



Full wwPDB X-ray Structure Validation Report ⓘ

Jul 2, 2019 – 11:14 AM EDT

PDB ID : 5YB0
Title : Crystal Structure of Wild Type Phosphoserine aminotransferase (PSAT) from *E. histolytica*
Authors : Singh, R.K.; Gourinath, S.
Deposited on : 2017-09-02
Resolution : 2.94 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

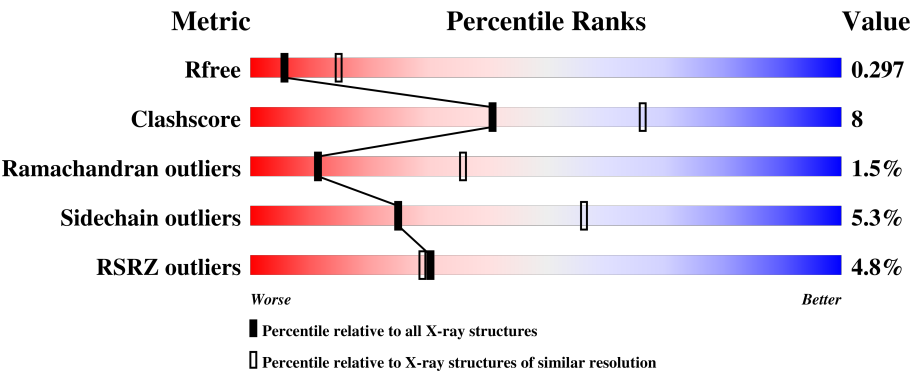
MolProbity : 4.02b-467
Mogul : 1.8.0 (224370), CSD as540be (2019)
Xtriage (Phenix) : 1.13
EDS : 2.3.2
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.3.2

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 2.94 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}	111664	2506 (2.98-2.90)
Clashscore	122126	2745 (2.98-2.90)
Ramachandran outliers	120053	2675 (2.98-2.90)
Sidechain outliers	120020	2677 (2.98-2.90)
RSRZ outliers	108989	2445 (2.98-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	358	
1	B	358	
1	C	358	
1	D	358	
1	E	358	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	358	
1	G	358	
1	H	358	
1	I	358	
1	J	358	
1	K	358	
1	L	358	

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	A	401	-	-	X	-
2	PLP	F	401	-	-	X	-

2 Entry composition

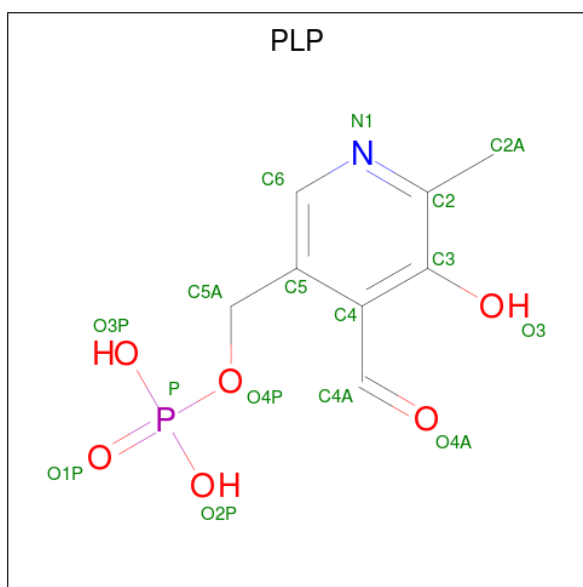
There are 4 unique types of molecules in this entry. The entry contains 27402 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Phosphoserine aminotransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	348	Total	C	N	O	S	0	0	0
			2751	1765	458	513	15			
1	B	349	Total	C	N	O	S	0	0	0
			2759	1771	459	514	15			
1	C	349	Total	C	N	O	S	0	0	0
			2703	1734	450	504	15			
1	D	345	Total	C	N	O	S	0	0	0
			2603	1666	438	485	14			
1	E	342	Total	C	N	O	S	0	0	0
			2477	1579	419	464	15			
1	F	322	Total	C	N	O	S	0	0	0
			2300	1466	380	442	12			
1	G	341	Total	C	N	O	S	0	0	0
			2506	1600	425	466	15			
1	H	349	Total	C	N	O	S	0	0	0
			2225	1401	394	419	11			
1	I	336	Total	C	N	O	S	0	0	0
			2246	1407	395	431	13			
1	J	253	Total	C	N	O	S	0	0	0
			1491	926	265	291	9			
1	K	316	Total	C	N	O	S	0	0	0
			1752	1075	326	347	4			
1	L	216	Total	C	N	O	S	0	0	0
			1269	790	230	245	4			

- 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
			16	8	1	6	1		
2	B	1	Total	C	N	O	P	0	0
			16	8	1	6	1		
2	C	1	Total	C	N	O	P	0	0
			16	8	1	6	1		
2	D	1	Total	C	N	O	P	0	0
			16	8	1	6	1		
2	E	1	Total	C	N	O	P	0	0
			16	8	1	6	1		
2	F	1	Total	C	N	O	P	0	0
			16	8	1	6	1		
2	G	1	Total	C	N	O	P	0	0
			16	8	1	6	1		
2	H	1	Total	C	N	O	P	0	0
			16	8	1	6	1		
2	I	1	Total	C	N	O	P	0	0
			16	8	1	6	1		
2	K	1	Total	C	N	O	P	0	0
			16	8	1	6	1		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Cl	0	0
			1	1		
3	A	1	Total	Cl	0	0
			1	1		

Continued on next page...

Continued from previous page...

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

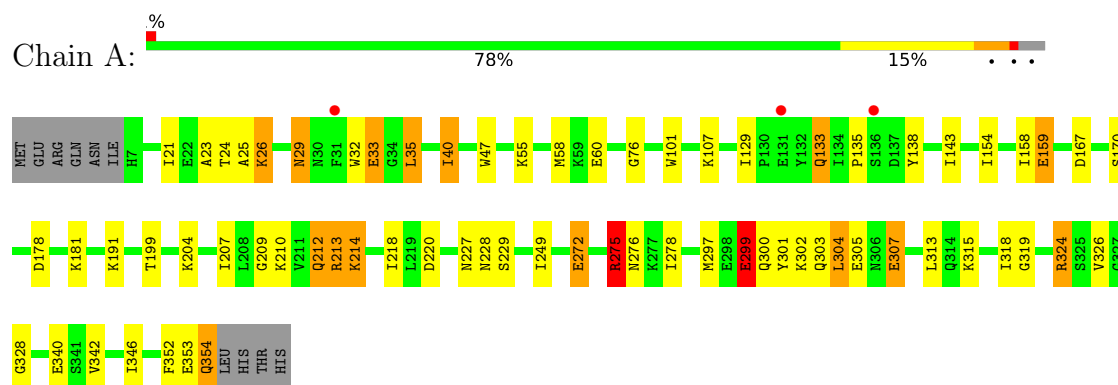
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	14	Total 14	O 14	0	0
4	B	12	Total 12	O 12	0	0
4	C	16	Total 16	O 16	0	0
4	D	11	Total 11	O 11	0	0
4	E	18	Total 18	O 18	0	0
4	F	9	Total 9	O 9	0	0
4	G	13	Total 13	O 13	0	0
4	H	19	Total 19	O 19	0	0
4	I	23	Total 23	O 23	0	0
4	J	10	Total 10	O 10	0	0
4	K	8	Total 8	O 8	0	0
4	L	2	Total 2	O 2	0	0

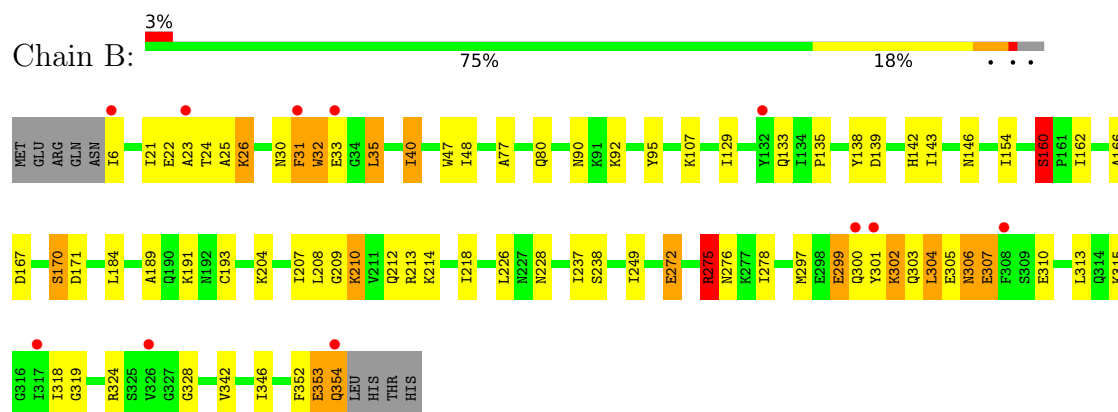
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

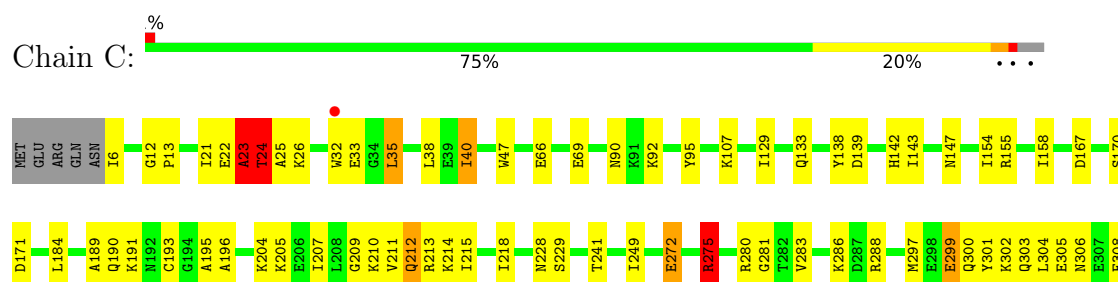
• Molecule 1: Phosphoserine aminotransferase

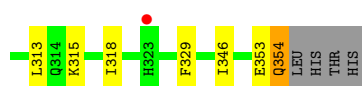


• Molecule 1: Phosphoserine aminotransferase

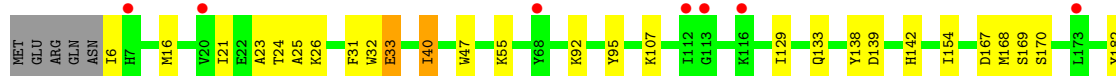
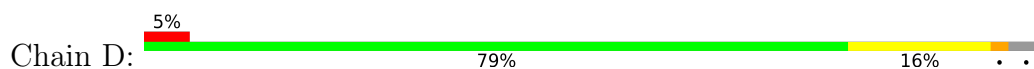


