



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 24, 2024 – 08:04 AM EDT

PDB ID : 6H65
Title : Crystal structure of the branched-chain-amino-acid aminotransferase from *Haliangium ochraceum*
Authors : Boyko, K.M.; Timofeev, V.I.; Bezsudnova, E.Y.; Nikolaeva, A.Y.; Rakitina, T.V.; Popov, V.O.
Deposited on : 2018-07-26
Resolution : 2.35 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

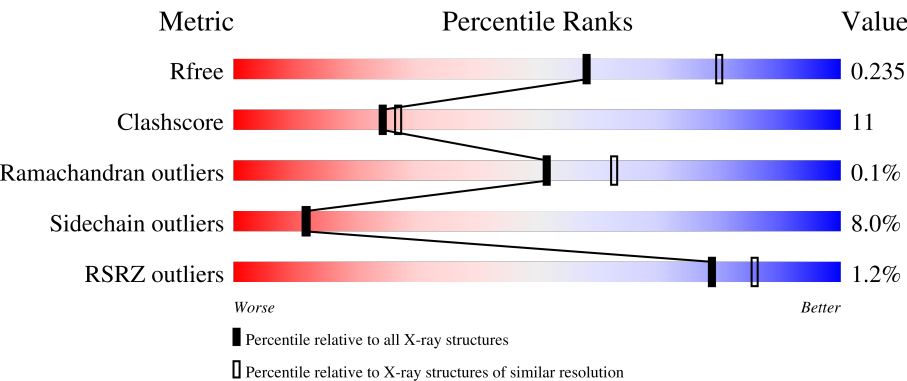
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.35 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	1164 (2.36-2.36)
Clashscore	141614	1232 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)
RSRZ outliers	127900	1150 (2.36-2.36)

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

Mol	Chain	Length	Quality of chain
1	A	317	<div><div>%</div><div><div></div><div>76%</div><div>14%</div><div>5%</div><div>...</div></div></div>
1	B	317	<div><div>2%</div><div><div></div><div>75%</div><div>16%</div><div>...</div></div></div>
1	C	317	<div><div>%</div><div><div></div><div>77%</div><div>15%</div><div>...</div></div></div>
1	D	317	<div><div>%</div><div><div></div><div>77%</div><div>15%</div><div>...</div></div></div>
1	E	317	<div><div>3%</div><div><div></div><div>76%</div><div>17%</div><div>...</div></div></div>

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Mol	Chain	Length	Quality of chain
1	F	317	 76% 15% . . .

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PLP	C	401	-	X	-	-
2	PLP	E	401	-	X	-	-

2 Entry composition [i](#)

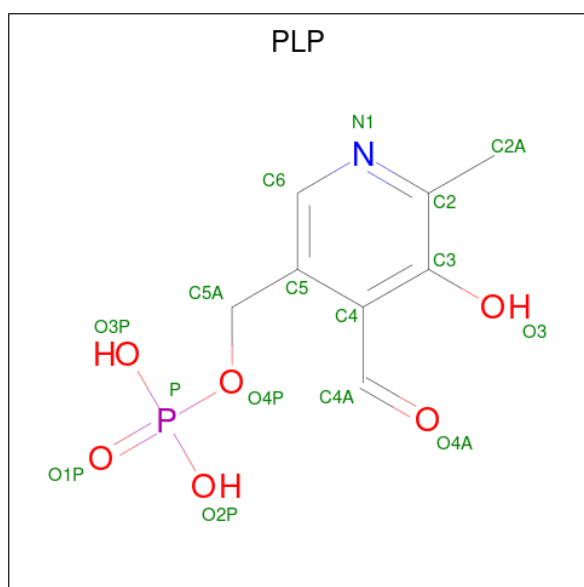
There are 3 unique types of molecules in this entry. The entry contains 14697 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Branched-chain-amino-acid aminotransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	305	Total	C	N	O	S	0	1	0
			2401	1518	419	450	14			
1	B	306	Total	C	N	O	S	0	1	0
			2419	1528	423	454	14			
1	C	308	Total	C	N	O	S	0	1	0
			2433	1536	425	458	14			
1	D	305	Total	C	N	O	S	0	1	0
			2408	1523	419	452	14			
1	E	307	Total	C	N	O	S	0	2	0
			2428	1530	427	457	14			
1	F	306	Total	C	N	O	S	0	1	0
			2407	1522	418	453	14			

- Molecule 2 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: C₈H₁₀NO₆P).



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		
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		

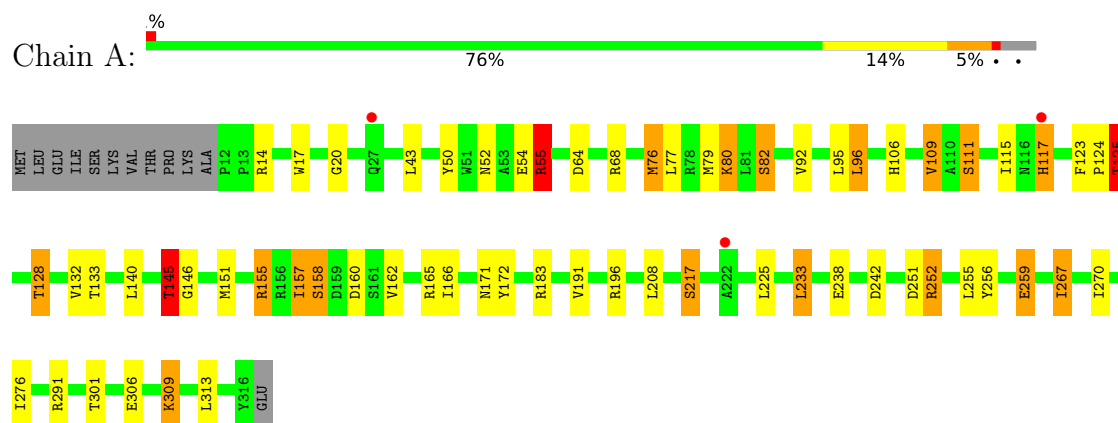
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	17	Total	O	0	0
			17	17		
3	B	21	Total	O	0	0
			21	21		
3	C	25	Total	O	0	0
			25	25		
3	D	16	Total	O	0	0
			16	16		
3	E	19	Total	O	0	0
			19	19		
3	F	13	Total	O	0	0
			13	13		

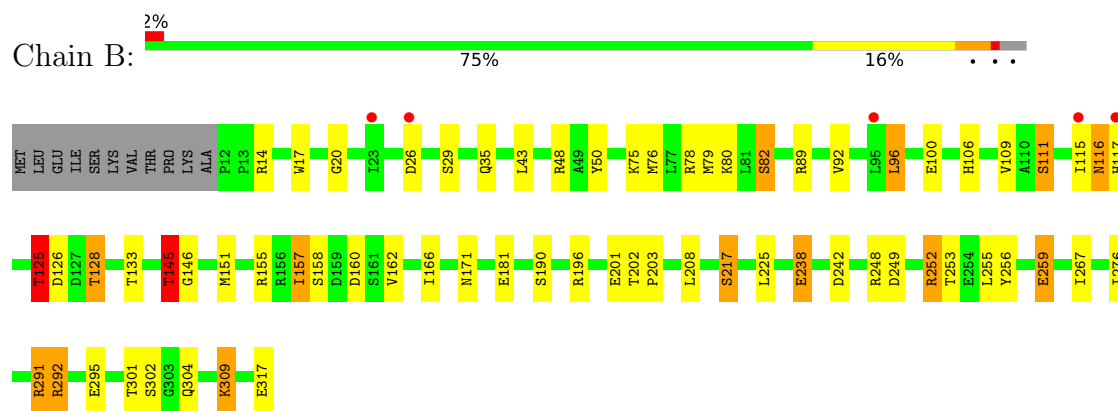
3 Residue-property plots [i](#)

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.

