Full wwPDB X-ray Structure Validation Report (i)

Jun 24, 2024 – 10:39 PM EDT

PDB ID	:	5O5C
Title	:	The crystal structure of DfoJ, the desferrioxamine biosynthetic pathway lysine decarboxylase from the fire blight disease pathogen Erwinia amylovora
Authors	:	Salomone-Stagni, M.; Bartho, J.D.; Polsinelli, I.; Bellini, D.; Walsh, M.A.; Demitri, N.; Benini, S.
Deposited on	:	2017-06-01
Resolution	:	2.10 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 (i)) were used in the production of this report:

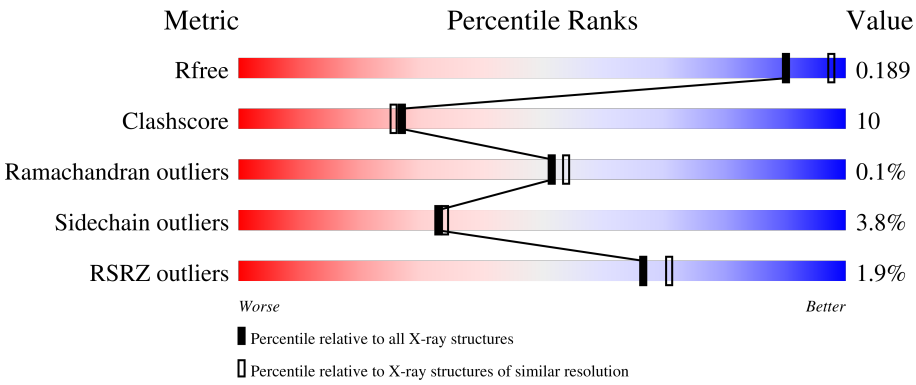
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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	519	3%, 68%, 18%, •, 11%
1	B	519	2%, 71%, 17%, •, 10%
1	C	519	2%, 68%, 18%, ••, 11%
1	D	519	2%, 72%, 17%, •, 10%
1	E	519	%, 74%, 13%, •, 12%

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Mol	Chain	Length	Quality of chain
1	F	519	% 72% 15% • 10%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 22003 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.

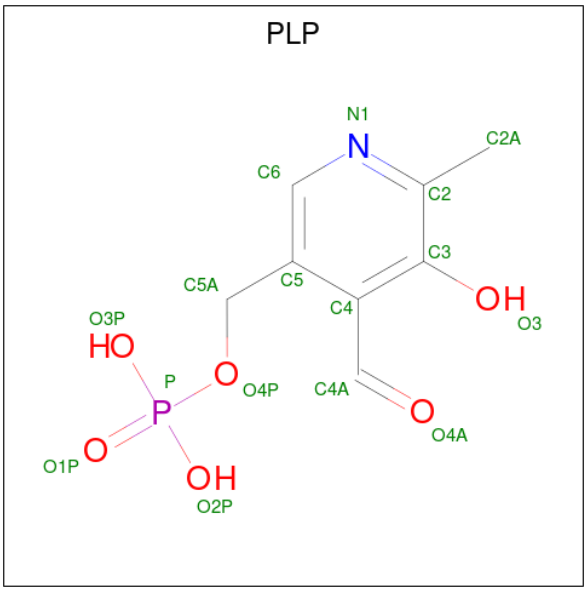
- Molecule 1 is a protein called Putative decarboxylase involved in desferrioxamine biosynthesis.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	464	3621	2302	641	661	17	0	0	0
1	B	468	3645	2316	645	667	17	0	0	0
1	C	462	3599	2289	635	658	17	0	0	0
1	D	468	3646	2317	645	667	17	0	0	0
1	E	457	3565	2266	631	651	17	0	0	0
1	F	467	3637	2312	644	664	17	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP D4I245
A	0	ALA	-	expression tag	UNP D4I245
B	-1	GLY	-	expression tag	UNP D4I245
B	0	ALA	-	expression tag	UNP D4I245
C	-1	GLY	-	expression tag	UNP D4I245
C	0	ALA	-	expression tag	UNP D4I245
D	-1	GLY	-	expression tag	UNP D4I245
D	0	ALA	-	expression tag	UNP D4I245
E	-1	GLY	-	expression tag	UNP D4I245
E	0	ALA	-	expression tag	UNP D4I245
F	-1	GLY	-	expression tag	UNP D4I245
F	0	ALA	-	expression tag	UNP D4I245

- 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		
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.

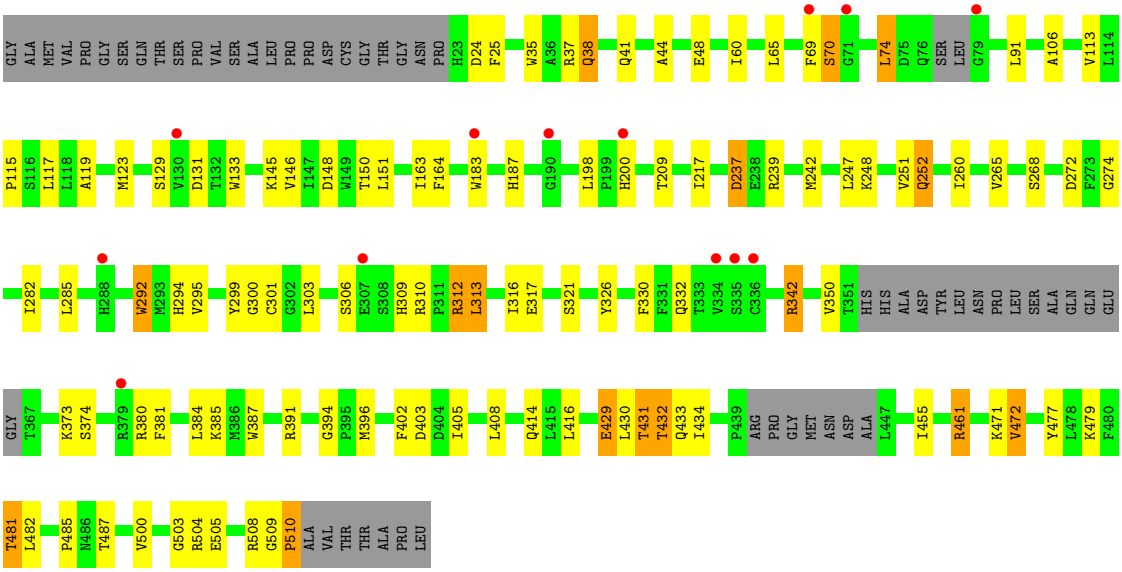
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	30	Total	O	0	0
			30	30		
3	B	31	Total	O	0	0
			31	31		
3	C	43	Total	O	0	0
			43	43		
3	D	42	Total	O	0	0
			42	42		
3	E	23	Total	O	0	0
			23	23		
3	F	31	Total	O	0	0
			31	31		

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.

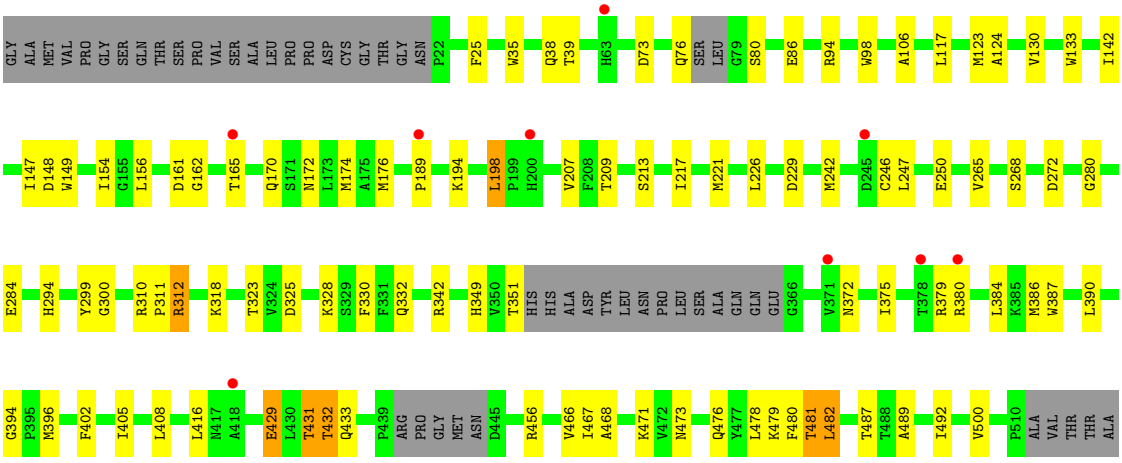
• Molecule 1: Putative decarboxylase involved in desferrioxamine biosynthesis

Chain A:



• Molecule 1: Putative decarboxylase involved in desferrioxamine biosynthesis

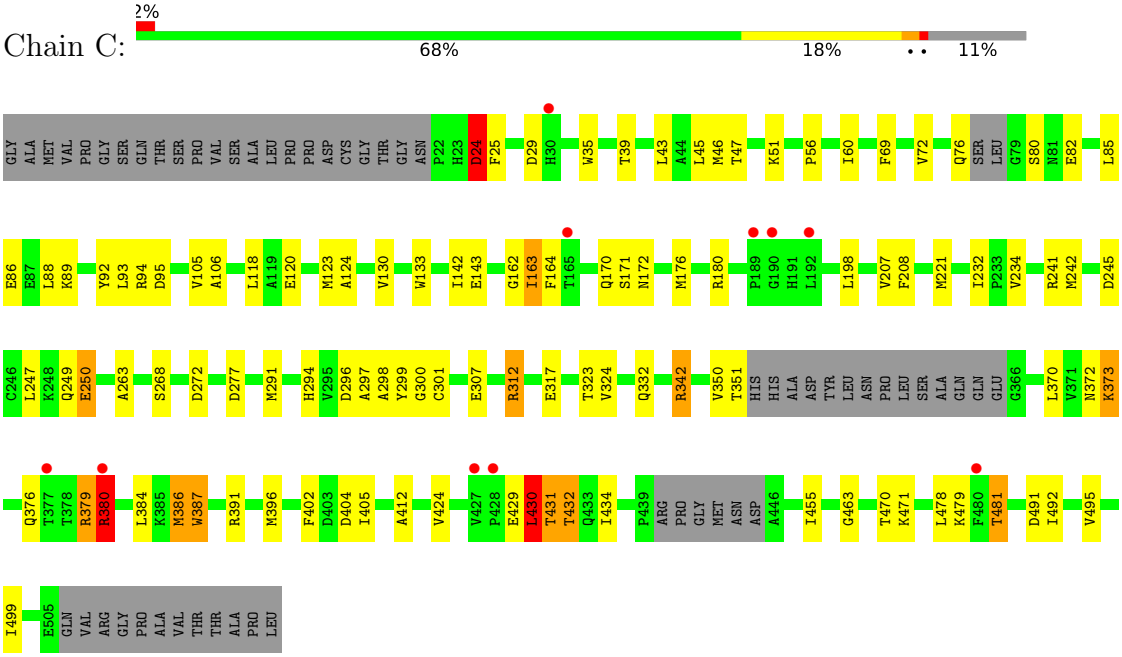
Chain B:



PRO
LEU

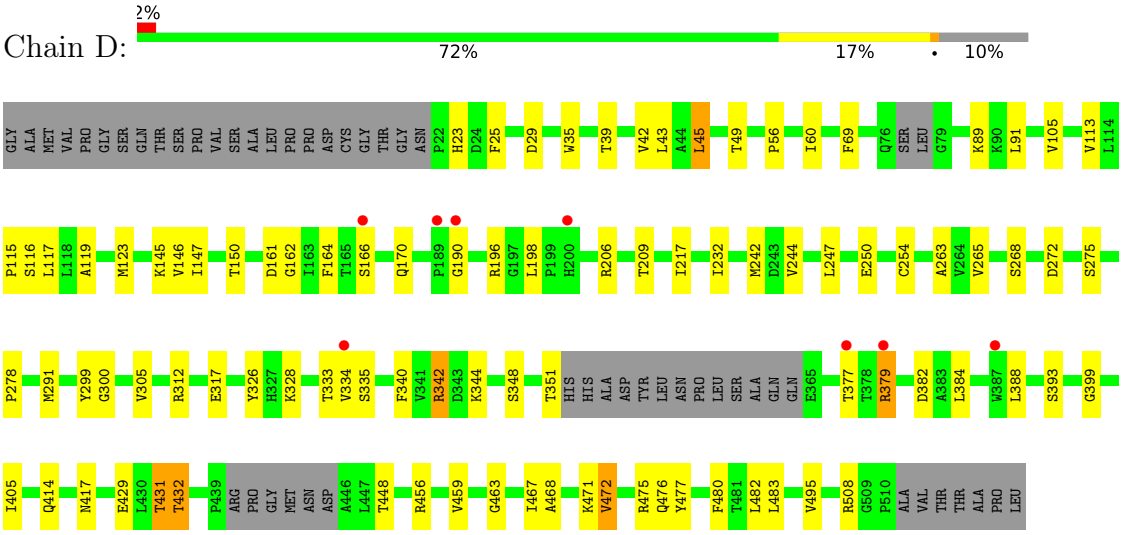
• Molecule 1: Putative decarboxylase involved in desferrioxamine biosynthesis

Chain C:



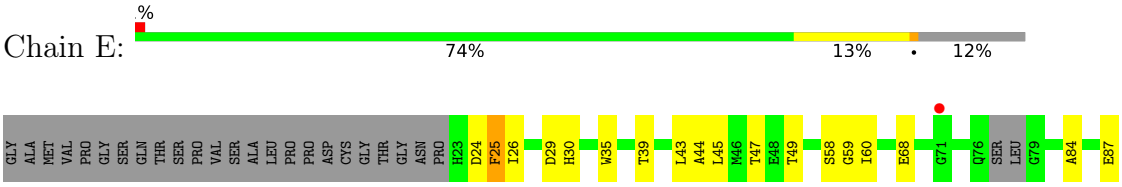
• Molecule 1: Putative decarboxylase involved in desferrioxamine biosynthesis

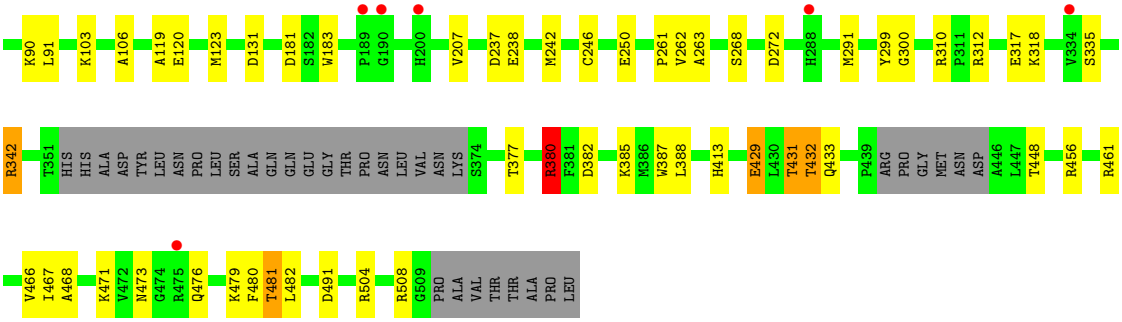
Chain D:



• Molecule 1: Putative decarboxylase involved in desferrioxamine biosynthesis

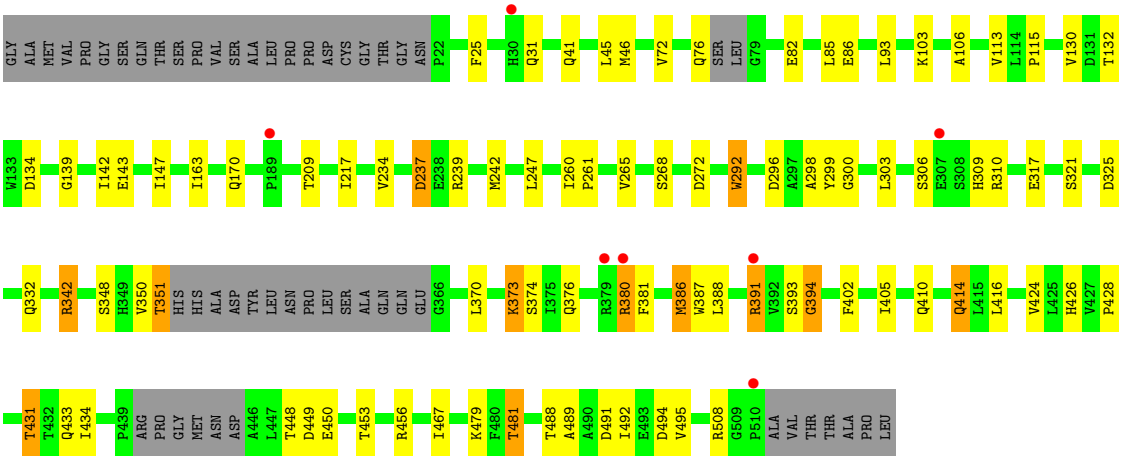
Chain E:





- Molecule 1: Putative decarboxylase involved in desferrioxamine biosynthesis

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α, β, γ	269.79Å 269.79Å 56.19Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	233.65 – 2.10 47.41 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.9 (233.65-2.10) 99.9 (47.41-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	110.40 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.165 , 0.187 0.169 , 0.189	Depositor DCC
R_{free} test set	13243 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å^2)	29.4	Xtriage
Anisotropy	0.035	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 45.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.000 for -h,-k,l 0.000 for h,-h-k,-l 0.036 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	22003	wwPDB-VP
Average B, all atoms (Å^2)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 23.63 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.4894e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 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	0.79	2/3704 (0.1%)	0.94	11/5031 (0.2%)
1	B	0.82	2/3729 (0.1%)	0.95	8/5065 (0.2%)
1	C	0.79	0/3682	1.00	17/5001 (0.3%)
1	D	0.75	0/3730	0.91	5/5066 (0.1%)
1	E	0.78	1/3646 (0.0%)	0.94	9/4950 (0.2%)
1	F	0.81	1/3721 (0.0%)	0.93	4/5054 (0.1%)
All	All	0.79	6/22212 (0.0%)	0.95	54/30167 (0.2%)

