



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:27 PM UTC

PDB ID : 1OHY / pdb_00001ohy
Title : 4-AMINO BUTYRATE-AMINOTRANSFERASE inactivated by gamma-ethynyl GABA
Authors : Storici, P.; Schirmer, T.
Deposited on : 2003-06-03
Resolution : 2.80 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

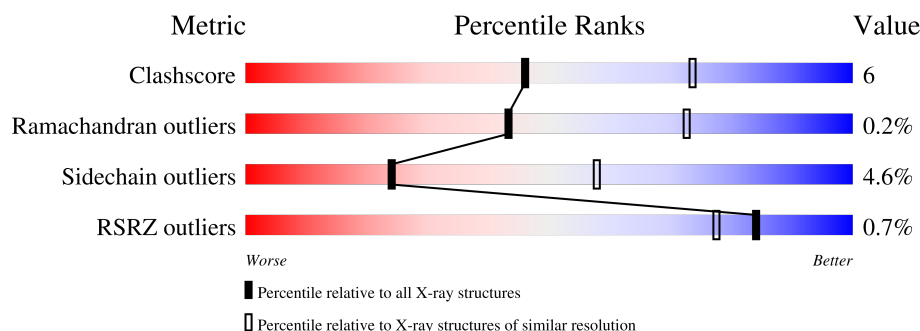
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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))
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	472	% 83% 13% ..
1	B	472	% 83% 14% ..
1	C	472	% 84% 12% ..
1	D	472	82% 14% ..

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
4	FES	A	800	-	-	X	-
4	FES	C	800	-	-	X	-

2 Entry composition [i](#)

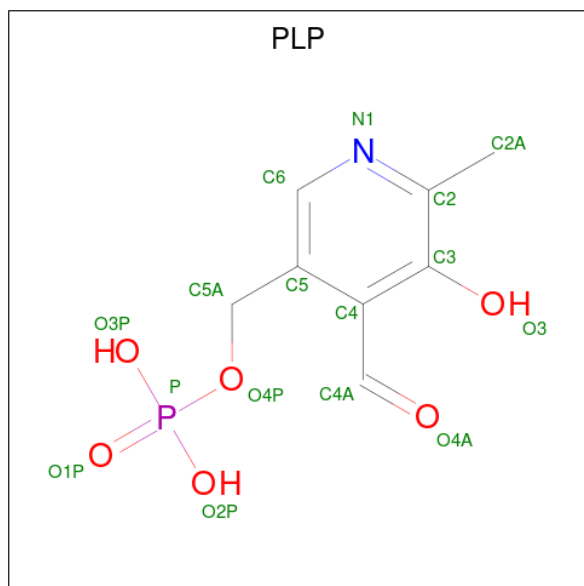
There are 5 unique types of molecules in this entry. The entry contains 14791 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 4-AMINO BUTYRATE AMINOTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	461	Total	C	N	O	S	0	0	0
			3600	2296	623	658	23			
1	B	461	Total	C	N	O	S	0	0	0
			3601	2296	624	658	23			
1	C	461	Total	C	N	O	S	0	0	0
			3601	2296	624	658	23			
1	D	461	Total	C	N	O	S	0	0	0
			3601	2296	624	658	23			

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



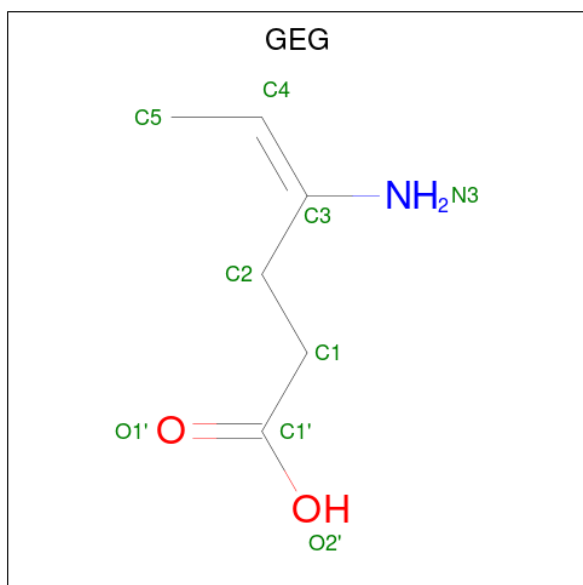
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	B	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

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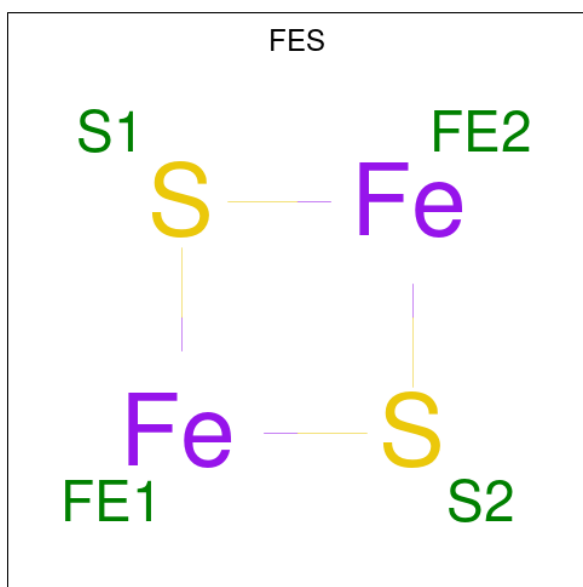
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	D	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