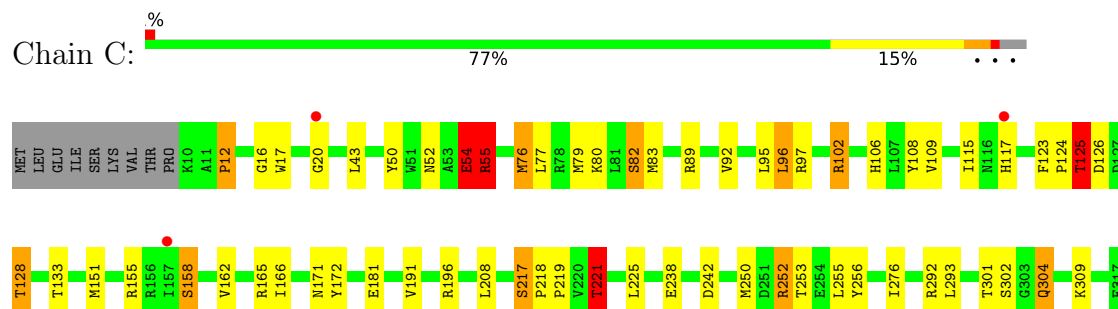
- Molecule 1: Branched-chain-amino-acid aminotransferase




- Molecule 1: Branched-chain-amino-acid aminotransferase



- Molecule 1: Branched-chain-amino-acid aminotransferase




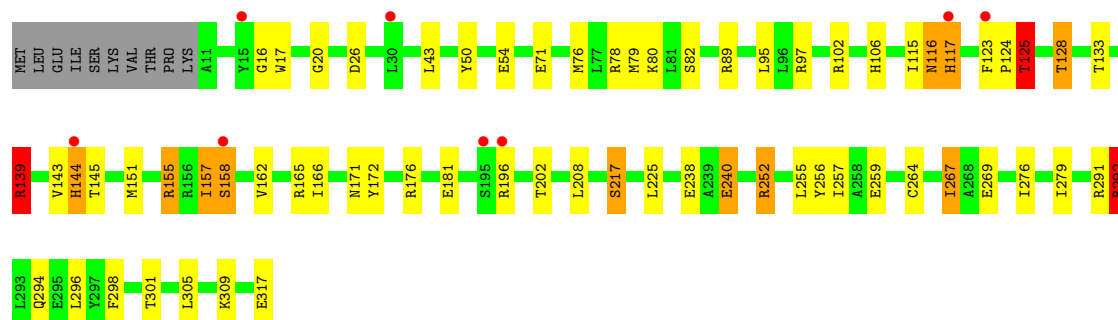
- Molecule 1: Branched-chain-amino-acid aminotransferase

Chain D:  77% 15% . . .



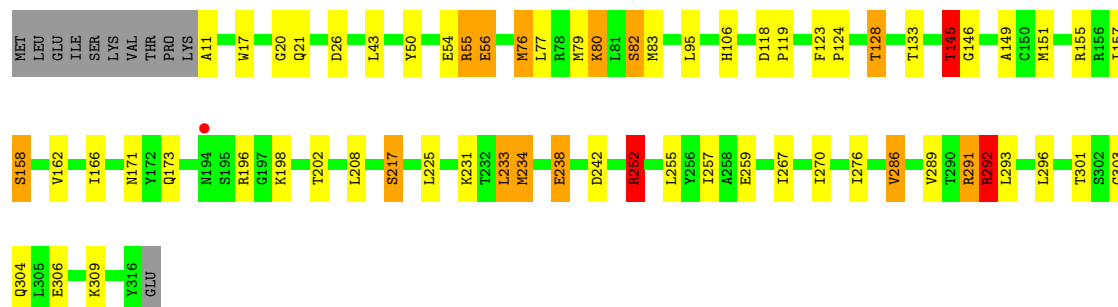
- Molecule 1: Branched-chain-amino-acid aminotransferase

Chain E:  76% 17% . . .



- Molecule 1: Branched-chain-amino-acid aminotransferase

Chain F:  76% 15% . . .



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	95.08Å 164.93Å 254.22Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.64 – 2.35 47.59 – 2.35	Depositor EDS
% Data completeness (in resolution range)	97.0 (47.64-2.35) 97.0 (47.59-2.35)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.46 (at 2.34Å)	Xtriage
Refinement program	REFMAC 5.8.0230	Depositor
R, R_{free}	0.199 , 0.235 0.199 , 0.235	Depositor DCC
R_{free} test set	3978 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	46.5	Xtriage
Anisotropy	0.510	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 33.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.048 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.048 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	14697	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.25% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.65	1/2458 (0.0%)	0.99	7/3342 (0.2%)
1	B	0.68	4/2477 (0.2%)	1.09	9/3365 (0.3%)
1	C	0.68	1/2490 (0.0%)	1.08	11/3384 (0.3%)
1	D	0.68	1/2465 (0.0%)	1.04	8/3351 (0.2%)
1	E	0.72	4/2492 (0.2%)	1.07	15/3386 (0.4%)
1	F	0.67	1/2463 (0.0%)	1.07	9/3350 (0.3%)
All	All	0.68	12/14845 (0.1%)	1.06	59/20178 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4
1	B	0	5
1	C	0	5
1	D	0	4
1	E	0	4
1	F	0	4
All	All	0	26

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	181	GLU	CD-OE1	8.27	1.34	1.25
1	D	181	GLU	CD-OE2	8.12	1.34	1.25
1	B	259	GLU	CD-OE2	7.68	1.34	1.25
1	E	181	GLU	CD-OE1	6.57	1.32	1.25
1	E	181	GLU	CD-OE2	6.09	1.32	1.25
1	E	71	GLU	CD-OE1	5.71	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	259	GLU	CD-OE1	5.57	1.31	1.25
1	A	259	GLU	CD-OE2	5.40	1.31	1.25
1	F	56	GLU	CD-OE2	5.24	1.31	1.25
1	B	181	GLU	CD-OE2	5.19	1.31	1.25
1	B	249	ASP	CG-OD1	5.16	1.37	1.25
1	E	317	GLU	CD-OE1	5.13	1.31	1.25