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	2
1	B	0	1
1	F	0	1
All	All	0	4

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	292	TRP	CB-CG	-9.63	1.32	1.50
1	E	237	ASP	CB-CG	-5.86	1.39	1.51
1	A	429	GLU	CG-CD	-5.33	1.44	1.51
1	B	133	TRP	CE3-CZ3	-5.33	1.29	1.38
1	F	394	GLY	N-CA	5.07	1.53	1.46
1	B	98	TRP	CB-CG	-5.01	1.41	1.50

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	380	ARG	NE-CZ-NH2	-15.33	112.64	120.30
1	C	380	ARG	NE-CZ-NH1	11.11	125.86	120.30
1	E	380	ARG	NE-CZ-NH2	-10.93	114.84	120.30
1	E	380	ARG	NE-CZ-NH1	10.70	125.65	120.30
1	A	380	ARG	NE-CZ-NH2	-10.07	115.26	120.30
1	F	342	ARG	NE-CZ-NH2	-9.57	115.52	120.30
1	E	342	ARG	NE-CZ-NH1	8.61	124.60	120.30
1	C	379	ARG	NE-CZ-NH2	-8.57	116.02	120.30
1	A	380	ARG	NE-CZ-NH1	8.35	124.48	120.30
1	F	386	MET	CG-SD-CE	7.93	112.89	100.20
1	A	237	ASP	CB-CG-OD2	-7.84	111.24	118.30
1	E	342	ARG	NE-CZ-NH2	-7.71	116.44	120.30
1	C	379	ARG	NE-CZ-NH1	7.13	123.86	120.30
1	A	342	ARG	NE-CZ-NH2	-7.10	116.75	120.30
1	C	277	ASP	CB-CG-OD1	6.66	124.30	118.30
1	D	379	ARG	NE-CZ-NH1	6.63	123.61	120.30
1	F	342	ARG	NE-CZ-NH1	6.62	123.61	120.30
1	A	342	ARG	NE-CZ-NH1	6.60	123.60	120.30
1	B	312	ARG	NE-CZ-NH1	6.56	123.58	120.30
1	D	342	ARG	NE-CZ-NH1	6.50	123.55	120.30
1	A	312	ARG	NE-CZ-NH1	6.42	123.51	120.30
1	B	148	ASP	CB-CG-OD1	6.41	124.07	118.30
1	A	312	ARG	NE-CZ-NH2	-6.38	117.11	120.30
1	C	277	ASP	CB-CG-OD2	-6.34	112.59	118.30
1	C	342	ARG	NE-CZ-NH2	-6.07	117.26	120.30
1	D	161	ASP	CB-CG-OD1	6.06	123.76	118.30
1	C	312	ARG	NE-CZ-NH1	6.03	123.31	120.30
1	C	312	ARG	NE-CZ-NH2	-6.02	117.29	120.30
1	D	379	ARG	NE-CZ-NH2	-6.02	117.29	120.30
1	B	380	ARG	NE-CZ-NH1	6.00	123.30	120.30
1	D	342	ARG	NE-CZ-NH2	-6.00	117.30	120.30
1	A	237	ASP	CB-CA-C	-5.87	98.66	110.40
1	E	480	PHE	CB-CA-C	-5.80	98.80	110.40
1	C	430	LEU	CA-CB-CG	5.80	128.63	115.30
1	E	237	ASP	CB-CA-C	-5.76	98.89	110.40
1	C	391	ARG	NE-CZ-NH2	-5.74	117.43	120.30
1	A	237	ASP	CB-CG-OD1	5.67	123.40	118.30
1	C	386	MET	CG-SD-CE	5.55	109.08	100.20
1	B	148	ASP	CB-CG-OD2	-5.50	113.35	118.30
1	C	85	LEU	CA-CB-CG	5.46	127.85	115.30
1	A	313	LEU	CA-CB-CG	5.45	127.83	115.30
1	C	180	ARG	NE-CZ-NH2	-5.39	117.60	120.30
1	E	242	MET	CG-SD-CE	5.39	108.82	100.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	272	ASP	CB-CG-OD1	5.38	123.14	118.30
1	E	181	ASP	CB-CG-OD1	5.31	123.08	118.30
1	B	229	ASP	CB-CG-OD2	-5.28	113.55	118.30
1	B	198	LEU	CA-CB-CG	5.24	127.35	115.30
1	E	480	PHE	CB-CG-CD2	-5.24	117.13	120.80
1	A	461	ARG	NE-CZ-NH1	5.15	122.88	120.30
1	C	391	ARG	NE-CZ-NH1	5.11	122.86	120.30
1	B	161	ASP	CB-CG-OD1	5.09	122.88	118.30
1	C	342	ARG	NE-CZ-NH1	5.06	122.83	120.30
1	C	163	ILE	CB-CA-C	-5.03	101.53	111.60
1	B	325	ASP	CB-CG-OD1	5.01	122.81	118.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	394	GLY	Peptide
1	A	509	GLY	Peptide
1	B	394	GLY	Peptide
1	F	394	GLY	Peptide

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	3621	0	3592	82	2
1	B	3645	0	3615	83	1
1	C	3599	0	3568	109	0
1	D	3646	0	3617	71	1
1	E	3565	0	3531	41	3
1	F	3637	0	3608	74	3
2	A	15	0	6	0	0
2	B	15	0	7	5	0
2	C	15	0	6	1	0
2	D	15	0	6	4	0
2	E	15	0	7	0	0
2	F	15	0	6	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	30	0	0	0	0
3	B	31	0	0	3	0
3	C	43	0	0	2	0
3	D	42	0	0	1	0
3	E	23	0	0	0	0
3	F	31	0	0	1	0
All	All	22003	0	21569	442	5