- Molecule 3 is (4E)-4-AMINOHEX-4-ENOIC ACID (CCD ID: GEG) (formula: C₆H₁₁NO₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			9	6	1	2		
3	B	1	Total	C	N	O	0	0
			9	6	1	2		
3	C	1	Total	C	N	O	0	0
			9	6	1	2		
3	D	1	Total	C	N	O	0	0
			9	6	1	2		

- Molecule 4 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe₂S₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	Fe	S	0	0
			4	2	2		
4	C	1	Total	Fe	S	0	0
			4	2	2		

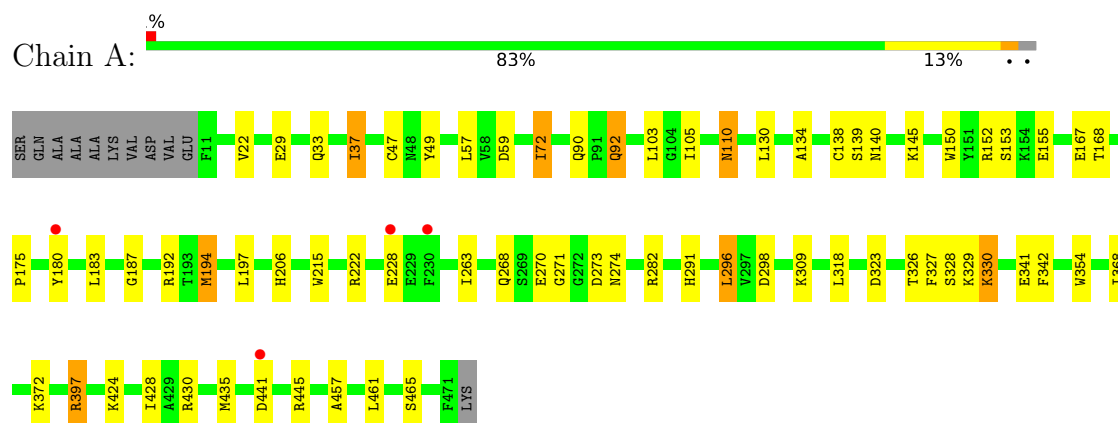
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	60	Total	O	0	0
			60	60		
5	B	55	Total	O	0	0
			55	55		
5	C	91	Total	O	0	0
			91	91		
5	D	78	Total	O	0	0
			78	78		

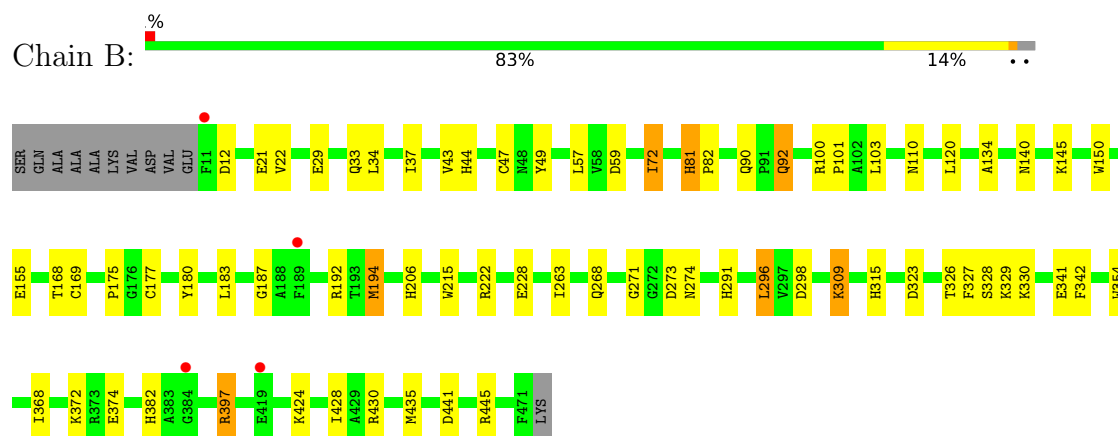
3 Residue-property plots [i](#)

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.

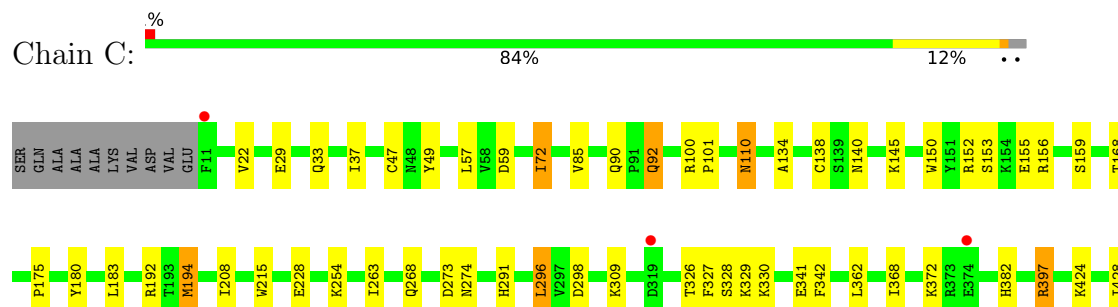
• Molecule 1: 4-AMINO BUTYRATE AMINOTRANSFERASE

