



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:34 PM UTC

PDB ID : 6FL5 / pdb_00006fl5
Title : Structure of human SHMT1-H135N-R137A-E168N mutant at 3.6 Ang. resolution
Authors : Giardina, G.; Cutruzzola, F.; Lucchi, R.
Deposited on : 2018-01-25
Resolution : 3.60 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

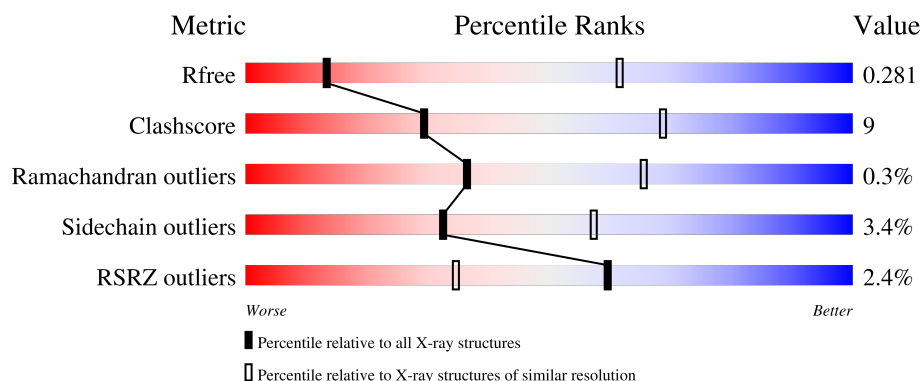
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.60 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}	180053	1747 (3.70-3.50)
Clashscore	190562	1827 (3.70-3.50)
Ramachandran outliers	187476	1773 (3.70-3.50)
Sidechain outliers	187428	1772 (3.70-3.50)
RSRZ outliers	180081	1745 (3.70-3.50)

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

Mol	Chain	Length	Quality of chain
1	A	471	
1	D	471	
1	G	471	
1	J	471	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 14389 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.

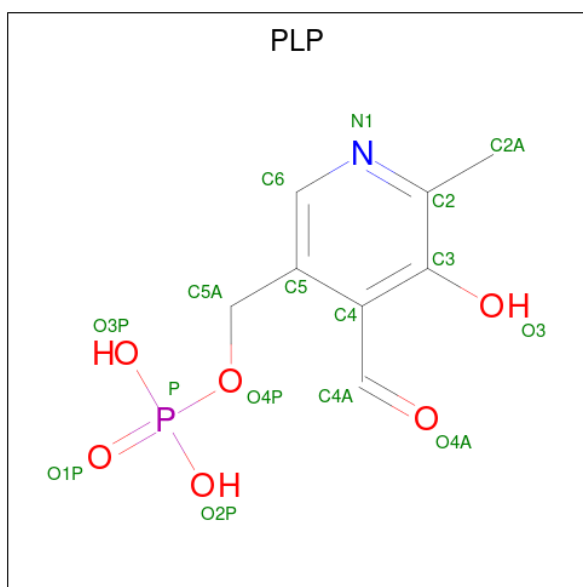
- Molecule 1 is a protein called Serine hydroxymethyltransferase, cytosolic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	471	Total	C	N	O	S	0	0	0
			3614	2282	632	682	18			
1	D	470	Total	C	N	O	S	0	0	0
			3603	2275	631	679	18			
1	G	467	Total	C	N	O	S	0	0	0
			3590	2266	628	678	18			
1	J	458	Total	C	N	O	S	0	0	0
			3518	2222	615	663	18			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	135	ASN	HIS	engineered mutation	UNP P34896
A	137	ALA	ARG	engineered mutation	UNP P34896
A	168	ASN	GLU	engineered mutation	UNP P34896
D	135	ASN	HIS	engineered mutation	UNP P34896
D	137	ALA	ARG	engineered mutation	UNP P34896
D	168	ASN	GLU	engineered mutation	UNP P34896
G	135	ASN	HIS	engineered mutation	UNP P34896
G	137	ALA	ARG	engineered mutation	UNP P34896
G	168	ASN	GLU	engineered mutation	UNP P34896
J	135	ASN	HIS	engineered mutation	UNP P34896
J	137	ALA	ARG	engineered mutation	UNP P34896
J	168	ASN	GLU	engineered mutation	UNP P34896

- Molecule 2 is PYRIDOXAL-5'-PHOSPHATE (CCD ID: PLP) (formula: C₈H₁₀NO₆P).



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

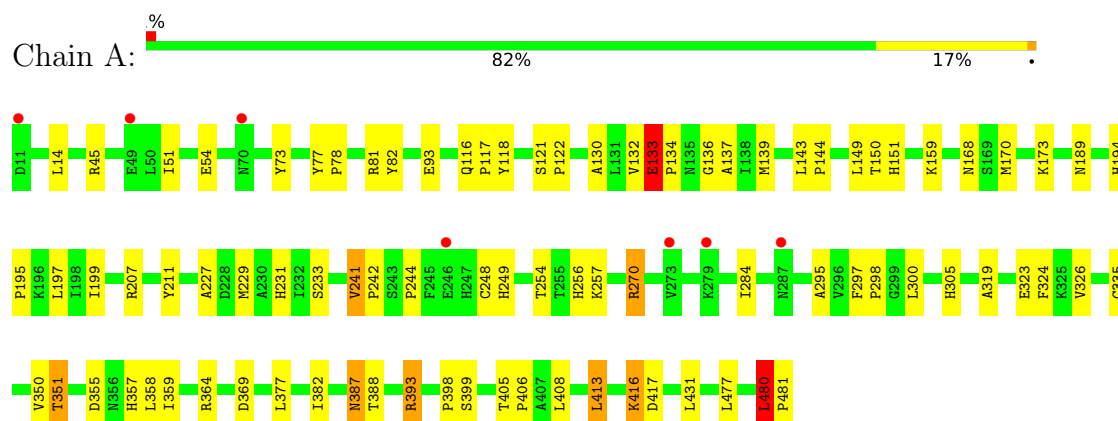
- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Cl	0	0
			2	2		
3	G	1	Total	Cl	0	0
			1	1		
3	J	1	Total	Cl	0	0
			1	1		