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 (442) 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:D:471:LYS:NZ	1:D:476:GLN:OE1	1.74	1.18
1:B:328:LYS:NZ	2:B:601:PLP:C4A	2.07	1.17
1:A:292:TRP:HH2	1:A:321:SER:OG	1.28	1.13
1:A:74:LEU:HD21	1:B:390:LEU:HD13	1.25	1.12
1:D:328:LYS:NZ	2:D:601:PLP:C4A	2.13	1.11
1:C:176:MET:HE1	1:C:207:VAL:HG11	1.32	1.08
1:A:292:TRP:CH2	1:A:321:SER:OG	2.01	1.06
1:C:60:ILE:HD12	1:C:95:ASP:OD1	1.55	1.06
1:D:209:THR:HG22	1:D:265:VAL:HB	1.38	1.02
1:B:328:LYS:HZ2	2:B:601:PLP:C4A	1.71	0.99
1:B:332:GLN:CG	1:B:386:MET:HE2	1.93	0.99
1:B:209:THR:HG22	1:B:265:VAL:HB	1.41	0.98
1:E:456:ARG:NH1	1:E:467:ILE:O	1.98	0.97
1:A:163:ILE:HD11	1:A:373:LYS:HE3	1.45	0.95
1:D:414:GLN:O	1:D:417:ASN:OD1	1.84	0.95
1:B:312:ARG:NH2	1:B:429:GLU:O	1.98	0.94
1:B:408:LEU:HD23	1:B:482:LEU:HD21	1.49	0.92
1:A:312:ARG:NH2	1:A:429:GLU:O	2.02	0.92
1:D:328:LYS:HZ1	2:D:601:PLP:C4A	1.77	0.91
1:C:299:TYR:OH	1:C:431:THR:HG22	1.69	0.90
1:B:328:LYS:HZ1	2:B:601:PLP:C4A	1.77	0.90
1:C:106:ALA:O	1:C:481:THR:HG23	1.70	0.90
1:D:113:VAL:HG12	1:D:115:PRO:HD2	1.54	0.88
1:F:292:TRP:HZ3	1:F:321:SER:HG	0.94	0.88
1:F:292:TRP:HZ3	1:F:321:SER:OG	1.56	0.88
1:D:190:GLY:O	1:D:196:ARG:NH2	2.07	0.87
1:A:317:GLU:O	1:A:342:ARG:NH2	2.07	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:328:LYS:HZ2	2:D:601:PLP:C4A	1.85	0.86
1:F:292:TRP:CZ3	1:F:321:SER:OG	2.26	0.86
1:D:146:VAL:O	1:D:150:THR:HG23	1.74	0.86
1:F:209:THR:HG22	1:F:265:VAL:HB	1.57	0.86
1:D:456:ARG:NH1	1:D:467:ILE:O	2.09	0.85
1:A:74:LEU:CD2	1:B:390:LEU:HD13	2.05	0.84
1:C:130:VAL:HG12	1:C:370:LEU:HD12	1.58	0.83
1:C:163:ILE:HD11	1:C:373:LYS:CD	2.09	0.83
1:D:312:ARG:NH2	1:D:429:GLU:O	2.12	0.83
1:F:103:LYS:NZ	1:F:494:ASP:OD2	2.12	0.82
1:B:332:GLN:HG3	1:B:386:MET:HE2	1.62	0.81
1:D:150:THR:HG21	1:D:326:TYR:OH	1.80	0.81
1:F:209:THR:HG21	1:F:217:ILE:HG21	1.60	0.81
1:E:312:ARG:NH2	1:E:429:GLU:O	2.14	0.81
1:C:294:HIS:CE1	1:C:323:THR:HG23	2.16	0.80
1:A:163:ILE:CD1	1:A:373:LYS:HE3	2.11	0.80
1:D:272:ASP:O	1:D:432:THR:HG21	1.81	0.80
1:B:294:HIS:HE1	1:B:323:THR:HG23	1.47	0.80
1:E:317:GLU:O	1:E:342:ARG:NH2	2.15	0.80
1:C:130:VAL:HG12	1:C:130:VAL:O	1.83	0.79
1:B:294:HIS:CE1	1:B:323:THR:HG23	2.18	0.77
1:C:272:ASP:O	1:C:432:THR:HG21	1.85	0.77
1:B:456:ARG:NH1	1:B:467:ILE:O	2.18	0.77
1:A:74:LEU:HD21	1:B:390:LEU:CD1	2.10	0.76
1:E:299:TYR:OH	1:E:431:THR:HG22	1.86	0.76
1:C:232:ILE:HG21	1:C:250:GLU:HG3	1.66	0.76
1:F:103:LYS:CE	1:F:494:ASP:OD2	2.33	0.76
1:B:332:GLN:CG	1:B:386:MET:CE	2.64	0.76
1:A:209:THR:HG22	1:A:265:VAL:HB	1.67	0.76
1:A:44:ALA:O	1:A:48:GLU:HG3	1.86	0.74
1:D:206:ARG:HD2	1:D:232:ILE:CD1	2.17	0.74
1:C:163:ILE:CD1	1:C:373:LYS:HE3	2.18	0.74
1:F:103:LYS:HE3	1:F:494:ASP:OD2	1.88	0.74
1:B:176:MET:CE	1:B:207:VAL:HG21	2.18	0.73
1:F:299:TYR:OH	1:F:431:THR:HG22	1.88	0.73
1:B:431:THR:HG23	1:B:482:LEU:O	1.89	0.73
1:B:416:LEU:HD12	1:B:433:GLN:HG2	1.70	0.72
1:A:123:MET:HE2	1:A:381:PHE:O	1.88	0.72
1:B:106:ALA:O	1:B:481:THR:CG2	2.38	0.72
1:A:35:TRP:HZ3	1:A:38:GLN:HE21	1.37	0.71
1:B:456:ARG:NH1	1:B:468:ALA:HA	2.06	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:272:ASP:O	1:E:432:THR:HG21	1.91	0.71
1:E:68:GLU:OE2	1:E:90:LYS:NZ	2.23	0.71
1:F:106:ALA:O	1:F:481:THR:CG2	2.39	0.70
1:E:45:LEU:O	1:E:49:THR:HG23	1.91	0.70
1:A:123:MET:HE2	1:A:384:LEU:HB3	1.73	0.69
1:D:232:ILE:CG2	1:D:250:GLU:HG2	2.22	0.69
1:B:408:LEU:HD23	1:B:482:LEU:CD2	2.22	0.69
1:F:306:SER:O	1:F:310:ARG:CG	2.41	0.69
1:A:150:THR:HG21	1:A:326:TYR:OH	1.93	0.69
1:C:143:GLU:OE1	1:C:379:ARG:NH2	2.25	0.69
1:C:242:MET:HE2	1:C:247:LEU:HB2	1.74	0.69
1:F:242:MET:HE2	1:F:247:LEU:HB2	1.75	0.69
1:C:332:GLN:CG	1:C:386:MET:CE	2.71	0.68
1:A:416:LEU:HD12	1:A:433:GLN:HG2	1.74	0.68
1:C:332:GLN:CD	1:C:386:MET:HE2	2.13	0.68
1:F:113:VAL:HG22	1:F:115:PRO:HD2	1.75	0.68
1:C:45:LEU:HD23	1:C:46:MET:HE2	1.76	0.67
1:C:242:MET:CE	1:C:247:LEU:HB2	2.24	0.67
1:F:494:ASP:OD1	1:F:495:VAL:N	2.28	0.67
1:C:299:TYR:CZ	1:C:430:LEU:HG	2.30	0.67
1:C:404:ASP:OD2	1:D:23:HIS:NE2	2.27	0.67
1:C:412:ALA:HB2	1:C:492:ILE:HD13	1.77	0.67
1:F:414:GLN:OE1	1:F:414:GLN:N	2.27	0.67
1:C:72:VAL:HG13	1:D:145:LYS:HE2	1.77	0.67
1:A:163:ILE:HG22	1:A:164:PHE:O	1.95	0.66
1:F:410:GLN:O	1:F:414:GLN:OE1	2.13	0.66
1:B:332:GLN:HG2	1:B:386:MET:CE	2.25	0.66
1:A:292:TRP:HZ3	1:A:294:HIS:HB2	1.61	0.66
1:A:472:VAL:HG12	1:A:477:TYR:CE1	2.31	0.66
1:C:120:GLU:OE2	1:C:380:ARG:NH2	2.26	0.66
1:C:163:ILE:HD11	1:C:373:LYS:CG	2.25	0.66
1:C:163:ILE:HD11	1:C:373:LYS:HE3	1.78	0.66
1:F:45:LEU:HD22	1:F:85:LEU:HD13	1.78	0.65
1:B:106:ALA:O	1:B:481:THR:HG22	1.95	0.65
1:C:332:GLN:CG	1:C:386:MET:HE3	2.27	0.65
1:B:431:THR:CG2	1:B:482:LEU:O	2.44	0.65
1:A:163:ILE:HD11	1:A:373:LYS:CE	2.22	0.65
1:C:130:VAL:CG1	1:C:370:LEU:HD12	2.27	0.65
1:C:163:ILE:HD11	1:C:373:LYS:CE	2.26	0.65
1:F:170:GLN:HE22	1:F:376:GLN:HG3	1.62	0.64
1:A:313:LEU:HD21	1:A:316:ILE:HG21	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:209:THR:HB	1:B:213:SER:OG	1.97	0.64
1:C:272:ASP:O	1:C:432:THR:CG2	2.46	0.64
1:B:242:MET:HE2	1:B:247:LEU:HB2	1.80	0.64
1:E:263:ALA:N	1:E:291:MET:HE2	2.12	0.64
1:B:351:THR:HB	1:B:372:ASN:O	1.99	0.63
1:D:105:VAL:HG23	1:D:467:ILE:HD13	1.81	0.63
1:C:263:ALA:N	1:C:291:MET:HE2	2.15	0.62
1:D:456:ARG:NH1	1:D:468:ALA:HA	2.13	0.62
1:F:130:VAL:HG12	1:F:130:VAL:O	2.00	0.62
1:D:263:ALA:N	1:D:291:MET:HE2	2.15	0.62
1:F:142:ILE:HG23	1:F:387:TRP:CD1	2.35	0.62
1:A:272:ASP:O	1:A:432:THR:HG21	2.01	0.61
1:A:313:LEU:CD2	1:A:316:ILE:HG21	2.30	0.61
1:B:473:ASN:OD1	1:D:508:ARG:O	2.17	0.61
1:B:332:GLN:CD	1:B:386:MET:HE2	2.20	0.61
1:F:106:ALA:O	1:F:481:THR:HG23	2.00	0.61
1:F:332:GLN:CG	1:F:386:MET:HE3	2.30	0.61
1:D:431:THR:HG23	1:D:482:LEU:O	1.99	0.61
1:D:467:ILE:HD11	1:D:495:VAL:CG1	2.31	0.61
1:A:106:ALA:O	1:A:481:THR:HG22	2.00	0.61
1:C:198:LEU:HD12	1:D:198:LEU:HD12	1.82	0.61
1:C:133:TRP:HH2	1:D:60:ILE:O	1.84	0.60
1:A:113:VAL:HG13	1:A:115:PRO:HD2	1.83	0.60
1:C:35:TRP:O	1:C:39:THR:HG23	2.01	0.60
1:C:351:THR:HG22	1:C:372:ASN:O	2.01	0.60
1:D:272:ASP:O	1:D:432:THR:CG2	2.49	0.60
1:C:172:ASN:OD1	1:C:323:THR:HG21	2.01	0.60
1:F:410:GLN:OE1	1:F:428:PRO:HG2	2.02	0.59
1:A:123:MET:CE	1:A:381:PHE:O	2.50	0.59
1:F:450:GLU:HA	1:F:453:THR:HG22	1.83	0.59
1:A:247:LEU:HD22	1:A:282:ILE:HD12	1.83	0.59
1:C:163:ILE:HD11	1:C:373:LYS:HD2	1.84	0.59
1:B:142:ILE:HG23	1:B:387:TRP:CD1	2.37	0.59
1:B:318:LYS:HA	1:B:342:ARG:HH12	1.67	0.59
1:C:45:LEU:HD23	1:C:46:MET:CE	2.32	0.59
1:B:170:GLN:HE21	1:B:174:MET:HE3	1.68	0.58
1:F:242:MET:HE1	1:F:247:LEU:HD13	1.85	0.58