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	126	ASP	CB-CA-C	-19.37	71.66	110.40
1	C	126	ASP	CB-CA-C	-18.89	72.62	110.40
1	D	292	ARG	CG-CD-NE	12.80	138.68	111.80
1	F	26	ASP	CB-CA-C	-12.15	86.09	110.40
1	D	56	GLU	CB-CA-C	9.70	129.81	110.40
1	E	26	ASP	CB-CA-C	-9.57	91.26	110.40
1	D	26	ASP	CB-CA-C	-9.53	91.34	110.40
1	E	139	ARG	CG-CD-NE	7.93	128.46	111.80
1	E	102	ARG	CB-CG-CD	7.55	131.24	111.60
1	E	78	ARG	NE-CZ-NH2	-7.54	116.53	120.30
1	C	54	GLU	CB-CA-C	7.37	125.14	110.40
1	B	111	SER	N-CA-CB	6.95	120.92	110.50
1	E	125	THR	CB-CA-C	-6.83	93.15	111.60
1	D	125	THR	CB-CA-C	-6.78	93.30	111.60
1	F	145	THR	CA-CB-OG1	-6.75	94.82	109.00
1	F	238	GLU	CB-CA-C	6.75	123.90	110.40
1	B	116	ASN	N-CA-CB	6.66	122.59	110.60
1	C	55	ARG	CB-CA-C	-6.64	97.12	110.40
1	F	291	ARG	CG-CD-NE	-6.59	97.96	111.80
1	A	125	THR	CB-CA-C	-6.52	94.00	111.60
1	A	145	THR	CA-CB-OG1	-6.51	95.32	109.00
1	C	125	THR	CB-CA-C	-6.50	94.04	111.60
1	B	238	GLU	CB-CA-C	6.49	123.38	110.40
1	C	292	ARG	CG-CD-NE	6.43	125.31	111.80
1	B	145	THR	CA-CB-OG1	-6.32	95.73	109.00
1	C	12	PRO	N-CA-CB	-6.29	95.68	102.60
1	C	221	THR	CA-CB-OG1	-6.28	95.81	109.00
1	D	145	THR	CA-CB-OG1	-6.15	96.08	109.00
1	C	304	GLN	CB-CG-CD	6.12	127.50	111.60
1	E	176	ARG	CB-CG-CD	6.11	127.48	111.60
1	E	139	ARG	NE-CZ-NH1	-6.08	117.26	120.30
1	D	292	ARG	CB-CG-CD	-6.07	95.83	111.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	125	THR	CB-CA-C	-6.06	95.23	111.60
1	F	234	MET	CG-SD-CE	5.99	109.78	100.20
1	C	89	ARG	NE-CZ-NH2	-5.91	117.35	120.30
1	A	111	SER	N-CA-CB	5.89	119.33	110.50
1	D	51	TRP	CA-CB-CG	-5.89	102.52	113.70
1	E	54	GLU	CB-CA-C	5.87	122.13	110.40
1	A	165	ARG	NE-CZ-NH2	-5.78	117.41	120.30
1	F	173	GLN	CB-CA-C	5.66	121.72	110.40
1	C	158	SER	N-CA-CB	-5.66	102.02	110.50
1	E	97	ARG	NE-CZ-NH1	-5.54	117.53	120.30
1	E	252	ARG	NE-CZ-NH2	-5.53	117.54	120.30
1	F	252	ARG	NE-CZ-NH1	5.53	123.06	120.30
1	E	291	ARG	CG-CD-NE	5.44	123.22	111.80
1	B	309	LYS	CB-CG-CD	5.39	125.61	111.60
1	F	158	SER	CB-CA-C	-5.33	99.98	110.10
1	A	68	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	B	116	ASN	CB-CA-C	5.23	120.86	110.40
1	A	252	ARG	NE-CZ-NH2	-5.23	117.69	120.30
1	C	221	THR	N-CA-CB	-5.22	100.38	110.30
1	B	248	ARG	NE-CZ-NH2	-5.22	117.69	120.30
1	E	292[A]	ARG	CG-CD-NE	5.15	122.62	111.80
1	E	292[B]	ARG	CG-CD-NE	5.15	122.62	111.80
1	D	78	ARG	NE-CZ-NH1	-5.14	117.73	120.30
1	A	155	ARG	CG-CD-NE	5.12	122.54	111.80
1	E	252	ARG	NE-CZ-NH1	5.11	122.86	120.30
1	F	55	ARG	NE-CZ-NH2	-5.02	117.79	120.30
1	E	155	ARG	CG-CD-NE	5.00	122.31	111.80

There are no chirality outliers.

All (26) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	14	ARG	Sidechain
1	A	155	ARG	Sidechain
1	A	183	ARG	Sidechain
1	A	291	ARG	Sidechain
1	B	155	ARG	Sidechain
1	B	252	ARG	Sidechain
1	B	291	ARG	Sidechain
1	B	292	ARG	Sidechain
1	B	89	ARG	Sidechain
1	C	102	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	C	155	ARG	Sidechain
1	C	165	ARG	Sidechain
1	C	252	ARG	Sidechain
1	C	97	ARG	Sidechain
1	D	155	ARG	Sidechain
1	D	292	ARG	Sidechain
1	D	55	ARG	Sidechain
1	D	68	ARG	Sidechain
1	E	139	ARG	Sidechain
1	E	155	ARG	Sidechain
1	E	292[A]	ARG	Sidechain
1	E	292[B]	ARG	Sidechain
1	F	11	ALA	Peptide
1	F	155	ARG	Sidechain
1	F	252	ARG	Sidechain
1	F	292	ARG	Sidechain

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	2401	0	2371	63	0
1	B	2419	0	2391	46	0
1	C	2433	0	2402	60	0
1	D	2408	0	2384	57	0
1	E	2428	0	2395	60	0
1	F	2407	0	2378	68	0
2	A	15	0	7	1	0
2	B	15	0	7	1	0
2	C	15	0	6	1	0
2	D	15	0	6	1	0
2	E	15	0	7	1	0
2	F	15	0	7	0	0
3	A	17	0	0	0	0
3	B	21	0	0	0	0
3	C	25	0	0	1	0
3	D	16	0	0	1	0
3	E	19	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	13	0	0	2	0
All	All	14697	0	14361	316	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 11.