3 Residue-property plots

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.

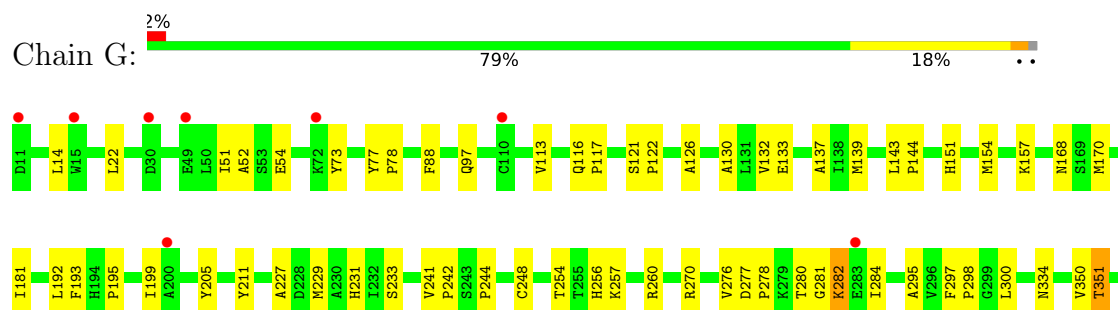
- Molecule 1: Serine hydroxymethyltransferase, cytosolic

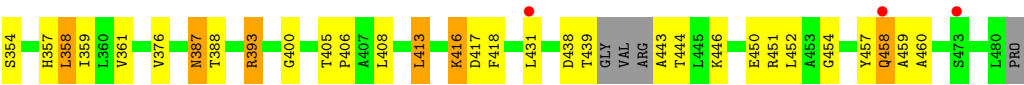


- Molecule 1: Serine hydroxymethyltransferase, cytosolic

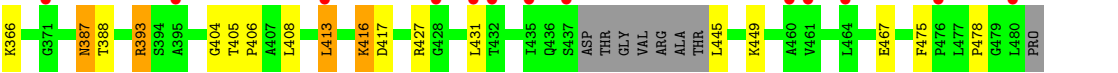
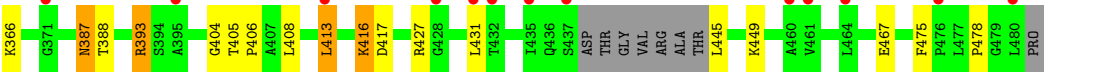
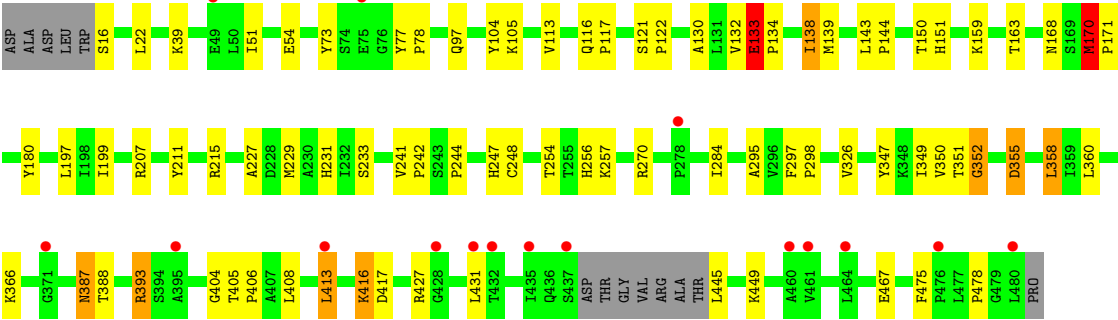
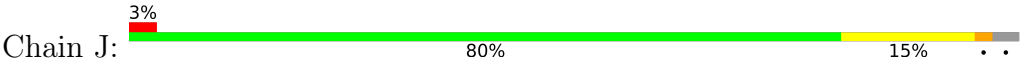


- Molecule 1: Serine hydroxymethyltransferase, cytosolic





● Molecule 1: Serine hydroxymethyltransferase, cytosolic



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	139.72Å 139.72Å 267.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.01 – 3.60 50.01 – 3.60	Depositor EDS
% Data completeness (in resolution range)	98.0 (50.01-3.60) 98.0 (50.01-3.60)	Depositor EDS
R_{merge}	0.31	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.98 (at 3.57Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.262 , 0.277 0.262 , 0.281	Depositor DCC
R_{free} test set	1545 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	72.1	Xtriage
Anisotropy	0.460	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 68.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	14389	wwPDB-VP
Average B, all atoms (Å ²)	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.53% 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: PLP, CL

