALA:HA	1:E:278:ARG:CZ	2.49	0.42
1:C:370:VAL:HG12	1:C:372:LEU:HG	2.02	0.42
1:F:285:MSE:HE2	1:F:287:ILE:CG1	2.46	0.42
1:F:332:TRP:HE3	1:F:335:LEU:HD12	1.85	0.42
1:A:328:HIS:HD2	1:A:331:VAL:N	2.08	0.42
1:C:14:LEU:HD23	1:C:402:TYR:CG	2.55	0.42
1:A:202:ASN:HD21	1:A:204:THR:HB	1.84	0.42
1:E:241:VAL:HG13	1:E:246:VAL:HB	2.02	0.42
1:C:67:ARG:HA	1:C:68:PRO:C	2.40	0.42
1:D:321:LEU:HB3	1:D:322:PRO:HD2	2.01	0.42
1:B:132:LEU:HD23	1:B:174:GLU:HA	2.00	0.42
1:F:246:VAL:O	1:F:246:VAL:HG12	2.18	0.41
1:E:236:GLN:HG2	1:E:237:GLN:O	2.19	0.41
1:E:303:TYR:HB2	1:E:357:MSE:HE1	2.01	0.41
1:A:385:MSE:SE	3:A:625:HOH:O	2.87	0.41
1:E:216:GLU:CD	1:E:216:GLU:H	2.22	0.41
1:E:45:GLY:HA3	3:E:497:HOH:O	2.20	0.41
1:F:308:GLN:HB2	1:F:320:VAL:HB	2.02	0.41
1:B:39:ARG:NH2	1:B:399:ASP:OD1	2.53	0.41
1:B:204:THR:HG22	1:B:236:GLN:HE22	1.84	0.41
1:E:50:LYS:HD2	1:E:386:MSE:HE3	2.01	0.41
1:E:302:THR:O	1:E:303:TYR:HB2	2.20	0.41
1:D:31:HIS:HE2	1:D:358:ALA:HB1	1.85	0.41
1:A:265:GLN:HA	3:A:628:HOH:O	2.20	0.41
1:B:107:TRP:CH2	1:B:359:ASN:HB3	2.55	0.41
1:B:374:GLU:HA	1:B:377:ARG:CZ	2.51	0.41
1:D:394:LEU:O	1:D:398:VAL:HG23	2.20	0.41
1:E:61:VAL:HG22	1:E:62:ILE:N	2.35	0.41
1:E:135:LYS:HE2	1:E:212:ARG:NH2	2.36	0.41
1:F:81:SER:OG	1:F:84:GLN:HG3	2.20	0.41
1:A:198:ARG:HD2	1:A:205:ARG:NH2	2.26	0.41
1:A:241:VAL:HG22	1:A:246:VAL:CG2	2.49	0.41
1:D:302:THR:O	1:D:303:TYR:HB2	2.21	0.41
1:D:45:GLY:HA3	3:D:561:HOH:O	2.20	0.41
1:F:246:VAL:HG22	1:F:251:VAL:HG13	2.02	0.41
1:B:357:MSE:HE2	3:B:746:HOH:O	2.20	0.41
1:F:228:ASN:HA	1:F:229:PRO:HD3	1.96	0.41
1:E:354:ARG:HA	1:E:354:ARG:HD3	1.76	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:91:ARG:HG3	1:F:92:GLN:CG	2.51	0.41
1:E:70:ILE:HG22	1:E:74:ARG:NH1	2.36	0.41
1:A:430:LEU:HD23	1:A:430:LEU:C	2.40	0.41
1:F:227:VAL:CG1	1:F:232:VAL:CG1	2.99	0.41
1:D:31:HIS:NE2	1:D:358:ALA:HB1	2.35	0.41
1:D:397:TRP:CZ2	1:D:427:LEU:HB2	2.56	0.41
1:A:165:LEU:N	1:A:165:LEU:CD1	2.84	0.41
1:E:328:HIS:HD2	1:E:331:VAL:HG23	1.84	0.41
1:A:103:ALA:C	1:A:105:PRO:HD2	2.41	0.41
1:D:319:LEU:HD11	1:D:345:ILE:HD13	2.03	0.41
1:F:303:TYR:CD1	1:F:357:MSE:HE1	2.56	0.41
1:A:61:VAL:HG22	1:A:62:ILE:N	2.36	0.41
1:C:378:ARG:HB3	1:C:378:ARG:HH11	1.82	0.41
1:F:91:ARG:HG3	1:F:92:GLN:HG3	2.03	0.41
1:D:195:VAL:HA	1:D:235:ALA:O	2.21	0.41
1:F:304:LEU:CD1	1:F:335:LEU:HD21	2.50	0.40
1:A:416:LEU:HD22	3:A:497:HOH:O	2.21	0.40
1:E:276:ASN:HD21	1:E:280:ARG:CD	2.34	0.40
1:F:247:PHE:HD1	1:F:248:HIS:CE1	2.39	0.40
1:D:367:ARG:HD2	1:D:367:ARG:C	2.41	0.40
1:C:204:THR:O	1:C:204:THR:HG22	2.21	0.40
1:A:158:LYS:HZ2	1:A:375:GLU:HB3	1.83	0.40
1:F:299:THR:HG23	1:F:305:PHE:HD1	1.86	0.40
1:A:251:VAL:HG12	1:A:251:VAL:O	2.22	0.40
1:F:83:GLU:HG2	1:F:414:PRO:HB3	2.02	0.40
1:C:218:SER:O	1:C:221:VAL:CG1	2.70	0.40
1:B:81:SER:OG	1:B:84:GLN:HG3	2.22	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	425/458 (93%)	411 (97%)	13 (3%)	1 (0%)	52	42
1	B	425/458 (93%)	412 (97%)	12 (3%)	1 (0%)	52	42
1	C	425/458 (93%)	412 (97%)	12 (3%)	1 (0%)	52	42
1	D	425/458 (93%)	411 (97%)	13 (3%)	1 (0%)	52	42
1	E	425/458 (93%)	413 (97%)	11 (3%)	1 (0%)	52	42
1	F	425/458 (93%)	413 (97%)	11 (3%)	1 (0%)	52	42
All	All	2550/2748 (93%)	2472 (97%)	72 (3%)	6 (0%)	52	42