• Molecule 1: Phosphoserine aminotransferase

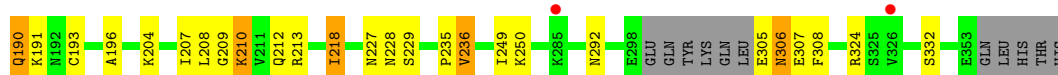
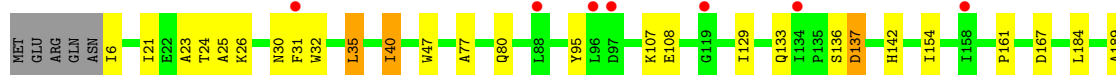
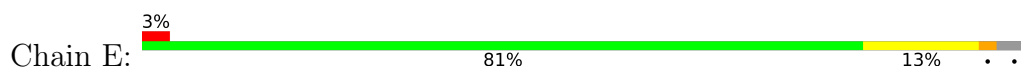




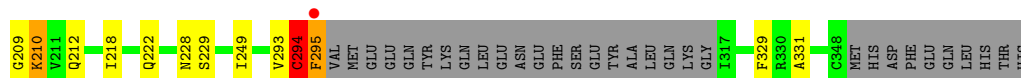
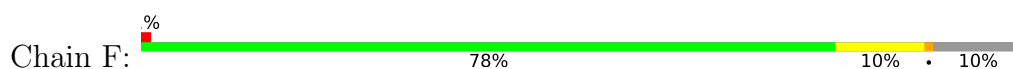
• Molecule 1: Phosphoserine aminotransferase



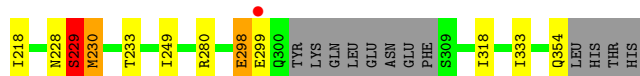
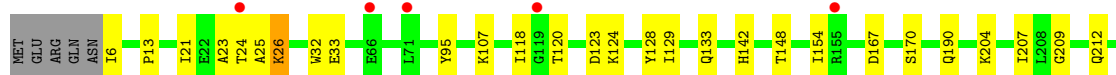
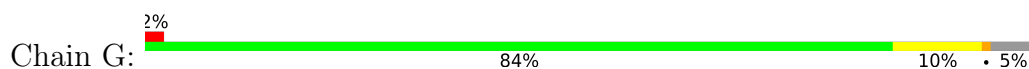
• Molecule 1: Phosphoserine aminotransferase



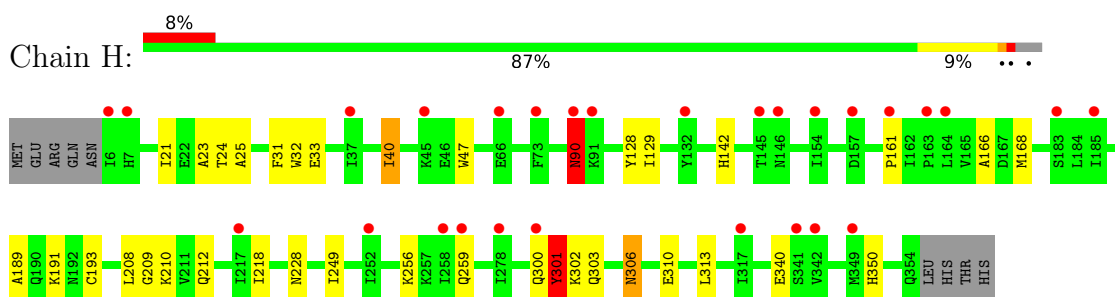
• Molecule 1: Phosphoserine aminotransferase



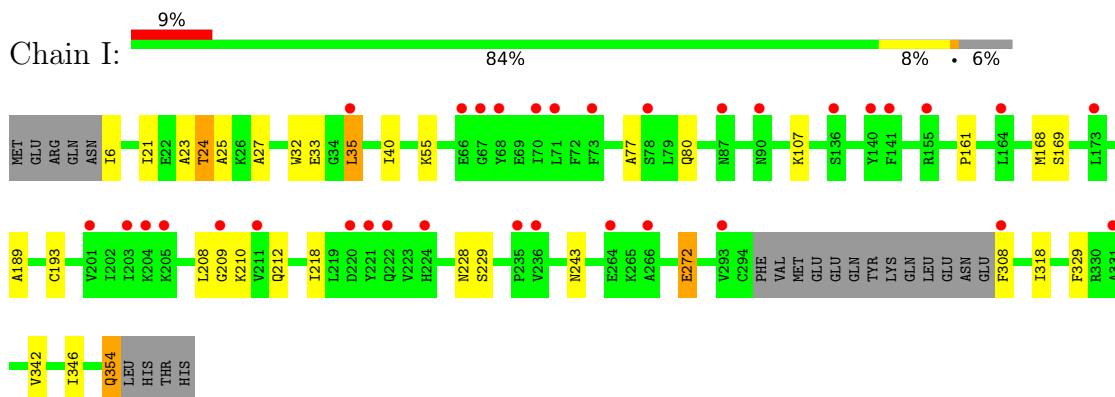
• Molecule 1: Phosphoserine aminotransferase



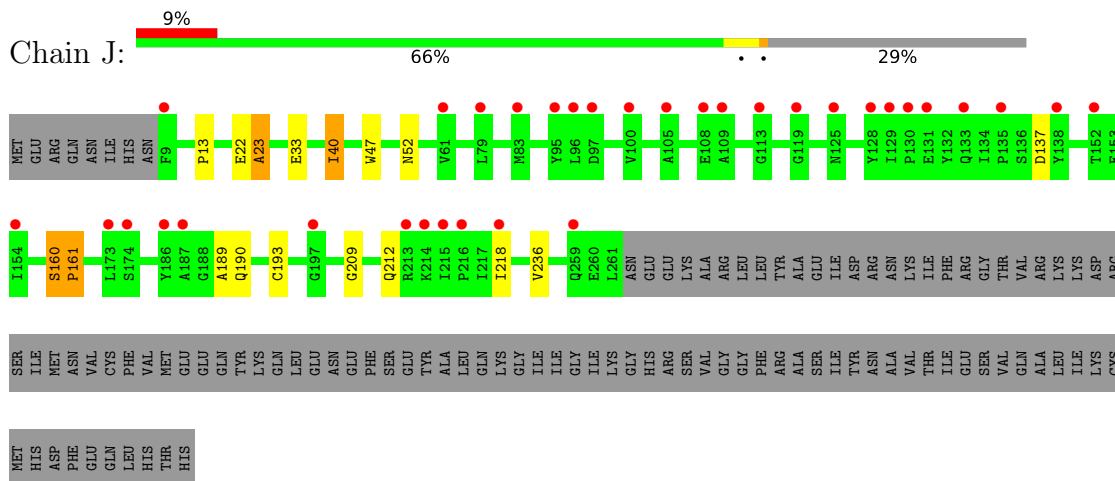
• Molecule 1: Phosphoserine aminotransferase



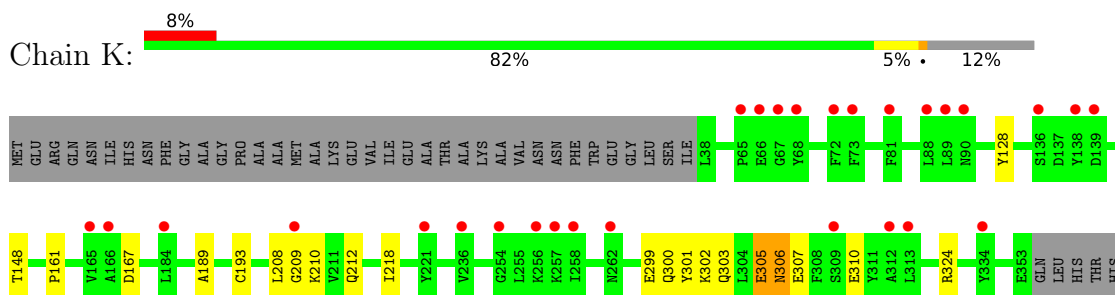
- Molecule 1: Phosphoserine aminotransferase



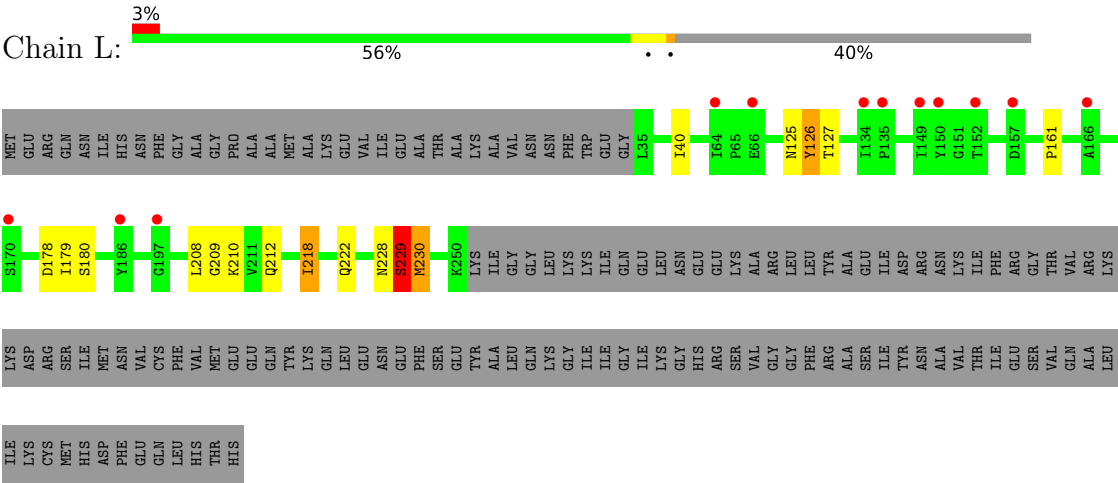
- Molecule 1: Phosphoserine aminotransferase



- Molecule 1: Phosphoserine aminotransferase



- Molecule 1: Phosphoserine aminotransferase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	66.45Å 134.07Å 139.06Å 62.85° 88.58° 74.92°	Depositor
Resolution (Å)	50.15 – 2.94 50.08 – 3.01	Depositor EDS
% Data completeness (in resolution range)	87.9 (50.15-2.94) 87.9 (50.08-3.01)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.49 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.265 , 0.301 0.259 , 0.297	Depositor DCC
R_{free} test set	3837 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	76.4	Xtriage
Anisotropy	0.199	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 56.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.044 for h,h-k,-l	Xtriage
Reported twinning fraction	0.888 for H, K, L 0.112 for H, H-K, -L	Depositor
Outliers	0 of 76766 reflections	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	27402	wwPDB-VP
Average B, all atoms (Å ²)	84.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.85% 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 ⓘ