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	0.30	0/3687	0.69	4/4992 (0.1%)
1	D	0.30	0/3675	0.67	2/4975 (0.0%)
1	G	0.30	0/3661	0.69	0/4954
1	J	0.29	0/3587	0.70	4/4851 (0.1%)
All	All	0.30	0/14610	0.69	10/19772 (0.1%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	133	GLU	CA-C-N	8.97	131.05	119.84
1	J	133	GLU	C-N-CA	8.97	131.05	119.84
1	J	170	MET	CA-C-N	7.14	127.56	119.92
1	J	170	MET	C-N-CA	7.14	127.56	119.92
1	A	477	LEU	CA-C-N	6.50	126.88	119.93
1	A	477	LEU	C-N-CA	6.50	126.88	119.93
1	A	133	GLU	CA-C-N	5.66	126.92	119.84
1	A	133	GLU	C-N-CA	5.66	126.92	119.84
1	D	133	GLU	CA-C-N	5.05	126.15	119.84
1	D	133	GLU	C-N-CA	5.05	126.15	119.84

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3614	0	3587	73	0
1	D	3603	0	3576	55	0
1	G	3590	0	3563	71	0
1	J	3518	0	3499	65	0
2	A	15	0	6	0	0
2	D	15	0	6	0	0
2	G	15	0	6	0	0
2	J	15	0	6	0	0
3	A	2	0	0	0	0
3	G	1	0	0	0	0
3	J	1	0	0	0	0
All	All	14389	0	14249	247	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (247) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:480:LEU:HB2	1:A:481:PRO:CD	1.71	1.20
1:A:480:LEU:CD1	1:A:481:PRO:HD2	1.75	1.14
1:A:480:LEU:HB2	1:A:481:PRO:HD3	1.34	1.09
1:A:480:LEU:HD12	1:A:481:PRO:HD2	1.11	1.07
1:G:438:ASP:OD2	1:G:457:TYR:OH	1.86	0.92
1:A:480:LEU:CB	1:A:481:PRO:CD	2.46	0.90
1:A:480:LEU:HD12	1:A:481:PRO:CD	2.02	0.84
1:A:480:LEU:HB2	1:A:481:PRO:HD2	1.58	0.84
1:G:14:LEU:HD23	1:J:326:VAL:HG21	1.58	0.83
1:G:454:GLY:O	1:G:458:GLN:NE2	2.15	0.79
1:J:254:THR:OG1	1:J:256:HIS:CE1	2.36	0.79
1:D:168:ASN:CG	1:J:168:ASN:HD21	1.93	0.77
1:A:350:VAL:O	1:A:351:THR:HG22	1.86	0.76
1:G:254:THR:OG1	1:G:256:HIS:CE1	2.41	0.74
1:J:121:SER:HB2	1:J:122:PRO:HD3	1.68	0.74
1:G:229:MET:HE2	1:G:233:SER:HA	1.70	0.73
1:G:350:VAL:O	1:G:351:THR:HG22	1.89	0.73
1:J:351:THR:HG22	1:J:351:THR:O	1.89	0.72
1:G:157:LYS:H	1:G:157:LYS:HD2	1.55	0.72
1:A:45:ARG:HB2	1:A:45:ARG:NH2	2.06	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:130:ALA:HB2	1:G:295:ALA:HB2	1.73	0.70
1:D:229:MET:HE2	1:D:233:SER:HA	1.73	0.69
1:G:121:SER:HB2	1:G:122:PRO:HD3	1.72	0.69
1:A:229:MET:HE2	1:A:233:SER:HA	1.74	0.69
1:G:277:ASP:OD1	1:G:278:PRO:HD2	1.93	0.68
1:J:405:THR:N	1:J:406:PRO:CD	2.57	0.67
1:A:405:THR:N	1:A:406:PRO:CD	2.59	0.66
1:G:405:THR:N	1:G:406:PRO:HD2	2.11	0.66
1:D:254:THR:OG1	1:D:256:HIS:CE1	2.49	0.66
1:A:480:LEU:CG	1:A:481:PRO:HD2	2.26	0.65
1:D:405:THR:N	1:D:406:PRO:CD	2.60	0.65
1:G:405:THR:N	1:G:406:PRO:CD	2.59	0.65
1:G:354:SER:HB2	1:G:359:ILE:HG22	1.78	0.64
1:D:416:LYS:H	1:D:416:LYS:HD3	1.62	0.64
1:D:121:SER:HB2	1:D:122:PRO:HD3	1.78	0.64
1:G:227:ALA:HB2	1:G:248:CYS:SG	2.39	0.63
1:A:121:SER:HB2	1:A:122:PRO:HD3	1.81	0.63
1:D:116:GLN:N	1:D:117:PRO:CD	2.61	0.63
1:A:326:VAL:HG21	1:D:14:LEU:HD23	1.80	0.62
1:J:229:MET:HE2	1:J:233:SER:HA	1.82	0.62
1:G:408:LEU:HB3	1:G:413:LEU:HG	1.81	0.62
1:A:254:THR:OG1	1:A:256:HIS:CE1	2.53	0.62
1:A:405:THR:N	1:A:406:PRO:HD2	2.14	0.62
1:D:168:ASN:CB	1:J:168:ASN:HD21	2.13	0.62
1:J:405:THR:N	1:J:406:PRO:HD2	2.15	0.61