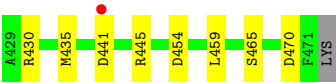


• Molecule 1: 4-AMINO BUTYRATE AMINOTRANSFERASE

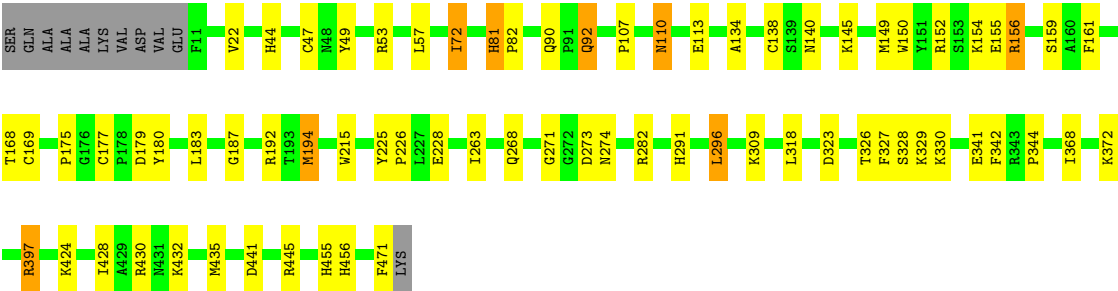
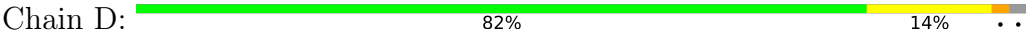


• Molecule 1: 4-AMINO BUTYRATE AMINOTRANSFERASE





● Molecule 1: 4-AMINO BUTYRATE AMINOTRANSFERASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	69.02Å 225.88Å 70.35Å 90.00° 108.51° 90.00°	Depositor
Resolution (Å)	30.00 – 2.80 30.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	84.8 (30.00-2.80) 84.7 (30.00-2.80)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.49 (at 2.80Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.198 , 0.229 0.205 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	27.0	Xtriage
Anisotropy	0.170	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 38.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.025 for l,-k,h	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	14791	wwPDB-VP
Average B, all atoms (Å ²)	10.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.37% 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: FES, PLP, GEG

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	0.77	6/3688 (0.2%)	0.97	1/4988 (0.0%)
1	B	0.79	10/3689 (0.3%)	0.97	0/4990
1	C	0.78	4/3689 (0.1%)	0.97	1/4990 (0.0%)
1	D	0.79	7/3689 (0.2%)	0.98	1/4990 (0.0%)
All	All	0.78	27/14755 (0.2%)	0.97	3/19958 (0.0%)

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	291	HIS	CG-ND1	13.35	1.52	1.38
1	C	291	HIS	CG-ND1	12.66	1.52	1.38
1	B	291	HIS	CG-ND1	10.81	1.50	1.38
1	D	291	HIS	CG-ND1	9.23	1.48	1.38
1	B	206	HIS	CG-ND1	8.80	1.48	1.38
1	A	291	HIS	CD2-NE2	8.53	1.47	1.37
1	C	291	HIS	CD2-NE2	8.41	1.47	1.37
1	A	206	HIS	CG-ND1	8.29	1.47	1.38
1	B	382	HIS	CG-ND1	8.00	1.47	1.38
1	D	44	HIS	CG-ND1	7.58	1.46	1.38
1	D	194	MET	SD-CE	-7.55	1.60	1.79
1	C	194	MET	SD-CE	-7.38	1.61	1.79
1	B	194	MET	SD-CE	-7.35	1.61	1.79
1	D	81	HIS	CG-ND1	7.12	1.46	1.38
1	A	291	HIS	CE1-NE2	7.09	1.39	1.32
1	B	206	HIS	CD2-NE2	7.00	1.45	1.37
1	B	291	HIS	CD2-NE2	6.85	1.45	1.37
1	A	206	HIS	CD2-NE2	6.47	1.45	1.37
1	A	194	MET	SD-CE	-6.32	1.63	1.79
1	D	44	HIS	CD2-NE2	6.18	1.44	1.37
1	B	44	HIS	CG-ND1	6.12	1.45	1.38
1	D	291	HIS	CD2-NE2	6.10	1.44	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	291	HIS	CE1-NE2	5.94	1.38	1.32
1	B	382	HIS	CD2-NE2	5.79	1.44	1.37
1	B	81	HIS	CG-ND1	5.78	1.44	1.38
1	B	291	HIS	CE1-NE2	5.39	1.38	1.32
1	D	81	HIS	CD2-NE2	5.32	1.43	1.37

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	291	HIS	ND1-CE1-NE2	-5.21	103.19	108.40
1	D	107	PRO	O-C-N	5.18	123.69	121.31
1	C	85	VAL	CB-CA-C	-5.06	105.50	111.97