All (316) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:218:PRO:HD3	1:C:250:MET:CE	1.62	1.29
1:C:218:PRO:CD	1:C:250:MET:CE	2.24	1.16
1:D:106:HIS:CE1	1:D:267:ILE:HD11	1.80	1.15
1:C:106:HIS:HE1	1:C:108:TYR:CZ	1.69	1.11
1:C:218:PRO:CD	1:C:250:MET:HE1	1.78	1.10
1:D:106:HIS:CE1	1:D:267:ILE:CD1	2.39	1.05
1:F:157:ILE:CD1	1:F:162:VAL:HB	1.93	0.99
1:D:157:ILE:HD12	1:D:158:SER:H	1.24	0.98
1:F:292:ARG:O	1:F:296:LEU:HD13	1.62	0.98
1:A:157:ILE:HD12	1:A:158:SER:H	1.25	0.96
1:F:76[B]:MET:CE	1:F:166:ILE:HD11	1.97	0.95
1:E:157:ILE:HD12	1:E:158:SER:H	1.31	0.94
1:B:157:ILE:HD12	1:B:158:SER:H	1.31	0.94
1:E:76[B]:MET:SD	1:E:166:ILE:HD11	2.09	0.92
1:B:35:GLN:HE21	1:B:116:ASN:HD22	0.94	0.92
1:A:54:GLU:O	1:A:55:ARG:HB2	1.66	0.92
1:F:157:ILE:HD11	1:F:162:VAL:HB	1.52	0.90
1:B:35:GLN:NE2	1:B:116:ASN:HD22	1.70	0.89
1:C:218:PRO:CD	1:C:250:MET:HE3	1.99	0.89
1:D:157:ILE:HG13	1:D:162:VAL:HB	1.56	0.88
1:A:162:VAL:HG12	1:A:171:ASN:OD1	1.74	0.88
1:D:76[A]:MET:HE3	1:D:77:LEU:HG	1.56	0.88
1:C:106:HIS:CE1	1:C:108:TYR:CZ	2.60	0.88
1:C:217:SER:CA	1:C:250:MET:HE2	2.04	0.87
1:A:55:ARG:CG	1:A:55:ARG:HH21	1.88	0.86
1:D:106:HIS:HE1	1:D:267:ILE:HD11	1.39	0.86
1:D:106:HIS:HE1	1:D:267:ILE:CD1	1.84	0.86
1:B:35:GLN:HE21	1:B:116:ASN:ND2	1.72	0.85
1:C:54:GLU:O	1:C:55:ARG:HB2	1.73	0.85
1:C:218:PRO:HD3	1:C:250:MET:HE1	0.89	0.85
1:C:217:SER:HA	1:C:250:MET:HE2	1.57	0.85
1:D:76[B]:MET:CE	1:D:166:ILE:HD11	2.06	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:157:ILE:HG13	1:B:162:VAL:HB	1.58	0.84
1:C:106:HIS:HE1	1:C:108:TYR:CE2	1.94	0.84
1:C:217:SER:HA	1:C:250:MET:CE	2.08	0.84
1:F:76[B]:MET:HE2	1:F:166:ILE:HD11	1.60	0.84
1:E:157:ILE:HG13	1:E:162:VAL:HB	1.60	0.83
1:E:139:ARG:NH1	1:E:298:PHE:CE1	2.47	0.82
1:A:157:ILE:HG13	1:A:162:VAL:HB	1.60	0.82
1:A:55:ARG:HH21	1:A:55:ARG:HG2	1.43	0.81
1:D:80:LYS:O	1:D:128:THR:HG21	1.80	0.81
1:F:80:LYS:O	1:F:128:THR:HG21	1.80	0.80
1:A:80:LYS:O	1:A:128:THR:HG21	1.81	0.80
1:B:80:LYS:O	1:B:128:THR:HG21	1.82	0.80
1:F:76[A]:MET:HE3	1:F:77:LEU:HG	1.61	0.80
1:E:80:LYS:O	1:E:128:THR:HG21	1.80	0.80
1:A:115:ILE:O	1:A:125:THR:HG21	1.82	0.80
1:C:76[A]:MET:HE3	1:C:77:LEU:HG	1.63	0.80
1:C:80:LYS:O	1:C:128:THR:HG21	1.83	0.79
1:C:218:PRO:N	1:C:250:MET:CE	2.46	0.79
1:F:286:VAL:HG13	1:F:291:ARG:NH2	1.98	0.78
1:A:76[A]:MET:CE	1:A:166:ILE:HG13	2.12	0.78
1:C:218:PRO:N	1:C:250:MET:HE3	1.98	0.78
1:A:76[A]:MET:HE3	1:A:77:LEU:HG	1.65	0.78
1:A:76[B]:MET:SD	1:A:166:ILE:HD11	2.24	0.77
1:D:76[A]:MET:CE	1:D:166:ILE:HG13	2.14	0.77
1:A:106:HIS:CE1	1:A:267:ILE:HG12	2.21	0.76
1:C:115:ILE:O	1:C:125:THR:HG21	1.85	0.76
1:D:157:ILE:HD12	1:D:158:SER:N	2.00	0.76
1:F:157:ILE:HD11	1:F:162:VAL:CB	2.15	0.76
1:D:76[B]:MET:HE3	1:D:166:ILE:HD11	1.66	0.76
1:A:157:ILE:HD12	1:A:158:SER:N	2.00	0.76
1:E:115:ILE:O	1:E:125:THR:HG21	1.86	0.75
1:D:115:ILE:O	1:D:125:THR:HG21	1.86	0.75
1:F:76[A]:MET:CE	1:F:166:ILE:HG13	2.16	0.75
1:E:172:TYR:OH	2:E:401:PLP:O3	2.05	0.74
1:E:106:HIS:CE1	1:E:267:ILE:HG12	2.22	0.73
1:B:157:ILE:HD12	1:B:158:SER:N	2.02	0.73
1:E:157:ILE:HD12	1:E:158:SER:N	2.03	0.73
1:B:115:ILE:O	1:B:125:THR:HG21	1.87	0.72
1:C:76[A]:MET:CE	1:C:166:ILE:HG13	2.19	0.72
1:A:76[A]:MET:HE2	1:A:166:ILE:HG13	1.71	0.72
1:C:106:HIS:CE1	1:C:108:TYR:CE2	2.79	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:144:HIS:HB3	1:F:55:ARG:HG2	1.73	0.70
1:E:139:ARG:NH1	1:E:298:PHE:CD1	2.62	0.68
1:F:145:THR:HG22	1:F:146:GLY:O	1.93	0.67
1:A:145:THR:HG22	1:A:146:GLY:O	1.94	0.67
1:D:145:THR:HG22	1:D:146:GLY:O	1.94	0.67
1:B:145:THR:HG22	1:B:146:GLY:O	1.94	0.67
1:A:55:ARG:HG2	1:A:55:ARG:NH2	2.10	0.66
1:E:144:HIS:ND1	1:F:55:ARG:CZ	2.58	0.66
1:A:54:GLU:O	1:A:55:ARG:CB	2.39	0.66
1:C:217:SER:C	1:C:250:MET:HE2	2.17	0.65
1:C:218:PRO:CG	1:C:250:MET:HE3	2.25	0.65
1:E:144:HIS:CB	1:F:55:ARG:HG2	2.26	0.65
1:D:76[A]:MET:HE1	1:D:166:ILE:HG13	1.79	0.64
1:B:106:HIS:CE1	1:B:267:ILE:HG22	2.33	0.64
1:B:255:LEU:HB3	1:B:276:ILE:HD12	1.80	0.64
1:F:76[A]:MET:CE	1:F:77:LEU:HG	2.27	0.64
1:F:76[A]:MET:HE2	1:F:166:ILE:HG13	1.79	0.64
1:F:286:VAL:CG1	1:F:291:ARG:HH21	2.10	0.64
1:C:217:SER:C	1:C:250:MET:CE	2.66	0.64
1:A:43:LEU:CB	1:A:79:MET:HE1	2.28	0.64
1:D:255:LEU:HB3	1:D:276:ILE:HD12	1.79	0.64
1:A:43:LEU:HB2	1:A:79:MET:HE1	1.78	0.64
1:E:255:LEU:HB3	1:E:276:ILE:HD12	1.79	0.63
1:B:291:ARG:O	1:B:295:GLU:HG2	1.98	0.63
1:F:106:HIS:CE1	1:F:267:ILE:HG22	2.33	0.63
1:C:217:SER:CA	1:C:250:MET:CE	2.73	0.63
1:F:118:ASP:OD1	1:F:119:PRO:HD2	1.99	0.63
1:A:306:GLU:OE2	1:A:309:LYS:HD2	2.00	0.62
1:D:76[A]:MET:CE	1:D:77:LEU:HG	2.29	0.62
1:A:140:LEU:HD12	1:A:140:LEU:H	1.65	0.62
1:F:76[B]:MET:HE1	1:F:166:ILE:HD11	1.78	0.61
1:E:144:HIS:CB	1:F:55:ARG:CG	2.79	0.60
1:A:151:MET:HE3	1:A:276:ILE:CG2	2.32	0.60
1:B:157:ILE:CG1	1:B:162:VAL:HB	2.31	0.60