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	0.67	0/2799	0.85	4/3771 (0.1%)
1	B	0.60	0/2807	0.86	4/3782 (0.1%)
1	C	0.57	0/2749	0.76	2/3710 (0.1%)
1	D	0.51	0/2644	0.70	1/3571 (0.0%)
1	E	0.54	0/2515	0.67	0/3410
1	F	1.04	8/2336 (0.3%)	0.82	9/3178 (0.3%)
1	G	0.48	0/2547	0.66	0/3448
1	H	0.47	1/2255 (0.0%)	0.72	5/3096 (0.2%)
1	I	0.43	0/2275	0.59	0/3100
1	J	0.50	0/1508	0.68	3/2082 (0.1%)
1	K	0.42	0/1769	0.63	0/2455
1	L	0.43	0/1285	0.63	1/1778 (0.1%)
All	All	0.59	9/27489 (0.0%)	0.73	29/37381 (0.1%)

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	4
1	C	0	2
1	D	0	2
1	E	0	2
1	F	0	2
1	G	0	1
1	H	0	5
1	I	0	1
1	J	0	2
1	K	0	2

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
1	L	0	2
All	All	0	27

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	295	PHE	CA-C	23.87	2.15	1.52
1	F	295	PHE	C-O	22.02	1.65	1.23
1	F	295	PHE	N-CA	17.75	1.81	1.46
1	F	294	CYS	CA-C	16.00	1.94	1.52
1	F	294	CYS	C-N	10.57	1.58	1.34
1	F	294	CYS	N-CA	9.87	1.66	1.46
1	F	295	PHE	CA-CB	8.36	1.72	1.53
1	H	128	TYR	C-O	-5.52	1.12	1.23
1	F	294	CYS	CA-CB	5.23	1.65	1.53

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	160	SER	C-N-CD	-17.05	83.08	120.60
1	F	294	CYS	N-CA-CB	-10.71	91.33	110.60
1	B	160	SER	C-N-CA	10.64	166.68	122.00
1	H	32	TRP	N-CA-C	-10.57	82.47	111.00
1	F	295	PHE	CA-C-O	-10.31	98.44	120.10
1	F	294	CYS	CA-C-N	10.25	139.75	117.20
1	F	32	TRP	N-CA-C	-10.06	83.84	111.00
1	F	294	CYS	CA-C-O	-9.37	100.43	120.10
1	F	294	CYS	C-N-CA	7.92	141.50	121.70
1	F	294	CYS	N-CA-C	7.54	131.36	111.00
1	H	301	TYR	N-CA-C	7.13	130.26	111.00
1	A	275	ARG	NE-CZ-NH1	6.95	123.77	120.30
1	B	275	ARG	NE-CZ-NH1	6.74	123.67	120.30
1	L	127	THR	N-CA-C	6.70	129.09	111.00
1	F	295	PHE	N-CA-CB	6.67	122.61	110.60
1	C	275	ARG	NE-CZ-NH1	6.17	123.39	120.30
1	B	160	SER	CB-CA-C	6.08	121.66	110.10
1	C	23	ALA	N-CA-C	-6.07	94.62	111.00
1	D	32	TRP	C-N-CA	6.06	136.86	121.70
1	H	128	TYR	N-CA-C	5.91	126.97	111.00
1	A	29	ASN	N-CA-C	5.85	126.80	111.00
1	H	90	ASN	N-CA-C	-5.73	95.53	111.00
1	J	23	ALA	N-CA-C	-5.73	95.53	111.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	161	PRO	N-CA-C	-5.66	97.38	112.10
1	F	294	CYS	CB-CA-C	5.57	121.53	110.40
1	H	32	TRP	CA-C-N	5.40	129.07	117.20
1	A	214	LYS	N-CA-CB	-5.25	101.15	110.60
1	J	160	SER	C-N-CA	5.23	143.96	122.00
1	A	159	GLU	CA-CB-CG	5.08	124.58	113.40

There are no chirality outliers.

All (27) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	212	GLN	Peptide
1	A	299	GLU	Peptide
1	B	160	SER	Peptide
1	B	212	GLN	Peptide
1	B	299	GLU	Peptide
1	B	353	GLU	Peptide
1	C	212	GLN	Peptide
1	C	305	GLU	Peptide
1	D	212	GLN	Peptide
1	D	302	LYS	Peptide
1	E	212	GLN	Peptide
1	E	213	ARG	Peptide
1	F	212	GLN	Peptide
1	F	294	CYS	Peptide
1	G	212	GLN	Peptide
1	H	212	GLN	Peptide
1	H	300	GLN	Peptide
1	H	301	TYR	Peptide
1	H	302	LYS	Peptide
1	H	90	ASN	Peptide
1	I	212	GLN	Peptide
1	J	160	SER	Peptide
1	J	212	GLN	Peptide
1	K	212	GLN	Peptide
1	K	299	GLU	Peptide
1	L	126	TYR	Peptide
1	L	212	GLN	Peptide

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	2751	0	2813	68	0
1	B	2759	0	2823	82	1
1	C	2703	0	2726	64	0
1	D	2603	0	2592	33	0
1	E	2477	0	2358	40	0
1	F	2300	0	2138	35	0
1	G	2506	0	2407	25	1
1	H	2225	0	1837	21	0
1	I	2246	0	1931	24	0
1	J	1491	0	1103	10	0
1	K	1752	0	1108	11	0
1	L	1269	0	893	8	0
2	A	16	0	7	9	0
2	B	16	0	8	4	0
2	C	16	0	7	3	0
2	D	16	0	8	3	0
2	E	16	0	8	3	0
2	F	16	0	8	6	0
2	G	16	0	7	1	0
2	H	16	0	7	4	0
2	I	16	0	8	0	0
2	K	16	0	7	2	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	1	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
4	A	14	0	0	1	0
4	B	12	0	0	0	0
4	C	16	0	0	2	0
4	D	11	0	0	0	0
4	E	18	0	0	1	0
4	F	9	0	0	2	0
4	G	13	0	0	2	0
4	H	19	0	0	6	0
4	I	23	0	0	3	0
4	J	10	0	0	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	K	8	0	0	2	0
4	L	2	0	0	0	0
All	All	27402	0	24804	400	1

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 8.

All (400) 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:F:295:PHE:CA	1:F:295:PHE:N	1.81	1.42
1:F:295:PHE:C	1:F:295:PHE:O	1.65	1.35
1:F:294:CYS:CA	1:F:294:CYS:C	1.94	1.35
1:B:354:GLN:NE2	1:B:354:GLN:O	1.62	1.33
1:F:295:PHE:C	1:F:295:PHE:CA	2.15	1.15
1:B:191:LYS:NZ	2:B:401:PLP:O3	1.79	1.13
1:H:301:TYR:O	1:H:303:GLN:HA	1.52	1.08
1:A:301:TYR:C	1:A:303:GLN:HA	1.77	1.05
1:A:278:ILE:HD11	1:A:353:GLU:HA	1.38	1.04
1:F:191:LYS:NZ	2:F:401:PLP:O3	1.92	1.03
1:B:278:ILE:HD11	1:B:353:GLU:HA	1.38	1.02
1:B:305:GLU:O	1:B:307:GLU:N	1.94	1.01
1:B:301:TYR:O	1:B:303:GLN:HG2	1.60	1.01
1:B:301:TYR:C	1:B:303:GLN:HA	1.83	0.99
1:B:354:GLN:CD	1:B:354:GLN:O	2.04	0.96
1:G:229:SER:O	1:G:230:MET:HG3	1.64	0.96
2:F:401:PLP:O3P	1:G:233:THR:OG1	1.83	0.96
1:C:301:TYR:C	1:C:303:GLN:HA	1.85	0.95
1:C:22:GLU:O	1:C:23:ALA:O	1.86	0.93
1:C:353:GLU:OE2	4:C:501:HOH:O	1.86	0.91
1:D:272:GLU:HG2	1:D:346:ILE:HG23	1.50	0.91
1:H:166:ALA:HB3	4:H:502:HOH:O	1.71	0.91
1:B:354:GLN:CD	1:B:354:GLN:C	2.29	0.91
1:A:133:GLN:OE1	1:A:133:GLN:HA	1.70	0.89
1:E:191:LYS:NZ	2:E:401:PLP:O3	2.06	0.88
1:G:229:SER:O	1:G:230:MET:CG	2.22	0.87
1:C:22:GLU:C	1:C:23:ALA:O	2.12	0.87
1:F:294:CYS:HA	1:F:294:CYS:C	1.95	0.86
1:H:142:HIS:CB	4:H:517:HOH:O	2.22	0.86
1:F:293:VAL:O	1:F:331:ALA:N	2.09	0.85
1:A:305:GLU:O	1:A:307:GLU:N	2.09	0.85