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	3600	0	3501	49	1
1	B	3601	0	3503	45	0
1	C	3601	0	3503	40	1
1	D	3601	0	3503	46	1
2	A	15	0	7	2	0
2	B	15	0	7	2	0
2	C	15	0	7	2	0
2	D	15	0	7	1	0
3	A	9	0	7	4	0
3	B	9	0	7	4	0
3	C	9	0	7	4	0
3	D	9	0	7	4	0
4	A	4	0	0	4	0
4	C	4	0	0	4	0
5	A	60	0	0	2	0
5	B	55	0	0	3	0
5	C	91	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	D	78	0	0	4	0
All	All	14791	0	14066	166	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (166) 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:B:374:GLU:HG3	5:B:2046:HOH:O	1.65	0.95
1:C:72:ILE:CG2	3:C:700:GEG:H5C2	2.12	0.79
1:B:72:ILE:CG2	3:B:700:GEG:H5C2	2.12	0.79
1:A:138:CYS:HB3	4:A:800:FES:S2	2.23	0.77
1:A:72:ILE:CG2	3:A:700:GEG:H5C2	2.14	0.77
1:D:72:ILE:CG2	3:D:700:GEG:H5C2	2.17	0.75
1:C:397:ARG:HG2	1:C:397:ARG:HH11	1.54	0.73
1:A:397:ARG:HH11	1:A:397:ARG:HG2	1.54	0.72
1:D:397:ARG:HH11	1:D:397:ARG:HG2	1.54	0.71
1:B:397:ARG:HG2	1:B:397:ARG:HH11	1.54	0.70
1:C:152:ARG:HD2	1:C:180:TYR:HE1	1.57	0.69
1:C:152:ARG:HD2	1:C:180:TYR:CE1	2.27	0.69
1:C:329:LYS:NZ	2:C:600:PLP:C4A	2.57	0.66
1:A:152:ARG:HD2	1:A:180:TYR:HE1	1.60	0.66
1:B:397:ARG:HH11	1:B:397:ARG:CG	2.12	0.63
1:C:397:ARG:HH11	1:C:397:ARG:CG	2.11	0.63
1:D:179:ASP:HB2	5:D:2028:HOH:O	1.98	0.63
1:D:397:ARG:HH11	1:D:397:ARG:CG	2.11	0.62
1:A:397:ARG:HH11	1:A:397:ARG:CG	2.12	0.61
1:B:309:LYS:HG3	1:B:315:HIS:CE1	2.35	0.61
1:C:382:HIS:NE2	1:C:454:ASP:OD2	2.33	0.61
1:A:134:ALA:HB3	4:A:800:FES:S1	2.41	0.60
1:A:22:VAL:HG11	1:A:430:ARG:HD3	1.84	0.60
1:D:471:PHE:C	5:D:2077:HOH:O	2.45	0.59
1:A:72:ILE:HG21	3:A:700:GEG:H5C2	1.84	0.59
1:B:22:VAL:HG11	1:B:430:ARG:HD3	1.84	0.59
1:A:152:ARG:HD2	1:A:180:TYR:CE1	2.38	0.58
1:C:22:VAL:HG11	1:C:430:ARG:HD3	1.84	0.58
1:D:22:VAL:HG11	1:D:430:ARG:HD3	1.84	0.58
1:C:72:ILE:HG21	3:C:700:GEG:H5C2	1.82	0.57
1:C:155:GLU:OE1	1:C:180:TYR:OH	2.19	0.57
1:C:138:CYS:HB3	4:C:800:FES:S2	2.45	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:194:MET:HE1	1:D:215:TRP:HH2	1.70	0.56
1:B:155:GLU:OE1	1:B:180:TYR:OH	2.23	0.56
1:A:155:GLU:OE1	1:A:180:TYR:OH	2.19	0.56
1:A:329:LYS:NZ	2:A:600:PLP:C4A	2.65	0.56
1:B:72:ILE:HG22	3:B:700:GEG:H5C2	1.88	0.55
1:B:329:LYS:NZ	2:B:600:PLP:C4A	2.70	0.55
1:A:194:MET:HE1	1:B:215:TRP:HH2	1.71	0.55
4:C:800:FES:S2	1:D:138:CYS:HB3	2.47	0.55
1:A:268:GLN:O	1:A:273:ASP:HA	2.08	0.54
1:B:72:ILE:HG21	3:B:700:GEG:H5C2	1.89	0.54
1:C:268:GLN:O	1:C:273:ASP:HA	2.08	0.54
1:D:90:GLN:HB3	1:D:92:GLN:NE2	2.24	0.53
1:B:268:GLN:O	1:B:273:ASP:HA	2.09	0.53
1:D:329:LYS:NZ	2:D:600:PLP:C4A	2.71	0.53
1:D:268:GLN:O	1:D:273:ASP:HA	2.08	0.52
1:A:90:GLN:HB3	1:A:92:GLN:NE2	2.25	0.52