1:C:76[A]:MET:CE	1:C:77:LEU:HG	2.30	0.60
1:C:128:THR:HG23	3:C:505:HOH:O	2.00	0.60
1:A:76[A]:MET:CE	1:A:77:LEU:HG	2.31	0.60
1:A:117:HIS:HB2	1:A:125:THR:CG2	2.32	0.60
1:D:106:HIS:HE1	1:D:267:ILE:HD12	1.67	0.59
1:C:54:GLU:O	1:C:55:ARG:CB	2.43	0.59
1:A:117:HIS:HB2	1:A:125:THR:HG22	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:139:ARG:NH2	1:F:56:GLU:HG3	2.17	0.59
1:A:157:ILE:CG1	1:A:162:VAL:HB	2.32	0.59
1:C:76[A]:MET:HE2	1:C:166:ILE:HG13	1.85	0.59
1:D:157:ILE:CG1	1:D:162:VAL:HB	2.31	0.59
1:D:253:THR:HB	1:F:76[B]:MET:CE	2.32	0.59
1:E:117:HIS:HB2	1:E:125:THR:CG2	2.33	0.59
1:C:172:TYR:OH	2:C:401:PLP:O3	2.14	0.59
1:D:76[A]:MET:HE2	1:D:166:ILE:HG13	1.83	0.58
1:D:76[B]:MET:CE	1:D:166:ILE:CD1	2.79	0.58
1:A:255:LEU:HB3	1:A:276:ILE:HD12	1.86	0.58
1:F:162:VAL:CG1	1:F:171:ASN:OD1	2.52	0.58
1:A:76[B]:MET:CE	1:F:257:ILE:CG2	2.81	0.58
1:A:82:SER:HB2	1:A:128:THR:HG22	1.86	0.57
1:D:76[B]:MET:HE3	1:D:166:ILE:CD1	2.34	0.57
1:A:95:LEU:HD22	1:A:132:VAL:HG12	1.86	0.57
1:B:92:VAL:O	1:B:96:LEU:HD22	2.04	0.57
1:E:157:ILE:CG1	1:E:162:VAL:HB	2.33	0.57
1:B:78:ARG:CZ	1:E:279:ILE:HD11	2.34	0.57
1:B:76[A]:MET:SD	1:B:166:ILE:HD11	2.44	0.57
1:D:92:VAL:O	1:D:96:LEU:HD22	2.05	0.57
1:B:82:SER:HB2	1:B:128:THR:HG22	1.87	0.57
1:A:313:LEU:HB2	1:B:317:GLU:HB2	1.86	0.57
1:C:217:SER:HA	1:C:250:MET:HE1	1.87	0.57
1:D:117:HIS:HB2	1:D:125:THR:CG2	2.35	0.56
1:E:151:MET:HE3	1:E:276:ILE:CG2	2.36	0.56
1:D:106:HIS:NE2	1:D:267:ILE:HD11	2.16	0.56
1:E:151:MET:HE3	1:E:276:ILE:HG21	1.87	0.56
1:D:162:VAL:CG1	1:D:171:ASN:OD1	2.54	0.55
1:C:162:VAL:CG1	1:C:171:ASN:OD1	2.54	0.55
1:E:82:SER:HB2	1:E:128:THR:HG22	1.88	0.55
1:F:128:THR:HG23	3:F:502:HOH:O	2.07	0.55
1:A:162:VAL:CG1	1:A:171:ASN:OD1	2.52	0.55
1:B:35:GLN:NE2	1:B:116:ASN:HB3	2.22	0.55
1:E:162:VAL:CG1	1:E:171:ASN:OD1	2.55	0.55
1:D:117:HIS:HB2	1:D:125:THR:HG22	1.89	0.54
1:B:253:THR:HB	1:C:76[B]:MET:CE	2.37	0.54
1:F:286:VAL:CG1	1:F:291:ARG:NH2	2.66	0.54
1:B:82:SER:CB	1:B:128:THR:HG22	2.38	0.54
1:B:162:VAL:CG1	1:B:171:ASN:OD1	2.55	0.54
1:F:157:ILE:HD11	1:F:162:VAL:CG2	2.37	0.54
1:D:253:THR:HB	1:F:76[B]:MET:HE3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:208:LEU:HG	1:D:217:SER:HB2	1.89	0.53
1:B:43:LEU:CD2	1:B:79:MET:HE3	2.39	0.53
1:A:82:SER:CB	1:A:128:THR:HG22	2.37	0.53
1:E:117:HIS:HB2	1:E:125:THR:HG22	1.89	0.53
1:F:157:ILE:CG1	1:F:162:VAL:HB	2.38	0.53
1:C:76[B]:MET:SD	1:C:166:ILE:HD11	2.49	0.53
1:F:208:LEU:HG	1:F:217:SER:HB2	1.91	0.53
1:C:218:PRO:HG3	1:C:250:MET:HE3	1.89	0.53
1:A:76[B]:MET:CE	1:F:257:ILE:HG21	2.39	0.53
1:A:109:VAL:HB	1:A:132:VAL:HG22	1.91	0.53
1:A:208:LEU:HG	1:A:217:SER:HB2	1.89	0.53
1:B:255:LEU:HB3	1:B:276:ILE:CD1	2.39	0.52
1:A:76[B]:MET:HE2	1:F:257:ILE:CG2	2.39	0.52
1:C:151:MET:HE3	1:C:276:ILE:HG21	1.92	0.52
1:A:76[A]:MET:HE1	1:A:166:ILE:HG13	1.90	0.52
1:A:76[B]:MET:HE1	1:F:257:ILE:CG2	2.39	0.52
1:D:56:GLU:OE1	1:D:56:GLU:C	2.47	0.52
1:F:157:ILE:CD1	1:F:162:VAL:CB	2.74	0.52
1:D:82:SER:HB2	1:D:128:THR:HG22	1.92	0.52
1:D:82:SER:CB	1:D:128:THR:HG22	2.40	0.52
1:A:76[B]:MET:CE	1:F:257:ILE:HG23	2.40	0.52
1:E:82:SER:CB	1:E:128:THR:HG22	2.39	0.52
1:E:294:GLN:CD	1:F:54:GLU:HG3	2.30	0.52
1:C:151:MET:HE3	1:C:276:ILE:CG2	2.40	0.52
1:D:76[B]:MET:HE2	1:D:166:ILE:HD11	1.90	0.51
1:C:92:VAL:O	1:C:96:LEU:HD22	2.11	0.51
1:D:106:HIS:CE1	1:D:267:ILE:CG1	2.93	0.51
1:D:43:LEU:CD2	1:D:79:MET:HE3	2.40	0.51
1:E:208:LEU:HG	1:E:217:SER:HB2	1.93	0.51
1:F:82:SER:CB	1:F:128:THR:HG22	2.41	0.51
1:F:289:VAL:O	1:F:293:LEU:HD23	2.10	0.51
1:E:151:MET:HG3	1:E:252:ARG:NE	2.26	0.51
1:E:240:GLU:HG2	1:E:296:LEU:HD22	1.93	0.51
1:A:151:MET:HE3	1:A:276:ILE:HG21	1.94	0.50
1:E:144:HIS:ND1	1:F:55:ARG:NH2	2.58	0.50
1:F:255:LEU:HB3	1:F:276:ILE:HD12	1.94	0.50
1:C:255:LEU:HB3	1:C:276:ILE:HD12	1.92	0.50
1:F:43:LEU:CD2	1:F:79:MET:HE3	2.42	0.50
1:F:76[A]:MET:HE1	1:F:166:ILE:HG13	1.92	0.50
1:C:218:PRO:CG	1:C:250:MET:CE	2.87	0.50
1:F:82:SER:HB2	1:F:128:THR:HG22	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:80:LYS:O	1:D:80:LYS:HG3	2.11	0.49
1:A:92:VAL:O	1:A:96:LEU:HD22	2.13	0.49
1:C:208:LEU:HG	1:C:217:SER:HB2	1.94	0.49
1:F:17:TRP:CZ2	1:F:20:GLY:HA2	2.48	0.49
1:A:52:ASN:OD1	1:A:54:GLU:O	2.31	0.48
1:E:43:LEU:CD2	1:E:79:MET:HE3	2.43	0.48
1:D:255:LEU:HB3	1:D:276:ILE:CD1	2.41	0.48
1:C:82:SER:HB2	1:C:128:THR:HG22	1.95	0.48
1:B:160:ASP:HB3	3:E:505:HOH:O	2.14	0.48
1:C:52:ASN:OD1	1:C:54:GLU:O	2.32	0.48
1:D:76[B]:MET:HE2	1:D:166:ILE:CD1	2.44	0.48
1:E:139:ARG:HH21	1:F:56:GLU:HG3	1.77	0.48
1:C:76[A]:MET:HE1	1:C:166:ILE:HG13	1.93	0.48
1:C:82:SER:CB	1:C:128:THR:HG22	2.43	0.47
1:D:17:TRP:CZ2	1:D:20:GLY:HA2	2.49	0.47
1:E:116:ASN:OD1	1:E:116:ASN:N	2.46	0.47
1:F:255:LEU:HB3	1:F:276:ILE:CD1	2.44	0.47
1:C:151:MET:CE	1:C:191:VAL:HB	2.44	0.47
