Full wwPDB X-ray Structure Validation Report (i)

Oct 23, 2023 – 07:52 PM EDT

PDB ID	:	2ZY4
Title	:	dodecameric L-aspartate beta-decarboxylase
Authors	:	Chen, H.-J.; Ko, T.-P.; Lee, C.-Y.; Wang, N.-C.; Wang, A.H.-J.
Deposited on	:	2009-01-13
Resolution	:	2.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

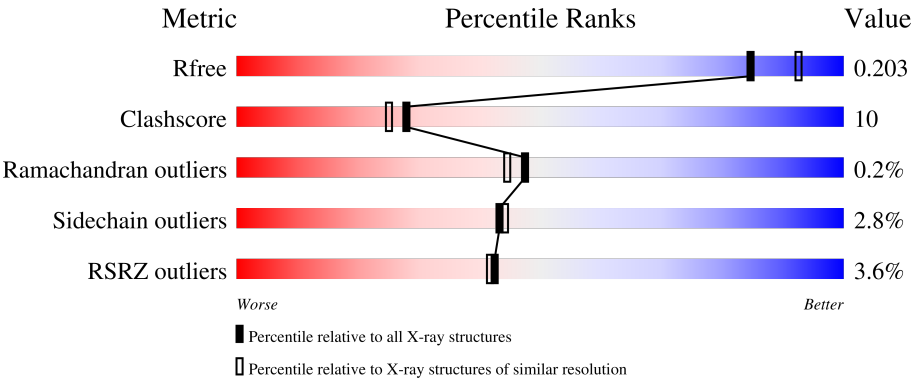
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.00 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}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	546	2% 80% 15% • •
1	B	546	2% 76% 16% • 6%
1	C	546	3% 75% 18% • 6%
1	D	546	3% 79% 15% • 6%
1	E	546	5% 73% 19% • 7%

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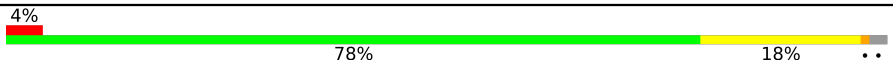
Mol	Chain	Length	Quality of chain
1	F	546	

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 27823 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 L-aspartate beta-decarboxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	524	Total	C	N	O	S	0	0	0
			4131	2630	701	782	18			
1	B	512	Total	C	N	O	S	0	0	0
			4032	2567	687	761	17			
1	C	511	Total	C	N	O	S	0	0	0
			4019	2557	685	760	17			
1	D	515	Total	C	N	O	S	0	0	0
			4046	2573	692	764	17			
1	E	509	Total	C	N	O	S	0	0	0
			4007	2551	683	756	17			
1	F	535	Total	C	N	O	S	0	0	0
			4202	2675	716	794	17			

There are 78 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	534	LYS	-	expression tag	UNP Q93QX0
A	535	LEU	-	expression tag	UNP Q93QX0
A	536	ALA	-	expression tag	UNP Q93QX0
A	537	ALA	-	expression tag	UNP Q93QX0
A	538	ALA	-	expression tag	UNP Q93QX0
A	539	LEU	-	expression tag	UNP Q93QX0
A	540	GLU	-	expression tag	UNP Q93QX0
A	541	HIS	-	expression tag	UNP Q93QX0
A	542	HIS	-	expression tag	UNP Q93QX0
A	543	HIS	-	expression tag	UNP Q93QX0
A	544	HIS	-	expression tag	UNP Q93QX0
A	545	HIS	-	expression tag	UNP Q93QX0
A	546	HIS	-	expression tag	UNP Q93QX0
B	534	LYS	-	expression tag	UNP Q93QX0
B	535	LEU	-	expression tag	UNP Q93QX0
B	536	ALA	-	expression tag	UNP Q93QX0
B	537	ALA	-	expression tag	UNP Q93QX0

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Chain	Residue	Modelled	Actual	Comment	Reference
B	538	ALA	-	expression tag	UNP Q93QX0
B	539	LEU	-	expression tag	UNP Q93QX0
B	540	GLU	-	expression tag	UNP Q93QX0
B	541	HIS	-	expression tag	UNP Q93QX0
B	542	HIS	-	expression tag	UNP Q93QX0
B	543	HIS	-	expression tag	UNP Q93QX0
B	544	HIS	-	expression tag	UNP Q93QX0
B	545	HIS	-	expression tag	UNP Q93QX0
B	546	HIS	-	expression tag	UNP Q93QX0
C	534	LYS	-	expression tag	UNP Q93QX0
C	535	LEU	-	expression tag	UNP Q93QX0
C	536	ALA	-	expression tag	UNP Q93QX0
C	537	ALA	-	expression tag	UNP Q93QX0
C	538	ALA	-	expression tag	UNP Q93QX0
C	539	LEU	-	expression tag	UNP Q93QX0
C	540	GLU	-	expression tag	UNP Q93QX0
C	541	HIS	-	expression tag	UNP Q93QX0
C	542	HIS	-	expression tag	UNP Q93QX0
C	543	HIS	-	expression tag	UNP Q93QX0
C	544	HIS	-	expression tag	UNP Q93QX0
C	545	HIS	-	expression tag	UNP Q93QX0
C	546	HIS	-	expression tag	UNP Q93QX0
D	534	LYS	-	expression tag	UNP Q93QX0
D	535	LEU	-	expression tag	UNP Q93QX0
D	536	ALA	-	expression tag	UNP Q93QX0
D	537	ALA	-	expression tag	UNP Q93QX0
D	538	ALA	-	expression tag	UNP Q93QX0
D	539	LEU	-	expression tag	UNP Q93QX0
D	540	GLU	-	expression tag	UNP Q93QX0
D	541	HIS	-	expression tag	UNP Q93QX0
D	542	HIS	-	expression tag	UNP Q93QX0
D	543	HIS	-	expression tag	UNP Q93QX0
D	544	HIS	-	expression tag	UNP Q93QX0
D	545	HIS	-	expression tag	UNP Q93QX0
D	546	HIS	-	expression tag	UNP Q93QX0
E	534	LYS	-	expression tag	UNP Q93QX0
E	535	LEU	-	expression tag	UNP Q93QX0
E	536	ALA	-	expression tag	UNP Q93QX0
E	537	ALA	-	expression tag	UNP Q93QX0
E	538	ALA	-	expression tag	UNP Q93QX0
E	539	LEU	-	expression tag	UNP Q93QX0
E	540	GLU	-	expression tag	UNP Q93QX0

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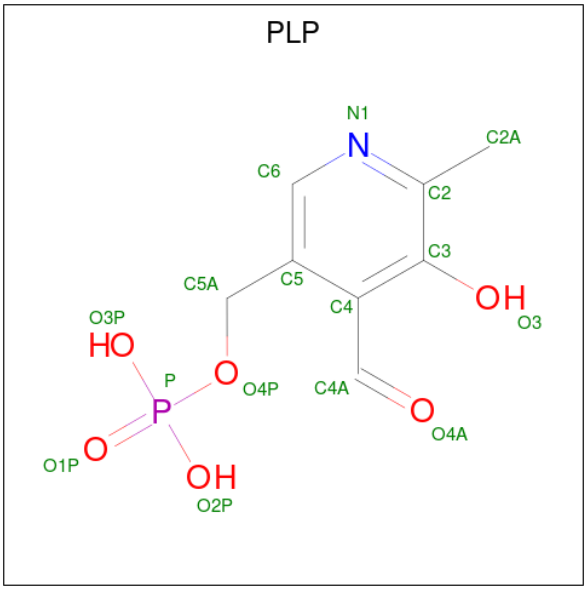
Chain	Residue	Modelled	Actual	Comment	Reference
E	541	HIS	-	expression tag	UNP Q93QX0
E	542	HIS	-	expression tag	UNP Q93QX0
E	543	HIS	-	expression tag	UNP Q93QX0
E	544	HIS	-	expression tag	UNP Q93QX0
E	545	HIS	-	expression tag	UNP Q93QX0
E	546	HIS	-	expression tag	UNP Q93QX0
F	534	LYS	-	expression tag	UNP Q93QX0
F	535	LEU	-	expression tag	UNP Q93QX0
F	536	ALA	-	expression tag	UNP Q93QX0
F	537	ALA	-	expression tag	UNP Q93QX0
F	538	ALA	-	expression tag	UNP Q93QX0
F	539	LEU	-	expression tag	UNP Q93QX0
F	540	GLU	-	expression tag	UNP Q93QX0
F	541	HIS	-	expression tag	UNP Q93QX0
F	542	HIS	-	expression tag	UNP Q93QX0
F	543	HIS	-	expression tag	UNP Q93QX0
F	544	HIS	-	expression tag	UNP Q93QX0
F	545	HIS	-	expression tag	UNP Q93QX0
F	546	HIS	-	expression tag	UNP Q93QX0

- Molecule 2 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: $C_8H_{10}NO_6P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	B	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	D	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	E	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	F	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 4 is water.