1:G:116:GLN:N	1:G:117:PRO:CD	2.63	0.61
1:J:116:GLN:N	1:J:117:PRO:CD	2.63	0.61
1:A:387:ASN:HD22	1:A:388:THR:N	1.98	0.61
1:A:357:HIS:HD1	1:A:357:HIS:H	1.49	0.61
1:A:480:LEU:CB	1:A:481:PRO:HD2	2.19	0.61
1:D:168:ASN:HB3	1:J:168:ASN:HD21	1.66	0.60
1:A:116:GLN:N	1:A:117:PRO:CD	2.65	0.60
1:D:405:THR:N	1:D:406:PRO:HD2	2.16	0.60
1:J:215:ARG:NH1	1:J:247:HIS:O	2.32	0.60
1:A:82:TYR:HE2	1:A:297:PHE:HE2	1.49	0.60
1:G:157:LYS:HD2	1:G:157:LYS:N	2.17	0.60
1:A:173:LYS:HD2	1:G:192:LEU:HD21	1.85	0.59
1:G:130:ALA:HB2	1:G:295:ALA:CB	2.32	0.59
1:J:408:LEU:HB3	1:J:413:LEU:HG	1.86	0.58
1:A:82:TYR:CE2	1:A:297:PHE:HE2	2.21	0.58
1:G:254:THR:HG21	1:G:257:LYS:HD2	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:413:LEU:HD13	1:J:417:ASP:HB3	1.85	0.58
1:G:357:HIS:HD1	1:G:357:HIS:H	1.52	0.57
1:D:387:ASN:HD22	1:D:388:THR:N	2.02	0.57
1:A:151:HIS:CD2	1:A:199:ILE:HG21	2.40	0.57
1:J:180:TYR:CE1	1:J:351:THR:HG23	2.40	0.57
1:G:452:LEU:C	1:G:454:GLY:H	2.13	0.57
1:J:138:ILE:HD11	1:J:163:THR:CG2	2.35	0.57
1:J:227:ALA:HB2	1:J:248:CYS:SG	2.45	0.57
1:A:408:LEU:HB3	1:A:413:LEU:HG	1.87	0.57
1:A:413:LEU:HD13	1:A:417:ASP:HB3	1.87	0.57
1:J:387:ASN:HD22	1:J:388:THR:N	2.02	0.57
1:J:138:ILE:HD11	1:J:163:THR:HG22	1.85	0.56
1:G:77:TYR:HB3	1:G:78:PRO:HD2	1.87	0.56
1:G:139:MET:HG3	1:G:195:PRO:HB3	1.88	0.56
1:J:393:ARG:CD	1:J:393:ARG:H	2.18	0.56
1:D:133:GLU:HB3	1:D:134:PRO:HD2	1.88	0.56
1:G:139:MET:HE3	1:G:170:MET:HE2	1.88	0.56
1:J:350:VAL:HG12	1:J:360:LEU:HB3	1.88	0.56
1:A:197:LEU:HD23	1:A:197:LEU:C	2.30	0.55
1:J:393:ARG:H	1:J:393:ARG:NE	2.03	0.55
1:G:277:ASP:CG	1:G:278:PRO:HD2	2.31	0.55
1:G:387:ASN:HD22	1:G:388:THR:N	2.04	0.55
1:G:393:ARG:H	1:G:393:ARG:CD	2.19	0.55
1:D:116:GLN:N	1:D:117:PRO:HD2	2.21	0.55
1:D:413:LEU:HD13	1:D:417:ASP:HB3	1.89	0.55
1:A:51:ILE:HB	1:A:54:GLU:HG3	1.88	0.55
1:D:241:VAL:HG13	1:D:242:PRO:HD2	1.89	0.55
1:D:408:LEU:HB3	1:D:413:LEU:HG	1.89	0.55
1:G:358:LEU:C	1:G:358:LEU:HD12	2.31	0.54
1:J:254:THR:HG21	1:J:257:LYS:HD2	1.88	0.54
1:J:416:LYS:H	1:J:416:LYS:HD3	1.72	0.54
1:J:132:VAL:HG21	1:J:138:ILE:CG2	2.38	0.54
1:A:77:TYR:HB3	1:A:78:PRO:HD2	1.90	0.53
1:D:211:TYR:CZ	1:D:244:PRO:HB3	2.44	0.53
1:D:254:THR:HG21	1:D:257:LYS:HD2	1.91	0.53
1:A:416:LYS:HD3	1:A:416:LYS:H	1.74	0.53
1:D:351:THR:HG23	1:D:351:THR:O	2.09	0.52
1:D:180:TYR:HE1	1:D:207:ARG:HG3	1.74	0.52
1:A:284:ILE:HD12	1:A:284:ILE:N	2.24	0.51
1:J:116:GLN:N	1:J:117:PRO:HD2	2.25	0.51
1:G:116:GLN:N	1:G:117:PRO:HD2	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:393:ARG:H	1:G:393:ARG:NE	2.08	0.51
1:J:130:ALA:HB2	1:J:295:ALA:HB2	1.93	0.51
1:J:207:ARG:CG	1:J:351:THR:HG21	2.40	0.51
1:G:282:LYS:O	1:G:284:ILE:HD12	2.11	0.50
1:G:413:LEU:HD13	1:G:417:ASP:HB3	1.92	0.50
1:G:277:ASP:OD2	1:G:280:THR:HG23	2.11	0.50
1:D:51:ILE:HB	1:D:54:GLU:HG3	1.94	0.50
1:J:51:ILE:HB	1:J:54:GLU:HG3	1.94	0.50
1:J:358:LEU:HD12	1:J:358:LEU:C	2.37	0.50
1:A:207:ARG:HE	1:A:351:THR:HG23	1.77	0.49
1:G:416:LYS:H	1:G:416:LYS:HD3	1.76	0.49
1:A:393:ARG:H	1:A:393:ARG:NE	2.10	0.49
1:A:45:ARG:HB2	1:A:45:ARG:HH21	1.77	0.49