1:C:17:TRP:CZ2	1:C:20:GLY:HA2	2.50	0.47
1:D:51:TRP:CE2	1:D:56:GLU:O	2.67	0.47
1:A:17:TRP:CZ2	1:A:20:GLY:HA2	2.49	0.47
1:E:17:TRP:CZ2	1:E:20:GLY:HA2	2.50	0.47
1:E:43:LEU:CB	1:E:79:MET:HE3	2.45	0.47
1:A:50:TYR:CD2	1:A:301:THR:HB	2.50	0.47
1:A:151:MET:CE	1:A:191:VAL:HB	2.45	0.47
1:B:75:LYS:NZ	1:E:256:TYR:O	2.38	0.47
1:A:55:ARG:HH21	1:A:55:ARG:HG3	1.76	0.47
1:A:151:MET:HG3	1:A:252:ARG:NE	2.29	0.46
1:E:16:GLY:HA2	1:E:95:LEU:HD11	1.96	0.46
1:B:17:TRP:CZ2	1:B:20:GLY:HA2	2.50	0.46
1:C:43:LEU:CD2	1:C:79:MET:HE3	2.45	0.46
1:B:208:LEU:HG	1:B:217:SER:HB2	1.97	0.46
1:D:51:TRP:NE1	1:D:56:GLU:O	2.48	0.46
1:E:89:ARG:HG2	1:E:89:ARG:HH11	1.81	0.46
1:B:117:HIS:N	1:B:125:THR:HG23	2.31	0.46
1:C:92:VAL:O	1:C:96:LEU:CD2	2.64	0.46
1:E:117:HIS:N	1:E:125:THR:HG23	2.31	0.46
1:D:253:THR:HB	1:F:76[B]:MET:HE1	1.98	0.46
1:E:117:HIS:H	1:E:125:THR:HG23	1.81	0.46
1:A:255:LEU:HB3	1:A:276:ILE:CD1	2.46	0.45
1:A:64:ASP:OD2	1:B:317:GLU:HA	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:106:HIS:CE1	1:D:267:ILE:HG13	2.52	0.45
1:B:43:LEU:CB	1:B:79:MET:HE3	2.47	0.45
1:F:233:LEU:HD11	1:F:270:ILE:HD11	1.98	0.45
1:A:76[B]:MET:HE1	1:F:257:ILE:HG21	1.99	0.45
1:B:302:SER:OG	1:B:304:GLN:HG3	2.16	0.45
1:A:233:LEU:HD11	1:A:270:ILE:HD11	1.99	0.45
1:D:172:TYR:OH	2:D:401:PLP:O3	2.28	0.45
1:E:144:HIS:HB2	1:F:55:ARG:CG	2.46	0.45
1:F:286:VAL:HG11	1:F:291:ARG:HH21	1.81	0.45
1:A:160:ASP:HB3	3:F:511:HOH:O	2.17	0.44
1:C:253:THR:OG1	1:E:165:ARG:HD2	2.18	0.44
1:B:50:TYR:CD2	1:B:301:THR:HB	2.53	0.44
1:E:144:HIS:HB2	1:F:55:ARG:HG3	2.00	0.44
1:C:219:PRO:HG2	1:C:221:THR:HG22	1.99	0.44
1:F:106:HIS:HE1	1:F:267:ILE:HG22	1.82	0.44
1:B:35:GLN:HE21	1:B:116:ASN:HB3	1.82	0.43
1:B:76[A]:MET:CE	1:E:257:ILE:CG2	2.96	0.43
1:C:16:GLY:HA2	1:C:95:LEU:HD11	1.99	0.43
1:D:264:CYS:HA	1:D:269:GLU:O	2.18	0.43
1:B:151:MET:HG3	1:B:252:ARG:NE	2.33	0.43
1:A:92:VAL:O	1:A:96:LEU:CD2	2.67	0.43
1:A:151:MET:HE2	1:A:191:VAL:HB	2.01	0.43
1:E:240:GLU:HG2	1:E:296:LEU:CD2	2.47	0.43
1:F:151:MET:HG3	1:F:252:ARG:NE	2.34	0.43
1:B:253:THR:HB	1:C:76[B]:MET:HE2	1.99	0.43
1:C:117:HIS:N	1:C:125:THR:HG23	2.34	0.43
1:D:16:GLY:HA2	1:D:95:LEU:HD11	2.00	0.43
1:F:231:LYS:HA	1:F:234:MET:HE2	2.01	0.43
1:A:251:ASP:HB3	1:D:159:ASP:OD2	2.19	0.43
1:B:76[A]:MET:HE1	1:E:257:ILE:CG2	2.49	0.43
1:A:117:HIS:N	1:A:125:THR:HG23	2.34	0.43
1:C:102:ARG:HH11	1:C:102:ARG:HG2	1.83	0.43
1:E:294:GLN:OE1	1:F:54:GLU:CG	2.67	0.42
1:A:76[A]:MET:HE2	1:A:166:ILE:CG1	2.47	0.42
1:D:92:VAL:O	1:D:96:LEU:CD2	2.66	0.42
1:D:233:LEU:HD21	1:D:270:ILE:HD11	2.01	0.42
1:A:172:TYR:OH	2:A:401:PLP:O3	2.02	0.42
1:E:16:GLY:HA2	1:E:95:LEU:CD1	2.50	0.42
1:E:144:HIS:HB3	1:F:55:ARG:CG	2.43	0.42
1:C:50:TYR:CD2	1:C:301:THR:HB	2.54	0.42
1:E:144:HIS:CE1	1:E:145:THR:CG2	3.03	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:123:PHE:CG	1:A:124:PRO:HD2	2.55	0.42
1:B:190:SER:O	1:B:203:PRO:HD3	2.20	0.42
1:B:292:ARG:HD2	1:B:292:ARG:HA	1.91	0.42
1:E:143:VAL:HG12	1:F:54:GLU:HB3	2.01	0.41
1:B:92:VAL:O	1:B:96:LEU:CD2	2.68	0.41
1:F:55:ARG:NH2	1:F:303:GLY:O	2.48	0.41
1:B:117:HIS:H	1:B:125:THR:HG23	1.84	0.41
1:D:267:ILE:HD13	3:D:513:HOH:O	2.20	0.41
1:A:106:HIS:CE1	1:A:267:ILE:CG1	2.97	0.41
1:B:201:GLU:OE1	2:B:401:PLP:N1	2.54	0.41
1:B:256:TYR:HB2	1:C:76[B]:MET:HG2	2.03	0.41
1:D:302:SER:OG	1:D:304:GLN:HG3	2.21	0.41
1:E:123:PHE:CG	1:E:124:PRO:HD2	2.56	0.41
1:F:198:LYS:HA	1:F:198:LYS:HD3	1.91	0.41
1:C:16:GLY:HA2	1:C:95:LEU:CD1	2.51	0.41
1:C:123:PHE:CG	1:C:124:PRO:HD2	2.56	0.41
1:D:43:LEU:HD23	1:D:79:MET:HE3	2.01	0.41
1:D:51:TRP:CZ2	1:D:56:GLU:O	2.74	0.41
1:D:241:LEU:HD21	1:D:292:ARG:HG2	2.03	0.41
1:D:299:GLY:HA3	1:D:305:LEU:HD22	2.01	0.41
1:F:123:PHE:CG	1:F:124:PRO:HD2	2.56	0.41
1:F:293:LEU:HD13	1:F:293:LEU:HA	1.86	0.41
1:B:76[A]:MET:CE	1:E:257:ILE:HG21	2.50	0.41
1:A:76[B]:MET:HE1	1:F:257:ILE:HG23	2.01	0.40
1:F:43:LEU:HD23	1:F:79:MET:HE3	2.03	0.40
1:F:50:TYR:CD2	1:F:301:THR:HB	2.57	0.40
1:F:157:ILE:HG12	1:F:162:VAL:HB	2.02	0.40
1:A:256:TYR:HB2	1:D:76[B]:MET:SD	2.62	0.40
1:C:256:TYR:HB2	1:E:76[B]:MET:HG2	2.02	0.40
1:E:144:HIS:NE2	1:E:145:THR:HG23	2.35	0.40
1:E:264:CYS:HA	1:E:269:GLU:O	2.21	0.40
1:B:76[A]:MET:HE1	1:E:257:ILE:HG21	2.04	0.40
1:C:151:MET:HG3	1:C:252:ARG:NE	2.36	0.40
1:C:302:SER:OG	1:C:304:GLN:HG3	2.21	0.40
1:E:43:LEU:HB2	1:E:79:MET:HE3	2.04	0.40
1:F:149:ALA:O	1:F:276:ILE:HA	2.21	0.40
1:E:50:TYR:CD2	1:E:301:THR:HB	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	304/317 (96%)	293 (96%)	10 (3%)	1 (0%)	41	47
1	B	305/317 (96%)	296 (97%)	9 (3%)	0	100	100
1	C	307/317 (97%)	297 (97%)	9 (3%)	1 (0%)	41	47
1	D	304/317 (96%)	296 (97%)	8 (3%)	0	100	100
1	E	307/317 (97%)	297 (97%)	10 (3%)	0	100	100
1	F	305/317 (96%)	294 (96%)	11 (4%)	0	100	100
All	All	1832/1902 (96%)	1773 (97%)	57 (3%)	2 (0%)	51	63