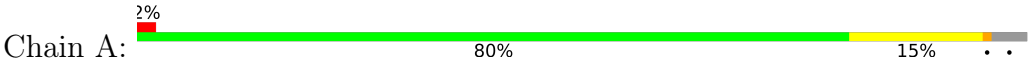
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	565	Total	O	0	0
			565	565		
4	B	611	Total	O	0	0
			611	611		
4	C	593	Total	O	0	0
			593	593		
4	D	573	Total	O	0	0
			573	573		
4	E	462	Total	O	0	0
			462	462		
4	F	486	Total	O	0	0
			486	486		

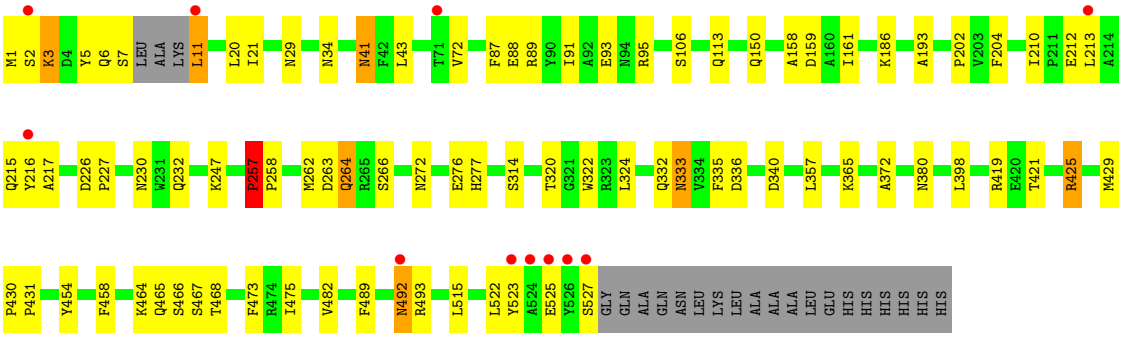
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: L-aspartate beta-decarboxylase

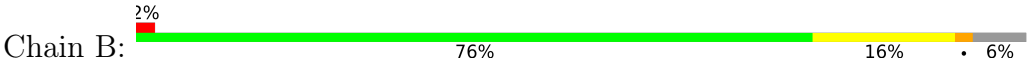
Chain A:

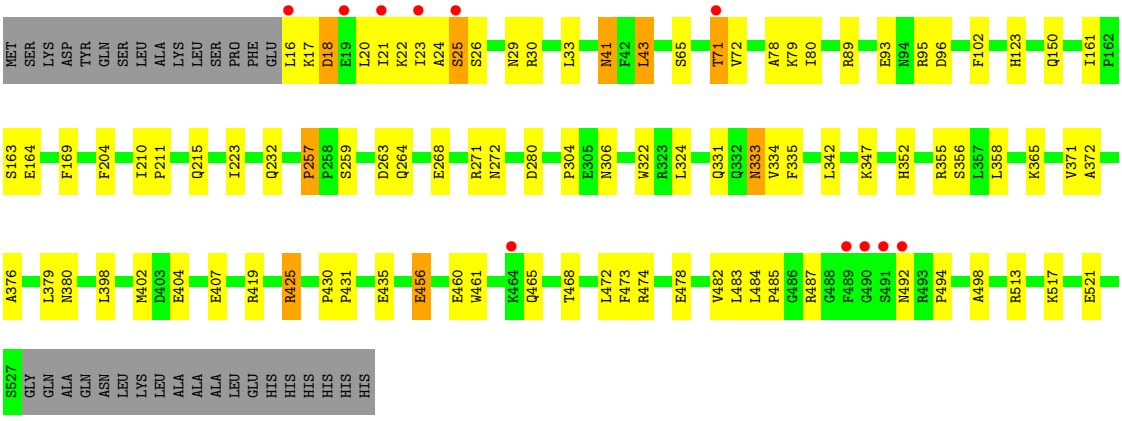




• Molecule 1: L-aspartate beta-decarboxylase

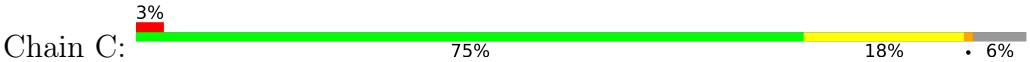
Chain B:

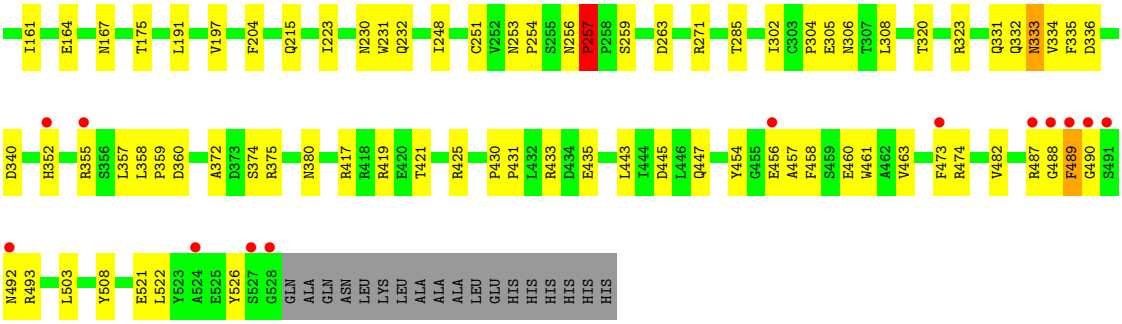




• Molecule 1: L-aspartate beta-decarboxylase

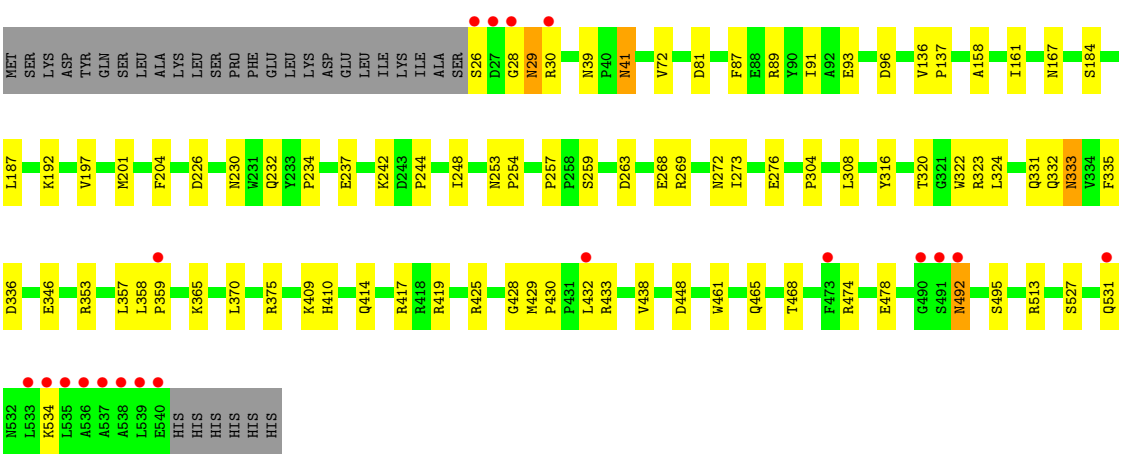
Chain C:





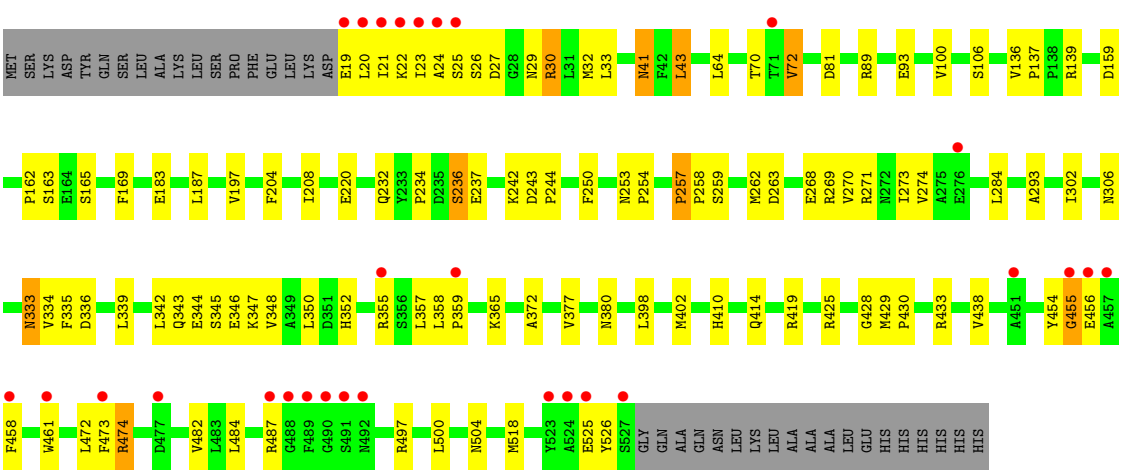
• Molecule 1: L-aspartate beta-decarboxylase

Chain D:



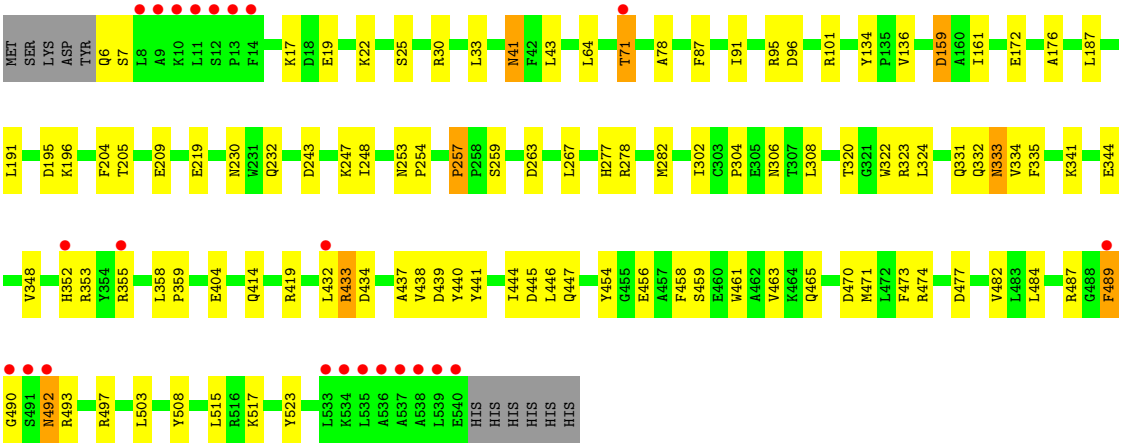
• Molecule 1: L-aspartate beta-decarboxylase

Chain E:



• Molecule 1: L-aspartate beta-decarboxylase

Chain F:


MET SER LYS ASP TYR Q6 S7 L8 A9 K10 L11 S12 P13 F14 K17 D18 E19 K22 S25 R30 L33 N41 F42 L43 L64 T71 A78 F87 I91 R95 D96 R101 Y134 P135 V136 D159 A160 I161 E172 A176 L187
L191 D195 K196 F204 T205 E209 E219 N230 W231 Q232 D243 K247 I248 N253 P254 P257 P258 S259 D263 L267 H277 R278 M282 I302 C303 P304 E305 N306 T307 L308 T320 G321 W322 R323 L324 Q331 Q332 N333 V334 F335 K341 E344
V348 H352 R353 Y354 R355 L358 P359 E404 Q414 R419 L432 R433 D434 A437 V438 D439 Y440 Y441 I444 D445 L446 Q447 Y454 G455 E456 A457 F458 S459 E460 W461 A462 V463 K464 Q465 D470 M471 L472 F473 R474 D477 V482 L483 L484 R487 G488 F489
G490 S491 N492 R493 R497 L503 Y508 L515 R516 K517 Y523 L533 K534 L535 A536 A537 A538 L539 E540 HIS HIS HIS HIS HIS HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	149.95Å 217.15Å 207.15Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.00 29.71 – 2.00	Depositor EDS
% Data completeness (in resolution range)	94.7 (30.00-2.00) 94.8 (29.71-2.00)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.58 (at 2.00Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.157 , 0.204 0.155 , 0.203	Depositor DCC
R_{free} test set	10656 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å^2)	19.3	Xtriage
Anisotropy	0.176	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 65.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	27823	wwPDB-VP
Average B, all atoms (Å^2)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.42% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CL, PLP

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	0.71	0/4215	0.80	2/5705 (0.0%)
1	B	0.72	0/4114	0.80	3/5571 (0.1%)
1	C	0.70	0/4101	0.79	2/5554 (0.0%)
1	D	0.70	0/4128	0.76	1/5591 (0.0%)
1	E	0.68	0/4089	0.78	2/5538 (0.0%)
1	F	0.70	0/4286	0.79	3/5803 (0.1%)
All	All	0.70	0/24933	0.79	13/33762 (0.0%)

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	257	PRO	N-CA-C	7.55	131.73	112.10
1	B	257	PRO	N-CA-C	7.18	130.77	112.10
1	D	257	PRO	N-CA-C	7.16	130.71	112.10
1	F	257	PRO	N-CA-C	6.68	129.48	112.10
1	E	257	PRO	N-CA-C	6.67	129.45	112.10
1	F	64	LEU	CA-CB-CG	6.64	130.56	115.30
1	A	257	PRO	N-CA-C	6.28	128.43	112.10
1	A	425	ARG	NE-CZ-NH2	-5.64	117.48	120.30
1	B	43	LEU	CA-CB-CG	5.61	128.21	115.30
1	C	223	ILE	N-CA-C	-5.57	95.97	111.00
1	F	440	TYR	N-CA-C	-5.46	96.27	111.00
1	E	43	LEU	CA-CB-CG	5.04	126.90	115.30
1	B	223	ILE	N-CA-C	-5.02	97.45	111.00

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	4131	0	4097	77	1
1	B	4032	0	4004	83	0
1	C	4019	0	3983	82	0
1	D	4046	0	4011	71	0
1	E	4007	0	3975	91	0
1	F	4202	0	4181	90	0
2	A	15	0	6	0	0
2	B	15	0	6	0	0
2	C	15	0	7	0	0
2	D	15	0	7	0	0
2	E	15	0	6	0	0
2	F	15	0	7	0	0
3	A	1	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	1	0	0	0	0
3	F	1	0	0	0	0
4	A	565	0	0	17	0
4	B	611	0	0	20	0
4	C	593	0	0	17	1
4	D	573	0	0	19	0
4	E	462	0	0	16	0
4	F	486	0	0	15	1
All	All	27823	0	24290	481	2

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 10.