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:272:GLU:HG2	1:B:346:ILE:HG23	1.57	0.84
1:A:302:LYS:N	1:A:303:GLN:HA	1.91	0.84
1:A:301:TYR:O	1:A:303:GLN:HG2	1.77	0.83
1:C:272:GLU:HG2	1:C:346:ILE:HG23	1.62	0.81
1:I:308:PHE:HB3	1:I:329:PHE:CZ	2.15	0.81
1:C:23:ALA:O	1:C:25:ALA:N	2.15	0.80
1:B:302:LYS:N	1:B:303:GLN:HA	1.95	0.80
1:I:272:GLU:HG2	1:I:346:ILE:HG23	1.63	0.79
1:C:212:GLN:NE2	4:C:502:HOH:O	2.14	0.79
1:D:305:GLU:O	1:D:307:GLU:N	2.17	0.77
1:L:229:SER:O	1:L:230:MET:CB	2.33	0.77
1:A:272:GLU:HG2	1:A:346:ILE:HG23	1.65	0.76
1:K:301:TYR:C	1:K:303:GLN:HA	2.05	0.76
1:E:32:TRP:CB	1:E:35:LEU:HB2	2.16	0.76
1:B:304:LEU:CD1	1:B:328:GLY:HA2	2.16	0.75
1:C:191:LYS:NZ	2:C:401:PLP:C3	2.45	0.75
1:B:278:ILE:CD1	1:B:353:GLU:HA	2.17	0.74
1:B:133:GLN:HA	1:B:133:GLN:OE1	1.85	0.74
1:A:32:TRP:CB	1:A:35:LEU:HB2	2.18	0.74
1:B:191:LYS:NZ	2:B:401:PLP:C3	2.50	0.74
1:C:297:MET:HG2	1:C:304:LEU:CB	2.18	0.73
1:H:301:TYR:O	1:H:303:GLN:CA	2.36	0.73
1:A:300:GLN:HB3	1:A:301:TYR:CD2	2.24	0.72
1:H:191:LYS:NZ	2:H:401:PLP:O4A	2.22	0.72
1:A:301:TYR:O	1:A:303:GLN:CG	2.37	0.72
1:G:133:GLN:OE1	1:G:133:GLN:HA	1.88	0.72
1:H:191:LYS:NZ	2:H:401:PLP:O3	2.24	0.71
1:C:32:TRP:CB	1:C:35:LEU:HB2	2.20	0.71
1:A:55:LYS:NZ	1:A:228:ASN:OD1	2.17	0.71
1:A:304:LEU:HD11	1:A:328:GLY:HA2	1.71	0.70
1:C:302:LYS:N	1:C:303:GLN:HA	2.06	0.70
1:D:208:LEU:O	1:D:210:LYS:N	2.22	0.70
1:A:191:LYS:HZ3	2:A:401:PLP:C4A	2.04	0.70
1:E:228:ASN:O	1:E:228:ASN:CG	2.29	0.70
1:H:228:ASN:O	1:H:228:ASN:CG	2.30	0.70
1:C:191:LYS:NZ	2:C:401:PLP:O3	2.25	0.69
1:H:23:ALA:O	1:H:25:ALA:N	2.25	0.69
1:B:30:ASN:C	1:B:31:PHE:O	2.30	0.69
1:E:305:GLU:O	1:E:307:GLU:N	2.25	0.69
1:A:301:TYR:O	1:A:303:GLN:HA	1.93	0.68
1:F:228:ASN:O	1:F:228:ASN:CG	2.32	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:55:LYS:NZ	1:I:228:ASN:OD1	2.17	0.68
1:I:32:TRP:CB	1:I:35:LEU:HB2	2.24	0.68
1:B:228:ASN:CG	1:B:228:ASN:O	2.29	0.68
1:D:191:LYS:NZ	2:D:401:PLP:C3	2.54	0.68
1:D:55:LYS:NZ	1:D:228:ASN:OD1	2.20	0.67
1:A:191:LYS:NZ	2:A:401:PLP:O4A	2.24	0.67
1:H:256:LYS:HA	4:H:501:HOH:O	1.95	0.67
1:F:133:GLN:OE1	1:F:133:GLN:HA	1.92	0.67
1:I:243:ASN:CB	4:I:512:HOH:O	2.42	0.67
1:B:191:LYS:HZ3	2:B:401:PLP:C3	2.08	0.67
1:A:304:LEU:CD1	1:A:328:GLY:HA2	2.24	0.66
1:A:191:LYS:NZ	2:A:401:PLP:C4A	2.58	0.66
1:C:23:ALA:O	1:C:24:THR:C	2.32	0.66
1:B:30:ASN:O	1:B:31:PHE:O	2.14	0.66
1:C:204:LYS:O	1:C:207:ILE:HG12	1.96	0.66
1:D:301:TYR:C	1:D:303:GLN:HA	2.16	0.66
1:C:66:GLU:HG2	1:J:52:ASN:ND2	2.11	0.65
1:C:133:GLN:OE1	1:C:133:GLN:HA	1.95	0.65
1:F:191:LYS:NZ	2:F:401:PLP:C3	2.60	0.65
1:E:189:ALA:HA	1:E:193:CYS:HB2	1.79	0.65
1:B:297:MET:HG3	1:B:304:LEU:N	2.12	0.64
1:G:228:ASN:O	1:G:229:SER:O	2.15	0.64
1:B:305:GLU:HG3	1:E:137:ASP:CG	2.16	0.64
1:I:308:PHE:HB3	1:I:329:PHE:CE2	2.32	0.64
1:B:40:ILE:HD11	1:B:47:TRP:HB2	1.80	0.64
1:B:31:PHE:O	1:B:32:TRP:CB	2.46	0.63
1:I:272:GLU:CG	1:I:346:ILE:HG23	2.28	0.63
1:K:301:TYR:O	1:K:303:GLN:HA	1.98	0.63
1:C:297:MET:CG	1:C:304:LEU:CB	2.77	0.63
1:F:33:GLU:O	1:G:6:ILE:HD13	1.99	0.62
1:J:40:ILE:HD11	1:J:47:TRP:HB2	1.81	0.62
1:C:6:ILE:HD13	1:D:33:GLU:O	1.99	0.62
1:B:297:MET:HG2	1:B:304:LEU:HB2	1.82	0.62
1:E:250:LYS:HE2	1:I:354:GLN:NE2	2.15	0.61
1:C:228:ASN:O	1:C:228:ASN:CG	2.36	0.61
1:A:133:GLN:NE2	1:C:283:VAL:C	2.53	0.61
1:B:300:GLN:O	1:B:301:TYR:C	2.37	0.61
1:H:40:ILE:HD11	1:H:47:TRP:HB2	1.83	0.61
1:B:272:GLU:CG	1:B:346:ILE:HG23	2.31	0.60
1:F:295:PHE:H	1:F:329:PHE:CB	2.13	0.60
1:A:275:ARG:HH11	1:A:275:ARG:HB3	1.67	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:278:ILE:HD13	1:A:352:PHE:HD1	1.67	0.59
1:B:307:GLU:HG3	1:B:352:PHE:HZ	1.67	0.59
1:H:23:ALA:C	1:H:25:ALA:H	2.06	0.59
1:C:40:ILE:HD11	1:C:47:TRP:HB2	1.85	0.59
1:K:306:ASN:O	1:K:310:GLU:N	2.35	0.58
1:B:299:GLU:OE2	1:B:300:GLN:NE2	2.26	0.58
1:G:229:SER:O	1:G:230:MET:CB	2.51	0.58
1:I:308:PHE:O	1:I:308:PHE:CG	2.56	0.58
1:B:301:TYR:O	1:B:303:GLN:CG	2.46	0.58
1:C:147:ASN:HB3	3:C:402:CL:CL	2.41	0.58
1:F:204:LYS:O	1:F:207:ILE:HG12	2.04	0.58
1:J:22:GLU:C	1:J:23:ALA:O	2.36	0.57
1:A:191:LYS:NZ	2:A:401:PLP:O3	2.37	0.57
1:A:299:GLU:HA	1:A:300:GLN:CB	2.32	0.57
1:B:275:ARG:HB3	1:B:275:ARG:HH11	1.69	0.57
1:G:280:ARG:HB2	1:G:298:GLU:OE2	2.05	0.57
1:A:307:GLU:HG3	1:A:352:PHE:HZ	1.70	0.57
1:C:297:MET:HG3	1:C:304:LEU:N	2.20	0.57
1:E:191:LYS:NZ	2:E:401:PLP:C3	2.66	0.57
1:A:191:LYS:NZ	2:A:401:PLP:C3	2.67	0.57
1:A:305:GLU:HA	1:F:137:ASP:CB	2.35	0.57
1:B:297:MET:HG3	1:B:304:LEU:CA	2.35	0.56
1:A:272:GLU:CG	1:A:346:ILE:HG23	2.33	0.56
1:E:23:ALA:C	1:E:25:ALA:H	2.08	0.56
1:E:40:ILE:HD11	1:E:47:TRP:HB2	1.87	0.56
1:A:297:MET:HG3	1:A:304:LEU:N	2.20	0.56
1:G:354:GLN:HA	1:G:354:GLN:NE2	2.20	0.56
1:D:191:LYS:NZ	2:D:401:PLP:O3	2.39	0.56
1:F:40:ILE:HD11	1:F:47:TRP:HB2	1.86	0.56
1:G:333:ILE:HG13	1:G:333:ILE:O	2.06	0.56
1:C:272:GLU:CG	1:C:346:ILE:HG23	2.34	0.56
1:A:60:GLU:HB2	4:A:506:HOH:O	2.05	0.56
1:B:304:LEU:HD11	1:B:328:GLY:HA2	1.87	0.56
1:F:210:LYS:O	1:F:210:LYS:HG2	2.06	0.56
1:A:278:ILE:HD11	1:A:353:GLU:CA	2.26	0.55
1:D:40:ILE:HD11	1:D:47:TRP:HB2	1.88	0.55
1:K:148:THR:OG1	2:K:401:PLP:H2A1	2.07	0.55
1:D:23:ALA:O	1:D:25:ALA:N	2.37	0.55
1:F:295:PHE:N	1:F:329:PHE:CB	2.70	0.55
1:F:18:LYS:HE3	4:F:509:HOH:O	2.07	0.55
1:I:228:ASN:CG	1:I:228:ASN:O	2.44	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:32:TRP:N	1:A:33:GLU:HA	2.22	0.55
1:B:307:GLU:OE1	1:B:307:GLU:HA	2.06	0.55
1:A:297:MET:HG3	1:A:304:LEU:CA	2.38	0.54
1:F:184:LEU:HD23	1:F:184:LEU:C	2.28	0.54
1:C:301:TYR:O	1:C:303:GLN:HA	2.08	0.54
1:F:294:CYS:CA	1:F:294:CYS:O	2.50	0.54
1:B:204:LYS:O	1:B:207:ILE:HG12	2.07	0.54
1:E:32:TRP:CB	1:E:35:LEU:H	2.20	0.54
1:A:275:ARG:HG3	1:A:276:ASN:N	2.23	0.54
1:G:148:THR:OG1	2:G:401:PLP:O3	2.24	0.54
1:A:228:ASN:CG	1:A:228:ASN:O	2.46	0.54
1:C:32:TRP:CB	1:C:35:LEU:H	2.21	0.54
1:G:6:ILE:HG23	1:G:318:ILE:HD12	1.90	0.54
1:A:129:ILE:HD13	1:A:154:ILE:HG13	1.88	0.53
1:C:95:TYR:CE2	1:C:142:HIS:CG	2.96	0.53
1:I:6:ILE:HD13	1:J:33:GLU:O	2.08	0.53
1:I:354:GLN:NE2	1:I:354:GLN:HA	2.24	0.53
1:L:228:ASN:C	1:L:229:SER:O	2.46	0.53
1:B:160:SER:HB3	1:B:162:ILE:O	2.07	0.53
1:C:33:GLU:O	1:D:6:ILE:HD13	2.08	0.53
1:A:204:LYS:O	1:A:207:ILE:HG12	2.08	0.53
1:C:12:GLY:HA2	1:C:13:PRO:C	2.28	0.53
1:A:40:ILE:HD11	1:A:47:TRP:HB2	1.91	0.52
2:F:401:PLP:H4A	2:F:401:PLP:O4P	2.09	0.52
1:J:236:VAL:HG12	4:J:401:HOH:O	2.09	0.52
1:E:23:ALA:O	1:E:25:ALA:N	2.35	0.52
1:B:23:ALA:C	1:B:25:ALA:H	2.11	0.52
1:B:23:ALA:O	1:B:25:ALA:N	2.37	0.52
1:C:354:GLN:NE2	1:C:354:GLN:HA	2.25	0.52
1:E:227:ASN:O	1:E:228:ASN:C	2.48	0.52
1:H:191:LYS:HZ1	2:H:401:PLP:C4A	2.16	0.52
1:E:324:ARG:CB	4:E:504:HOH:O	2.58	0.52
1:H:259:GLN:HB3	4:H:501:HOH:O	2.09	0.52
1:A:101:TRP:CZ2	2:A:401:PLP:C4A	2.93	0.52
1:A:23:ALA:O	1:A:26:LYS:HD3	2.09	0.52
1:A:354:GLN:HA	1:A:354:GLN:NE2	2.25	0.51
1:B:324:ARG:NE	1:E:210:LYS:HA	2.25	0.51
1:C:171:ASP:C	1:C:171:ASP:OD1	2.46	0.51
1:B:305:GLU:HG3	1:E:137:ASP:OD1	2.11	0.51
1:F:125:ASN:HB2	4:F:503:HOH:O	2.10	0.51
1:H:208:LEU:O	1:H:210:LYS:N	2.40	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:189:ALA:HA	1:I:193:CYS:HB2	1.92	0.51
1:B:143:ILE:O	1:B:166:ALA:HA	2.11	0.51
1:D:129:ILE:HD13	1:D:154:ILE:HG13	1.92	0.50
1:G:95:TYR:CE2	1:G:142:HIS:CG	2.99	0.50
1:K:189:ALA:HA	1:K:193:CYS:HB2	1.92	0.50
1:D:272:GLU:CG	1:D:346:ILE:HG23	2.34	0.50
1:A:23:ALA:C	1:A:25:ALA:H	2.15	0.50
1:A:301:TYR:O	1:A:303:GLN:CA	2.59	0.49
1:C:301:TYR:O	1:C:303:GLN:CB	2.60	0.49
1:I:23:ALA:O	1:I:25:ALA:N	2.38	0.49
1:C:69:GLU:HG3	1:C:205:LYS:HD3	1.94	0.49
1:H:168:MET:HG3	4:H:502:HOH:O	2.11	0.49
1:A:297:MET:HG2	1:A:304:LEU:HB2	1.94	0.49
1:C:275:ARG:HH11	1:C:275:ARG:CG	2.26	0.49
1:D:204:LYS:O	1:D:207:ILE:HG12	2.11	0.49
1:H:189:ALA:HA	1:H:193:CYS:HB2	1.94	0.49
1:E:204:LYS:O	1:E:207:ILE:HG12	2.12	0.49
1:L:208:LEU:O	1:L:210:LYS:N	2.41	0.49
1:A:300:GLN:HB3	1:A:301:TYR:HD2	1.73	0.49
1:D:23:ALA:C	1:D:25:ALA:H	2.14	0.49
