



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 16, 2020 – 06:56 PM BST

PDB ID : 7JH3  
Title : Crystal structure of 4-aminobutyrate aminotransferase PuuE from Escherichia coli in complex with PLP  
Authors : Valteau, D.; Evdokimova, E.; Stogios, P.J.; Di Leo, R.; Savchenko, A.; Joachimiak, A.; Satchell, K.J.F.; Center for Structural Genomics of Infectious Diseases (CSGID)  
Deposited on : 2020-07-20  
Resolution : 2.68 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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.13.1  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.13.1

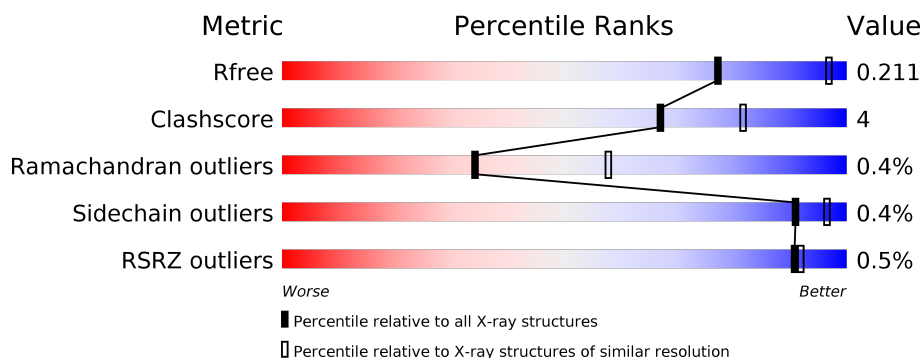
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.68 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	3863 (2.70-2.66)
Clashscore	141614	4210 (2.70-2.66)
Ramachandran outliers	138981	4141 (2.70-2.66)
Sidechain outliers	138945	4141 (2.70-2.66)
RSRZ outliers	127900	3780 (2.70-2.66)

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  $\geq 3$ , 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	421	<div> <div>90%</div> <div>9%</div> </div>
1	B	421	<div> <div>89%</div> <div>10%</div> </div>
1	C	421	<div> <div>2%</div> <div>88%</div> <div>11%</div> </div>
1	D	421	<div> <div>89%</div> <div>10%</div> </div>
1	E	421	<div> <div>89%</div> <div>11%</div> </div>
1	F	421	<div> <div>89%</div> <div>11%</div> </div>

## 2 Entry composition [i](#)

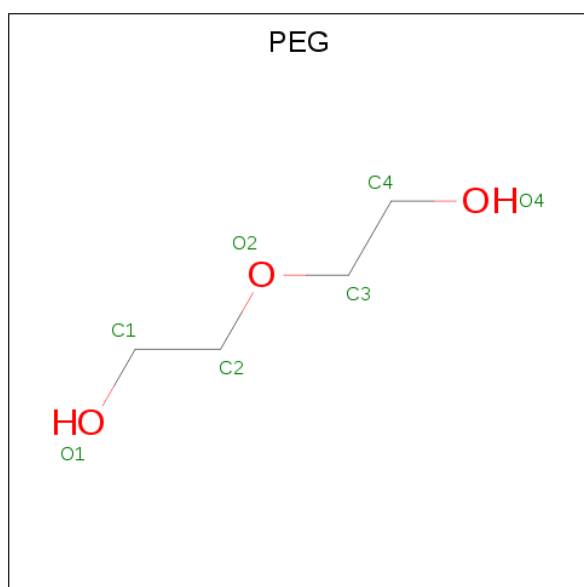
There are 3 unique types of molecules in this entry. The entry contains 19411 atoms, of which 20 are hydrogens and 0 are deuteriums.