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	184	GLY
1	B	184	GLY
1	D	184	GLY
1	E	184	GLY
1	C	184	GLY
1	F	184	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	357/368 (97%)	349 (98%)	8 (2%)	60	53
1	B	357/368 (97%)	346 (97%)	11 (3%)	47	37
1	C	357/368 (97%)	347 (97%)	10 (3%)	51	41
1	D	357/368 (97%)	350 (98%)	7 (2%)	63	57
1	E	357/368 (97%)	346 (97%)	11 (3%)	47	37
1	F	357/368 (97%)	342 (96%)	15 (4%)	36	24
All	All	2142/2208 (97%)	2080 (97%)	62 (3%)	50	40

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	GLN
1	A	208	ARG
1	A	264	GLN
1	A	280	ARG
1	A	323	GLN
1	A	367	ARG
1	A	375	GLU
1	A	416	LEU
1	B	9	ASP
1	B	32	ARG
1	B	91	ARG
1	B	223	ARG
1	B	264	GLN
1	B	323	GLN
1	B	348	LEU
1	B	357	MSE
1	B	367	ARG
1	B	386	MSE
1	B	430	LEU
1	C	9	ASP
1	C	83	GLU
1	C	204	THR
1	C	230	GLN
1	C	247	PHE
1	C	313	ASP
1	C	321	LEU
1	C	353	LEU
1	C	367	ARG
1	C	390	LEU
1	D	9	ASP
1	D	198	ARG
1	D	276	ASN
1	D	277	LEU
1	D	321	LEU
1	D	353	LEU
1	D	367	ARG
1	E	9	ASP
1	E	86	LEU
1	E	205	ARG
1	E	241	VAL
1	E	276	ASN
1	E	280	ARG
1	E	321	LEU

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Mol	Chain	Res	Type
1	E	367	ARG
1	E	375	GLU
1	E	378	ARG
1	E	430	LEU
1	F	9	ASP
1	F	14	LEU
1	F	34	GLN
1	F	39	ARG
1	F	46	LEU
1	F	165	LEU
1	F	228	ASN
1	F	241	VAL
1	F	319	LEU
1	F	321	LEU
1	F	324	GLU
1	F	332	TRP
1	F	367	ARG
1	F	375	GLU
1	F	405	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (50) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2	ASN
1	A	202	ASN
1	A	236	GLN
1	A	323	GLN
1	A	328	HIS
1	A	415	GLN
1	B	2	ASN
1	B	34	GLN
1	B	202	ASN
1	B	228	ASN
1	B	236	GLN
1	B	323	GLN
1	B	328	HIS
1	B	392	ASN
1	B	432	ASN
1	C	2	ASN
1	C	154	ASN
1	C	230	GLN
1	C	231	GLN