1:E:218:ILE:HD12	1:E:218:ILE:O	2.13	0.49
1:B:92:LYS:HB3	1:B:138:TYR:CD1	2.47	0.49
2:F:401:PLP:O3P	1:G:233:THR:CB	2.59	0.49
1:D:303:GLN:O	1:D:307:GLU:CB	2.61	0.48
1:F:208:LEU:O	1:F:210:LYS:N	2.39	0.48
1:I:23:ALA:C	1:I:25:ALA:H	2.16	0.48
1:B:90:ASN:HB3	1:B:139:ASP:OD2	2.14	0.48
1:A:167:ASP:OD2	2:A:401:PLP:N1	2.47	0.48
1:B:342:VAL:O	1:B:346:ILE:HG13	2.13	0.48
1:A:191:LYS:NZ	2:A:401:PLP:C4	2.75	0.48
1:G:118:ILE:HG12	4:G:503:HOH:O	2.13	0.48
1:B:275:ARG:HG3	1:B:276:ASN:N	2.28	0.48
1:I:6:ILE:HG23	1:I:318:ILE:HD12	1.94	0.48
1:D:133:GLN:HA	1:D:133:GLN:OE1	2.12	0.48
1:K:302:LYS:N	1:K:303:GLN:HA	2.29	0.48
1:C:275:ARG:HH11	1:C:275:ARG:HB3	1.77	0.48
1:D:92:LYS:HB3	1:D:138:TYR:CD1	2.48	0.48
1:E:6:ILE:HD13	1:H:33:GLU:O	2.14	0.48
1:B:278:ILE:HG22	1:B:297:MET:HE3	1.95	0.47
1:A:354:GLN:HA	1:A:354:GLN:HE21	1.78	0.47
1:E:95:TYR:CE2	1:E:142:HIS:CG	3.02	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:6:ILE:N	4:G:502:HOH:O	2.47	0.47
1:B:226:LEU:HD11	1:F:222:GLN:O	2.14	0.47
1:B:6:ILE:HG23	1:B:318:ILE:HD12	1.96	0.47
1:C:300:GLN:O	1:C:301:TYR:C	2.52	0.47
1:E:190:GLN:HB3	1:E:196:ALA:HA	1.97	0.47
1:G:204:LYS:O	1:G:207:ILE:HG12	2.14	0.47
1:A:220:ASP:OD1	1:A:220:ASP:C	2.53	0.47
1:A:301:TYR:O	1:A:303:GLN:CB	2.63	0.47
1:D:167:ASP:OD2	2:D:401:PLP:N1	2.48	0.47
1:I:77:ALA:O	1:I:80:GLN:N	2.47	0.47
1:E:208:LEU:O	1:E:210:LYS:N	2.38	0.47
1:E:30:ASN:O	1:E:32:TRP:N	2.47	0.47
1:A:191:LYS:HZ1	2:A:401:PLP:C4	2.28	0.47
1:B:306:ASN:O	1:B:310:GLU:N	2.44	0.47
1:E:305:GLU:O	1:E:306:ASN:C	2.53	0.46
1:C:143:ILE:HD13	1:C:158:ILE:HD12	1.97	0.46
1:K:305:GLU:O	1:K:306:ASN:CB	2.64	0.46
1:A:300:GLN:O	1:A:301:TYR:C	2.52	0.46
1:C:66:GLU:HG2	1:J:52:ASN:HD22	1.79	0.46
1:G:129:ILE:HD13	1:G:154:ILE:HG13	1.96	0.46
1:G:13:PRO:HA	1:G:190:GLN:O	2.15	0.46
1:L:228:ASN:O	1:L:229:SER:O	2.34	0.46
1:D:92:LYS:O	1:D:139:ASP:HB2	2.15	0.46
1:C:155:ARG:NH1	1:C:286:LYS:O	2.49	0.46
1:E:305:GLU:C	1:E:307:GLU:N	2.68	0.46
1:I:354:GLN:HE21	1:I:354:GLN:HA	1.80	0.46
1:B:32:TRP:CB	1:B:35:LEU:H	2.28	0.46
1:B:305:GLU:CG	1:E:137:ASP:CG	2.82	0.46
1:A:297:MET:CG	1:A:304:LEU:HB2	2.46	0.46
1:C:190:GLN:HB3	1:C:196:ALA:HA	1.98	0.45
1:E:133:GLN:OE1	1:E:133:GLN:HA	2.16	0.45
1:K:128:TYR:CB	4:K:505:HOH:O	2.63	0.45
1:B:354:GLN:O	1:B:354:GLN:CG	2.64	0.45
1:C:13:PRO:HA	1:C:190:GLN:O	2.17	0.45
1:J:236:VAL:O	4:J:401:HOH:O	2.21	0.45
1:A:227:ASN:O	1:A:228:ASN:C	2.54	0.45
1:L:218:ILE:HD12	1:L:218:ILE:O	2.16	0.45
1:A:275:ARG:HH11	1:A:275:ARG:CG	2.30	0.45
1:B:32:TRP:CB	1:B:35:LEU:HB2	2.47	0.45
1:A:342:VAL:O	1:A:346:ILE:HG13	2.17	0.45
1:B:189:ALA:HA	1:B:193:CYS:HB2	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:292:ASN:ND2	1:E:332:SER:OG	2.49	0.45
1:B:146:ASN:HB2	1:B:171:ASP:OD2	2.17	0.45
1:B:306:ASN:HD21	1:E:136:SER:H	1.64	0.45
1:B:302:LYS:N	1:B:303:GLN:CA	2.74	0.45
1:D:189:ALA:HA	1:D:193:CYS:HB2	1.99	0.45
1:D:6:ILE:HG23	1:D:318:ILE:HD12	1.99	0.45
1:I:27:ALA:N	4:I:501:HOH:O	2.45	0.45
1:A:302:LYS:N	1:A:303:GLN:CA	2.73	0.44
1:B:297:MET:CG	1:B:304:LEU:HB2	2.44	0.44
1:C:184:LEU:HD23	1:C:184:LEU:C	2.37	0.44
1:E:167:ASP:OD2	2:E:401:PLP:N1	2.50	0.44
1:B:32:TRP:CB	1:B:33:GLU:CA	2.94	0.44
1:C:167:ASP:OD2	2:C:401:PLP:N1	2.51	0.44
1:C:6:ILE:HG23	1:C:318:ILE:HD12	1.99	0.44
1:F:295:PHE:HA	1:F:295:PHE:N	2.11	0.44
1:B:275:ARG:CG	1:B:275:ARG:HH11	2.30	0.44
1:B:32:TRP:N	1:B:33:GLU:HA	2.32	0.44
1:D:354:GLN:HA	1:D:354:GLN:NE2	2.33	0.44
1:B:135:PRO:HG2	1:B:138:TYR:CD2	2.53	0.44
1:H:191:LYS:CE	2:H:401:PLP:O4A	2.65	0.44
1:A:318:ILE:HG22	1:A:319:GLY:N	2.33	0.44
1:B:208:LEU:O	1:B:210:LYS:N	2.45	0.44
1:D:218:ILE:O	1:D:218:ILE:HD12	2.17	0.44
1:F:32:TRP:CB	1:F:35:LEU:HB2	2.48	0.44
1:B:129:ILE:HD13	1:B:154:ILE:HG13	1.98	0.44
1:C:275:ARG:HH11	1:C:275:ARG:HG2	1.82	0.44
1:C:280:ARG:HD2	1:C:281:GLY:O	2.16	0.44
1:L:178:ASP:O	1:L:180:SER:N	2.51	0.44
1:A:76:GLY:HA2	1:A:199:THR:OG1	2.17	0.44
1:B:184:LEU:C	1:B:184:LEU:HD23	2.38	0.44
1:E:210:LYS:HG2	1:E:210:LYS:O	2.18	0.44
1:F:294:CYS:HB3	1:F:329:PHE:O	2.18	0.44
1:B:22:GLU:O	1:B:23:ALA:C	2.54	0.44
1:B:26:LYS:HG3	1:B:30:ASN:HA	2.00	0.44
1:E:228:ASN:OD1	1:E:228:ASN:O	2.35	0.44
1:A:135:PRO:HG2	1:A:138:TYR:CD2	2.52	0.43
1:B:299:GLU:OE2	1:B:300:GLN:HB2	2.17	0.43
1:C:32:TRP:N	1:C:33:GLU:HA	2.33	0.43
1:F:167:ASP:OD2	2:F:401:PLP:N1	2.50	0.43
1:L:125:ASN:O	1:L:126:TYR:C	2.56	0.43
1:A:307:GLU:HG3	1:A:352:PHE:CZ	2.51	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:342:VAL:O	1:D:346:ILE:HG13	2.18	0.43
1:H:350:HIS:CB	4:H:516:HOH:O	2.66	0.43
1:I:342:VAL:O	1:I:346:ILE:HG13	2.18	0.43
1:F:129:ILE:HD13	1:F:154:ILE:HG13	2.01	0.43
1:G:23:ALA:O	1:G:26:LYS:HD3	2.18	0.43
1:A:212:GLN:HG3	1:A:213:ARG:HE	1.82	0.43
1:C:23:ALA:C	1:C:25:ALA:H	2.22	0.43
1:D:95:TYR:CE2	1:D:142:HIS:CG	3.07	0.43
1:A:178:ASP:OD2	1:A:181:LYS:HE2	2.17	0.43
1:B:352:PHE:O	1:B:354:GLN:HA	2.19	0.43
1:C:283:VAL:HG23	1:C:288:ARG:HG2	1.99	0.43
1:C:23:ALA:C	1:C:25:ALA:N	2.72	0.43
1:C:308:PHE:HB3	1:C:329:PHE:CZ	2.53	0.43
1:G:23:ALA:C	1:G:25:ALA:H	2.22	0.43
1:G:32:TRP:N	1:G:33:GLU:HA	2.33	0.43
1:B:77:ALA:O	1:B:80:GLN:N	2.52	0.43
1:C:301:TYR:O	1:C:303:GLN:CA	2.67	0.43
1:C:92:LYS:HB3	1:C:138:TYR:CD1	2.54	0.43
1:C:129:ILE:HD13	1:C:154:ILE:HG13	2.01	0.43
1:D:333:ILE:HG13	1:D:333:ILE:O	2.19	0.43
1:H:306:ASN:O	1:H:310:GLU:N	2.47	0.43
1:B:48:ILE:HD13	1:F:206:GLU:CD	2.38	0.43
1:E:129:ILE:HD13	1:E:154:ILE:HG13	2.01	0.43
1:F:23:ALA:C	1:F:25:ALA:H	2.21	0.43
1:G:95:TYR:CD2	1:G:142:HIS:HB3	2.54	0.43
1:I:208:LEU:O	1:I:210:LYS:N	2.46	0.43
1:I:24:THR:HG22	4:I:501:HOH:O	2.18	0.43
1:J:189:ALA:HA	1:J:193:CYS:HB2	2.00	0.42
1:C:299:GLU:HA	1:C:300:GLN:HA	1.58	0.42
1:H:23:ALA:C	1:H:25:ALA:N	2.72	0.42
1:B:95:TYR:CE2	1:B:142:HIS:CG	3.07	0.42
1:B:299:GLU:N	1:B:300:GLN:HA	2.30	0.42
1:B:297:MET:CG	1:B:304:LEU:CA	2.97	0.42
1:K:167:ASP:OD2	2:K:401:PLP:N1	2.52	0.42
1:E:305:GLU:O	1:E:308:PHE:N	2.51	0.42
1:B:278:ILE:HG22	1:B:297:MET:CE	2.49	0.42
1:C:12:GLY:CA	1:C:13:PRO:C	2.88	0.42
1:C:297:MET:HG3	1:C:304:LEU:CA	2.49	0.42
1:E:77:ALA:O	1:E:80:GLN:N	2.52	0.42
1:F:228:ASN:O	1:F:228:ASN:OD1	2.38	0.42
1:B:353:GLU:O	1:B:354:GLN:C	2.58	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:168:MET:CE	1:D:182:TYR:CE1	3.03	0.42
1:A:23:ALA:O	1:A:25:ALA:N	2.51	0.42
1:B:305:GLU:HG3	1:E:137:ASP:OD2	2.20	0.42
1:C:189:ALA:HA	1:C:193:CYS:HB2	2.00	0.42
1:G:123:ASP:OD2	1:G:124:LYS:HE3	2.19	0.42
1:J:13:PRO:HA	1:J:190:GLN:O	2.19	0.42
1:A:299:GLU:HA	1:A:300:GLN:HB2	2.02	0.41
1:D:320:ILE:HA	1:D:330:ARG:O	2.20	0.41
1:A:76:GLY:CA	1:A:199:THR:OG1	2.69	0.41
1:A:324:ARG:HD3	1:F:210:LYS:O	2.20	0.41
1:B:146:ASN:HD22	1:B:170:SER:HB3	1.84	0.41
1:C:211:VAL:HG11	1:C:215:ILE:HD11	2.02	0.41
1:C:297:MET:HG3	1:C:304:LEU:H	1.86	0.41
1:I:168:MET:O	1:I:169:SER:C	2.59	0.41
1:I:32:TRP:N	1:I:33:GLU:HA	2.35	0.41
1:B:237:ILE:HG23	1:B:238:SER:N	2.36	0.41
1:J:137:ASP:CB	4:J:407:HOH:O	2.67	0.41
1:C:90:ASN:HB3	1:C:139:ASP:OD2	2.20	0.41
1:F:189:ALA:HA	1:F:193:CYS:HB2	2.01	0.41
1:A:278:ILE:HG22	1:A:297:MET:HE3	2.01	0.41
1:C:69:GLU:CG	1:C:205:LYS:HD3	2.50	0.41
1:G:167:ASP:C	1:G:167:ASP:OD1	2.59	0.41
1:K:324:ARG:N	4:K:501:HOH:O	2.53	0.41
1:E:184:LEU:C	1:E:184:LEU:HD23	2.41	0.41
1:K:208:LEU:O	1:K:210:LYS:N	2.50	0.41
1:B:32:TRP:CB	1:B:33:GLU:C	2.89	0.41
1:A:278:ILE:HG22	1:A:297:MET:CE	2.51	0.41
1:E:108:GLU:OE2	1:E:108:GLU:HA	2.21	0.41
1:F:57:LEU:O	1:F:58:MET:C	2.60	0.41
1:B:167:ASP:OD2	2:B:401:PLP:N1	2.54	0.40
1:A:143:ILE:HD13	1:A:158:ILE:HD12	2.03	0.40
1:B:318:ILE:HG22	1:B:319:GLY:N	2.36	0.40
1:D:167:ASP:HB2	1:D:186:TYR:CZ	2.56	0.40
1:B:306:ASN:HD21	1:E:136:SER:N	2.20	0.40
1:C:195:ALA:HB2	1:C:241:THR:HG21	2.04	0.40
1:C:38:LEU:HB2	1:D:16:MET:SD	2.61	0.40
1:F:13:PRO:HA	1:F:190:GLN:O	2.21	0.40
1:D:226:LEU:HD21	1:L:222:GLN:CB	2.51	0.40
1:B:135:PRO:HG2	1:B:138:TYR:HD2	1.86	0.40
1:D:168:MET:O	1:D:169:SER:C	2.60	0.40
1:E:235:PRO:O	1:E:236:VAL:C	2.60	0.40