1:A:192:ARG:HB3	1:B:145:LYS:NZ	2.26	0.51
1:B:90:GLN:HB3	1:B:92:GLN:NE2	2.25	0.51
1:D:72:ILE:HG21	3:D:700:GEG:H5C2	1.90	0.51
1:C:183:LEU:C	1:C:183:LEU:HD23	2.36	0.51
1:A:183:LEU:C	1:A:183:LEU:HD23	2.35	0.51
1:C:192:ARG:HB3	1:D:145:LYS:NZ	2.25	0.51
1:D:183:LEU:C	1:D:183:LEU:HD23	2.36	0.51
1:C:90:GLN:HB3	1:C:92:GLN:NE2	2.26	0.50
1:A:192:ARG:HB3	1:B:145:LYS:HZ3	1.77	0.50
1:B:183:LEU:C	1:B:183:LEU:HD23	2.36	0.50
1:D:155:GLU:OE1	1:D:180:TYR:OH	2.30	0.50
1:D:22:VAL:CG1	1:D:430:ARG:HD3	2.43	0.49
1:A:150:TRP:CD2	1:A:342:PHE:CE2	3.01	0.49
1:C:150:TRP:CD2	1:C:342:PHE:CE2	3.01	0.49
1:C:22:VAL:CG1	1:C:430:ARG:HD3	2.43	0.49
1:D:150:TRP:CD2	1:D:342:PHE:CE2	3.00	0.49
1:A:22:VAL:CG1	1:A:430:ARG:HD3	2.43	0.49
1:B:150:TRP:CD2	1:B:342:PHE:CE2	3.01	0.49
1:C:215:TRP:HH2	1:D:194:MET:HE1	1.78	0.49
1:B:22:VAL:CG1	1:B:430:ARG:HD3	2.43	0.48
1:A:138:CYS:CB	4:A:800:FES:S2	2.93	0.48
1:A:298:ASP:OD1	2:A:600:PLP:N1	2.46	0.48
1:A:72:ILE:HB	3:A:700:GEG:C5	2.44	0.47
1:A:215:TRP:HH2	1:B:194:MET:HE1	1.79	0.47
1:D:168:THR:HG21	1:D:175:PRO:HD2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:168:THR:HG21	1:A:175:PRO:HD2	1.96	0.47
1:C:47:CYS:HB2	1:C:49:TYR:CE2	2.49	0.47
1:C:192:ARG:HB3	1:D:145:LYS:HZ3	1.80	0.47
1:A:47:CYS:HB2	1:A:49:TYR:CE2	2.49	0.47
1:C:57:LEU:HD23	1:C:435:MET:SD	2.54	0.47
1:C:168:THR:HG21	1:C:175:PRO:HD2	1.96	0.47
1:D:81:HIS:ND1	1:D:82:PRO:HD2	2.30	0.47
1:C:298:ASP:OD1	2:C:600:PLP:N1	2.47	0.46
1:B:168:THR:HG21	1:B:175:PRO:HD2	1.96	0.46
1:A:37:ILE:HG21	1:B:120:LEU:HD21	1.97	0.46
1:B:57:LEU:HD23	1:B:435:MET:SD	2.56	0.46
1:C:362:LEU:O	5:C:2073:HOH:O	2.21	0.46
1:B:47:CYS:HB2	1:B:49:TYR:CE2	2.50	0.46
4:C:800:FES:S1	1:D:134:ALA:HB3	2.56	0.46
1:D:47:CYS:HB2	1:D:49:TYR:CE2	2.51	0.46
1:D:152:ARG:HD2	1:D:180:TYR:CE1	2.51	0.45
1:D:155:GLU:OE2	1:D:180:TYR:OH	2.35	0.45
1:B:263:ILE:HA	1:B:296:LEU:O	2.17	0.45
1:C:263:ILE:HA	1:C:296:LEU:O	2.17	0.45
1:A:330:LYS:HD3	5:A:2035:HOH:O	2.17	0.45
1:B:100:ARG:HA	1:B:101:PRO:HD3	1.81	0.45
1:C:268:GLN:HB2	1:C:274:ASN:HB2	1.98	0.44
1:D:263:ILE:HA	1:D:296:LEU:O	2.17	0.44
1:A:57:LEU:HD23	1:A:435:MET:SD	2.57	0.44
1:A:268:GLN:HB2	1:A:274:ASN:HB2	1.99	0.44
1:B:435:MET:HE2	1:B:435:MET:HB3	1.88	0.44
1:A:270:GLU:HG2	5:A:2059:HOH:O	2.17	0.44
1:B:424:LYS:O	1:B:428:ILE:HG12	2.18	0.44
1:A:263:ILE:HA	1:A:296:LEU:O	2.17	0.44
1:C:72:ILE:HB	3:C:700:GEG:C5	2.47	0.44
1:A:397:ARG:CG	1:A:397:ARG:NH1	2.79	0.44
1:B:374:GLU:CG	5:B:2046:HOH:O	2.44	0.44
1:A:457:ALA:O	1:A:461:LEU:HG	2.17	0.44
1:B:81:HIS:HA	1:B:82:PRO:HD3	1.87	0.44
1:B:140:ASN:OD1	1:B:326:THR:HG21	2.18	0.44
1:B:268:GLN:HB2	1:B:274:ASN:HB2	1.99	0.43