1:G:51:ILE:HB	1:G:54:GLU:HG3	1.95	0.49
1:G:284:ILE:HD12	1:G:284:ILE:N	2.27	0.49
1:G:376:VAL:HG22	1:G:452:LEU:HD13	1.95	0.49
1:D:358:LEU:C	1:D:358:LEU:HD12	2.37	0.48
1:G:211:TYR:CZ	1:G:244:PRO:HB3	2.47	0.48
1:A:358:LEU:HD12	1:A:358:LEU:C	2.37	0.48
1:J:351:THR:O	1:J:352:GLY:C	2.56	0.48
1:G:151:HIS:CD2	1:G:199:ILE:HG21	2.48	0.48
1:J:130:ALA:HB2	1:J:295:ALA:CB	2.44	0.48
1:J:77:TYR:HB3	1:J:78:PRO:HD2	1.95	0.48
1:J:351:THR:O	1:J:351:THR:CG2	2.61	0.48
1:A:143:LEU:HB3	1:A:144:PRO:HD3	1.95	0.48
1:G:361:VAL:O	1:G:400:GLY:HA2	2.14	0.48
1:A:45:ARG:HH21	1:A:45:ARG:CB	2.27	0.48
1:G:22:LEU:HB3	1:J:478:PRO:HB3	1.96	0.48
1:J:151:HIS:CD2	1:J:199:ILE:HG21	2.49	0.48
1:A:116:GLN:N	1:A:117:PRO:HD2	2.29	0.47
1:A:14:LEU:HD23	1:D:326:VAL:HG21	1.97	0.47
1:D:151:HIS:CD2	1:D:199:ILE:HG21	2.50	0.47
1:D:393:ARG:H	1:D:393:ARG:NE	2.13	0.47
1:G:297:PHE:CD1	1:G:298:PRO:HA	2.50	0.47
1:A:207:ARG:HE	1:A:351:THR:CG2	2.27	0.47
1:A:207:ARG:NH1	1:A:355:ASP:OD1	2.44	0.47
1:D:350:VAL:O	1:D:351:THR:HG22	2.15	0.47
1:G:358:LEU:C	1:G:358:LEU:CD1	2.88	0.47
1:J:170:MET:HA	1:J:171:PRO:HD2	1.76	0.47
1:A:81:ARG:NH2	1:A:93:GLU:OE1	2.45	0.47
1:D:143:LEU:N	1:D:144:PRO:HD2	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:297:PHE:CG	1:G:298:PRO:HA	2.50	0.46
1:J:143:LEU:N	1:J:144:PRO:HD2	2.31	0.46
1:A:249:HIS:HA	1:A:270:ARG:HG3	1.98	0.46
1:J:358:LEU:C	1:J:358:LEU:CD1	2.89	0.46
1:A:143:LEU:N	1:A:144:PRO:HD2	2.30	0.46
1:A:335:CYS:SG	1:A:359:ILE:HG23	2.56	0.46
1:D:168:ASN:ND2	1:J:168:ASN:HD21	2.14	0.46
1:G:157:LYS:H	1:G:157:LYS:CD	2.26	0.46
1:D:180:TYR:CE1	1:D:207:ARG:HG3	2.51	0.46
1:J:297:PHE:CG	1:J:298:PRO:HA	2.51	0.46
1:J:358:LEU:HD12	1:J:358:LEU:O	2.15	0.46
1:D:354:SER:HB2	1:D:359:ILE:HG22	1.96	0.45
1:D:439:THR:O	1:D:443:ALA:HB2	2.16	0.45
1:D:132:VAL:O	1:D:133:GLU:HB2	2.17	0.45
1:G:88:PHE:CE1	1:J:39:LYS:HD3	2.51	0.45
1:D:323:GLU:OE1	1:D:323:GLU:N	2.43	0.45
1:D:180:TYR:HE1	1:D:207:ARG:CG	2.29	0.45
1:D:207:ARG:NH1	1:D:355:ASP:OD1	2.49	0.45
1:G:132:VAL:O	1:G:133:GLU:HB2	2.16	0.45
1:G:143:LEU:N	1:G:144:PRO:HD2	2.32	0.45
1:A:130:ALA:HB2	1:A:295:ALA:HB2	1.98	0.45
1:D:284:ILE:N	1:D:284:ILE:HD12	2.32	0.45
1:J:284:ILE:N	1:J:284:ILE:HD12	2.31	0.45
1:A:170:MET:HE1	1:A:189:ASN:HB3	1.99	0.45
1:J:121:SER:HA	1:J:150:THR:HG21	1.99	0.45
1:D:168:ASN:HB3	1:J:168:ASN:ND2	2.31	0.44
1:A:254:THR:HG21	1:A:257:LYS:HD2	1.99	0.44
1:D:118:TYR:CE1	1:D:305:HIS:CD2	3.05	0.44
1:G:260:ARG:CZ	1:J:22:LEU:HD21	2.46	0.44
1:J:139:MET:HG2	1:J:170:MET:O	2.18	0.44
1:A:194:HIS:CD2	1:G:154:MET:HG3	2.53	0.44
1:A:387:ASN:HD22	1:A:387:ASN:C	2.26	0.44
1:D:106:LEU:HD11	1:D:245:PHE:CE2	2.52	0.44
1:G:446:LYS:NZ	1:G:450:GLU:OE2	2.39	0.44
1:J:445:LEU:HG	1:J:449:LYS:HE3	1.99	0.44
1:D:256:HIS:ND1	1:D:263:ARG:HA	2.33	0.44
1:J:427:ARG:HH22	1:J:467:GLU:CD	2.26	0.44
1:G:143:LEU:HB3	1:G:144:PRO:HD3	2.00	0.44
1:G:458:GLN:HE21	1:G:458:GLN:HB2	1.54	0.44
1:J:241:VAL:HG13	1:J:242:PRO:HD2	1.99	0.44
1:A:323:GLU:OE1	1:A:323:GLU:N	2.41	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:361:VAL:O	1:D:400:GLY:HA2	2.18	0.43