1:D:467:ILE:HD11	1:D:495:VAL:HG11	1.85	0.58
1:F:41:GLN:O	1:F:45:LEU:HD13	2.03	0.58
1:F:46:MET:HE1	1:F:93:LEU:HD11	1.85	0.58
1:B:328:LYS:HZ2	2:B:601:PLP:C4	2.16	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:317:GLU:O	1:F:342:ARG:NH2	2.35	0.58
1:C:332:GLN:CG	1:C:386:MET:HE2	2.34	0.57
1:F:491:ASP:O	1:F:494:ASP:OD1	2.22	0.57
1:C:317:GLU:O	1:C:342:ARG:NH2	2.38	0.57
1:F:234:VAL:HG21	1:F:242:MET:HE3	1.86	0.57
1:A:113:VAL:CG1	1:A:115:PRO:HD2	2.35	0.57
1:F:306:SER:O	1:F:310:ARG:HG3	2.04	0.57
1:A:431:THR:HG23	1:A:482:LEU:O	2.04	0.57
1:C:332:GLN:HG2	1:C:386:MET:HE3	1.86	0.56
1:B:402:PHE:O	1:B:405:ILE:HG13	2.04	0.56
1:F:130:VAL:O	1:F:130:VAL:CG1	2.54	0.56
1:C:130:VAL:O	1:C:130:VAL:CG1	2.53	0.56
1:F:170:GLN:HE22	1:F:376:GLN:CG	2.18	0.56
1:C:170:GLN:HE22	1:C:376:GLN:HG3	1.70	0.56
1:C:39:THR:HG22	3:D:726:HOH:O	2.05	0.56
1:A:129:SER:OG	1:A:131:ASP:OD1	2.20	0.56
1:B:123:MET:HG3	1:B:384:LEU:HD23	1.89	0.55
1:C:69:PHE:O	1:C:72:VAL:HG12	2.06	0.55
1:A:402:PHE:O	1:A:405:ILE:HG13	2.06	0.55
1:A:74:LEU:HD22	1:B:149:TRP:CG	2.41	0.55
1:A:106:ALA:O	1:A:481:THR:CG2	2.54	0.55
1:C:380:ARG:HD2	1:D:334:VAL:O	2.07	0.55
1:C:123:MET:HG3	1:C:384:LEU:HD23	1.89	0.55
1:C:272:ASP:OD2	1:C:470:THR:HG21	2.06	0.55
1:D:232:ILE:HG21	1:D:250:GLU:HG2	1.88	0.55
1:C:24:ASP:OD1	1:C:24:ASP:N	2.40	0.55
1:F:163:ILE:HG13	1:F:373:LYS:HB2	1.89	0.55
1:C:434:ILE:CD1	1:C:479:LYS:HG3	2.37	0.55
1:F:449:ASP:O	1:F:453:THR:HG22	2.06	0.55
1:A:60:ILE:CD1	1:A:65:LEU:HB2	2.37	0.54
1:F:237:ASP:HB3	1:F:239:ARG:H	1.73	0.54
1:B:328:LYS:NZ	2:B:601:PLP:C4	2.70	0.54
1:E:456:ARG:NH1	1:E:468:ALA:HA	2.22	0.54
1:F:292:TRP:HH2	1:F:321:SER:HB3	1.73	0.54
1:F:492:ILE:O	1:F:495:VAL:HG22	2.07	0.54
1:A:163:ILE:HG13	1:A:373:LYS:HB2	1.89	0.54
1:E:25:PHE:CD1	1:E:26:ILE:HD12	2.43	0.54
1:F:306:SER:O	1:F:310:ARG:HG2	2.07	0.54
1:D:275:SER:HA	1:D:429:GLU:OE1	2.08	0.54
1:C:88:LEU:HD12	1:D:388:LEU:HD21	1.90	0.53
1:A:508:ARG:HB2	1:A:510:PRO:HD3	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:105:VAL:HG12	1:C:105:VAL:O	2.08	0.53
1:C:143:GLU:CD	1:C:379:ARG:HH22	2.11	0.53
1:E:207:VAL:HG22	1:E:263:ALA:HB3	1.90	0.53
1:A:268:SER:O	1:A:300:GLY:HA3	2.08	0.53
1:B:408:LEU:HD11	1:B:492:ILE:HD11	1.90	0.53
1:E:246:CYS:O	1:E:250:GLU:OE1	2.26	0.53
1:B:272:ASP:O	1:B:432:THR:HG21	2.09	0.53
1:C:124:ALA:HB1	1:D:117:LEU:HD22	1.90	0.53
1:D:56:PRO:HD2	1:D:463:GLY:O	2.09	0.53
1:D:209:THR:HG21	1:D:217:ILE:HG21	1.90	0.53
1:C:242:MET:HE1	1:C:247:LEU:HD22	1.91	0.52
3:C:742:HOH:O	1:D:333:THR:HG21	2.09	0.52
1:B:35:TRP:O	1:B:39:THR:HG23	2.10	0.52
1:D:35:TRP:O	1:D:39:THR:HG23	2.09	0.52
1:D:299:TYR:OH	1:D:431:THR:HG22	2.08	0.52
1:F:242:MET:CE	1:F:247:LEU:HD13	2.40	0.52
1:B:209:THR:CG2	1:B:265:VAL:HB	2.27	0.52
1:B:246:CYS:O	1:B:250:GLU:OE1	2.26	0.52
1:D:431:THR:CG2	1:D:482:LEU:O	2.57	0.52
1:A:35:TRP:CH2	1:B:117:LEU:HB3	2.45	0.52
1:C:434:ILE:HD13	1:C:479:LYS:HG3	1.91	0.52
1:F:303:LEU:HD22	1:F:309:HIS:HB3	1.91	0.52
1:D:242:MET:HE3	1:D:247:LEU:HD22	1.91	0.52
1:D:328:LYS:NZ	2:D:601:PLP:C4	2.70	0.52
1:E:103:LYS:HE3	1:E:491:ASP:HB2	1.91	0.52
1:F:450:GLU:HA	1:F:453:THR:CG2	2.40	0.51
1:B:176:MET:HE1	1:B:207:VAL:HG21	1.92	0.51
1:A:123:MET:CE	1:A:384:LEU:HB3	2.39	0.51
1:C:120:GLU:CD	1:C:380:ARG:HH22	2.14	0.51
1:D:39:THR:O	1:D:43:LEU:HG	2.11	0.51
1:C:294:HIS:NE2	1:C:323:THR:HG23	2.25	0.51
1:A:505:GLU:HA	1:A:510:PRO:HD2	1.93	0.51
1:E:504:ARG:O	1:E:508:ARG:HG3	2.10	0.51
1:A:37:ARG:O	1:A:41:GLN:HG3	2.11	0.51
1:C:105:VAL:O	1:C:105:VAL:CG1	2.59	0.51
1:D:232:ILE:HG21	1:D:250:GLU:CG	2.41	0.51
1:D:456:ARG:O	1:D:459:VAL:HG22	2.11	0.50
1:F:388:LEU:HA	1:F:391:ARG:HG2	1.92	0.50
1:D:45:LEU:O	1:D:49:THR:HG23	2.11	0.50
1:B:330:PHE:HB3	1:B:386:MET:CE	2.41	0.50
1:C:43:LEU:O	1:C:47:THR:OG1	2.22	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:456:ARG:HG3	1:F:467:ILE:HG23	1.92	0.50
1:F:467:ILE:HG22	3:F:729:HOH:O	2.12	0.50
1:A:306:SER:OG	1:A:403:ASP:OD1	2.28	0.49
1:B:310:ARG:HB3	1:B:311:PRO:HD3	1.94	0.49
1:B:147:ILE:HD13	1:B:162:GLY:O	2.12	0.49
1:C:272:ASP:OD1	1:C:479:LYS:NZ	2.42	0.49
1:C:299:TYR:CE2	1:C:430:LEU:HG	2.46	0.49
1:D:45:LEU:HD13	1:D:89:LYS:HE2	1.94	0.49
1:D:467:ILE:HD12	1:D:480:PHE:HE1	1.77	0.49
1:F:143:GLU:HG2	1:F:147:ILE:HD12	1.93	0.49
1:C:47:THR:HG22	1:C:51:LYS:HE2	1.95	0.49
1:A:301:CYS:HG	1:A:330:PHE:HE1	1.60	0.49
1:C:88:LEU:HD21	1:C:92:TYR:HD2	1.77	0.49
1:F:130:VAL:CG1	1:F:370:LEU:HD12	2.42	0.49
1:F:139:GLY:HA2	1:F:381:PHE:CZ	2.47	0.49
1:C:294:HIS:HE1	1:C:323:THR:HG23	1.72	0.49
1:A:117:LEU:CD2	1:B:124:ALA:O	2.61	0.49
1:C:176:MET:HE1	1:C:207:VAL:CG1	2.23	0.49
1:B:299:TYR:OH	1:B:431:THR:HG22	2.13	0.49
1:B:467:ILE:HD11	1:B:478:LEU:HD13	1.95	0.49
1:E:413:HIS:HB2	1:E:433:GLN:OE1	2.13	0.49
1:C:332:GLN:NE2	1:C:386:MET:CE	2.76	0.49
1:D:242:MET:CE	1:D:247:LEU:HD22	2.42	0.49
1:A:183:TRP:CZ2	1:A:260:ILE:HG21	2.48	0.48
1:E:272:ASP:O	1:E:432:THR:CG2	2.60	0.48
1:C:234:VAL:HG11	1:C:242:MET:HE3	1.95	0.48
1:F:41:GLN:HE22	1:F:82:GLU:CD	2.15	0.48
1:F:387:TRP:CZ3	1:F:391:ARG:HD2	2.48	0.48
1:A:248:LYS:O	1:A:252:GLN:NE2	2.41	0.48
1:C:332:GLN:HG3	1:C:386:MET:CE	2.41	0.48
1:D:206:ARG:HD2	1:D:232:ILE:HD13	1.95	0.48
1:D:209:THR:CG2	1:D:265:VAL:HB	2.28	0.48
1:A:148:ASP:O	1:A:151:LEU:HB3	2.13	0.48
1:E:43:LEU:O	1:E:47:THR:HG23	2.13	0.48
1:B:172:ASN:OD1	1:B:323:THR:HG21	2.14	0.48
1:C:80:SER:HB2	1:C:82:GLU:OE1	2.13	0.48
1:B:330:PHE:HB3	1:B:386:MET:HE3	1.94	0.48
1:B:268:SER:O	1:B:300:GLY:HA3	2.13	0.48
1:F:46:MET:CE	1:F:93:LEU:HD11	2.43	0.48
1:A:209:THR:HG21	1:A:217:ILE:HG21	1.96	0.48
1:B:165:THR:HG22	1:B:174:MET:HE1	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:163:ILE:HD11	1:C:373:LYS:HB2	1.95	0.48
1:C:245:ASP:O	1:C:249:GLN:HG2	2.14	0.48
1:A:198:LEU:HD12	1:B:198:LEU:HD12	1.95	0.47
1:A:242:MET:HE2	1:A:247:LEU:HB2	1.97	0.47
1:A:434:ILE:HD13	1:A:479:LYS:HG3	1.95	0.47
1:C:46:MET:HE1	1:C:93:LEU:HD13	1.96	0.47
1:B:500:VAL:HG23	3:B:722:HOH:O	2.15	0.47
1:D:268:SER:O	1:D:300:GLY:HA3	2.15	0.47
1:B:416:LEU:CD1	1:B:433:GLN:HG2	2.40	0.47
1:A:416:LEU:CD1	1:A:433:GLN:HG2	2.41	0.47
1:C:332:GLN:NE2	1:C:386:MET:HE2	2.30	0.47
1:D:105:VAL:CG2	1:D:467:ILE:HD13	2.44	0.47
1:D:414:GLN:C	1:D:417:ASN:OD1	2.51	0.47
1:C:56:PRO:HD2	1:C:463:GLY:O	2.15	0.47
1:E:120:GLU:OE2	1:E:380:ARG:NH2	2.47	0.47
1:C:299:TYR:OH	1:C:431:THR:CG2	2.54	0.47
1:D:69:PHE:CZ	1:D:91:LEU:HB3	2.49	0.47
1:E:318:LYS:HA	1:E:342:ARG:NH2	2.29	0.47
1:B:330:PHE:CB	1:B:386:MET:HE3	2.45	0.46
1:C:263:ALA:CA	1:C:291:MET:HE2	2.45	0.46
1:E:26:ILE:HD12	1:E:26:ILE:N	2.30	0.46