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-aminobutyrate aminotransferase PuuE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	420	Total	C	N	O	P	S	0	0	0
			3152	1993	546	597	1	15			
1	B	420	Total	C	N	O	P	S	0	0	0
			3152	1993	546	597	1	15			
1	C	420	Total	C	N	O	P	S	0	0	0
			3152	1993	546	597	1	15			
1	D	420	Total	C	N	O	P	S	0	0	0
			3152	1993	546	597	1	15			
1	E	420	Total	C	N	O	P	S	0	0	0
			3152	1993	546	597	1	15			
1	F	420	Total	C	N	O	P	S	0	0	0
			3152	1993	546	597	1	15			

- Molecule 2 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	H	O	0	0
			17	4	10	3		
2	D	1	Total	C	H	O	0	0
			17	4	10	3		

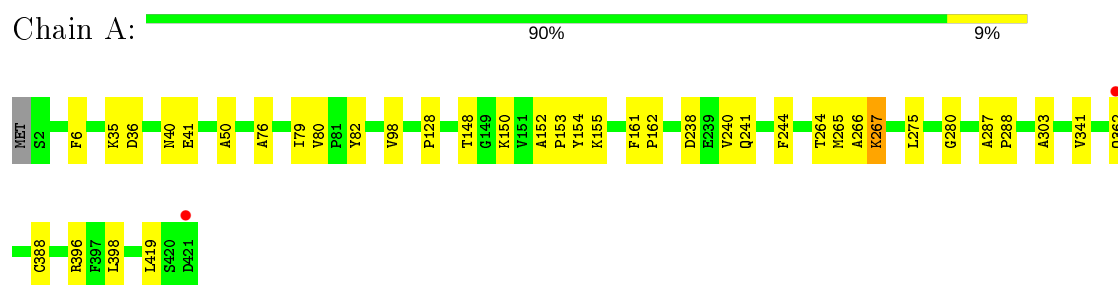
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	85	Total	O	0	0
			85	85		
3	B	73	Total	O	0	0
			73	73		
3	C	60	Total	O	0	0
			60	60		
3	D	89	Total	O	0	0
			89	89		
3	E	89	Total	O	0	0
			89	89		
3	F	69	Total	O	0	0
			69	69		

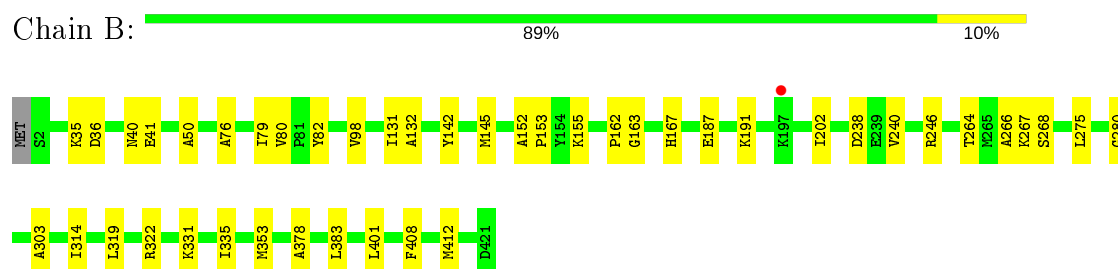
### 3 Residue-property plots

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.

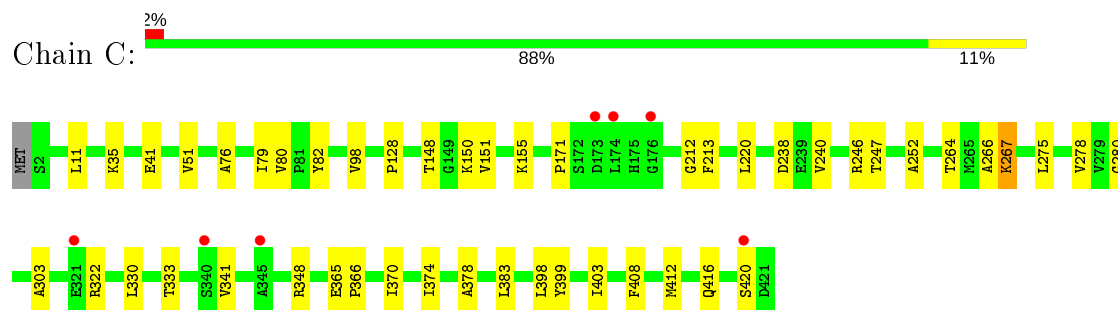
- Molecule 1: 4-aminobutyrate aminotransferase PuuE