1:A:121:SER:HA	1:A:150:THR:HG21	2.01	0.43
1:A:241:VAL:HG13	1:A:242:PRO:HD2	2.00	0.43
1:G:137:ALA:HB1	1:G:193:PHE:CE2	2.53	0.43
1:G:241:VAL:HG13	1:G:242:PRO:HD2	1.99	0.43
1:A:211:TYR:CZ	1:A:244:PRO:HB3	2.53	0.43
1:G:116:GLN:O	1:G:117:PRO:C	2.62	0.43
1:J:350:VAL:CG1	1:J:360:LEU:HB3	2.48	0.43
1:D:75:GLU:HB3	1:D:297:PHE:CZ	2.54	0.43
1:D:121:SER:HA	1:D:150:THR:HG21	2.00	0.43
1:G:181:ILE:HG13	1:G:205:TYR:CE1	2.54	0.43
1:G:280:THR:OG1	1:G:281:GLY:N	2.51	0.43
1:A:118:TYR:CE1	1:A:305:HIS:CD2	3.07	0.43
1:A:393:ARG:H	1:A:393:ARG:CD	2.32	0.43
1:A:364:ARG:HG3	1:A:399:SER:HB3	2.00	0.43
1:D:77:TYR:HB3	1:D:78:PRO:HD2	2.00	0.43
1:A:168:ASN:CG	1:G:168:ASN:ND2	2.77	0.42
1:A:116:GLN:O	1:A:117:PRO:C	2.62	0.42
1:D:328:GLN:O	1:D:331:VAL:HB	2.19	0.42
1:G:52:ALA:CB	1:G:358:LEU:HD23	2.49	0.42
1:G:459:ALA:O	1:G:460:ALA:C	2.63	0.42
1:J:349:ILE:HB	1:J:352:GLY:HA2	2.01	0.42
1:A:132:VAL:O	1:A:133:GLU:HB2	2.19	0.42
1:G:350:VAL:O	1:G:351:THR:CG2	2.64	0.42
1:J:413:LEU:HD22	1:J:475:PHE:CE2	2.54	0.42
1:D:50:LEU:HB2	1:D:383:ALA:O	2.19	0.42
1:J:143:LEU:HB3	1:J:144:PRO:HD3	2.01	0.42
1:A:377:LEU:HB3	1:A:382:ILE:HB	2.00	0.42
1:G:334:ASN:HB3	1:G:418:PHE:CD2	2.55	0.42
1:J:197:LEU:C	1:J:197:LEU:HD23	2.44	0.42
1:D:143:LEU:HB3	1:D:144:PRO:HD3	2.02	0.42
1:J:138:ILE:CD1	1:J:163:THR:CG2	2.97	0.42
1:J:350:VAL:O	1:J:350:VAL:HG13	2.19	0.42
1:A:168:ASN:CG	1:G:168:ASN:HD21	2.28	0.42
1:D:227:ALA:HB2	1:D:248:CYS:SG	2.60	0.42
1:A:139:MET:HG3	1:A:195:PRO:HB3	2.02	0.41
1:J:355:ASP:OD1	1:J:355:ASP:N	2.53	0.41
1:J:211:TYR:CZ	1:J:244:PRO:HB3	2.55	0.41
1:A:227:ALA:HB2	1:A:248:CYS:SG	2.60	0.41
1:J:132:VAL:O	1:J:133:GLU:HB2	2.19	0.41
1:A:149:LEU:HD13	1:D:298:PRO:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:451:ARG:HD3	1:G:451:ARG:HA	1.91	0.41
1:A:137:ALA:HA	1:A:168:ASN:O	2.20	0.41
1:G:452:LEU:C	1:G:454:GLY:N	2.77	0.41
1:J:347:TYR:CE2	1:J:366:LYS:HG3	2.55	0.41
1:A:45:ARG:NH2	1:A:45:ARG:CB	2.78	0.41
1:A:297:PHE:CG	1:A:298:PRO:HA	2.56	0.41
1:A:300:LEU:HD23	1:D:162:ALA:CB	2.51	0.41
1:A:319:ALA:HA	1:A:324:PHE:CG	2.56	0.41
1:D:249:HIS:HA	1:D:270:ARG:HG3	2.03	0.41
1:J:404:GLY:C	1:J:406:PRO:HD2	2.46	0.41
1:G:77:TYR:HB3	1:G:78:PRO:CD	2.50	0.41
1:A:351:THR:HG23	1:A:351:THR:O	2.21	0.40
1:J:104:TYR:O	1:J:105:LYS:C	2.64	0.40
1:A:132:VAL:HG12	1:A:136:GLY:HA3	2.02	0.40
1:D:429:ILE:O	1:D:432:THR:HB	2.22	0.40
1:G:97:GLN:HB2	1:G:113:VAL:HG13	2.03	0.40
1:G:126:ALA:HA	1:G:300:LEU:CD1	2.51	0.40
1:J:97:GLN:HB2	1:J:113:VAL:CG1	2.52	0.40
1:D:251:VAL:HB	1:D:268:PHE:HB2	2.03	0.40
1:A:369:ASP:HB2	1:A:398:PRO:O	2.20	0.40
1:D:181:ILE:HG13	1:D:205:TYR:CZ	2.57	0.40
1:G:439:THR:O	1:G:443:ALA:CB	2.69	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	469/471 (100%)	451 (96%)	15 (3%)	3 (1%)	21	54
1	D	468/471 (99%)	449 (96%)	19 (4%)	0	100	100
1	G	463/471 (98%)	443 (96%)	20 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	J	454/471 (96%)	437 (96%)	14 (3%)	3 (1%)	18	51
All	All	1854/1884 (98%)	1780 (96%)	68 (4%)	6 (0%)	36	65