1:A:332:GLN:OE1	1:A:385:LYS:HB3	2.16	0.46
1:A:251:VAL:HG21	1:A:285:LEU:HD21	1.97	0.46
1:B:489:ALA:HA	1:B:492:ILE:HD12	1.98	0.46
1:F:268:SER:O	1:F:300:GLY:HA3	2.14	0.46
1:A:35:TRP:CZ3	1:A:38:GLN:NE2	2.84	0.46
1:B:332:GLN:HG3	1:B:386:MET:CE	2.38	0.46
1:C:46:MET:HE3	1:C:93:LEU:HD11	1.97	0.46
1:C:142:ILE:HG23	1:C:387:TRP:CD1	2.51	0.46
1:A:119:ALA:O	1:A:123:MET:HG3	2.15	0.46
1:C:118:LEU:HD12	1:D:42:VAL:HG21	1.98	0.46
1:F:350:VAL:CG1	1:F:374:SER:O	2.64	0.46
1:B:242:MET:HE1	1:B:247:LEU:HD13	1.98	0.46
1:B:467:ILE:HG22	3:B:730:HOH:O	2.15	0.46
1:F:296:ASP:OD2	2:F:601:PLP:N1	2.49	0.46
1:D:335:SER:O	1:D:382:ASP:CG	2.54	0.46
1:E:58:SER:OG	1:E:60:ILE:HG12	2.16	0.46
1:F:332:GLN:NE2	1:F:386:MET:CE	2.79	0.46
1:A:146:VAL:O	1:A:150:THR:HG23	2.16	0.45
1:D:305:VAL:O	1:D:399:GLY:HA3	2.16	0.45
1:D:472:VAL:HG13	1:D:477:TYR:CD1	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:455:ILE:HD11	1:A:503:GLY:CA	2.46	0.45
1:E:183:TRP:CD2	1:E:262:VAL:HG22	2.50	0.45
1:E:35:TRP:O	1:E:39:THR:HG23	2.17	0.45
1:F:292:TRP:CH2	1:F:321:SER:HB3	2.51	0.45
1:C:491:ASP:O	1:C:495:VAL:HG23	2.16	0.45
1:A:209:THR:CG2	1:A:265:VAL:HB	2.42	0.45
1:A:505:GLU:HA	1:A:510:PRO:CD	2.46	0.45
1:B:471:LYS:HG3	1:B:476:GLN:OE1	2.17	0.45
1:C:208:PHE:HD1	1:C:291:MET:HE1	1.81	0.45
1:B:408:LEU:HD22	1:B:487:THR:O	2.16	0.45
1:B:242:MET:HE1	1:B:247:LEU:HD22	1.99	0.45
1:C:208:PHE:CD1	1:C:291:MET:HE1	2.52	0.45
1:C:272:ASP:OD2	1:C:470:THR:CG2	2.65	0.45
1:D:467:ILE:CD1	1:D:480:PHE:HE1	2.30	0.45
1:F:332:GLN:HG2	1:F:386:MET:HE3	1.99	0.45
1:A:145:LYS:HG2	1:A:387:TRP:HZ3	1.81	0.44
1:A:299:TYR:OH	1:A:431:THR:HG22	2.17	0.44
1:B:209:THR:HG21	1:B:217:ILE:HG21	1.99	0.44
1:A:274:GLY:O	1:A:429:GLU:HB3	2.17	0.44
1:B:130:VAL:HG23	1:B:379:ARG:NH2	2.32	0.44
1:E:68:GLU:CD	1:E:90:LYS:NZ	2.69	0.44
1:B:242:MET:CE	1:B:247:LEU:HD13	2.48	0.44
1:C:171:SER:HB3	1:C:323:THR:HG22	2.00	0.44
1:D:244:VAL:CG2	1:D:278:PRO:HG2	2.48	0.44
1:B:221:MET:CE	1:B:226:LEU:HD12	2.47	0.44
1:C:124:ALA:O	1:D:117:LEU:HD21	2.18	0.44
1:D:166:SER:H	1:D:170:GLN:NE2	2.15	0.44
1:C:88:LEU:HD23	1:C:93:LEU:HG	2.00	0.44
1:C:470:THR:HG22	1:C:471:LYS:N	2.33	0.44
1:D:348:SER:HA	1:D:351:THR:HG22	1.99	0.44
1:D:317:GLU:O	1:D:342:ARG:NH2	2.50	0.44
1:F:132:THR:OG1	1:F:134:ASP:OD1	2.26	0.44
1:F:402:PHE:HA	1:F:405:ILE:HG12	2.00	0.44
1:F:242:MET:HE1	1:F:247:LEU:HD22	1.99	0.44
1:A:313:LEU:HD23	1:A:316:ILE:CG2	2.48	0.44
1:A:381:PHE:CE2	1:A:384:LEU:HB2	2.53	0.44
1:F:488:THR:HG22	1:F:489:ALA:H	1.83	0.44
1:B:402:PHE:CD1	1:B:405:ILE:HD11	2.53	0.43
1:B:500:VAL:CG2	3:B:722:HOH:O	2.66	0.43
1:C:163:ILE:HD12	1:C:163:ILE:HG23	1.65	0.43
1:D:164:PHE:HB2	1:D:379:ARG:NH2	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:103:LYS:HE3	1:E:491:ASP:CB	2.49	0.43
1:F:434:ILE:HD13	1:F:479:LYS:HG3	2.00	0.43
1:B:479:LYS:HG2	1:B:480:PHE:N	2.33	0.43
1:C:232:ILE:CG2	1:C:250:GLU:HG3	2.44	0.43
1:C:241:ARG:HH21	1:C:429:GLU:CD	2.21	0.43
1:F:424:VAL:CG2	1:F:433:GLN:OE1	2.67	0.43
1:C:332:GLN:CD	1:C:386:MET:CE	2.84	0.43
1:A:434:ILE:CD1	1:A:479:LYS:HG3	2.49	0.43
1:B:142:ILE:HG23	1:B:387:TRP:CG	2.54	0.43
1:C:88:LEU:CD2	1:C:93:LEU:HG	2.48	0.43
1:E:471:LYS:HG3	1:E:476:GLN:NE2	2.33	0.43
1:B:280:GLY:O	1:B:284:GLU:HG3	2.18	0.43
1:E:106:ALA:O	1:E:481:THR:HG22	2.18	0.43
1:E:471:LYS:HG3	1:E:476:GLN:HE21	1.82	0.43
1:A:237:ASP:HB3	1:A:239:ARG:H	1.84	0.43
1:A:242:MET:CE	1:A:247:LEU:HD13	2.49	0.42
1:A:431:THR:CG2	1:A:482:LEU:O	2.66	0.42
1:C:176:MET:CE	1:C:221:MET:SD	3.07	0.42
1:F:488:THR:HG22	1:F:489:ALA:N	2.34	0.42
1:B:194:LYS:HD2	1:B:349:HIS:O	2.19	0.42
1:C:163:ILE:HD11	1:C:373:LYS:CB	2.49	0.42
1:D:123:MET:HG3	1:D:384:LEU:HD23	2.01	0.42
1:D:405:ILE:HG21	1:D:483:LEU:HA	2.01	0.42
1:A:183:TRP:CE2	1:A:187:HIS:ND1	2.87	0.42
3:C:742:HOH:O	1:D:333:THR:CG2	2.64	0.42
1:B:73:ASP:OD1	1:B:73:ASP:C	2.58	0.42
1:C:162:GLY:O	1:C:163:ILE:HD13	2.20	0.42
1:C:163:ILE:HG13	1:C:373:LYS:HB2	2.00	0.42
1:E:106:ALA:O	1:E:481:THR:CG2	2.67	0.42
1:C:164:PHE:HB2	1:C:379:ARG:NH2	2.35	0.42
1:E:238:GLU:H	1:E:238:GLU:CD	2.23	0.42
1:E:131:ASP:HB3	1:E:377:THR:O	2.19	0.42
1:E:468:ALA:HB3	1:E:479:LYS:HB3	2.02	0.42
1:A:60:ILE:HD12	1:A:65:LEU:HB2	2.01	0.42
1:C:176:MET:HE2	1:C:221:MET:SD	2.60	0.42
1:E:119:ALA:HB3	1:E:385:LYS:HG2	2.00	0.42
1:A:350:VAL:CG1	1:A:374:SER:O	2.67	0.42
1:F:292:TRP:CH2	1:F:321:SER:CB	3.03	0.42
1:C:60:ILE:HD12	1:C:95:ASP:CG	2.32	0.42
1:C:296:ASP:OD2	2:C:601:PLP:N1	2.53	0.42
1:E:59:GLY:HA3	1:E:461:ARG:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:242:MET:CE	1:A:247:LEU:HD22	2.49	0.41
1:A:408:LEU:HD21	1:A:487:THR:HB	2.01	0.41
1:B:154:ILE:CG2	1:B:156:LEU:HG	2.50	0.41
1:C:297:ALA:O	1:C:298:ALA:C	2.59	0.41
1:A:303:LEU:HD22	1:A:309:HIS:HB3	2.01	0.41
1:A:500:VAL:CG1	1:A:504:ARG:CZ	2.99	0.41
1:C:163:ILE:CG1	1:C:373:LYS:HB2	2.50	0.41
1:F:298:ALA:O	1:F:325:ASP:HB2	2.20	0.41
1:F:426:HIS:CD2	1:F:426:HIS:N	2.88	0.41
1:B:106:ALA:HB2	1:B:466:VAL:HG12	2.01	0.41
1:C:242:MET:HE1	1:C:247:LEU:HD13	2.02	0.41
1:A:119:ALA:HB1	1:A:123:MET:HE3	2.03	0.41
1:E:261:PRO:HB2	1:E:291:MET:HE3	2.03	0.41
1:D:150:THR:OG1	1:D:340:PHE:CE2	2.64	0.41
1:E:44:ALA:O	1:E:47:THR:OG1	2.36	0.41
1:F:416:LEU:HD12	1:F:433:GLN:HG2	2.02	0.41
1:A:163:ILE:CG1	1:A:373:LYS:HB2	2.50	0.41
1:C:86:GLU:O	1:C:89:LYS:HB2	2.20	0.41
1:C:301:CYS:SG	1:C:324:VAL:HG13	2.61	0.41
1:B:467:ILE:HD13	1:B:467:ILE:HG21	1.80	0.41
1:C:312:ARG:NH2	1:C:429:GLU:O	2.52	0.41
1:A:242:MET:CE	1:A:247:LEU:HB2	2.51	0.41
1:B:176:MET:HE1	1:B:207:VAL:CG2	2.51	0.41
1:C:402:PHE:HA	1:C:405:ILE:HG12	2.03	0.41
1:C:455:ILE:HG21	1:C:499:ILE:HG23	2.03	0.41
1:D:119:ALA:O	1:D:123:MET:HG3	2.21	0.41
1:D:244:VAL:O	1:D:244:VAL:HG12	2.20	0.41
1:E:268:SER:O	1:E:300:GLY:HA3	2.21	0.41
1:F:106:ALA:O	1:F:481:THR:HG22	2.19	0.41
1:E:387:TRP:CZ3	1:E:388:LEU:CD2	3.04	0.41
1:C:268:SER:O	1:C:300:GLY:HA3	2.20	0.40
1:D:147:ILE:HD13	1:D:162:GLY:O	2.21	0.40
1:E:123:MET:HE1	1:E:382:ASP:HA	2.03	0.40
1:F:332:GLN:CD	1:F:386:MET:CE	2.89	0.40
1:A:117:LEU:HD22	1:B:124:ALA:HB1	2.02	0.40
1:A:295:VAL:HG11	1:A:316:ILE:HG13	2.03	0.40
1:F:348:SER:HA	1:F:351:THR:HG23	2.03	0.40
1:F:209:THR:HG22	1:F:265:VAL:CB	2.40	0.40
1:A:69:PHE:CZ	1:A:91:LEU:HB3	2.55	0.40
1:B:170:GLN:HG3	1:B:375:ILE:HD11	2.03	0.40
1:C:163:ILE:CD1	1:C:373:LYS:HB2	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:260:ILE:HA	1:F:261:PRO:HD3	1.99	0.40
1:B:408:LEU:CD2	1:B:482:LEU:HD21	2.35	0.40
1:E:87:GLU:HG2	1:E:91:LEU:CD1	2.52	0.40
1:E:106:ALA:HB2	1:E:466:VAL:HG12	2.02	0.40
1:F:142:ILE:HG23	1:F:387:TRP:CG	2.56	0.40