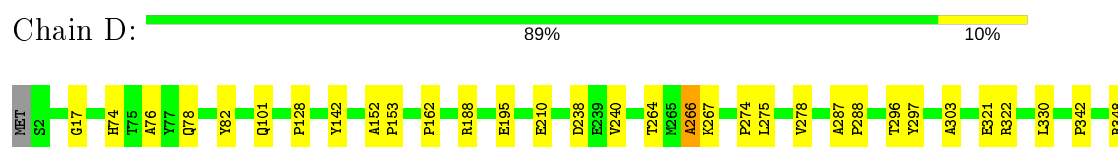
- Molecule 1: 4-aminobutyrate aminotransferase PuuE



- Molecule 1: 4-aminobutyrate aminotransferase PuuE



- Molecule 1: 4-aminobutyrate aminotransferase PuuE





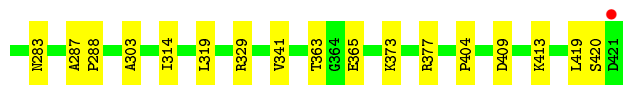
- Molecule 1: 4-aminobutyrate aminotransferase PuuE

Chain E: 89% 11%



- Molecule 1: 4-aminobutyrate aminotransferase PuuE

Chain F: 89% 11%



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	198.64Å 78.84Å 164.98Å 90.00° 112.82° 90.00°	Depositor
Resolution (Å)	24.88 – 2.68 24.88 – 2.66	Depositor EDS
% Data completeness (in resolution range)	93.8 (24.88-2.68) 92.3 (24.88-2.66)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.42 (at 2.68Å)	Xtriage
Refinement program	PHENIX 1.17.1 _3660	Depositor
R, $R_{free}$	0.178 , 0.211 0.178 , 0.211	Depositor DCC
$R_{free}$ test set	2000 reflections (2.98%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	36.5	Xtriage
Anisotropy	0.302	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 27.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	19411	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.21% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: PEG, LLP

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	0.34	0/3190	0.48	0/4330
1	B	0.31	0/3190	0.47	0/4330
1	C	0.30	0/3190	0.47	0/4330
1	D	0.29	0/3190	0.47	0/4330
1	E	0.33	0/3190	0.48	0/4330
1	F	0.30	0/3190	0.48	0/4330
All	All	0.31	0/19140	0.47	0/25980

There are no bond length outliers.

There are no bond angle outliers.

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	3152	0	3122	21	0
1	B	3152	0	3122	24	0
1	C	3152	0	3122	25	0
1	D	3152	0	3122	27	0
1	E	3152	0	3122	27	0
1	F	3152	0	3122	27	0
2	B	7	10	10	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	7	10	10	2	0
3	A	85	0	0	1	0
3	B	73	0	0	0	0
3	C	60	0	0	1	0
3	D	89	0	0	5	0
3	E	89	0	0	2	0
3	F	69	0	0	5	0
All	All	19391	20	18752	146	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 4.