1:B:327:PHE:CD1	1:B:327:PHE:C	2.96	0.43
1:C:145:LYS:NZ	1:D:192:ARG:HB3	2.33	0.43
1:D:57:LEU:HD23	1:D:435:MET:SD	2.58	0.43
1:A:105:ILE:HA	1:B:43:VAL:HA	1.99	0.43
1:A:145:LYS:NZ	1:B:192:ARG:HB3	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:424:LYS:O	1:C:428:ILE:HG12	2.18	0.43
1:C:59:ASP:OD1	1:C:59:ASP:C	2.61	0.43
1:A:72:ILE:CB	3:A:700:GEG:H5C2	2.49	0.43
1:D:179:ASP:CB	5:D:2028:HOH:O	2.62	0.43
1:D:327:PHE:CD1	1:D:327:PHE:C	2.96	0.43
1:B:29:GLU:OE2	1:B:33:GLN:NE2	2.50	0.43
1:C:208:ILE:HD13	1:D:161:PHE:CD2	2.53	0.43
1:A:424:LYS:O	1:A:428:ILE:HG12	2.18	0.43
1:B:145:LYS:NZ	5:B:2017:HOH:O	2.50	0.43
1:D:268:GLN:HB2	1:D:274:ASN:HB2	1.99	0.43
1:A:327:PHE:CD1	1:A:327:PHE:C	2.97	0.43
1:C:327:PHE:CD1	1:C:327:PHE:C	2.97	0.43
1:D:113:GLU:CB	5:D:2016:HOH:O	2.65	0.43
1:C:100:ARG:HA	1:C:101:PRO:HD3	1.80	0.43
1:C:140:ASN:OD1	1:C:326:THR:HG21	2.18	0.43
1:B:298:ASP:OD1	2:B:600:PLP:N1	2.52	0.42
1:B:59:ASP:OD1	1:B:59:ASP:C	2.60	0.42
1:A:59:ASP:OD1	1:A:59:ASP:C	2.62	0.42
1:D:72:ILE:HG22	3:D:700:GEG:H5C2	1.98	0.42
1:D:225:TYR:HA	1:D:226:PRO:C	2.43	0.42
1:B:169:CYS:HA	1:B:177:CYS:SG	2.59	0.42
1:C:153:SER:HA	1:C:156:ARG:HG2	2.01	0.42
1:D:140:ASN:OD1	1:D:326:THR:HG21	2.19	0.42
1:D:424:LYS:O	1:D:428:ILE:HG12	2.19	0.42
4:A:800:FES:S1	1:B:134:ALA:HB3	2.60	0.42
1:C:134:ALA:HB3	4:C:800:FES:S1	2.60	0.42
1:A:29:GLU:OE2	1:A:33:GLN:NE2	2.51	0.42
1:D:187:GLY:O	1:D:271:GLY:HA3	2.20	0.42
1:D:72:ILE:HB	3:D:700:GEG:C5	2.50	0.41
1:C:110:ASN:ND2	1:C:110:ASN:C	2.79	0.41
1:B:72:ILE:HB	3:B:700:GEG:C5	2.50	0.41
1:A:140:ASN:OD1	1:A:326:THR:HG21	2.21	0.41
1:A:323:ASP:HB3	1:A:342:PHE:CE1	2.56	0.41
1:B:187:GLY:O	1:B:271:GLY:HA3	2.21	0.41
1:C:29:GLU:OE2	1:C:33:GLN:NE2	2.50	0.41
1:A:110:ASN:ND2	1:A:110:ASN:C	2.77	0.41
1:D:149:MET:HE1	1:D:344:PRO:HB3	2.03	0.41
1:D:169:CYS:HA	1:D:177:CYS:SG	2.61	0.41
1:D:323:ASP:HB3	1:D:342:PHE:CE1	2.56	0.41
1:D:397:ARG:HG2	1:D:397:ARG:NH1	2.30	0.41
1:A:130:LEU:HB3	1:B:37:ILE:HG23	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:110:ASN:ND2	1:D:110:ASN:C	2.78	0.41
1:D:455:HIS:NE2	1:D:456:HIS:CE1	2.89	0.41
1:A:282:ARG:CD	1:A:318:LEU:HD21	2.51	0.40
1:A:435:MET:HE2	1:A:435:MET:HB3	1.87	0.40
1:A:103:LEU:HD12	1:A:354:TRP:O	2.22	0.40
1:A:187:GLY:O	1:A:271:GLY:HA3	2.21	0.40
1:A:197:LEU:HD12	1:A:197:LEU:HA	1.94	0.40
1:B:323:ASP:HB3	1:B:342:PHE:CE1	2.55	0.40
1:D:282:ARG:CD	1:D:318:LEU:HD21	2.51	0.40
1:B:103:LEU:HD12	1:B:354:TRP:O	2.21	0.40
1:C:72:ILE:CB	3:C:700:GEG:H5C2	2.51	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:156:ARG:O	1:D:432:LYS:NZ[1_455]	2.02	0.18
1:A:167:GLU:OE2	1:C:254:LYS:CE[2_647]	2.06	0.14