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Mol	Chain	Res	Type
1	C	238	ASN
1	C	282	ASN
1	C	415	GLN
1	D	2	ASN
1	D	75	GLN
1	D	84	GLN
1	D	92	GLN
1	D	202	ASN
1	D	226	GLN
1	D	276	ASN
1	D	282	ASN
1	D	323	GLN
1	D	328	HIS
1	E	2	ASN
1	E	95	HIS
1	E	154	ASN
1	E	226	GLN
1	E	231	GLN
1	E	265	GLN
1	E	276	ASN
1	E	328	HIS
1	F	2	ASN
1	F	34	GLN
1	F	226	GLN
1	F	228	ASN
1	F	230	GLN
1	F	256	ASN
1	F	323	GLN
1	F	328	HIS
1	F	336	ASN
1	F	359	ASN

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 6 ligands modelled in this entry, 6 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	420/458 (91%)	-0.37	3 (0%)	89	90	10, 22, 37, 50	0
1	B	420/458 (91%)	-0.38	1 (0%)	95	95	10, 22, 36, 51	0
1	C	420/458 (91%)	-0.28	7 (1%)	73	76	13, 25, 39, 51	0
1	D	420/458 (91%)	-0.07	18 (4%)	39	42	12, 27, 42, 52	0
1	E	420/458 (91%)	-0.27	5 (1%)	81	83	13, 26, 40, 51	0
1	F	420/458 (91%)	-0.09	13 (3%)	52	56	12, 27, 42, 52	0
All	All	2520/2748 (91%)	-0.24	47 (1%)	70	73	10, 25, 40, 52	0

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	201	GLY	8.7
1	F	201	GLY	6.4
1	D	19	ALA	4.8
1	F	19	ALA	4.6
1	F	326	ARG	4.5
1	D	203	ASP	3.8
1	A	210	PRO	3.7
1	F	332	TRP	3.6
1	D	332	TRP	3.4
1	F	203	ASP	3.3
1	C	201	GLY	3.2
1	F	294	VAL	3.1
1	D	210	PRO	3.1
1	D	209	TYR	3.0
1	C	123	GLY	2.9
1	D	326	ARG	2.7
1	D	294	VAL	2.7
1	A	19	ALA	2.6
1	D	2	ASN	2.5

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Mol	Chain	Res	Type	RSRZ
1	F	292	THR	2.5
1	D	340	ALA	2.5
1	C	31	HIS	2.5
1	D	331	VAL	2.5
1	D	292	THR	2.5
1	F	331	VAL	2.4
1	F	209	TYR	2.4
1	C	230	GLN	2.3
1	D	206	PRO	2.3
1	F	4	TRP	2.3
1	E	31	HIS	2.3
1	D	290	PRO	2.3
1	B	203	ASP	2.3
1	F	210	PRO	2.3
1	D	121	LEU	2.2
1	E	19	ALA	2.2
1	C	19	ALA	2.2
1	D	208	ARG	2.2
1	A	201	GLY	2.2
1	E	275	ALA	2.1
1	E	201	GLY	2.1
1	C	210	PRO	2.1
1	E	33	PHE	2.1
1	D	4	TRP	2.1
1	C	268	ALA	2.0
1	F	339	LEU	2.0
1	F	281	VAL	2.0
1	D	301	SER	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 (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	K	F	448	1/1	0.94	0.07	-1.71	51,51,51,51	0
2	K	E	448	1/1	0.98	0.07	-1.73	27,27,27,27	0
2	K	D	448	1/1	0.94	0.06	-1.75	63,63,63,63	0
2	K	B	448	1/1	1.00	0.06	-3.22	24,24,24,24	0
2	K	C	448	1/1	0.99	0.05	-3.65	31,31,31,31	0
2	K	A	448	1/1	1.00	0.04	-8.23	24,24,24,24	0

6.5 Other polymers (i)

There are no such residues in this entry.