All (5) 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)
1:A:70:SER:OG	1:B:76:GLN:OE1[1_556]	1.66	0.54
1:E:335:SER:OG	1:F:380:ARG:NH1[1_556]	1.73	0.47
1:D:475:ARG:NH2	1:F:508:ARG:O[1_556]	1.80	0.40
1:E:84:ALA:O	1:F:391:ARG:NH1[1_556]	1.86	0.34
1:A:508:ARG:O	1:E:473:ASN:ND2[2_664]	2.03	0.17

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	456/519 (88%)	439 (96%)	17 (4%)	0	100	100
1	B	460/519 (89%)	436 (95%)	22 (5%)	2 (0%)	34	32
1	C	454/519 (88%)	428 (94%)	25 (6%)	1 (0%)	47	49
1	D	460/519 (89%)	435 (95%)	25 (5%)	0	100	100
1	E	449/519 (86%)	423 (94%)	26 (6%)	0	100	100
1	F	459/519 (88%)	432 (94%)	26 (6%)	1 (0%)	47	49
All	All	2738/3114 (88%)	2593 (95%)	141 (5%)	4 (0%)	51	54

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	24	ASP
1	F	237	ASP
1	B	80	SER
1	B	189	PRO

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	390/432 (90%)	369 (95%)	21 (5%)	22	20
1	B	392/432 (91%)	382 (97%)	10 (3%)	46	50
1	C	387/432 (90%)	369 (95%)	18 (5%)	26	25
1	D	392/432 (91%)	380 (97%)	12 (3%)	40	43
1	E	382/432 (88%)	370 (97%)	12 (3%)	40	43
1	F	391/432 (90%)	376 (96%)	15 (4%)	33	34
All	All	2334/2592 (90%)	2246 (96%)	88 (4%)	33	34

All (88) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	ASP
1	A	25	PHE
1	A	38	GLN
1	A	70	SER
1	A	74	LEU
1	A	133	TRP
1	A	200	HIS
1	A	252	GLN
1	A	310	ARG
1	A	391	ARG
1	A	396	MET
1	A	414	GLN
1	A	430	LEU
1	A	431	THR
1	A	432	THR