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	480	LEU
1	J	352	GLY
1	J	134	PRO
1	A	134	PRO
1	J	133	GLU
1	A	133	GLU

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	383/387 (99%)	371 (97%)	12 (3%)	35	59
1	D	381/387 (98%)	369 (97%)	12 (3%)	35	59
1	G	381/387 (98%)	367 (96%)	14 (4%)	30	56
1	J	374/387 (97%)	360 (96%)	14 (4%)	30	56
All	All	1519/1548 (98%)	1467 (97%)	52 (3%)	32	57

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	73	TYR
1	A	159	LYS
1	A	231	HIS
1	A	241	VAL
1	A	270	ARG
1	A	351	THR
1	A	387	ASN
1	A	393	ARG

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Mol	Chain	Res	Type
1	A	413	LEU
1	A	416	LYS
1	A	431	LEU
1	A	480	LEU
1	D	73	TYR
1	D	159	LYS
1	D	170	MET
1	D	231	HIS
1	D	241	VAL
1	D	270	ARG
1	D	351	THR
1	D	387	ASN
1	D	393	ARG
1	D	413	LEU
1	D	416	LYS
1	D	431	LEU
1	G	73	TYR
1	G	231	HIS
1	G	270	ARG
1	G	276	VAL
1	G	282	LYS
1	G	351	THR
1	G	358	LEU
1	G	387	ASN
1	G	393	ARG
1	G	413	LEU
1	G	416	LYS
1	G	431	LEU
1	G	444	THR
1	G	458	GLN
1	J	16	SER
1	J	73	TYR
1	J	138	ILE
1	J	159	LYS
1	J	170	MET
1	J	231	HIS
1	J	270	ARG
1	J	355	ASP
1	J	358	LEU
1	J	387	ASN
1	J	393	ARG
1	J	413	LEU

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Mol	Chain	Res	Type
1	J	416	LYS
1	J	431	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	71	ASN
1	A	80	GLN
1	A	97	GLN
1	A	109	GLN
1	A	168	ASN
1	A	231	HIS
1	A	256	HIS
1	A	305	HIS
1	A	318	GLN
1	A	387	ASN
1	A	458	GLN
1	D	97	GLN
1	D	109	GLN
1	D	168	ASN
1	D	189	ASN
1	D	221	ASN
1	D	231	HIS
1	D	247	HIS
1	D	256	HIS
1	D	318	GLN
1	D	387	ASN
1	D	458	GLN
1	G	80	GLN
1	G	97	GLN
1	G	109	GLN
1	G	168	ASN
1	G	231	HIS
1	G	256	HIS
1	G	318	GLN
1	G	387	ASN
1	G	458	GLN
1	J	80	GLN
1	J	97	GLN
1	J	109	GLN
1	J	168	ASN
1	J	231	HIS

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Mol	Chain	Res	Type
1	J	256	HIS
1	J	305	HIS
1	J	318	GLN
1	J	329	HIS
1	J	330	GLN
1	J	458	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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	G	501	1	15,15,16	3.07	3 (20%)	21,22,23	1.26	2 (9%)
2	PLP	D	500	1	15,15,16	3.12	3 (20%)	21,22,23	1.30	4 (19%)
2	PLP	J	501	1	15,15,16	3.10	3 (20%)	21,22,23	1.24	2 (9%)
2	PLP	A	501	1	15,15,16	3.04	3 (20%)	21,22,23	1.28	2 (9%)