All (1) 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:B:33:GLU:OE1	1:G:128:TYR:OH[1_455]	2.17	0.03

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	346/358 (97%)	321 (93%)	21 (6%)	4 (1%)	14	42
1	B	347/358 (97%)	319 (92%)	22 (6%)	6 (2%)	10	32
1	C	347/358 (97%)	327 (94%)	15 (4%)	5 (1%)	12	38
1	D	341/358 (95%)	318 (93%)	17 (5%)	6 (2%)	9	31
1	E	338/358 (94%)	314 (93%)	17 (5%)	7 (2%)	8	27
1	F	318/358 (89%)	301 (95%)	15 (5%)	2 (1%)	27	60
1	G	337/358 (94%)	321 (95%)	11 (3%)	5 (2%)	11	36
1	H	347/358 (97%)	322 (93%)	18 (5%)	7 (2%)	8	28
1	I	332/358 (93%)	314 (95%)	15 (4%)	3 (1%)	19	50
1	J	251/358 (70%)	237 (94%)	12 (5%)	2 (1%)	21	53
1	K	314/358 (88%)	294 (94%)	14 (4%)	6 (2%)	9	30
1	L	214/358 (60%)	201 (94%)	8 (4%)	5 (2%)	7	25
All	All	3832/4296 (89%)	3589 (94%)	185 (5%)	58 (2%)	11	36

All (58) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	299	GLU
1	B	31	PHE
1	B	32	TRP
1	B	160	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	306	ASN
1	C	23	ALA
1	C	24	THR
1	D	24	THR
1	D	33	GLU
1	D	306	ASN
1	E	24	THR
1	E	306	ASN
1	G	230	MET
1	H	24	THR
1	I	24	THR
1	J	161	PRO
1	K	300	GLN
1	L	229	SER
1	A	24	THR
1	A	29	ASN
1	B	24	THR
1	C	299	GLU
1	D	209	GLY
1	E	209	GLY
1	G	229	SER
1	G	299	GLU
1	K	306	ASN
1	L	179	ILE
1	L	230	MET
1	C	306	ASN
1	E	31	PHE
1	G	24	THR
1	H	90	ASN
1	I	209	GLY
1	J	209	GLY
1	L	209	GLY
1	A	209	GLY
1	B	209	GLY
1	D	31	PHE
1	E	190	GLN
1	E	236	VAL
1	F	24	THR
1	H	31	PHE
1	I	161	PRO
1	K	305	GLU
1	K	307	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	H	306	ASN
1	K	209	GLY
1	H	129	ILE
1	H	161	PRO
1	H	209	GLY
1	C	209	GLY
1	D	236	VAL
1	F	209	GLY
1	G	209	GLY
1	K	161	PRO
1	L	161	PRO
1	E	161	PRO

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	299/310 (96%)	273 (91%)	26 (9%)	11	31
1	B	300/310 (97%)	280 (93%)	20 (7%)	18	45
1	C	286/310 (92%)	268 (94%)	18 (6%)	20	48
1	D	267/310 (86%)	250 (94%)	17 (6%)	19	47
1	E	235/310 (76%)	225 (96%)	10 (4%)	32	64
1	F	214/310 (69%)	206 (96%)	8 (4%)	37	70
1	G	242/310 (78%)	233 (96%)	9 (4%)	37	70
1	H	159/310 (51%)	153 (96%)	6 (4%)	36	69
1	I	179/310 (58%)	171 (96%)	8 (4%)	30	63
1	J	86/310 (28%)	84 (98%)	2 (2%)	53	81
1	K	67/310 (22%)	66 (98%)	1 (2%)	67	88
1	L	66/310 (21%)	63 (96%)	3 (4%)	30	63
All	All	2400/3720 (64%)	2272 (95%)	128 (5%)	25	56