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Mol	Chain	Res	Type
1	A	461	ARG
1	A	471	LYS
1	A	472	VAL
1	A	481	THR
1	A	485	PRO
1	A	510	PRO
1	B	25	PHE
1	B	38	GLN
1	B	86	GLU
1	B	94	ARG
1	B	396	MET
1	B	429	GLU
1	B	431	THR
1	B	432	THR
1	B	481	THR
1	B	482	LEU
1	C	24	ASP
1	C	25	PHE
1	C	29	ASP
1	C	76	GLN
1	C	94	ARG
1	C	250	GLU
1	C	307	GLU
1	C	350	VAL
1	C	373	LYS
1	C	380	ARG
1	C	387	TRP
1	C	396	MET
1	C	424	VAL
1	C	430	LEU
1	C	431	THR
1	C	432	THR
1	C	478	LEU
1	C	481	THR
1	D	25	PHE
1	D	29	ASP
1	D	45	LEU
1	D	116	SER
1	D	254	CYS
1	D	344	LYS
1	D	377	THR
1	D	393	SER

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Mol	Chain	Res	Type
1	D	431	THR
1	D	432	THR
1	D	448	THR
1	D	472	VAL
1	E	24	ASP
1	E	25	PHE
1	E	29	ASP
1	E	30	HIS
1	E	310	ARG
1	E	380	ARG
1	E	429	GLU
1	E	431	THR
1	E	432	THR
1	E	448	THR
1	E	481	THR
1	E	482	LEU
1	F	25	PHE
1	F	31	GLN
1	F	72	VAL
1	F	76	GLN
1	F	86	GLU
1	F	292	TRP
1	F	351	THR
1	F	373	LYS
1	F	380	ARG
1	F	391	ARG
1	F	393	SER
1	F	414	GLN
1	F	431	THR
1	F	448	THR
1	F	481	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	170	GLN

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	F	601	1	15,15,16	2.82	4 (26%)	20,22,23	1.57	5 (25%)
2	PLP	A	601	1	15,15,16	3.04	3 (20%)	20,22,23	1.46	4 (20%)
2	PLP	D	601	-	15,15,16	2.53	3 (20%)	20,22,23	1.62	6 (30%)
2	PLP	C	601	1	15,15,16	3.07	3 (20%)	20,22,23	1.18	1 (5%)
2	PLP	B	601	-	15,15,16	2.58	3 (20%)	20,22,23	1.69	4 (20%)
2	PLP	E	601	1	15,15,16	2.98	3 (20%)	20,22,23	1.34	3 (15%)

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	F	601	1	-	0/6/6/8	0/1/1/1
2	PLP	A	601	1	-	0/6/6/8	0/1/1/1
2	PLP	D	601	-	-	1/6/6/8	0/1/1/1
2	PLP	C	601	1	-	0/6/6/8	0/1/1/1
2	PLP	B	601	-	-	0/6/6/8	0/1/1/1
2	PLP	E	601	1	-	0/6/6/8	0/1/1/1

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	PLP	C5-C4	8.50	1.49	1.40
2	C	601	PLP	C3-C2	8.26	1.49	1.40
2	E	601	PLP	C5-C4	7.74	1.49	1.40
2	F	601	PLP	C3-C2	7.32	1.48	1.40
2	C	601	PLP	C5-C4	7.00	1.48	1.40
2	E	601	PLP	C3-C2	6.99	1.47	1.40
2	B	601	PLP	C3-C2	6.52	1.47	1.40
2	D	601	PLP	C3-C2	6.42	1.47	1.40
2	A	601	PLP	C3-C2	6.32	1.47	1.40
2	F	601	PLP	C5-C4	6.18	1.47	1.40
2	B	601	PLP	C5-C4	5.75	1.46	1.40
2	D	601	PLP	C5-C4	5.26	1.46	1.40
2	D	601	PLP	C3-C4	4.55	1.49	1.40
2	A	601	PLP	C3-C4	4.25	1.49	1.40
2	F	601	PLP	C3-C4	4.19	1.48	1.40
2	B	601	PLP	C3-C4	4.16	1.48	1.40
2	C	601	PLP	C3-C4	4.11	1.48	1.40
2	E	601	PLP	C3-C4	4.07	1.48	1.40
2	F	601	PLP	C4A-C4	-2.57	1.46	1.51

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	601	PLP	C6-N1-C2	3.63	125.89	119.17
2	B	601	PLP	C6-N1-C2	3.53	125.71	119.17
2	F	601	PLP	C6-N1-C2	3.29	125.26	119.17
2	B	601	PLP	O4P-C5A-C5	-2.93	103.76	109.35
2	C	601	PLP	C6-N1-C2	2.87	124.48	119.17
2	B	601	PLP	C4-C3-C2	-2.72	116.06	120.07
2	A	601	PLP	C6-N1-C2	2.67	124.11	119.17
2	E	601	PLP	C6-N1-C2	2.67	124.11	119.17
2	F	601	PLP	C4A-C4-C5	-2.61	118.24	120.94
2	D	601	PLP	C4A-C4-C5	-2.45	118.42	120.94
2	F	601	PLP	C4-C3-C2	-2.36	116.59	120.07
2	D	601	PLP	C3-C2-N1	-2.33	117.75	120.77
2	D	601	PLP	C5A-C5-C6	2.32	123.20	119.37
2	A	601	PLP	C2A-C2-C3	-2.23	118.13	120.89
2	F	601	PLP	O3-C3-C2	2.22	122.33	117.49
2	E	601	PLP	C4-C3-C2	-2.22	116.79	120.07
2	A	601	PLP	O3P-P-O2P	2.18	115.97	107.64
2	D	601	PLP	C2A-C2-N1	2.15	121.87	117.67
2	F	601	PLP	C5A-C5-C6	2.15	122.91	119.37
2	B	601	PLP	C4A-C4-C5	-2.08	118.80	120.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	601	PLP	O3P-P-O2P	2.05	115.48	107.64
2	A	601	PLP	O3-C3-C4	2.04	123.48	118.10
2	D	601	PLP	O3-C3-C4	2.03	123.44	118.10

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	601	PLP	C5A-O4P-P-O1P

There are no ring outliers.

4 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	601	PLP	1	0
2	D	601	PLP	4	0
2	C	601	PLP	1	0
2	B	601	PLP	5	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 (i)

6.1 Protein, DNA and RNA chains (i)

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	464/519 (89%)	-0.11	13 (2%)	53	59	19, 31, 49, 76	0
1	B	468/519 (90%)	-0.18	9 (1%)	66	71	16, 28, 45, 64	0
1	C	462/519 (89%)	-0.17	10 (2%)	62	66	16, 28, 45, 62	0
1	D	468/519 (90%)	-0.15	8 (1%)	70	74	17, 30, 49, 63	0
1	E	457/519 (88%)	-0.22	7 (1%)	73	77	15, 28, 46, 72	0
1	F	467/519 (89%)	-0.27	7 (1%)	73	77	16, 28, 43, 67	0
All	All	2786/3114 (89%)	-0.18	54 (1%)	66	71	15, 29, 47, 76	0

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	71	GLY	6.8
1	F	391	ARG	5.0
1	E	71	GLY	4.7
1	D	200	HIS	4.2
1	C	480	PHE	4.1
1	A	183	TRP	3.7
1	C	428	PRO	3.7
1	A	288	HIS	3.6
1	A	69	PHE	3.6
1	D	190	GLY	3.5
1	A	307	GLU	3.4
1	B	245	ASP	3.3
1	D	379	ARG	2.8
1	D	334	VAL	2.8
1	C	427	VAL	2.7
1	B	380	ARG	2.7
1	B	189	PRO	2.6
1	B	418	ALA	2.6
1	D	189	PRO	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	334	VAL	2.5
1	D	377	THR	2.5
1	C	189	PRO	2.5
1	E	200	HIS	2.5
1	C	192	LEU	2.4
1	E	189	PRO	2.4
1	E	334	VAL	2.4
1	C	30	HIS	2.4
1	A	190	GLY	2.4
1	C	190	GLY	2.4
1	A	200	HIS	2.3
1	B	200	HIS	2.3
1	F	189	PRO	2.3
1	D	387	TRP	2.3
1	C	380	ARG	2.3
1	C	165	THR	2.2
1	A	335	SER	2.2
1	A	130	VAL	2.1
1	E	288	HIS	2.1
1	F	380	ARG	2.1
1	B	378	THR	2.1
1	C	377	THR	2.1
1	A	79	GLY	2.1
1	A	336	CYS	2.1
1	E	190	GLY	2.1
1	F	379	ARG	2.1
1	B	63	HIS	2.1
1	B	165	THR	2.0
1	F	307	GLU	2.0
1	A	379	ARG	2.0
1	E	475	ARG	2.0
1	D	166	SER	2.0
1	F	510	PRO	2.0
1	F	30	HIS	2.0
1	B	371	VAL	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	D	601	15/16	0.96	0.21	39,42,47,48	0
2	PLP	F	601	15/16	0.97	0.18	36,37,41,42	0
2	PLP	B	601	15/16	0.98	0.22	35,37,40,41	0
2	PLP	E	601	15/16	0.98	0.20	35,41,46,49	0
2	PLP	C	601	15/16	0.98	0.20	29,39,42,44	0
2	PLP	A	601	15/16	0.99	0.20	35,40,42,42	0

6.5 Other polymers (i)

There are no such residues in this entry.