All (481) 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:A:429:MET:HG3	4:A:2840:HOH:O	1.35	1.26
1:F:332:GLN:HG2	4:F:3116:HOH:O	1.54	1.08
1:E:26:SER:HB3	1:E:29:ASN:HB2	1.41	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:17:LYS:HE3	1:F:487:ARG:HH22	1.27	0.97
1:D:448:ASP:HB2	4:D:1323:HOH:O	1.64	0.94
1:E:359:PRO:HD2	4:E:2955:HOH:O	1.68	0.91
1:D:417:ARG:HH21	1:D:433:ARG:HH21	1.18	0.90
1:D:417:ARG:NH2	1:D:433:ARG:HH21	1.70	0.89
1:A:29:ASN:HD21	1:A:482:VAL:H	1.20	0.87
1:C:306:ASN:ND2	1:C:334:VAL:HG11	1.89	0.87
1:B:333:ASN:HD22	1:B:335:PHE:H	1.23	0.86
1:B:41:ASN:HD21	1:B:419:ARG:HH22	1.23	0.86
1:F:447:GLN:HB3	1:F:493:ARG:HH21	1.41	0.86
1:B:96:ASP:HB3	4:B:2096:HOH:O	1.73	0.85
1:B:264:GLN:O	1:B:268:GLU:HG2	1.76	0.84
1:D:332:GLN:HG2	4:D:2937:HOH:O	1.75	0.83
1:B:24:ALA:HB3	1:B:482:VAL:HG23	1.59	0.83
1:E:64:LEU:HD23	4:E:2811:HOH:O	1.77	0.82
1:C:41:ASN:HD21	1:C:419:ARG:HH22	1.20	0.82
1:E:357:LEU:HD23	4:E:2634:HOH:O	1.79	0.81
1:F:17:LYS:HE3	1:F:487:ARG:NH2	1.94	0.81
1:A:7:SER:C	4:A:1922:HOH:O	2.21	0.79
1:C:490:GLY:HA3	4:C:3235:HOH:O	1.81	0.78
1:B:89:ARG:NH1	1:B:93:GLU:HG3	2.00	0.76
1:F:7:SER:N	4:F:2793:HOH:O	2.18	0.76
1:D:161:ILE:HD11	1:D:304:PRO:HG3	1.68	0.76
1:A:2:SER:H	1:A:34:ASN:ND2	1.83	0.75
1:A:5:TYR:OH	1:A:20:LEU:HD23	1.85	0.75
1:C:232:GLN:HE22	1:C:263:ASP:H	1.33	0.74
1:E:365:LYS:HE3	4:E:1522:HOH:O	1.88	0.74
1:B:435:GLU:HG2	4:B:3214:HOH:O	1.88	0.73
1:F:33:LEU:HD11	1:F:482:VAL:HG11	1.70	0.72
4:A:2061:HOH:O	1:B:71:THR:HB	1.88	0.72
1:E:333:ASN:HD22	1:E:335:PHE:H	1.37	0.72
1:F:446:LEU:HB2	1:F:471:MET:CE	2.20	0.72
1:B:232:GLN:HE22	1:B:263:ASP:H	1.38	0.71
1:D:41:ASN:HD21	1:D:419:ARG:HH22	1.38	0.71
1:F:41:ASN:HD21	1:F:419:ARG:HH22	1.37	0.71
1:B:20:LEU:HB3	1:B:482:VAL:HG11	1.71	0.71
1:E:232:GLN:NE2	1:E:263:ASP:H	1.89	0.71
1:A:333:ASN:HD22	1:A:335:PHE:H	1.39	0.70
1:C:37:ARG:NH2	4:C:2971:HOH:O	2.15	0.70
1:F:490:GLY:HA2	4:F:2952:HOH:O	1.90	0.70
1:C:473:PHE:HD1	4:C:791:HOH:O	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:17:LYS:HE2	4:B:2886:HOH:O	1.91	0.70
1:C:232:GLN:NE2	1:C:263:ASP:H	1.88	0.70
1:D:232:GLN:HE22	1:D:263:ASP:H	1.37	0.70
1:D:357:LEU:HD23	4:D:2261:HOH:O	1.92	0.69
1:E:41:ASN:HD21	1:E:419:ARG:HH22	1.39	0.69
1:A:232:GLN:HE22	1:A:263:ASP:H	1.38	0.69
1:D:492:ASN:HB3	4:D:1370:HOH:O	1.91	0.69
1:E:24:ALA:HB3	1:E:482:VAL:CG2	2.22	0.69
1:A:41:ASN:HD21	1:A:419:ARG:HH22	1.41	0.68
1:A:464:LYS:HG2	4:A:1914:HOH:O	1.93	0.68
1:D:26:SER:HB3	1:D:29:ASN:HB2	1.75	0.68
1:E:89:ARG:NH1	1:E:93:GLU:HG3	2.07	0.68
1:E:433:ARG:HD3	4:E:3024:HOH:O	1.92	0.68
1:B:468:THR:O	1:B:472:LEU:HG	1.94	0.68
1:C:333:ASN:HD22	1:C:335:PHE:H	1.39	0.68
1:C:87:PHE:CE2	1:C:91:ILE:HD11	2.30	0.67
1:B:41:ASN:ND2	1:B:419:ARG:HH22	1.92	0.66
1:A:492:ASN:HD22	1:A:492:ASN:N	1.94	0.66
1:C:430:PRO:HD3	4:C:1175:HOH:O	1.95	0.66
1:A:11:LEU:N	1:A:11:LEU:HD23	2.11	0.66
1:F:433:ARG:HD3	1:F:434:ASP:O	1.95	0.66
1:B:24:ALA:HB3	1:B:482:VAL:CG2	2.25	0.66
1:B:232:GLN:NE2	1:B:263:ASP:H	1.93	0.66
1:B:23:ILE:HD13	1:B:473:PHE:CD1	2.30	0.65
1:A:88:GLU:OE1	4:A:2810:HOH:O	2.13	0.65
1:F:447:GLN:HG3	1:F:459:SER:OG	1.97	0.65
1:E:232:GLN:HE22	1:E:263:ASP:H	1.45	0.65
1:E:456:GLU:H	1:E:456:GLU:CD	2.00	0.65
1:A:272:ASN:ND2	1:A:276:GLU:HG3	2.11	0.65
1:C:23:ILE:HD13	1:C:473:PHE:CE1	2.31	0.65
1:C:435:GLU:HG2	4:C:3182:HOH:O	1.97	0.65
1:B:487:ARG:HD2	4:B:3209:HOH:O	1.95	0.64
1:F:25:SER:OG	1:F:30:ARG:NH2	2.29	0.64
1:A:272:ASN:HD21	1:A:276:GLU:HG3	1.63	0.64
1:E:23:ILE:HG23	4:E:2651:HOH:O	1.97	0.64
1:D:417:ARG:CZ	1:D:433:ARG:HE	2.11	0.64
1:E:25:SER:HB2	1:E:30:ARG:HH21	1.63	0.63
1:F:19:GLU:O	1:F:22:LYS:HB3	1.98	0.63
1:A:475:ILE:HD11	1:A:515:LEU:HD13	1.79	0.63
1:B:425:ARG:HD2	4:B:2205:HOH:O	1.98	0.63
1:B:41:ASN:HD21	1:B:419:ARG:NH2	1.94	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3:LYS:HE2	1:B:356:SER:HB3	1.79	0.63
1:C:443:LEU:HD21	1:C:489:PHE:HZ	1.63	0.63
1:C:447:GLN:HB2	1:C:463:VAL:HG21	1.80	0.63
1:F:446:LEU:HB2	1:F:471:MET:HE3	1.80	0.63
1:D:465:GLN:HG2	4:D:3012:HOH:O	1.99	0.63
1:B:333:ASN:HD22	1:B:335:PHE:N	1.93	0.62
1:C:433:ARG:HG2	1:C:433:ARG:HH11	1.64	0.62
1:D:30:ARG:HG3	1:D:30:ARG:HH11	1.65	0.62
1:B:306:ASN:ND2	1:B:334:VAL:HG11	2.15	0.62
1:E:234:PRO:HG2	1:E:237:GLU:HG2	1.80	0.62
1:D:417:ARG:NH2	1:D:433:ARG:NH2	2.46	0.61
1:E:344:GLU:O	1:E:348:VAL:HG23	2.00	0.61
1:A:11:LEU:N	4:A:1924:HOH:O	2.32	0.61
1:D:89:ARG:O	1:D:93:GLU:HG2	2.01	0.61
1:D:232:GLN:NE2	1:D:263:ASP:H	1.98	0.61
1:C:333:ASN:HD22	1:C:335:PHE:N	1.97	0.61
1:E:81:ASP:HB3	4:E:2541:HOH:O	1.99	0.61
1:D:417:ARG:NH2	1:D:433:ARG:HE	1.97	0.61
1:B:89:ARG:O	1:B:93:GLU:HG2	2.01	0.61
1:F:257:PRO:HB2	1:F:497:ARG:HD2	1.82	0.61
1:A:106:SER:HB2	1:A:398:LEU:HD13	1.83	0.61
1:C:305:GLU:HG2	1:C:332:GLN:O	2.01	0.60
1:E:343:GLN:HB2	1:E:346:GLU:HG3	1.83	0.60
1:B:16:LEU:CA	4:B:3287:HOH:O	2.48	0.60
1:F:71:THR:HA	4:F:2778:HOH:O	2.01	0.60
1:B:18:ASP:O	1:B:22:LYS:HG2	2.01	0.60
1:F:433:ARG:HG2	1:F:437:ALA:CB	2.32	0.60
1:C:421:THR:O	1:C:425:ARG:HG3	2.02	0.59
1:C:35:ALA:HB1	1:C:37:ARG:HH11	1.67	0.59
1:D:333:ASN:HD22	1:D:335:PHE:H	1.50	0.59
1:D:474:ARG:O	1:D:478:GLU:HG3	2.02	0.59
1:B:372:ALA:HA	1:B:380:ASN:HD22	1.66	0.59
1:C:25:SER:OG	1:C:30:ARG:NH2	2.35	0.59
1:F:333:ASN:HD22	1:F:335:PHE:H	1.51	0.59
1:A:232:GLN:NE2	1:A:263:ASP:H	1.99	0.59
1:E:487:ARG:NE	4:E:3271:HOH:O	2.34	0.59
1:A:89:ARG:NH1	1:A:93:GLU:HG3	2.17	0.59
1:C:340:ASP:OD1	4:C:2983:HOH:O	2.17	0.59
1:D:28:GLY:HA2	4:D:2319:HOH:O	2.01	0.59
1:A:158:ALA:HB1	1:A:161:ILE:HD12	1.85	0.58
1:B:306:ASN:HA	1:B:334:VAL:HG22	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:365:LYS:NZ	4:D:1342:HOH:O	2.25	0.58
1:A:492:ASN:N	1:A:492:ASN:ND2	2.50	0.58
1:C:41:ASN:ND2	1:C:419:ARG:HH22	1.98	0.58
1:A:333:ASN:HD22	1:A:335:PHE:N	2.01	0.58
1:F:433:ARG:HG2	1:F:437:ALA:HB3	1.86	0.58
1:A:2:SER:HA	1:A:34:ASN:HD22	1.69	0.57
1:B:483:LEU:HD22	1:B:498:ALA:HB2	1.85	0.57
1:F:341:LYS:NZ	4:F:3114:HOH:O	2.38	0.57
1:F:232:GLN:HE22	1:F:263:ASP:H	1.50	0.57
1:D:425:ARG:NH1	1:F:159:ASP:O	2.38	0.57
1:A:333:ASN:ND2	1:A:336:ASP:H	2.03	0.57
1:B:474:ARG:O	1:B:478:GLU:HG3	2.04	0.57
1:E:81:ASP:CB	4:E:2541:HOH:O	2.51	0.57
1:A:340:ASP:OD1	4:A:2035:HOH:O	2.17	0.57
1:A:6:GLN:HA	1:A:6:GLN:NE2	2.20	0.56
1:B:268:GLU:OE1	1:B:271:ARG:NH1	2.39	0.56
1:A:2:SER:CB	1:A:21:ILE:HD13	2.36	0.56
1:B:271:ARG:NH1	4:B:604:HOH:O	2.27	0.56
1:B:16:LEU:N	4:B:3287:HOH:O	2.37	0.56
1:D:425:ARG:CZ	1:F:159:ASP:O	2.54	0.56
1:E:19:GLU:HA	1:E:22:LYS:NZ	2.21	0.56
1:E:333:ASN:HD22	1:E:335:PHE:N	2.03	0.56
1:A:150:GLN:HE22	1:E:425:ARG:HH22	1.53	0.56
1:B:25:SER:OG	1:B:30:ARG:NH1	2.39	0.56
1:F:445:ASP:OD2	1:F:493:ARG:NH2	2.39	0.56
1:E:41:ASN:ND2	1:E:419:ARG:HH22	2.04	0.56
1:A:3:LYS:HE2	1:B:356:SER:CB	2.36	0.55
1:E:271:ARG:HB2	1:E:302:ILE:CG2	2.36	0.55
1:F:195:ASP:CG	1:F:247:LYS:HD3	2.27	0.55
1:B:20:LEU:HB3	1:B:482:VAL:CG1	2.36	0.55
1:C:167:ASN:HD21	1:C:331:GLN:HE21	1.53	0.55
1:F:33:LEU:CD1	1:F:482:VAL:HG11	2.34	0.55
1:B:365:LYS:NZ	4:B:572:HOH:O	2.39	0.55
1:C:41:ASN:HD21	1:C:419:ARG:NH2	1.97	0.55
1:C:33:LEU:HD11	1:C:482:VAL:HG11	1.88	0.55