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	55	ARG
1	C	55	ARG

5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	263/276 (95%)	239 (91%)	24 (9%)	9	8
1	B	265/276 (96%)	243 (92%)	22 (8%)	11	11
1	C	266/276 (96%)	246 (92%)	20 (8%)	13	13
1	D	265/276 (96%)	242 (91%)	23 (9%)	10	9
1	E	265/276 (96%)	247 (93%)	18 (7%)	16	16

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	263/276 (95%)	239 (91%)	24 (9%)	9	8
All	All	1587/1656 (96%)	1456 (92%)	131 (8%)	12	11

All (131) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	55	ARG
1	A	76[A]	MET
1	A	76[B]	MET
1	A	80	LYS
1	A	82	SER
1	A	96	LEU
1	A	109	VAL
1	A	111	SER
1	A	117	HIS
1	A	125	THR
1	A	128	THR
1	A	133	THR
1	A	145	THR
1	A	157	ILE
1	A	158	SER
1	A	196	ARG
1	A	217	SER
1	A	225	LEU
1	A	233	LEU
1	A	238	GLU
1	A	242	ASP
1	A	259	GLU
1	A	267	ILE
1	A	309	LYS
1	B	14	ARG
1	B	26	ASP
1	B	29	SER
1	B	48	ARG
1	B	82	SER
1	B	96	LEU
1	B	100	GLU
1	B	109	VAL
1	B	111	SER
1	B	125	THR
1	B	128	THR
1	B	133	THR

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Mol	Chain	Res	Type
1	B	145	THR
1	B	157	ILE
1	B	196	ARG
1	B	202	THR
1	B	217	SER
1	B	225	LEU
1	B	238	GLU
1	B	242	ASP
1	B	259	GLU
1	B	309	LYS
1	C	12	PRO
1	C	54	GLU
1	C	76[A]	MET
1	C	76[B]	MET
1	C	82	SER
1	C	83	MET
1	C	96	LEU
1	C	109	VAL
1	C	125	THR
1	C	128	THR
1	C	133	THR
1	C	158	SER
1	C	196	ARG
1	C	217	SER
1	C	221	THR
1	C	225	LEU
1	C	238	GLU
1	C	242	ASP
1	C	293	LEU
1	C	309	LYS
1	D	48	ARG
1	D	54	GLU
1	D	56	GLU
1	D	76[A]	MET
1	D	76[B]	MET
1	D	82	SER
1	D	96	LEU
1	D	116	ASN
1	D	117	HIS
1	D	125	THR
1	D	128	THR
1	D	133	THR

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Mol	Chain	Res	Type
1	D	157	ILE
1	D	196	ARG
1	D	202	THR
1	D	217	SER
1	D	225	LEU
1	D	238	GLU
1	D	242	ASP
1	D	259	GLU
1	D	292	ARG
1	D	304	GLN
1	D	305	LEU
1	E	116	ASN
1	E	117	HIS
1	E	125	THR
1	E	128	THR
1	E	133	THR
1	E	144	HIS
1	E	157	ILE
1	E	158	SER
1	E	196	ARG
1	E	202	THR
1	E	217	SER
1	E	225	LEU
1	E	238	GLU
1	E	240	GLU
1	E	259	GLU
1	E	267	ILE
1	E	305	LEU
1	E	309	LYS
1	F	21	GLN
1	F	76[A]	MET
1	F	76[B]	MET
1	F	80	LYS
1	F	82	SER
1	F	83	MET
1	F	95	LEU
1	F	128	THR
1	F	133	THR
1	F	145	THR
1	F	158	SER
1	F	196	ARG
1	F	202	THR

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Mol	Chain	Res	Type
1	F	217	SER
1	F	225	LEU
1	F	233	LEU
1	F	238	GLU
1	F	242	ASP
1	F	259	GLU
1	F	286	VAL
1	F	292	ARG
1	F	304	GLN
1	F	306	GLU
1	F	309	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	106	HIS
1	B	106	HIS
1	B	116	ASN
1	C	106	HIS
1	D	21	GLN
1	D	106	HIS
1	E	106	HIS
1	F	106	HIS

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](#)

6 ligands are modelled in this entry.

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	D	401	1	15,15,16	3.61	5 (33%)	20,22,23	2.65	11 (55%)
2	PLP	E	401	1	15,15,16	2.83	4 (26%)	20,22,23	3.61	11 (55%)
2	PLP	A	401	1	15,15,16	3.37	3 (20%)	20,22,23	1.97	11 (55%)
2	PLP	C	401	1	15,15,16	3.72	7 (46%)	20,22,23	3.82	12 (60%)
2	PLP	B	401	1	15,15,16	3.93	6 (40%)	20,22,23	2.72	10 (50%)
2	PLP	F	401	1	15,15,16	3.00	5 (33%)	20,22,23	3.04	10 (50%)

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	D	401	1	-	0/6/6/8	0/1/1/1
2	PLP	E	401	1	-	5/6/6/8	0/1/1/1
2	PLP	A	401	1	-	0/6/6/8	0/1/1/1
2	PLP	C	401	1	-	0/6/6/8	0/1/1/1
2	PLP	B	401	1	-	0/6/6/8	0/1/1/1
2	PLP	F	401	1	-	0/6/6/8	0/1/1/1

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	PLP	C3-C2	10.10	1.51	1.40
2	D	401	PLP	C5-C4	10.06	1.51	1.40
2	C	401	PLP	C3-C2	9.81	1.50	1.40
2	B	401	PLP	C5-C4	9.75	1.51	1.40
2	E	401	PLP	C3-C2	8.29	1.49	1.40
2	A	401	PLP	C5-C4	8.17	1.49	1.40
2	A	401	PLP	C3-C2	8.04	1.49	1.40
2	D	401	PLP	C3-C2	7.55	1.48	1.40
2	F	401	PLP	C3-C2	7.42	1.48	1.40
2	F	401	PLP	C5-C4	7.02	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	401	PLP	C5-C4	6.68	1.47	1.40
2	E	401	PLP	C5-C4	5.84	1.47	1.40
2	A	401	PLP	C3-C4	4.56	1.49	1.40
2	C	401	PLP	P-O1P	4.40	1.64	1.50
2	C	401	PLP	C2A-C2	3.63	1.56	1.50
2	C	401	PLP	C3-C4	3.55	1.47	1.40
2	F	401	PLP	C3-C4	3.42	1.47	1.40
2	D	401	PLP	C4A-C4	-3.36	1.44	1.51
2	B	401	PLP	C4A-C4	-3.03	1.45	1.51
2	F	401	PLP	C6-N1	-2.88	1.28	1.34
2	B	401	PLP	C6-N1	2.60	1.39	1.34
2	C	401	PLP	C6-C5	2.56	1.43	1.37
2	B	401	PLP	C3-C4	2.48	1.45	1.40
2	D	401	PLP	P-O3P	-2.37	1.45	1.54
2	F	401	PLP	C2-N1	2.35	1.38	1.33
2	E	401	PLP	C3-C4	2.30	1.44	1.40
2	D	401	PLP	C3-C4	2.29	1.44	1.40
2	B	401	PLP	C6-C5	2.26	1.42	1.37
2	C	401	PLP	C2-N1	2.22	1.38	1.33
2	E	401	PLP	P-O4P	-2.08	1.53	1.60