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	459/472 (97%)	434 (95%)	24 (5%)	1 (0%)	43	72
1	B	459/472 (97%)	436 (95%)	22 (5%)	1 (0%)	43	72
1	C	459/472 (97%)	432 (94%)	26 (6%)	1 (0%)	43	72
1	D	459/472 (97%)	436 (95%)	22 (5%)	1 (0%)	43	72
All	All	1836/1888 (97%)	1738 (95%)	94 (5%)	4 (0%)	43	72

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	328	SER
1	B	328	SER
1	C	328	SER
1	D	328	SER

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	383/408 (94%)	365 (95%)	18 (5%)	23	57
1	B	383/408 (94%)	366 (96%)	17 (4%)	25	59
1	C	383/408 (94%)	365 (95%)	18 (5%)	23	57
1	D	383/408 (94%)	366 (96%)	17 (4%)	25	59
All	All	1532/1632 (94%)	1462 (95%)	70 (5%)	24	58

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	ILE
1	A	72	ILE
1	A	92	GLN
1	A	110	ASN
1	A	139	SER
1	A	153	SER
1	A	222	ARG
1	A	228	GLU
1	A	296	LEU
1	A	309	LYS
1	A	330	LYS
1	A	341	GLU
1	A	368	ILE
1	A	372	LYS
1	A	397	ARG
1	A	441	ASP
1	A	445	ARG
1	A	465	SER

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Mol	Chain	Res	Type
1	B	12	ASP
1	B	21	GLU
1	B	34	LEU
1	B	72	ILE
1	B	92	GLN
1	B	110	ASN
1	B	222	ARG
1	B	228	GLU
1	B	296	LEU
1	B	309	LYS
1	B	330	LYS
1	B	341	GLU
1	B	368	ILE
1	B	372	LYS
1	B	397	ARG
1	B	441	ASP
1	B	445	ARG
1	C	37	ILE
1	C	72	ILE
1	C	92	GLN
1	C	110	ASN
1	C	159	SER
1	C	228	GLU
1	C	296	LEU
1	C	309	LYS
1	C	330	LYS
1	C	341	GLU
1	C	368	ILE
1	C	372	LYS
1	C	397	ARG
1	C	441	ASP
1	C	445	ARG
1	C	459	LEU
1	C	465	SER
1	C	470	ASP
1	D	53	ARG
1	D	72	ILE
1	D	92	GLN
1	D	110	ASN
1	D	154	LYS
1	D	156	ARG
1	D	159	SER

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Mol	Chain	Res	Type
1	D	228	GLU
1	D	296	LEU
1	D	309	LYS
1	D	330	LYS
1	D	341	GLU
1	D	368	ILE
1	D	372	LYS
1	D	397	ARG
1	D	441	ASP
1	D	445	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	92	GLN
1	A	110	ASN
1	A	268	GLN
1	A	274	ASN
1	A	315	HIS
1	B	92	GLN
1	B	110	ASN
1	B	268	GLN
1	B	274	ASN
1	C	92	GLN
1	C	110	ASN
1	C	268	GLN
1	C	274	ASN
1	C	379	ASN
1	C	458	HIS
1	D	38	GLN
1	D	92	GLN
1	D	110	ASN
1	D	268	GLN
1	D	274	ASN
1	D	315	HIS
1	D	456	HIS

5.3.3 RNA ⓘ

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

10 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	A	600	3	15,15,16	1.11	1 (6%)	21,22,23	1.05	2 (9%)
3	GEG	B	700	2,1	7,8,8	2.78	2 (28%)	5,9,9	1.51	1 (20%)
3	GEG	D	700	2,1	7,8,8	2.42	2 (28%)	5,9,9	1.26	0
2	PLP	C	600	3	15,15,16	1.06	1 (6%)	21,22,23	1.58	3 (14%)
4	FES	A	800	1	0,4,4	-	-	-	-	-
2	PLP	B	600	3	15,15,16	0.99	2 (13%)	21,22,23	1.38	2 (9%)
3	GEG	A	700	2,1	7,8,8	2.61	2 (28%)	5,9,9	1.78	2 (40%)
2	PLP	D	600	3	15,15,16	1.10	2 (13%)	21,22,23	1.15	2 (9%)
3	GEG	C	700	2,1	7,8,8	2.48	2 (28%)	5,9,9	1.47	1 (20%)
4	FES	C	800	1	0,4,4	-	-	-	-	-

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	600	3	-	0/6/6/8	0/1/1/1
3	GEG	B	700	2,1	-	3/6/7/7	-
3	GEG	D	700	2,1	-	5/6/7/7	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PLP	C	600	3	-	0/6/6/8	0/1/1/1
4	FES	A	800	1	-	-	0/1/1/1
2	PLP	B	600	3	-	0/6/6/8	0/1/1/1
3	GEG	A	700	2,1	-	4/6/7/7	-
2	PLP	D	600	3	-	0/6/6/8	0/1/1/1
3	GEG	C	700	2,1	-	4/6/7/7	-
4	FES	C	800	1	-	-	0/1/1/1