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	G	501	1	-	2/6/6/8	0/1/1/1
2	PLP	D	500	1	-	3/6/6/8	0/1/1/1
2	PLP	J	501	1	-	2/6/6/8	0/1/1/1
2	PLP	A	501	1	-	2/6/6/8	0/1/1/1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	500	PLP	C5-C4	7.90	1.49	1.40
2	J	501	PLP	C5-C4	7.77	1.49	1.40
2	G	501	PLP	C5-C4	7.65	1.49	1.40
2	D	500	PLP	C3-C2	7.63	1.48	1.41
2	A	501	PLP	C5-C4	7.52	1.49	1.40
2	J	501	PLP	C3-C2	7.49	1.48	1.41
2	A	501	PLP	C3-C2	7.44	1.48	1.41
2	G	501	PLP	C3-C2	7.38	1.48	1.41
2	G	501	PLP	C3-C4	4.50	1.48	1.40
2	J	501	PLP	C3-C4	4.42	1.48	1.40
2	A	501	PLP	C3-C4	4.39	1.48	1.40
2	D	500	PLP	C3-C4	4.24	1.48	1.40

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	501	PLP	O4P-C5A-C5	2.74	114.49	109.36
2	J	501	PLP	C6-N1-C2	2.48	123.70	119.20
2	A	501	PLP	O4P-C5A-C5	2.45	113.95	109.36
2	A	501	PLP	C6-N1-C2	2.44	123.63	119.20
2	J	501	PLP	O4P-C5A-C5	2.44	113.93	109.36
2	D	500	PLP	C6-N1-C2	2.43	123.61	119.20
2	G	501	PLP	C6-N1-C2	2.36	123.48	119.20
2	D	500	PLP	C4A-C4-C5	2.15	123.16	120.94
2	D	500	PLP	O4P-C5A-C5	2.09	113.28	109.36
2	D	500	PLP	O3-C3-C2	2.03	121.80	117.58

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	PLP	C5A-O4P-P-O2P
2	D	500	PLP	C4-C5-C5A-O4P
2	D	500	PLP	C6-C5-C5A-O4P
2	G	501	PLP	C4-C5-C5A-O4P
2	G	501	PLP	C6-C5-C5A-O4P
2	J	501	PLP	C4-C5-C5A-O4P
2	J	501	PLP	C6-C5-C5A-O4P
2	A	501	PLP	C5A-O4P-P-O3P
2	D	500	PLP	C5A-O4P-P-O1P

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	471/471 (100%)	0.49	7 (1%) 72 44	46, 64, 102, 151	0
1	D	470/471 (99%)	0.51	11 (2%) 61 35	47, 66, 108, 150	0
1	G	467/471 (99%)	0.59	11 (2%) 59 34	56, 74, 105, 128	0
1	J	458/471 (97%)	0.68	16 (3%) 47 27	54, 83, 137, 159	0
All	All	1866/1884 (99%)	0.56	45 (2%) 59 34	46, 71, 117, 159	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	J	432	THR	4.7
1	J	480	LEU	3.7
1	J	461	VAL	3.3
1	A	49	GLU	3.2
1	J	371	GLY	3.2
1	A	11	ASP	3.2
1	J	437	SER	3.0
1	D	70	ASN	2.9
1	J	460	ALA	2.8
1	A	70	ASN	2.8
1	D	457	TYR	2.7
1	G	11	ASP	2.6
1	G	283	GLU	2.6
1	J	49	GLU	2.6
1	G	200	ALA	2.5
1	G	431	LEU	2.5
1	G	49	GLU	2.4
1	D	480	LEU	2.4
1	D	439	THR	2.4
1	J	395	ALA	2.4
1	D	440	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	279	LYS	2.3
1	G	15	TRP	2.3
1	G	110	CYS	2.3
1	D	188	GLU	2.3
1	D	49	GLU	2.2
1	J	278	PRO	2.2
1	G	72	LYS	2.2
1	G	458	GLN	2.2
1	J	75	GLU	2.2
1	A	246	GLU	2.1
1	J	464	LEU	2.1
1	A	287	ASN	2.1
1	J	435	ILE	2.1
1	D	68	CYS	2.1
1	J	413	LEU	2.1
1	D	445	LEU	2.1
1	G	30	ASP	2.1
1	J	476	PRO	2.1
1	J	428	GLY	2.0
1	G	473	SER	2.0
1	D	279	LYS	2.0
1	D	431	LEU	2.0
1	A	273	VAL	2.0
1	J	431	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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($\text{\AA}^2$)	Q<0.9
2	PLP	G	501	15/16	0.89	0.13	67,69,73,73	0
2	PLP	J	501	15/16	0.89	0.12	69,71,72,72	0
2	PLP	D	500	15/16	0.90	0.12	62,65,65,66	0
3	CL	G	502	1/1	0.94	0.09	42,42,42,42	0
2	PLP	A	501	15/16	0.95	0.10	59,60,61,61	0
3	CL	A	503	1/1	0.96	0.13	32,32,32,32	0
3	CL	J	502	1/1	0.97	0.05	20,20,20,20	0
3	CL	A	502	1/1	0.99	0.05	19,19,19,19	0

6.5 Other polymers [i](#)

There are no such residues in this entry.