All (146) 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:142:TYR:CZ	1:B:162:PRO:HD3	2.31	0.65
1:D:275:LEU:HB2	1:D:303:ALA:HB1	1.78	0.65
1:B:142:TYR:CE2	1:B:162:PRO:HD3	2.34	0.63
1:A:35:LYS:HG2	1:A:41:GLU:HG2	1.80	0.62
1:D:162:PRO:HA	2:D:501:PEG:H42	1.83	0.61
1:B:162:PRO:HA	2:B:501:PEG:H12	1.83	0.60
1:C:51:VAL:HG22	1:C:267:LLP:HG3	1.84	0.60
1:F:275:LEU:HB2	1:F:303:ALA:HB1	1.83	0.59
1:E:18:VAL:HG23	3:E:574:HOH:O	2.03	0.58
1:A:275:LEU:HB2	1:A:303:ALA:HB1	1.84	0.58
1:A:241:GLN:OE1	1:A:396:ARG:NH2	2.36	0.57
1:F:329:ARG:NH2	1:F:409:ASP:OD1	2.37	0.57
1:B:275:LEU:HB2	1:B:303:ALA:HB1	1.86	0.57
1:D:240:VAL:HG13	1:D:266:ALA:HB3	1.87	0.57
1:B:240:VAL:HG13	1:B:266:ALA:HB3	1.86	0.57
1:C:98:VAL:HG11	1:C:280:GLY:HA2	1.85	0.57
1:B:35:LYS:HG2	1:B:41:GLU:HG2	1.86	0.56
1:E:240:VAL:HG13	1:E:266:ALA:HB3	1.85	0.56
1:E:275:LEU:HB2	1:E:303:ALA:HB1	1.87	0.55
1:A:240:VAL:HG13	1:A:266:ALA:HB3	1.89	0.55
1:D:274:PRO:HG2	1:E:274:PRO:HG2	1.89	0.55
1:C:79:ILE:HG22	1:C:80:VAL:HG23	1.87	0.55
1:F:341:VAL:HG21	1:F:419:LEU:HB3	1.89	0.55
1:C:264:THR:HG22	1:C:278:VAL:HG22	1.88	0.55
1:D:142:TYR:CZ	1:D:162:PRO:HD3	2.42	0.55
2:D:501:PEG:H41	1:E:163:GLY:H	1.71	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:240:VAL:HG13	1:F:266:ALA:HB3	1.89	0.54
1:E:377:ARG:NH2	1:E:421:ASP:HA	2.23	0.54
1:D:373:LYS:NZ	1:D:421:ASP:OD2	2.40	0.54
1:E:35:LYS:HG2	1:E:41:GLU:HG2	1.89	0.54
1:D:322:ARG:NH2	1:D:403:ILE:O	2.35	0.53
1:C:341:VAL:CG2	1:C:420:SER:HA	2.38	0.53
1:A:50:ALA:HB2	1:A:398:LEU:HD22	1.89	0.53
1:F:145:MET:O	1:F:155:LYS:HE2	2.08	0.53
1:B:98:VAL:HG11	1:B:280:GLY:HA2	1.91	0.52
1:C:275:LEU:HB2	1:C:303:ALA:HB1	1.92	0.51
1:A:161:PHE:HB3	1:A:162:PRO:HD2	1.93	0.51
1:C:333:THR:HG23	1:C:416:GLN:HE21	1.76	0.51
1:F:142:TYR:CZ	1:F:162:PRO:HD3	2.45	0.51
1:D:330:LEU:HD21	1:D:397:PHE:CD2	2.47	0.50
1:E:142:TYR:CZ	1:E:162:PRO:HD3	2.46	0.50
1:C:171:PRO:HG2	1:C:220:LEU:HD22	1.92	0.50
1:C:247:THR:HG21	1:C:252:ALA:HB2	1.93	0.50
1:B:378:ALA:HB1	1:B:383:LEU:HB3	1.93	0.49
1:C:246:ARG:NH2	1:C:399:TYR:O	2.35	0.49
1:D:377:ARG:HG2	1:D:418:ALA:HA	1.94	0.49