1:E:70:THR:OG1	1:E:72:VAL:HG23	2.05	0.55
1:D:527:SER:O	1:D:531:GLN:HG3	2.07	0.55
1:B:358:LEU:N	1:B:358:LEU:HD23	2.22	0.54
1:F:187:LEU:HD13	1:F:353:ARG:NH2	2.23	0.54
1:B:333:ASN:ND2	1:B:335:PHE:H	1.98	0.54
1:D:461:TRP:CH2	1:D:465:GLN:HG3	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:474:ARG:HH21	1:F:517:LYS:HE3	1.71	0.54
1:B:65:SER:OG	1:B:79:LYS:HE2	2.07	0.54
1:A:159:ASP:O	1:E:425:ARG:HG2	2.08	0.54
1:A:322:TRP:HB3	1:A:324:LEU:HG	1.90	0.54
1:E:343:GLN:O	1:E:346:GLU:N	2.40	0.54
1:F:454:TYR:HB2	1:F:458:PHE:CD2	2.43	0.54
1:F:333:ASN:HD22	1:F:335:PHE:N	2.06	0.54
1:F:446:LEU:HB2	1:F:471:MET:HE1	1.90	0.54
1:A:193:ALA:HA	1:A:217:ALA:HB3	1.89	0.53
1:D:41:ASN:ND2	1:D:419:ARG:HH22	2.06	0.53
1:F:358:LEU:HD23	1:F:358:LEU:N	2.23	0.53
1:D:89:ARG:NH1	1:D:93:GLU:HG3	2.23	0.53
1:E:497:ARG:HD2	4:E:3256:HOH:O	2.07	0.53
1:B:95:ARG:NH2	4:B:2815:HOH:O	2.39	0.53
1:F:344:GLU:O	1:F:348:VAL:HG23	2.07	0.53
1:F:306:ASN:ND2	1:F:334:VAL:HG11	2.23	0.53
1:A:89:ARG:O	1:A:93:GLU:HG2	2.09	0.53
1:A:41:ASN:ND2	1:A:419:ARG:HH22	2.05	0.53
1:D:417:ARG:HH21	1:D:433:ARG:NH2	1.98	0.53
1:E:41:ASN:HD21	1:E:419:ARG:NH2	2.06	0.53
1:F:96:ASP:HB2	4:F:969:HOH:O	2.08	0.53
1:E:461:TRP:HH2	1:E:525:GLU:HG3	1.74	0.53
1:F:41:ASN:ND2	1:F:419:ARG:HH22	2.05	0.52
1:F:447:GLN:OE1	1:F:463:VAL:HG21	2.09	0.52
1:A:6:GLN:HA	1:A:6:GLN:HE21	1.74	0.52
1:B:487:ARG:NH1	4:B:2086:HOH:O	2.42	0.52
1:F:159:ASP:CG	4:F:3108:HOH:O	2.47	0.52
1:E:474:ARG:HG3	1:E:518:MET:CE	2.40	0.52
1:D:333:ASN:HD22	1:D:335:PHE:N	2.08	0.52
1:A:365:LYS:HE3	4:A:3167:HOH:O	2.08	0.52
1:C:445:ASP:OD1	1:C:493:ARG:NH2	2.43	0.52
1:D:41:ASN:HD21	1:D:419:ARG:NH2	2.08	0.52
1:A:41:ASN:HD21	1:A:419:ARG:NH2	2.06	0.51
1:D:268:GLU:HG2	4:D:1337:HOH:O	2.10	0.51
1:C:490:GLY:HA2	4:C:1092:HOH:O	2.09	0.51
1:F:254:PRO:HB3	1:F:438:VAL:HG21	1.93	0.51
1:C:503:LEU:HB2	1:C:508:TYR:CZ	2.46	0.51
1:C:473:PHE:C	1:C:473:PHE:CD2	2.84	0.51
1:B:331:GLN:NE2	4:B:578:HOH:O	2.34	0.51
1:D:333:ASN:ND2	1:D:336:ASP:H	2.09	0.50
1:F:322:TRP:HB3	1:F:324:LEU:HG	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:429:MET:CG	4:A:2840:HOH:O	2.19	0.50
1:C:161:ILE:HD13	1:C:304:PRO:HB3	1.93	0.50
1:C:461:TRP:CZ3	1:C:526:TYR:HB2	2.46	0.50
1:C:21:ILE:HG13	1:C:33:LEU:HD12	1.94	0.50
1:E:89:ARG:O	1:E:93:GLU:HG2	2.12	0.50
1:D:158:ALA:HB1	1:D:161:ILE:HD12	1.92	0.50
1:D:425:ARG:NE	1:F:159:ASP:O	2.45	0.50
1:A:11:LEU:N	1:A:11:LEU:CD2	2.75	0.50
1:C:333:ASN:ND2	1:C:336:ASP:H	2.10	0.50
1:A:186:LYS:HD2	1:A:216:TYR:CD2	2.47	0.50
1:B:513:ARG:NH1	4:B:2931:HOH:O	2.44	0.50
1:C:358:LEU:HB2	1:C:359:PRO:HD2	1.93	0.50
1:D:167:ASN:HD21	1:D:331:GLN:HE21	1.60	0.49
1:E:306:ASN:ND2	1:E:334:VAL:HG11	2.27	0.49
1:F:78:ALA:HB1	4:F:2674:HOH:O	2.12	0.49
1:F:161:ILE:CD1	1:F:304:PRO:HB3	2.42	0.49
1:C:487:ARG:HD2	4:C:2039:HOH:O	2.11	0.49
1:D:320:THR:O	1:D:323:ARG:HD2	2.12	0.49
1:B:26:SER:OG	1:B:29:ASN:HB2	2.12	0.49
1:F:41:ASN:HD21	1:F:419:ARG:NH2	2.08	0.49
1:C:95:ARG:NH1	4:C:967:HOH:O	2.44	0.49
1:C:89:ARG:HD2	4:F:899:HOH:O	2.13	0.49
1:B:484:LEU:HD22	1:B:487:ARG:HH22	1.77	0.49
1:C:89:ARG:O	1:C:93:GLU:HG2	2.13	0.48
1:E:106:SER:HB2	1:E:398:LEU:HD13	1.95	0.48
1:E:269:ARG:O	1:E:273:ILE:HG13	2.12	0.48
1:E:474:ARG:HG3	1:E:474:ARG:NH1	2.27	0.48
1:E:236:SER:HB2	4:E:3099:HOH:O	2.12	0.48
1:F:253:ASN:HA	1:F:254:PRO:C	2.33	0.48
1:A:458:PHE:CE1	1:A:523:TYR:HA	2.49	0.48
1:B:33:LEU:HD11	1:B:482:VAL:HG11	1.95	0.48
1:C:161:ILE:CD1	1:C:304:PRO:HB3	2.43	0.48
1:B:517:LYS:O	1:B:521:GLU:HG3	2.14	0.48
1:D:304:PRO:HD2	4:D:2498:HOH:O	2.14	0.48
1:F:358:LEU:HB2	1:F:359:PRO:HD2	1.96	0.48
1:D:429:MET:HG2	4:D:2514:HOH:O	2.14	0.48
1:D:433:ARG:HD2	4:D:3034:HOH:O	2.13	0.48
1:E:352:HIS:CE1	1:E:355:ARG:HH12	2.32	0.48
1:E:474:ARG:HG3	1:E:474:ARG:HH11	1.78	0.48
1:B:483:LEU:CD2	1:B:498:ALA:HB2	2.43	0.47
1:C:334:VAL:HG12	4:C:2359:HOH:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:32:MET:O	1:E:484:LEU:HD21	2.14	0.47
1:F:232:GLN:NE2	1:F:263:ASP:H	2.10	0.47
1:B:322:TRP:HB3	1:B:324:LEU:HG	1.95	0.47
1:E:461:TRP:CH2	1:E:525:GLU:HG3	2.49	0.47
1:F:332:GLN:HA	1:F:332:GLN:NE2	2.28	0.47
1:F:447:GLN:HB2	1:F:463:VAL:CG2	2.44	0.47
1:C:253:ASN:HA	1:C:254:PRO:C	2.35	0.47
1:E:20:LEU:HB3	1:E:482:VAL:HG11	1.95	0.47
1:A:2:SER:OG	1:A:21:ILE:CG2	2.62	0.47
1:D:30:ARG:HG3	1:D:30:ARG:NH1	2.28	0.47
1:E:208:ILE:O	1:E:220:GLU:OE2	2.33	0.47
1:C:87:PHE:HZ	1:C:103:LEU:HB3	1.80	0.47
1:D:136:VAL:HA	1:D:137:PRO:C	2.34	0.47
1:F:489:PHE:CE2	1:F:493:ARG:HD3	2.50	0.47
1:C:474:ARG:HH22	1:C:521:GLU:CD	2.18	0.47
1:D:96:ASP:HB3	4:D:1231:HOH:O	2.14	0.47
1:D:254:PRO:HB3	1:D:438:VAL:HG21	1.95	0.47
1:F:247:LYS:HG3	4:F:2700:HOH:O	2.15	0.47
1:A:468:THR:HB	1:A:489:PHE:HA	1.97	0.47
1:E:242:LYS:O	1:E:244:PRO:HD3	2.15	0.47
1:E:100:VAL:HG12	4:E:2547:HOH:O	2.16	0.47
1:F:243:ASP:OD1	1:F:243:ASP:C	2.54	0.47
1:A:430:PRO:HA	1:A:431:PRO:HD3	1.79	0.46
1:C:430:PRO:HA	1:C:431:PRO:HD3	1.76	0.46
1:F:444:ILE:HG21	1:F:515:LEU:CD1	2.44	0.46
1:C:489:PHE:CD2	1:C:493:ARG:HD3	2.50	0.46
1:A:2:SER:HB2	1:A:21:ILE:HD13	1.97	0.46
1:B:280:ASP:HB3	4:B:676:HOH:O	2.14	0.46
1:C:271:ARG:HB2	1:C:302:ILE:CG2	2.46	0.46
1:B:71:THR:O	1:B:71:THR:HG23	2.15	0.46
1:E:472:LEU:HD23	1:E:472:LEU:N	2.31	0.46
1:E:525:GLU:O	1:E:526:TYR:C	2.54	0.46
1:B:150:GLN:NE2	1:B:163:SER:OG	2.49	0.46
1:B:164:GLU:CD	1:B:164:GLU:H	2.18	0.46
1:E:27:ASP:HA	1:E:30:ARG:NH1	2.31	0.46
1:E:293:ALA:HB2	1:E:438:VAL:HG22	1.97	0.46
1:C:357:LEU:HD11	1:C:372:ALA:HB2	1.96	0.46
1:D:359:PRO:HG2	4:D:797:HOH:O	2.15	0.46
1:F:196:LYS:HE2	1:F:219:GLU:OE2	2.16	0.46
1:A:210:ILE:HD11	1:B:379:LEU:HD11	1.97	0.46
1:A:454:TYR:HB2	1:A:458:PHE:CD2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:175:THR:HG22	1:D:375:ARG:HD2	1.98	0.46
1:E:136:VAL:HA	1:E:137:PRO:C	2.36	0.46
1:A:202:PRO:HG2	1:A:258:PRO:CG	2.46	0.46
1:E:253:ASN:HA	1:E:254:PRO:C	2.35	0.46
1:A:113:GLN:HE22	1:E:504:ASN:ND2	2.13	0.45
1:B:398:LEU:O	1:B:402:MET:HG3	2.16	0.45
1:D:414:GLN:HG2	4:D:2509:HOH:O	2.15	0.45
1:A:262:MET:HE3	1:A:266:SER:HB3	1.98	0.45
1:B:23:ILE:HD13	1:B:473:PHE:CE1	2.51	0.45
1:B:352:HIS:O	1:B:355:ARG:HG2	2.15	0.45
1:D:333:ASN:ND2	1:D:335:PHE:HB2	2.32	0.45
1:E:21:ILE:HG12	1:E:33:LEU:CD1	2.47	0.45
1:E:234:PRO:HG2	1:E:237:GLU:CG	2.45	0.45
1:A:276:GLU:HB2	1:A:277:HIS:HD2	1.82	0.45
1:C:72:VAL:HG12	1:C:74:VAL:HG23	1.98	0.45
1:D:461:TRP:CZ2	1:D:465:GLN:HG3	2.51	0.45
1:A:87:PHE:O	1:A:91:ILE:HG12	2.17	0.45
1:C:215:GLN:NE2	4:C:2354:HOH:O	2.47	0.45
1:B:23:ILE:HD13	1:B:473:PHE:HD1	1.77	0.45
1:B:24:ALA:CB	1:B:482:VAL:HG23	2.38	0.45
1:C:23:ILE:HD13	1:C:473:PHE:HE1	1.80	0.45
1:B:468:THR:OG1	1:B:494:PRO:HA	2.17	0.45
1:C:355:ARG:HE	1:C:355:ARG:HB2	1.63	0.45
1:D:432:LEU:HD23	4:D:3244:HOH:O	2.17	0.45
1:C:443:LEU:HD21	1:C:489:PHE:CZ	2.48	0.45
1:D:253:ASN:HA	1:D:254:PRO:C	2.37	0.45
1:E:345:SER:HB2	4:E:2629:HOH:O	2.16	0.45
1:E:454:TYR:HB2	1:E:458:PHE:CD2	2.52	0.45
1:F:458:PHE:CE1	1:F:523:TYR:HA	2.52	0.45
1:A:421:THR:O	1:A:425:ARG:HG3	2.17	0.44
1:F:461:TRP:O	1:F:465:GLN:HG2	2.17	0.44
1:A:213:LEU:HD11	1:B:376:ALA:O	2.17	0.44