All (128) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	ILE
1	A	26	LYS
1	A	33	GLU
1	A	35	LEU
1	A	40	ILE
1	A	58	MET
1	A	107	LYS
1	A	133	GLN
1	A	159	GLU
1	A	170	SER
1	A	210	LYS
1	A	213	ARG
1	A	214	LYS
1	A	218	ILE
1	A	229	SER
1	A	249	ILE
1	A	272	GLU
1	A	275	ARG
1	A	304	LEU
1	A	307	GLU
1	A	313	LEU
1	A	315	LYS
1	A	324	ARG
1	A	326	VAL
1	A	340	GLU
1	A	354	GLN
1	B	21	ILE
1	B	26	LYS
1	B	35	LEU
1	B	40	ILE
1	B	107	LYS
1	B	160	SER
1	B	170	SER
1	B	210	LYS
1	B	213	ARG
1	B	214	LYS
1	B	218	ILE
1	B	249	ILE
1	B	272	GLU
1	B	275	ARG
1	B	302	LYS
1	B	304	LEU
1	B	307	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	313	LEU
1	B	315	LYS
1	B	354	GLN
1	C	21	ILE
1	C	24	THR
1	C	26	LYS
1	C	35	LEU
1	C	40	ILE
1	C	107	LYS
1	C	170	SER
1	C	210	LYS
1	C	213	ARG
1	C	214	LYS
1	C	218	ILE
1	C	229	SER
1	C	249	ILE
1	C	272	GLU
1	C	275	ARG
1	C	313	LEU
1	C	315	LYS
1	C	354	GLN
1	D	21	ILE
1	D	26	LYS
1	D	40	ILE
1	D	107	LYS
1	D	170	SER
1	D	210	LYS
1	D	213	ARG
1	D	214	LYS
1	D	218	ILE
1	D	233	THR
1	D	249	ILE
1	D	272	GLU
1	D	296	VAL
1	D	313	LEU
1	D	315	LYS
1	D	340	GLU
1	D	354	GLN
1	E	21	ILE
1	E	26	LYS
1	E	35	LEU
1	E	40	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	107	LYS
1	E	137	ASP
1	E	210	LYS
1	E	218	ILE
1	E	229	SER
1	E	249	ILE
1	F	21	ILE
1	F	35	LEU
1	F	40	ILE
1	F	107	LYS
1	F	210	LYS
1	F	218	ILE
1	F	229	SER
1	F	249	ILE
1	G	21	ILE
1	G	26	LYS
1	G	107	LYS
1	G	120	THR
1	G	170	SER
1	G	218	ILE
1	G	229	SER
1	G	249	ILE
1	G	298	GLU
1	H	21	ILE
1	H	40	ILE
1	H	218	ILE
1	H	249	ILE
1	H	313	LEU
1	H	340	GLU
1	I	21	ILE
1	I	35	LEU
1	I	40	ILE
1	I	107	LYS
1	I	218	ILE
1	I	229	SER
1	I	272	GLU
1	I	354	GLN
1	J	40	ILE
1	J	218	ILE
1	K	218	ILE
1	L	40	ILE
1	L	218	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	L	229	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	350	HIS
1	A	354	GLN
1	B	303	GLN
1	B	350	HIS
1	C	354	GLN
1	D	354	GLN
1	E	52	ASN
1	E	292	ASN
1	G	350	HIS
1	G	354	GLN
1	I	354	GLN
1	J	52	ASN
1	K	350	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 15 ligands modelled in this entry, 5 are monoatomic - leaving 10 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	401	-	16,16,16	2.97	3 (18%)	20,23,23	1.73	6 (30%)
2	PLP	B	401	1	16,16,16	3.53	3 (18%)	20,23,23	2.13	5 (25%)
2	PLP	C	401	1	16,16,16	3.46	3 (18%)	20,23,23	1.57	6 (30%)
2	PLP	D	401	1	16,16,16	3.26	3 (18%)	20,23,23	1.90	4 (20%)
2	PLP	E	401	1	16,16,16	3.36	3 (18%)	20,23,23	2.28	8 (40%)
2	PLP	F	401	1	16,16,16	3.24	3 (18%)	20,23,23	2.01	6 (30%)
2	PLP	G	401	1	16,16,16	3.04	3 (18%)	20,23,23	1.87	5 (25%)
2	PLP	H	401	-	16,16,16	3.13	4 (25%)	20,23,23	2.37	6 (30%)
2	PLP	I	401	1	16,16,16	3.84	3 (18%)	20,23,23	1.96	5 (25%)
2	PLP	K	401	-	16,16,16	3.44	3 (18%)	20,23,23	1.82	6 (30%)

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	401	-	-	3/8/8/8	0/1/1/1
2	PLP	B	401	1	-	0/8/8/8	0/1/1/1
2	PLP	C	401	1	-	0/8/8/8	0/1/1/1
2	PLP	D	401	1	-	0/8/8/8	0/1/1/1
2	PLP	E	401	1	-	0/8/8/8	0/1/1/1
2	PLP	F	401	1	-	3/8/8/8	0/1/1/1
2	PLP	G	401	1	-	0/8/8/8	0/1/1/1
2	PLP	H	401	-	-	1/8/8/8	0/1/1/1
2	PLP	I	401	1	-	0/8/8/8	0/1/1/1
2	PLP	K	401	-	-	0/8/8/8	0/1/1/1

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	401	PLP	C3-C2	13.41	1.50	1.40
2	B	401	PLP	C3-C2	12.09	1.49	1.40
2	K	401	PLP	C3-C2	11.61	1.48	1.40
2	C	401	PLP	C3-C2	11.59	1.48	1.40
2	D	401	PLP	C3-C2	10.91	1.48	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	401	PLP	C3-C2	10.30	1.47	1.40
2	F	401	PLP	C3-C2	9.94	1.47	1.40
2	G	401	PLP	C3-C2	9.65	1.47	1.40
2	A	401	PLP	C3-C2	9.09	1.47	1.40
2	H	401	PLP	C3-C2	9.07	1.47	1.40
2	E	401	PLP	C4-C3	6.75	1.51	1.40
2	F	401	PLP	C4-C3	6.56	1.50	1.40
2	H	401	PLP	C4-C3	6.18	1.50	1.40
2	C	401	PLP	C4-C3	5.95	1.49	1.40
2	A	401	PLP	C4-C3	5.75	1.49	1.40
2	B	401	PLP	C4-C3	5.56	1.49	1.40
2	H	401	PLP	C4-C5	5.35	1.48	1.42
2	I	401	PLP	C4-C5	5.06	1.48	1.42
2	G	401	PLP	C4-C3	5.01	1.48	1.40
2	K	401	PLP	C4-C3	5.00	1.48	1.40
2	D	401	PLP	C4-C3	4.93	1.48	1.40
2	E	401	PLP	C4-C5	4.92	1.48	1.42
2	G	401	PLP	C4-C5	4.86	1.48	1.42
2	K	401	PLP	C4-C5	4.80	1.48	1.42
2	D	401	PLP	C4-C5	4.70	1.47	1.42
2	I	401	PLP	C4-C3	4.68	1.48	1.40
2	F	401	PLP	C4-C5	4.63	1.47	1.42
2	B	401	PLP	C4-C5	4.38	1.47	1.42
2	A	401	PLP	C4-C5	4.28	1.47	1.42
2	C	401	PLP	C4-C5	4.10	1.47	1.42
2	H	401	PLP	C4-C4A	2.07	1.51	1.46

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	401	PLP	C3-C4-C4A	6.48	129.01	119.83
2	E	401	PLP	C4-C3-C2	-5.98	116.48	120.15
2	B	401	PLP	C4-C3-C2	-5.94	116.50	120.15
2	D	401	PLP	C4-C3-C2	-5.74	116.62	120.15
2	I	401	PLP	C4-C3-C2	-4.95	117.11	120.15
2	H	401	PLP	C3-C4-C5	-4.95	114.47	118.27
2	F	401	PLP	C4-C3-C2	-4.52	117.38	120.15
2	G	401	PLP	C4-C3-C2	-4.22	117.56	120.15
2	K	401	PLP	O4P-C5A-C5	4.18	117.31	109.35
2	E	401	PLP	O4P-C5A-C5	4.17	117.29	109.35
2	I	401	PLP	O3-C3-C2	3.47	125.05	117.78
2	B	401	PLP	O3P-P-O4P	-3.46	97.52	106.73

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	401	PLP	O3P-P-O4P	-3.39	97.72	106.73
2	E	401	PLP	C3-C4-C4A	3.37	124.61	119.83
2	I	401	PLP	O4A-C4A-C4	-3.37	117.57	124.96
2	F	401	PLP	O4P-C5A-C5	3.32	115.68	109.35
2	C	401	PLP	C4-C3-C2	-3.30	118.12	120.15
2	K	401	PLP	C4-C3-C2	-3.29	118.13	120.15
2	A	401	PLP	C6-N1-C2	3.26	125.34	119.17
2	D	401	PLP	O4A-C4A-C4	-3.24	117.86	124.96
2	F	401	PLP	O4A-C4A-C4	-3.17	118.02	124.96
2	C	401	PLP	C3-C4-C4A	3.08	124.19	119.83
2	I	401	PLP	O3P-P-O2P	3.03	119.33	107.57
2	H	401	PLP	C4-C3-C2	-2.96	118.33	120.15
2	B	401	PLP	C3-C4-C4A	2.91	123.96	119.83
2	E	401	PLP	C6-N1-C2	2.88	124.62	119.17
2	A	401	PLP	C4-C3-C2	-2.79	118.44	120.15
2	G	401	PLP	O3P-P-O2P	2.78	118.37	107.57
2	E	401	PLP	O3P-P-O4P	-2.77	99.35	106.73
2	K	401	PLP	C3-C4-C5	-2.75	116.16	118.27
2	F	401	PLP	C6-N1-C2	2.74	124.36	119.17
2	D	401	PLP	C6-N1-C2	2.73	124.33	119.17
2	H	401	PLP	O3-C3-C4	2.73	126.96	119.60
2	B	401	PLP	C6-N1-C2	2.63	124.14	119.17
2	G	401	PLP	O4A-C4A-C4	-2.61	119.23	124.96
2	B	401	PLP	O4A-C4A-C4	-2.60	119.27	124.96
2	A	401	PLP	O4A-C4A-C4	-2.59	119.29	124.96
2	E	401	PLP	O4A-C4A-C4	-2.49	119.50	124.96
2	C	401	PLP	O3P-P-O4P	-2.48	100.13	106.73
2	K	401	PLP	C6-N1-C2	2.48	123.86	119.17
2	C	401	PLP	C3-C4-C5	-2.45	116.39	118.27
2	D	401	PLP	O3P-P-O1P	2.42	120.09	110.53
2	G	401	PLP	C6-N1-C2	2.35	123.62	119.17
2	F	401	PLP	O2P-P-O4P	-2.35	100.48	106.73
2	H	401	PLP	O3P-P-O2P	2.33	116.62	107.57
2	E	401	PLP	O3-C3-C4	2.26	125.71	119.60
2	K	401	PLP	O4A-C4A-C4	-2.23	120.07	124.96
2	A	401	PLP	C2A-C2-N1	2.22	122.08	117.82
2	K	401	PLP	O3P-P-O2P	2.22	116.19	107.57
2	I	401	PLP	C6-N1-C2	2.17	123.28	119.17
2	H	401	PLP	C6-N1-C2	2.16	123.26	119.17
2	A	401	PLP	O3P-P-O2P	2.13	115.87	107.57
2	A	401	PLP	C3-C4-C4A	2.12	122.84	119.83
2	F	401	PLP	C3-C4-C4A	2.10	122.81	119.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	401	PLP	O3P-P-O2P	2.05	115.53	107.57
2	C	401	PLP	O3P-P-O2P	2.03	115.47	107.57
2	C	401	PLP	O4A-C4A-C4	-2.01	120.56	124.96

There are no chirality outliers.