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	700	GEG	C3-N3	6.31	1.46	1.33
3	A	700	GEG	C3-N3	6.05	1.46	1.33
3	C	700	GEG	C3-N3	5.77	1.45	1.33
3	D	700	GEG	C3-N3	5.43	1.44	1.33
3	B	700	GEG	C2-C3	3.20	1.54	1.50
3	A	700	GEG	C2-C3	2.82	1.54	1.50
3	D	700	GEG	C2-C3	2.71	1.53	1.50
2	D	600	PLP	C2-N1	2.53	1.38	1.33
3	C	700	GEG	C2-C3	2.41	1.53	1.50
2	A	600	PLP	C2-N1	2.38	1.38	1.33
2	C	600	PLP	C2-N1	2.30	1.38	1.33
2	B	600	PLP	C2-N1	2.26	1.37	1.33
2	D	600	PLP	C6-N1	2.20	1.38	1.34
2	B	600	PLP	C6-N1	2.03	1.38	1.34

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	600	PLP	C4A-C4-C5	-4.78	116.01	120.94
2	B	600	PLP	C4A-C4-C5	-3.86	116.96	120.94
3	A	700	GEG	O2'-C1'-C1	3.03	123.56	114.00
2	D	600	PLP	C4A-C4-C5	-2.90	117.95	120.94
2	C	600	PLP	C5-C6-N1	-2.74	119.38	123.83
3	B	700	GEG	O2'-C1'-C1	2.50	121.89	114.00
2	B	600	PLP	C5-C6-N1	-2.43	119.89	123.83
3	C	700	GEG	O2'-C1'-C1	2.40	121.59	114.00
2	D	600	PLP	C5-C6-N1	-2.33	120.04	123.83
2	A	600	PLP	C5-C6-N1	-2.15	120.33	123.83
2	C	600	PLP	C3-C4-C5	2.12	121.14	118.59
3	A	700	GEG	O1'-C1'-C1	-2.12	116.37	123.09
2	A	600	PLP	C4A-C4-C5	-2.08	118.80	120.94

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	700	GEG	C1'-C1-C2-C3
3	A	700	GEG	C1-C2-C3-C4
3	B	700	GEG	C1'-C1-C2-C3
3	B	700	GEG	C1-C2-C3-C4
3	D	700	GEG	C1-C2-C3-C4
3	C	700	GEG	C1'-C1-C2-C3
3	D	700	GEG	C1'-C1-C2-C3
3	C	700	GEG	C1-C2-C3-N3
3	A	700	GEG	C1-C2-C3-N3
3	B	700	GEG	C1-C2-C3-N3
3	D	700	GEG	C1-C2-C3-N3
3	D	700	GEG	C2-C1-C1'-O1'
3	D	700	GEG	C2-C1-C1'-O2'
3	C	700	GEG	C2-C1-C1'-O1'
3	C	700	GEG	C2-C1-C1'-O2'
3	A	700	GEG	C2-C1-C1'-O2'

There are no ring outliers.

10 monomers are involved in 31 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	600	PLP	2	0
3	B	700	GEG	4	0
3	D	700	GEG	4	0
2	C	600	PLP	2	0
4	A	800	FES	4	0
2	B	600	PLP	2	0
3	A	700	GEG	4	0
2	D	600	PLP	1	0
3	C	700	GEG	4	0
4	C	800	FES	4	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	461/472 (97%)	0.05	4 (0%) 81 74	10, 11, 11, 11	0
1	B	461/472 (97%)	0.16	4 (0%) 81 74	10, 11, 11, 11	0
1	C	461/472 (97%)	-0.08	4 (0%) 81 74	10, 11, 11, 11	0
1	D	461/472 (97%)	-0.19	0 100 100	10, 11, 11, 12	0
All	All	1844/1888 (97%)	-0.01	12 (0%) 84 77	10, 11, 11, 12	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	11	PHE	4.1
1	C	319	ASP	2.8
1	C	374	GLU	2.7
1	A	441	ASP	2.6
1	A	230	PHE	2.6
1	B	189	PHE	2.5
1	C	441	ASP	2.5
1	A	228	GLU	2.4
1	B	419	GLU	2.4
1	C	11	PHE	2.3
1	A	180	TYR	2.2
1	B	384	GLY	2.1

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(Å ²)	Q<0.9
3	GEG	D	700	9/9	0.90	0.13	11,11,11,11	0
3	GEG	C	700	9/9	0.93	0.12	11,11,11,11	0
2	PLP	B	600	15/16	0.95	0.14	10,11,11,11	0
3	GEG	A	700	9/9	0.95	0.14	11,11,11,11	0
3	GEG	B	700	9/9	0.96	0.14	11,11,12,12	0
2	PLP	A	600	15/16	0.97	0.10	10,11,11,11	0
4	FES	A	800	4/4	0.97	0.19	13,14,14,15	0
2	PLP	D	600	15/16	0.98	0.07	10,11,11,11	0
2	PLP	C	600	15/16	0.98	0.07	10,11,11,11	0
4	FES	C	800	4/4	0.98	0.16	13,13,13,15	0

6.5 Other polymers [i](#)

There are no such residues in this entry.