1:C:352:HIS:O	1:C:355:ARG:HG2	2.16	0.44
1:C:357:LEU:HD21	1:C:380:ASN:CB	2.47	0.44
1:E:183:GLU:HG3	1:E:187:LEU:HD11	1.98	0.44
1:F:33:LEU:HD11	1:F:482:VAL:CG1	2.44	0.44
1:F:95:ARG:O	1:F:101:ARG:HD3	2.17	0.44
4:A:2061:HOH:O	1:B:71:THR:CB	2.57	0.44
1:D:316:TYR:OH	1:D:409:LYS:HB2	2.17	0.44
1:D:358:LEU:N	1:D:358:LEU:HD23	2.32	0.44
1:A:226:ASP:HA	1:A:227:PRO:HD3	1.84	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:320:THR:O	1:C:323:ARG:HD2	2.18	0.44
1:C:334:VAL:CG1	4:C:2359:HOH:O	2.65	0.44
1:E:19:GLU:HA	1:E:22:LYS:HZ3	1.81	0.44
1:D:197:VAL:HG23	1:D:248:ILE:HG23	1.99	0.44
1:E:474:ARG:HG3	1:E:518:MET:HE3	2.00	0.44
1:A:522:LEU:HD23	1:A:522:LEU:HA	1.87	0.44
1:B:215:GLN:HB2	4:B:2123:HOH:O	2.18	0.44
1:E:243:ASP:HA	1:E:244:PRO:HD2	1.86	0.44
1:A:464:LYS:HE3	4:A:1914:HOH:O	2.16	0.43
1:B:161:ILE:HD11	1:B:304:PRO:HB3	2.00	0.43
1:E:454:TYR:O	1:E:458:PHE:HB3	2.17	0.43
1:F:95:ARG:HA	4:F:2290:HOH:O	2.18	0.43
1:B:232:GLN:HE22	1:B:263:ASP:N	2.12	0.43
1:D:184:SER:CB	1:D:370:LEU:HD23	2.48	0.43
1:E:257:PRO:HG2	1:E:258:PRO:HD3	2.00	0.43
1:B:342:LEU:O	1:B:347:LYS:HE3	2.18	0.43
1:E:254:PRO:HB3	1:E:438:VAL:HG21	1.99	0.43
1:F:267:LEU:HB3	1:F:302:ILE:HG13	2.00	0.43
1:F:484:LEU:HB2	1:F:497:ARG:HB2	2.00	0.43
1:C:256:ASN:HA	1:C:257:PRO:HA	1.90	0.43
1:C:374:SER:O	1:C:375:ARG:HD3	2.18	0.43
1:A:340:ASP:CG	4:A:735:HOH:O	2.57	0.43
1:F:473:PHE:O	1:F:477:ASP:HB2	2.18	0.43
1:D:322:TRP:HB3	1:D:324:LEU:HG	2.01	0.43
1:B:102:PHE:CE1	1:B:402:MET:CE	3.01	0.43
1:F:439:ASP:HA	1:F:441:TYR:O	2.18	0.43
1:A:264:GLN:HE21	1:A:264:GLN:HB2	1.56	0.43
1:C:41:ASN:C	1:C:41:ASN:HD22	2.21	0.43
1:F:444:ILE:HG21	1:F:515:LEU:HD13	2.00	0.43
1:B:210:ILE:HB	1:B:211:PRO:HD3	2.01	0.43
1:C:191:LEU:HD23	1:C:191:LEU:HA	1.76	0.43
1:C:358:LEU:N	1:C:358:LEU:HD23	2.34	0.43
1:E:23:ILE:HD13	1:E:473:PHE:CD1	2.54	0.43
1:E:429:MET:CE	4:E:564:HOH:O	2.67	0.43
1:F:432:LEU:HA	1:F:432:LEU:HD12	1.80	0.43
1:B:407:GLU:HG2	4:B:732:HOH:O	2.18	0.43
1:C:231:TRP:CZ3	1:C:488:GLY:HA3	2.54	0.43
1:E:25:SER:HB2	1:E:30:ARG:NH2	2.33	0.43
1:F:503:LEU:HB2	1:F:508:TYR:CZ	2.53	0.43
1:A:43:LEU:C	1:A:43:LEU:HD12	2.40	0.42
1:B:272:ASN:ND2	4:B:666:HOH:O	2.47	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:920:HOH:O	1:F:404:GLU:HB3	2.19	0.42
1:D:226:ASP:HB2	1:D:234:PRO:HG3	2.01	0.42
1:D:234:PRO:HD2	1:D:237:GLU:HB2	2.01	0.42
1:D:468:THR:HG23	1:D:495:SER:O	2.18	0.42
1:A:525:GLU:C	1:A:527:SER:H	2.21	0.42
1:E:139:ARG:HG3	1:E:169:PHE:HA	2.01	0.42
1:F:161:ILE:HD13	1:F:304:PRO:HB3	2.00	0.42
1:F:333:ASN:HD22	1:F:333:ASN:C	2.23	0.42
1:C:72:VAL:HG12	1:C:74:VAL:CG2	2.49	0.42
1:F:6:GLN:HA	4:F:2793:HOH:O	2.18	0.42
1:F:25:SER:CB	1:F:30:ARG:HH21	2.30	0.42
1:A:247:LYS:HA	1:A:247:LYS:HD3	1.70	0.42
1:A:276:GLU:HB2	1:A:277:HIS:CD2	2.55	0.42
1:E:352:HIS:CE1	1:E:355:ARG:NH1	2.87	0.42
1:A:357:LEU:HD23	4:A:816:HOH:O	2.19	0.42
1:C:522:LEU:HD23	1:C:522:LEU:HA	1.88	0.42
1:E:243:ASP:C	1:E:243:ASP:OD1	2.56	0.42
1:C:84:GLU:O	1:C:88:GLU:HG3	2.20	0.42
1:D:308:LEU:HD23	1:D:308:LEU:HA	1.92	0.42
1:D:430:PRO:HD3	4:D:2513:HOH:O	2.20	0.42
1:E:398:LEU:HB3	1:E:402:MET:HE2	2.02	0.42
1:F:41:ASN:C	1:F:41:ASN:HD22	2.22	0.42
1:B:169:PHE:CD1	1:B:371:VAL:HG22	2.55	0.42
1:B:474:ARG:HH22	1:B:521:GLU:CD	2.23	0.42
1:C:24:ALA:HB3	1:C:482:VAL:HG23	2.01	0.42
1:C:417:ARG:HA	1:C:417:ARG:HD3	1.81	0.42
1:D:242:LYS:O	1:D:244:PRO:HD3	2.20	0.42
1:D:448:ASP:CB	4:D:1323:HOH:O	2.44	0.42
1:E:162:PRO:HG2	1:E:165:SER:OG	2.20	0.42
1:E:352:HIS:CD2	1:E:355:ARG:NH1	2.88	0.42
1:A:257:PRO:CD	1:A:258:PRO:HD3	2.50	0.42
1:E:23:ILE:CG2	4:E:2651:HOH:O	2.63	0.42
1:F:87:PHE:O	1:F:91:ILE:HG12	2.20	0.42
1:F:461:TRP:CH2	1:F:465:GLN:HG3	2.54	0.42
1:A:493:ARG:HB3	4:A:1910:HOH:O	2.19	0.42
1:B:80:ILE:HG13	1:B:123:HIS:HB2	2.01	0.42
1:B:456:GLU:O	1:B:460:GLU:HG3	2.19	0.42
1:C:308:LEU:HD23	1:C:308:LEU:HA	1.97	0.42
1:C:456:GLU:O	1:C:460:GLU:HG3	2.20	0.42
1:D:425:ARG:NH1	1:F:161:ILE:O	2.49	0.42
1:E:20:LEU:O	1:E:23:ILE:HB	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:205:THR:O	1:F:209:GLU:HG3	2.19	0.42
1:F:308:LEU:HD23	1:F:308:LEU:HA	1.92	0.42
1:A:492:ASN:ND2	4:A:2794:HOH:O	2.53	0.41
1:B:404:GLU:HG3	1:F:414:GLN:HG2	2.02	0.41
1:B:21:ILE:HD11	4:B:2058:HOH:O	2.20	0.41
1:B:215:GLN:CB	4:B:2123:HOH:O	2.69	0.41
1:D:187:LEU:HD13	1:D:353:ARG:NH2	2.35	0.41
1:D:410:HIS:HD2	4:D:2733:HOH:O	2.03	0.41
1:A:230:ASN:CG	4:A:1872:HOH:O	2.58	0.41
1:E:220:GLU:HG3	4:E:3092:HOH:O	2.20	0.41
1:E:358:LEU:HB2	1:E:359:PRO:CD	2.51	0.41
1:E:429:MET:HB3	1:E:430:PRO:HD2	2.03	0.41
1:C:251:CYS:O	1:C:285:THR:HA	2.20	0.41
1:D:269:ARG:O	1:D:273:ILE:HG13	2.20	0.41
1:D:428:GLY:O	1:D:429:MET:HB2	2.21	0.41
1:F:134:TYR:O	1:F:136:VAL:HG23	2.20	0.41
1:B:78:ALA:HB1	4:B:2100:HOH:O	2.20	0.41
1:C:64:LEU:HD11	4:F:873:HOH:O	2.20	0.41
1:C:454:TYR:HB2	1:C:458:PHE:CD2	2.56	0.41
1:C:457:ALA:HB3	4:C:1194:HOH:O	2.19	0.41
1:E:500:LEU:HD23	1:E:500:LEU:HA	1.92	0.41
1:A:95:ARG:HA	4:A:1985:HOH:O	2.21	0.41
1:C:164:GLU:CG	4:C:1035:HOH:O	2.67	0.41
1:E:372:ALA:HA	1:E:380:ASN:HD22	1.85	0.41
1:E:454:TYR:O	1:E:455:GLY:O	2.39	0.41
1:A:466:SER:HB3	1:A:467:SER:H	1.71	0.41
1:E:270:VAL:O	1:E:274:VAL:HG23	2.21	0.41
1:B:461:TRP:CH2	1:B:465:GLN:HG3	2.56	0.41
1:D:81:ASP:HB2	4:D:849:HOH:O	2.20	0.41
1:E:21:ILE:HG12	1:E:33:LEU:HD12	2.03	0.41
1:E:350:LEU:HA	1:E:350:LEU:HD23	1.78	0.41
1:A:212:GLU:OE2	1:A:212:GLU:HA	2.21	0.41
1:B:306:ASN:HA	1:B:334:VAL:CG2	2.50	0.41
1:C:18:ASP:N	4:C:3289:HOH:O	2.52	0.41
1:C:359:PRO:HG2	1:C:360:ASP:H	1.85	0.41
1:D:192:LYS:NZ	1:D:346:GLU:OE1	2.53	0.41
1:F:172:GLU:HB2	1:F:176:ALA:HB2	2.03	0.41
1:F:191:LEU:HD23	1:F:191:LEU:HA	1.95	0.41
1:F:248:ILE:HA	1:F:282:MET:O	2.20	0.41
1:F:333:ASN:ND2	1:F:335:PHE:H	2.16	0.41
1:B:355:ARG:HG3	1:B:356:SER:N	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:35:ALA:HB1	1:C:37:ARG:NH1	2.33	0.41
1:E:342:LEU:O	1:E:347:LYS:HE3	2.20	0.41
1:E:410:HIS:O	1:E:414:GLN:HG3	2.21	0.41
1:F:358:LEU:N	1:F:358:LEU:CD2	2.84	0.41
1:A:464:LYS:HA	1:A:464:LYS:HD3	1.78	0.40
1:D:272:ASN:O	1:D:276:GLU:HG2	2.21	0.40
1:F:6:GLN:NE2	4:F:2766:HOH:O	2.53	0.40
1:A:314:SER:HB3	1:A:320:THR:HG22	2.03	0.40
1:B:430:PRO:HA	1:B:431:PRO:HD3	1.98	0.40
1:C:95:ARG:HA	1:C:95:ARG:HD2	1.96	0.40
1:E:232:GLN:HE22	1:E:262:MET:HA	1.87	0.40
1:E:250:PHE:CD1	1:E:284:LEU:HD23	2.56	0.40
1:F:461:TRP:CZ2	1:F:465:GLN:HG3	2.56	0.40
1:A:41:ASN:HD21	1:A:419:ARG:HH12	1.68	0.40
1:A:372:ALA:HA	1:A:380:ASN:HD22	1.86	0.40
1:C:197:VAL:HG23	1:C:248:ILE:HG23	2.02	0.40
1:D:87:PHE:O	1:D:91:ILE:HG12	2.21	0.40
1:E:428:GLY:O	1:E:429:MET:HB2	2.21	0.40
1:C:19:GLU:HG3	4:C:791:HOH:O	2.22	0.40
1:C:357:LEU:HD11	1:C:372:ALA:CB	2.52	0.40
1:F:320:THR:O	1:F:323:ARG:HD2	2.22	0.40
1:F:352:HIS:O	1:F:355:ARG:HG2	2.22	0.40
1:A:20:LEU:HD11	1:A:473:PHE:HA	2.04	0.40
1:B:472:LEU:HD11	1:B:485:PRO:HA	2.03	0.40
1:E:336:ASP:HA	1:E:339:LEU:HD12	2.03	0.40
1:F:277:HIS:O	1:F:278:ARG:HD2	2.21	0.40
1:F:456:GLU:OE1	4:F:3261:HOH:O	2.22	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:1730:HOH:O	4:F:1730:HOH:O[4_566]	2.09	0.11
1:A:425:ARG:NH2	4:C:1033:HOH:O[4_566]	2.15	0.05