All (7) torsion outliers are listed below:

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

There are no ring outliers.

9 monomers are involved in 35 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	PLP	9	0
2	B	401	PLP	4	0
2	C	401	PLP	3	0
2	D	401	PLP	3	0
2	E	401	PLP	3	0
2	F	401	PLP	6	0
2	G	401	PLP	1	0
2	H	401	PLP	4	0
2	K	401	PLP	2	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	348/358 (97%)	-0.19	3 (0%) 84 85	36, 60, 97, 137	0
1	B	349/358 (97%)	-0.08	11 (3%) 47 46	37, 66, 111, 163	0
1	C	349/358 (97%)	-0.10	2 (0%) 89 89	35, 68, 102, 127	0
1	D	345/358 (96%)	0.14	17 (4%) 29 28	42, 86, 125, 153	0
1	E	342/358 (95%)	-0.09	9 (2%) 56 55	45, 75, 115, 131	0
1	F	322/358 (89%)	-0.11	4 (1%) 79 79	43, 78, 121, 146	0
1	G	341/358 (95%)	0.06	6 (1%) 68 69	48, 90, 125, 155	0
1	H	349/358 (97%)	0.20	28 (8%) 12 10	62, 100, 136, 160	0
1	I	336/358 (93%)	0.36	33 (9%) 7 6	55, 94, 137, 156	0
1	J	253/358 (70%)	0.50	34 (13%) 3 2	61, 100, 158, 199	0
1	K	316/358 (88%)	0.29	28 (8%) 9 8	68, 104, 143, 163	0
1	L	216/358 (60%)	0.16	12 (5%) 24 22	58, 107, 146, 165	0
All	All	3866/4296 (89%)	0.08	187 (4%) 30 29	35, 85, 133, 199	0

All (187) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	187	ALA	11.1
1	F	295	PHE	8.2
1	A	31	PHE	8.0
1	I	35	LEU	7.0
1	I	224	HIS	6.4
1	L	134	ILE	5.8
1	J	95	TYR	5.7
1	B	308	PHE	5.7
1	H	342	VAL	5.4
1	B	31	PHE	5.4
1	I	308	PHE	5.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	J	100	VAL	5.3
1	F	156	LYS	5.3
1	J	9	PHE	4.9
1	L	135	PRO	4.9
1	J	83	MET	4.8
1	I	221	TYR	4.8
1	E	326	VAL	4.7
1	J	119	GLY	4.7
1	J	129	ILE	4.5
1	H	258	ILE	4.4
1	H	349	MET	4.3
1	D	258	ILE	4.3
1	E	134	ILE	4.3
1	K	67	GLY	4.2
1	K	90	ASN	4.2
1	J	105	ALA	4.2
1	K	72	PHE	4.1
1	J	138	TYR	4.0
1	I	71	LEU	4.0
1	K	88	LEU	3.9
1	J	259	GLN	3.8
1	I	140	TYR	3.7
1	H	252	ILE	3.6
1	F	7	HIS	3.6
1	K	68	TYR	3.5
1	I	220	ASP	3.5
1	J	133	GLN	3.5
1	J	61	VAL	3.5
1	L	170	SER	3.4
1	I	235	PRO	3.4
1	D	252	ILE	3.4
1	J	214	LYS	3.4
1	B	317	ILE	3.4
1	H	154	ILE	3.4
1	K	313	LEU	3.3
1	K	165	VAL	3.3
1	B	6	ILE	3.3
1	J	216	PRO	3.3
1	G	119	GLY	3.2
1	K	257	LYS	3.2
1	H	7	HIS	3.2
1	D	326	VAL	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	K	334	TYR	3.1
1	D	113	GLY	3.1
1	L	150	TYR	3.1
1	I	141	PHE	3.1
1	I	66	GLU	3.1
1	J	108	GLU	3.1
1	G	66	GLU	3.1
1	L	197	GLY	3.0
1	I	164	LEU	3.0
1	I	73	PHE	3.0
1	L	64	ILE	3.0
1	K	138	TYR	3.0
1	E	119	GLY	3.0
1	J	174	SER	3.0
1	K	65	PRO	3.0
1	I	155	ARG	3.0
1	B	326	VAL	3.0
1	J	128	TYR	2.9
1	H	91	LYS	2.9
1	J	79	LEU	2.9
1	K	166	ALA	2.9
1	H	300	GLN	2.9
1	H	157	ASP	2.9
1	D	116	LYS	2.8
1	I	205	LYS	2.8
1	I	266	ALA	2.8
1	B	132	TYR	2.8
1	I	136	SER	2.8
1	J	97	ASP	2.8
1	K	254	GLY	2.8
1	J	109	ALA	2.8
1	J	186	TYR	2.8
1	J	213	ARG	2.8
1	J	113	GLY	2.8
1	I	203	ILE	2.8
1	H	341	SER	2.8
1	K	209	GLY	2.7
1	J	130	PRO	2.7
1	D	304	LEU	2.7
1	C	32	TRP	2.7
1	D	112	ILE	2.7
1	L	152	THR	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	I	209	GLY	2.7
1	K	73	PHE	2.7
1	I	201	VAL	2.7
1	D	270	TYR	2.7
1	H	90	ASN	2.7
1	I	264	GLU	2.7
1	K	66	GLU	2.7
1	I	87	ASN	2.6
1	I	222	GLN	2.6
1	C	323	HIS	2.6
1	I	68	TYR	2.6
1	K	309	SER	2.6
1	K	256	LYS	2.6
1	G	71	LEU	2.5
1	K	89	LEU	2.5
1	H	183	SER	2.5
1	L	149	ILE	2.5
1	H	45	LYS	2.5
1	H	259	GLN	2.5
1	D	173	LEU	2.5
1	J	125	ASN	2.5
1	H	6	ILE	2.5
1	I	211	VAL	2.5
1	K	312	ALA	2.5
1	I	173	LEU	2.5
1	D	7	HIS	2.4
1	E	96	LEU	2.4
1	J	218	ILE	2.4
1	F	31	PHE	2.4
1	I	90	ASN	2.4
1	E	285	LYS	2.4
1	J	197	GLY	2.4
1	H	146	ASN	2.4
1	K	184	LEU	2.4
1	I	236	VAL	2.4
1	E	158	ILE	2.4
1	K	236	VAL	2.4
1	H	217	ILE	2.4
1	H	161	PRO	2.3
1	B	23	ALA	2.3
1	E	88	LEU	2.3
1	J	215	ILE	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	301	TYR	2.3
1	H	132	TYR	2.3
1	D	68	TYR	2.3
1	H	163	PRO	2.3
1	B	301	TYR	2.3
1	I	331	ALA	2.3
1	L	66	GLU	2.3
1	K	136	SER	2.3
1	H	185	ILE	2.3
1	B	354	GLN	2.3
1	G	299	GLU	2.3
1	K	139	ASP	2.3
1	J	96	LEU	2.3
1	K	221	TYR	2.3
1	A	131	GLU	2.3
1	G	24	THR	2.2
1	J	152	THR	2.2
1	D	266	ALA	2.2
1	K	258	ILE	2.2
1	J	173	LEU	2.2
1	D	308	PHE	2.2
1	E	97	ASP	2.2
1	H	164	LEU	2.2
1	I	70	ILE	2.2
1	I	67	GLY	2.2
1	I	78	SER	2.2
1	D	244	GLN	2.2
1	H	145	THR	2.2
1	H	37	ILE	2.2
1	D	20	VAL	2.2
1	B	33	GLU	2.1
1	H	66	GLU	2.1
1	L	186	TYR	2.1
1	K	262	ASN	2.1
1	D	254	GLY	2.1
1	G	155	ARG	2.1
1	I	204	LYS	2.1
1	E	31	PHE	2.1
1	J	131	GLU	2.1
1	J	135	PRO	2.1
1	H	278	ILE	2.1
1	H	317	ILE	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	I	293	VAL	2.0
1	A	136	SER	2.0
1	J	154	ILE	2.0
1	K	81	PHE	2.0
1	H	73	PHE	2.0
1	L	157	ASP	2.0
1	L	166	ALA	2.0
1	B	300	GLN	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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	I	401	16/16	0.89	0.16	75,89,94,97	0
2	PLP	A	401	16/16	0.91	0.24	56,75,92,101	0
2	PLP	H	401	16/16	0.91	0.26	75,85,94,97	0
3	CL	A	402	1/1	0.92	0.09	74,74,74,74	0
3	CL	E	402	1/1	0.93	0.12	92,92,92,92	0
2	PLP	C	401	16/16	0.93	0.15	61,69,76,79	0
2	PLP	G	401	16/16	0.93	0.24	69,86,89,91	0
3	CL	C	402	1/1	0.94	0.28	81,81,81,81	0
2	PLP	K	401	16/16	0.95	0.12	62,70,73,74	0
2	PLP	E	401	16/16	0.95	0.20	64,71,78,79	0
2	PLP	F	401	16/16	0.96	0.17	64,71,74,75	0
2	PLP	D	401	16/16	0.96	0.21	57,86,93,95	0
2	PLP	B	401	16/16	0.96	0.15	49,64,70,75	0
3	CL	D	402	1/1	0.97	0.14	78,78,78,78	0
3	CL	B	402	1/1	0.98	0.16	67,67,67,67	0

6.5 Other polymers [i](#)

There are no such residues in this entry.