All (65) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	401	PLP	C4A-C4-C5	11.30	132.58	120.94
2	C	401	PLP	O2P-P-O4P	-7.87	85.80	106.73
2	C	401	PLP	C4A-C4-C5	6.61	127.74	120.94
2	F	401	PLP	C6-C5-C4	6.52	123.29	118.16
2	C	401	PLP	O4P-C5A-C5	5.83	120.45	109.35
2	F	401	PLP	C5A-C5-C6	-5.76	109.89	119.37
2	D	401	PLP	C4A-C4-C5	5.75	126.86	120.94
2	F	401	PLP	C4A-C4-C5	5.72	126.83	120.94
2	C	401	PLP	C3-C2-N1	-5.42	113.77	120.77
2	C	401	PLP	C3-C4-C5	-5.40	112.91	118.74
2	F	401	PLP	C3-C4-C5	-5.16	113.17	118.74
2	C	401	PLP	O3P-P-O4P	-4.99	93.45	106.73
2	B	401	PLP	C4A-C4-C5	4.88	125.96	120.94
2	B	401	PLP	C2A-C2-C3	-4.47	115.36	120.89
2	B	401	PLP	O3P-P-O2P	4.42	124.55	107.64
2	E	401	PLP	C3-C4-C5	-4.41	113.97	118.74
2	E	401	PLP	C4A-C4-C3	-4.19	113.41	120.50
2	B	401	PLP	O3P-P-O1P	4.07	126.63	110.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	401	PLP	O2P-P-O4P	-4.07	95.91	106.73
2	D	401	PLP	C6-C5-C4	4.00	121.31	118.16
2	E	401	PLP	C6-C5-C4	3.96	121.27	118.16
2	B	401	PLP	O2P-P-O1P	-3.95	95.22	110.68
2	C	401	PLP	C4-C3-C2	3.94	125.89	120.07
2	D	401	PLP	C5A-C5-C6	-3.81	113.10	119.37
2	A	401	PLP	C6-N1-C2	3.68	125.98	119.17
2	E	401	PLP	O2P-P-O1P	3.64	124.93	110.68
2	D	401	PLP	C6-N1-C2	3.49	125.63	119.17
2	E	401	PLP	C5A-C5-C6	-3.46	113.68	119.37
2	E	401	PLP	O3-C3-C2	3.41	124.93	117.49
2	E	401	PLP	C6-N1-C2	3.25	125.18	119.17
2	C	401	PLP	C2A-C2-N1	3.24	124.00	117.67
2	D	401	PLP	C3-C4-C5	-2.98	115.52	118.74
2	B	401	PLP	C6-C5-C4	2.95	120.48	118.16
2	C	401	PLP	C5-C6-N1	2.95	128.73	123.82
2	F	401	PLP	C2A-C2-C3	-2.92	117.28	120.89
2	B	401	PLP	C2A-C2-N1	2.90	123.34	117.67
2	E	401	PLP	C3-C2-N1	-2.90	117.02	120.77
2	B	401	PLP	O4P-C5A-C5	2.83	114.75	109.35
2	A	401	PLP	O3P-P-O1P	2.77	121.53	110.68
2	F	401	PLP	C2A-C2-N1	2.76	123.07	117.67
2	D	401	PLP	O2P-P-O1P	2.67	121.11	110.68
2	F	401	PLP	O3P-P-O4P	-2.65	99.68	106.73
2	F	401	PLP	O3-C3-C4	2.60	124.95	118.10
2	B	401	PLP	O3P-P-O4P	-2.59	99.84	106.73
2	D	401	PLP	O3P-P-O2P	2.59	117.53	107.64
2	C	401	PLP	O2P-P-O1P	2.56	120.69	110.68
2	E	401	PLP	O3P-P-O2P	2.55	117.38	107.64
2	F	401	PLP	O3P-P-O1P	2.49	120.42	110.68
2	C	401	PLP	O4P-P-O1P	2.46	113.37	106.47
2	B	401	PLP	C3-C4-C5	-2.38	116.17	118.74
2	A	401	PLP	C2A-C2-N1	2.37	122.31	117.67
2	A	401	PLP	O3-C3-C2	2.34	122.60	117.49
2	A	401	PLP	C6-C5-C4	-2.33	116.32	118.16
2	E	401	PLP	O3P-P-O1P	-2.31	101.64	110.68
2	A	401	PLP	O4P-P-O1P	-2.31	100.00	106.47
2	A	401	PLP	C3-C2-N1	-2.30	117.79	120.77
2	C	401	PLP	O3P-P-O2P	2.26	116.27	107.64
2	A	401	PLP	O2P-P-O4P	2.24	112.69	106.73
2	A	401	PLP	C4-C3-C2	-2.22	116.79	120.07
2	A	401	PLP	O4P-C5A-C5	2.15	113.45	109.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	401	PLP	C6-N1-C2	2.12	123.10	119.17
2	D	401	PLP	O3P-P-O4P	-2.12	101.09	106.73
2	D	401	PLP	C2A-C2-N1	2.10	121.78	117.67
2	A	401	PLP	C4A-C4-C3	-2.02	117.08	120.50
2	D	401	PLP	C5-C6-N1	-2.01	120.47	123.82

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	401	PLP	C4-C5-C5A-O4P
2	E	401	PLP	C6-C5-C5A-O4P
2	E	401	PLP	C5A-O4P-P-O2P
2	E	401	PLP	C5A-O4P-P-O3P
2	E	401	PLP	C5A-O4P-P-O1P

There are no ring outliers.

5 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	401	PLP	1	0
2	E	401	PLP	1	0
2	A	401	PLP	1	0
2	C	401	PLP	1	0
2	B	401	PLP	1	0

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	305/317 (96%)	0.06	3 (0%) 82 88	37, 57, 82, 110	0
1	B	306/317 (96%)	0.06	5 (1%) 72 80	36, 55, 73, 108	0
1	C	308/317 (97%)	0.02	3 (0%) 82 88	36, 53, 78, 121	0
1	D	305/317 (96%)	-0.02	2 (0%) 87 92	35, 54, 81, 114	0
1	E	307/317 (96%)	0.09	8 (2%) 56 65	34, 53, 82, 115	0
1	F	306/317 (96%)	-0.06	1 (0%) 94 97	35, 53, 83, 100	0
All	All	1837/1902 (96%)	0.03	22 (1%) 79 86	34, 54, 81, 121	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	117	HIS	4.9
1	D	117	HIS	4.6
1	E	117	HIS	4.2
1	A	117	HIS	3.9
1	E	144	HIS	3.5
1	E	195	SER	2.9
1	D	51	TRP	2.6
1	B	23	ILE	2.5
1	A	222	ALA	2.4
1	B	117	HIS	2.4
1	E	158	SER	2.4
1	E	15	TYR	2.4
1	B	115	ILE	2.3
1	E	123	PHE	2.3
1	A	27	GLN	2.3
1	B	95	LEU	2.1
1	C	20	GLY	2.1
1	B	26	ASP	2.1
1	F	194	ASN	2.0

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Mol	Chain	Res	Type	RSRZ
1	E	196	ARG	2.0
1	C	157	ILE	2.0
1	E	30	LEU	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	PLP	E	401	15/16	0.97	0.13	41,44,48,48	0
2	PLP	B	401	15/16	0.98	0.10	41,49,53,55	0
2	PLP	C	401	15/16	0.98	0.11	41,47,49,53	0
2	PLP	D	401	15/16	0.98	0.12	45,48,53,53	0
2	PLP	A	401	15/16	0.98	0.11	46,49,52,54	0
2	PLP	F	401	15/16	0.99	0.10	39,42,44,46	0

6.5 Other polymers [i](#)

There are no such residues in this entry.