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	520/546 (95%)	509 (98%)	11 (2%)	0	100	100
1	B	510/546 (93%)	500 (98%)	9 (2%)	1 (0%)	47	44
1	C	509/546 (93%)	493 (97%)	15 (3%)	1 (0%)	47	44
1	D	513/546 (94%)	504 (98%)	8 (2%)	1 (0%)	47	44
1	E	507/546 (93%)	481 (95%)	24 (5%)	2 (0%)	34	30
1	F	533/546 (98%)	522 (98%)	10 (2%)	1 (0%)	47	44
All	All	3092/3276 (94%)	3009 (97%)	77 (2%)	6 (0%)	47	44

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	492	ASN
1	D	492	ASN
1	E	455	GLY
1	C	492	ASN
1	F	492	ASN
1	E	377	VAL

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	439/455 (96%)	426 (97%)	13 (3%)	41	41
1	B	427/455 (94%)	415 (97%)	12 (3%)	43	44

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	C	425/455 (93%)	415 (98%)	10 (2%)	49 51
1	D	426/455 (94%)	415 (97%)	11 (3%)	46 48
1	E	424/455 (93%)	411 (97%)	13 (3%)	40 40
1	F	444/455 (98%)	431 (97%)	13 (3%)	42 43
All	All	2585/2730 (95%)	2513 (97%)	72 (3%)	43 44

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	3	LYS
1	A	11	LEU
1	A	41	ASN
1	A	72	VAL
1	A	204	PHE
1	A	215	GLN
1	A	257	PRO
1	A	264	GLN
1	A	332	GLN
1	A	333	ASN
1	A	465	GLN
1	A	492	ASN
1	B	18	ASP
1	B	25	SER
1	B	41	ASN
1	B	43	LEU
1	B	71	THR
1	B	72	VAL
1	B	204	PHE
1	B	257	PRO
1	B	259	SER
1	B	333	ASN
1	B	425	ARG
1	B	456	GLU
1	C	41	ASN
1	C	43	LEU
1	C	71	THR
1	C	81	ASP
1	C	204	PHE
1	C	230	ASN
1	C	257	PRO

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Mol	Chain	Res	Type
1	C	259	SER
1	C	333	ASN
1	C	489	PHE
1	D	29	ASN
1	D	39	ASN
1	D	41	ASN
1	D	72	VAL
1	D	201	MET
1	D	204	PHE
1	D	230	ASN
1	D	259	SER
1	D	333	ASN
1	D	513	ARG
1	D	534	LYS
1	E	30	ARG
1	E	41	ASN
1	E	43	LEU
1	E	72	VAL
1	E	159	ASP
1	E	163	SER
1	E	197	VAL
1	E	204	PHE
1	E	236	SER
1	E	259	SER
1	E	268	GLU
1	E	333	ASN
1	E	474	ARG
1	F	41	ASN
1	F	43	LEU
1	F	71	THR
1	F	159	ASP
1	F	204	PHE
1	F	230	ASN
1	F	259	SER
1	F	331	GLN
1	F	333	ASN
1	F	433	ARG
1	F	470	ASP
1	F	489	PHE
1	F	492	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (69) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	GLN
1	A	29	ASN
1	A	34	ASN
1	A	41	ASN
1	A	150	GLN
1	A	167	ASN
1	A	232	GLN
1	A	264	GLN
1	A	272	ASN
1	A	277	HIS
1	A	332	GLN
1	A	333	ASN
1	A	352	HIS
1	A	380	ASN
1	A	410	HIS
1	A	492	ASN
1	A	504	ASN
1	B	34	ASN
1	B	41	ASN
1	B	150	GLN
1	B	232	GLN
1	B	333	ASN
1	B	352	HIS
1	B	380	ASN
1	B	447	GLN
1	B	504	ASN
1	C	34	ASN
1	C	41	ASN
1	C	150	GLN
1	C	167	ASN
1	C	232	GLN
1	C	331	GLN
1	C	332	GLN
1	C	333	ASN
1	C	343	GLN
1	C	380	ASN
1	C	447	GLN
1	D	29	ASN
1	D	34	ASN
1	D	41	ASN
1	D	167	ASN
1	D	230	ASN
1	D	232	GLN

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Mol	Chain	Res	Type
1	D	264	GLN
1	D	333	ASN
1	D	380	ASN
1	D	504	ASN
1	E	34	ASN
1	E	41	ASN
1	E	150	GLN
1	E	232	GLN
1	E	331	GLN
1	E	333	ASN
1	E	380	ASN
1	E	381	HIS
1	E	504	ASN
1	F	6	GLN
1	F	34	ASN
1	F	41	ASN
1	F	230	ASN
1	F	232	GLN
1	F	264	GLN
1	F	277	HIS
1	F	331	GLN
1	F	332	GLN
1	F	333	ASN
1	F	465	GLN
1	F	504	ASN
1	F	532	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 12 ligands modelled in this entry, 6 are monoatomic - leaving 6 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	PLP	A	900	1	15,15,16	2.58	6 (40%)	20,22,23	1.87	4 (20%)
2	PLP	B	900	1	15,15,16	2.21	7 (46%)	20,22,23	1.69	5 (25%)
2	PLP	E	900	1	15,15,16	2.83	7 (46%)	20,22,23	1.41	2 (10%)
2	PLP	C	900	1	15,15,16	2.18	7 (46%)	20,22,23	1.63	3 (15%)
2	PLP	D	900	1	15,15,16	2.26	5 (33%)	20,22,23	2.06	4 (20%)
2	PLP	F	900	1	15,15,16	2.71	6 (40%)	20,22,23	2.02	4 (20%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PLP	A	900	1	-	1/6/6/8	0/1/1/1
2	PLP	B	900	1	-	0/6/6/8	0/1/1/1
2	PLP	E	900	1	-	0/6/6/8	0/1/1/1
2	PLP	C	900	1	-	0/6/6/8	0/1/1/1
2	PLP	D	900	1	-	0/6/6/8	0/1/1/1
2	PLP	F	900	1	-	0/6/6/8	0/1/1/1

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	900	PLP	C2A-C2	6.85	1.62	1.50
2	A	900	PLP	C3-C2	-6.01	1.34	1.40
2	F	900	PLP	C5-C4	5.39	1.46	1.40
2	F	900	PLP	C4A-C4	5.36	1.62	1.51
2	E	900	PLP	C5-C4	4.59	1.45	1.40
2	D	900	PLP	C2-N1	4.53	1.42	1.33
2	B	900	PLP	C4A-C4	4.46	1.60	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	900	PLP	O4P-C5A	4.44	1.61	1.45
2	C	900	PLP	O4P-C5A	4.40	1.61	1.45
2	F	900	PLP	C2A-C2	4.31	1.57	1.50
2	B	900	PLP	O4P-C5A	4.15	1.60	1.45
2	A	900	PLP	C5A-C5	3.99	1.61	1.50
2	F	900	PLP	C6-N1	3.83	1.42	1.34
2	E	900	PLP	C2-N1	3.62	1.40	1.33
2	C	900	PLP	C5A-C5	3.51	1.60	1.50
2	D	900	PLP	C5-C4	3.44	1.44	1.40
2	D	900	PLP	C2A-C2	3.16	1.55	1.50
2	D	900	PLP	O4P-C5A	3.11	1.56	1.45
2	D	900	PLP	C5A-C5	3.10	1.59	1.50
2	B	900	PLP	P-O3P	-3.03	1.43	1.54
2	E	900	PLP	C6-N1	3.03	1.40	1.34
2	A	900	PLP	P-O3P	-2.86	1.43	1.54
2	E	900	PLP	C4A-C4	2.82	1.57	1.51
2	C	900	PLP	C6-N1	2.64	1.40	1.34
2	C	900	PLP	C3-C2	-2.60	1.38	1.40
2	C	900	PLP	C2A-C2	2.52	1.54	1.50
2	B	900	PLP	C5A-C5	2.50	1.57	1.50
2	A	900	PLP	C2A-C2	2.48	1.54	1.50
2	B	900	PLP	C6-N1	2.47	1.39	1.34
2	C	900	PLP	P-O2P	-2.43	1.45	1.54
2	A	900	PLP	P-O4P	-2.35	1.52	1.60
2	E	900	PLP	P-O4P	-2.28	1.52	1.60
2	F	900	PLP	P-O3P	-2.13	1.46	1.54
2	F	900	PLP	O4P-C5A	2.13	1.52	1.45
2	C	900	PLP	C2-N1	2.11	1.37	1.33
2	B	900	PLP	C5-C4	2.06	1.42	1.40
2	E	900	PLP	P-O3P	-2.05	1.47	1.54
2	B	900	PLP	P-O4P	-2.04	1.53	1.60

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	900	PLP	C4A-C4-C5	6.92	128.07	120.94
2	D	900	PLP	C4A-C4-C5	5.41	126.51	120.94
2	A	900	PLP	C4A-C4-C5	5.25	126.34	120.94
2	B	900	PLP	C4A-C4-C5	5.01	126.09	120.94
2	C	900	PLP	C4A-C4-C5	4.87	125.95	120.94
2	D	900	PLP	C6-C5-C4	3.95	121.26	118.16
2	A	900	PLP	C5A-C5-C6	-3.81	113.11	119.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	900	PLP	C4A-C4-C3	-3.77	114.10	120.50
2	D	900	PLP	C4A-C4-C3	-3.62	114.37	120.50
2	D	900	PLP	C5A-C5-C6	-3.38	113.81	119.37
2	E	900	PLP	C4A-C4-C5	2.97	123.99	120.94
2	E	900	PLP	C5A-C5-C6	-2.88	114.64	119.37
2	F	900	PLP	C5A-C5-C6	-2.85	114.68	119.37
2	C	900	PLP	C4A-C4-C3	-2.83	115.71	120.50
2	C	900	PLP	C5A-C5-C6	-2.65	115.02	119.37
2	A	900	PLP	C4A-C4-C3	-2.40	116.43	120.50
2	B	900	PLP	C4A-C4-C3	-2.35	116.51	120.50
2	B	900	PLP	C5A-C5-C6	-2.32	115.56	119.37
2	B	900	PLP	O3P-P-O2P	2.29	116.39	107.64
2	F	900	PLP	O4P-C5A-C5	-2.13	105.30	109.35
2	B	900	PLP	O2P-P-O4P	-2.06	101.26	106.73
2	A	900	PLP	O3P-P-O1P	2.05	118.69	110.68

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	900	PLP	C6-C5-C5A-O4P

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

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	524/546 (95%)	-0.32	11 (2%)	63	62	10, 20, 42, 65	0
1	B	512/546 (93%)	-0.38	11 (2%)	63	62	9, 19, 43, 81	0
1	C	511/546 (93%)	-0.33	19 (3%)	41	41	9, 20, 46, 76	0
1	D	515/546 (94%)	-0.32	19 (3%)	41	41	9, 21, 43, 76	0
1	E	509/546 (93%)	-0.01	29 (5%)	23	23	11, 25, 57, 88	0
1	F	535/546 (97%)	-0.22	23 (4%)	35	34	9, 22, 52, 78	0
All	All	3106/3276 (94%)	-0.26	112 (3%)	42	42	9, 21, 48, 88	0

All (112) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	490	GLY	11.0
1	E	490	GLY	9.3
1	C	490	GLY	8.0
1	F	491	SER	7.2
1	D	490	GLY	7.1
1	E	489	PHE	6.8
1	F	490	GLY	6.6
1	B	492	ASN	6.1
1	F	539	LEU	5.9
1	F	536	ALA	5.6
1	E	21	ILE	5.6
1	E	23	ILE	5.4
1	C	492	ASN	5.4
1	D	538	ALA	5.1
1	B	23	ILE	5.0
1	E	487	ARG	5.0
1	D	535	LEU	5.0
1	D	539	LEU	4.8
1	D	537	ALA	4.8

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Mol	Chain	Res	Type	RSRZ
1	C	23	ILE	4.6
1	E	491	SER	4.4
1	E	71	THR	4.4
1	D	28	GLY	4.3
1	B	71	THR	4.2
1	F	10	LYS	4.0
1	E	473	PHE	3.9
1	E	455	GLY	3.9
1	A	524	ALA	3.8
1	E	25	SER	3.8
1	E	524	ALA	3.8
1	E	456	GLU	3.6
1	F	535	LEU	3.6
1	B	491	SER	3.5
1	D	432	LEU	3.5
1	C	491	SER	3.5
1	D	533	LEU	3.5
1	F	11	LEU	3.5
1	C	487	ARG	3.4
1	D	491	SER	3.4
1	F	534	LYS	3.4
1	E	488	GLY	3.4
1	F	538	ALA	3.3
1	A	525	GLU	3.3
1	D	536	ALA	3.2
1	D	30	ARG	3.2
1	E	492	ASN	3.2
1	F	537	ALA	3.2
1	B	489	PHE	3.2
1	C	489	PHE	3.1
1	F	432	LEU	3.1
1	A	523	TYR	3.1
1	D	540	GLU	3.1
1	C	355	ARG	3.1
1	C	527	SER	3.1
1	E	457	ALA	3.1
1	C	22	LYS	3.0
1	A	11	LEU	3.0
1	E	20	LEU	3.0
1	E	22	LYS	3.0
1	F	12	SER	3.0
1	E	461	TRP	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	531	GLN	2.9
1	A	213	LEU	2.8
1	A	526	TYR	2.8
1	A	492	ASN	2.8
1	D	26	SER	2.8
1	E	355	ARG	2.8
1	C	528	GLY	2.7
1	C	25	SER	2.7
1	E	359	PRO	2.7
1	E	276	GLU	2.7
1	E	527	SER	2.7
1	B	16	LEU	2.6
1	D	534	LYS	2.6
1	A	216	TYR	2.6
1	D	492	ASN	2.6
1	F	533	LEU	2.6
1	F	492	ASN	2.6
1	C	24	ALA	2.5
1	B	19	GLU	2.5
1	C	524	ALA	2.5
1	E	523	TYR	2.4
1	F	13	PRO	2.4
1	D	473	PHE	2.4
1	F	9	ALA	2.4
1	C	352	HIS	2.4
1	A	2	SER	2.4
1	C	19	GLU	2.3
1	F	355	ARG	2.3
1	F	14	PHE	2.3
1	E	451	ALA	2.3
1	F	8	LEU	2.3
1	C	456	GLU	2.3
1	E	19	GLU	2.3
1	F	540	GLU	2.2
1	E	24	ALA	2.2
1	E	477	ASP	2.2
1	C	473	PHE	2.2
1	A	527	SER	2.2
1	B	21	ILE	2.2
1	D	27	ASP	2.2
1	C	488	GLY	2.1
1	B	25	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	359	PRO	2.1
1	F	352	HIS	2.1
1	E	525	GLU	2.1
1	F	71	THR	2.1
1	B	464	LYS	2.1
1	E	458	PHE	2.1
1	F	489	PHE	2.1
1	A	71	THR	2.0
1	C	21	ILE	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 monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	B-factors(Å^2)	Q<0.9
2	PLP	E	900	15/16	0.98	0.09	17,21,23,24	0
3	CL	D	4004	1/1	0.98	0.06	21,21,21,21	0
3	CL	F	4006	1/1	0.98	0.05	24,24,24,24	0
2	PLP	D	900	15/16	0.99	0.11	14,16,17,18	0
2	PLP	A	900	15/16	0.99	0.08	14,15,18,18	0
2	PLP	F	900	15/16	0.99	0.08	13,15,18,18	0
3	CL	A	4001	1/1	0.99	0.05	18,18,18,18	0
3	CL	B	4002	1/1	0.99	0.04	20,20,20,20	0
3	CL	C	4003	1/1	0.99	0.04	19,19,19,19	0
2	PLP	B	900	15/16	0.99	0.08	12,15,17,18	0
3	CL	E	4005	1/1	0.99	0.05	20,20,20,20	0
2	PLP	C	900	15/16	0.99	0.09	13,15,17,17	0

6.5 Other polymers (i)

There are no such residues in this entry.