1:C:365:GLU:HG3	1:C:366:PRO:HD2	1.93	0.49
1:F:66:GLU:O	1:F:70:GLN:NE2	2.45	0.49
1:A:150:LYS:HD3	1:A:154:TYR:HE2	1.78	0.49
1:C:408:PHE:O	1:C:412:MET:HG2	2.12	0.49
1:E:329:ARG:NH2	1:E:405:ASP:OD1	2.44	0.49
1:E:219:GLU:CD	1:E:219:GLU:H	2.17	0.48
1:F:202:ILE:HG13	1:F:233:ILE:HG21	1.96	0.48
1:D:188:ARG:NE	1:F:169:PRO:HG3	2.28	0.48
1:E:249:LYS:HD3	1:E:254:ASP:HB3	1.95	0.48
1:E:50:ALA:HB2	1:E:398:LEU:HD22	1.94	0.48
1:F:377:ARG:NH1	1:F:420:SER:O	2.46	0.48
1:B:187:GLU:OE2	1:B:191:LYS:HE3	2.13	0.48
1:B:408:PHE:O	1:B:412:MET:HG2	2.13	0.48
1:D:238:ASP:HA	1:D:264:THR:OG1	2.14	0.48
1:A:79:ILE:HG22	1:A:80:VAL:HG23	1.95	0.47
1:E:145:MET:O	1:E:155:LYS:HD3	2.15	0.47
1:A:98:VAL:HG11	1:A:280:GLY:HA2	1.96	0.47
1:B:163:GLY:H	2:B:501:PEG:H12	1.78	0.47
1:B:79:ILE:HG22	1:B:80:VAL:HG23	1.95	0.47
1:B:322:ARG:HD3	1:B:401:LEU:O	2.14	0.47
1:D:210:GLU:HB3	3:D:630:HOH:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:225:ARG:NH1	1:F:259:LYS:O	2.43	0.47
3:A:504:HOH:O	1:F:17:GLY:N	2.42	0.47
1:C:370:ILE:O	1:C:374:ILE:HG12	2.15	0.46
1:D:348:ARG:NH1	1:D:357:GLU:OE1	2.37	0.46
1:F:29:ALA:HB2	1:F:34:LEU:HD12	1.96	0.46
1:B:131:ILE:HB	1:B:202:ILE:HG12	1.96	0.46
3:D:609:HOH:O	1:E:17:GLY:N	2.46	0.46
1:B:50:ALA:O	1:B:268:SER:OG	2.28	0.46
1:F:413:LYS:HD2	3:F:566:HOH:O	2.16	0.46
1:B:314:ILE:HG12	1:B:319:LEU:HD12	1.98	0.45
1:D:287:ALA:HB3	1:D:288:PRO:HD3	1.98	0.45
1:D:74:HIS:HE1	1:D:296:THR:O	1.98	0.45
1:D:388:CYS:O	1:D:394:VAL:HB	2.17	0.45
1:F:373:LYS:HD2	1:F:377:ARG:HH21	1.79	0.45
1:C:378:ALA:HB1	1:C:383:LEU:HB3	1.98	0.45
1:C:322:ARG:NH2	1:C:403:ILE:O	2.37	0.45
1:A:240:VAL:HG13	1:A:267:LLP:HG2	1.99	0.45
1:B:331:LYS:O	1:B:335:ILE:HG12	2.16	0.45
1:F:404:PRO:HA	3:F:548:HOH:O	2.16	0.45
1:A:6:PHE:CD1	3:F:515:HOH:O	2.56	0.44
1:F:188:ARG:HG2	3:F:568:HOH:O	2.15	0.44
1:D:78:GLN:HB3	3:E:574:HOH:O	2.17	0.44
1:A:240:VAL:CG1	1:A:267:LLP:HG2	2.48	0.44
1:E:97:PRO:O	1:E:260:PRO:HD2	2.18	0.44
1:A:36:ASP:OD2	1:A:40:ASN:N	2.50	0.44
1:B:145:MET:O	1:B:155:LYS:HD3	2.17	0.44
1:E:287:ALA:HB3	1:E:288:PRO:HD3	1.99	0.44
1:A:362:GLN:HA	1:A:362:GLN:OE1	2.18	0.44
1:D:195:GLU:HG2	3:D:677:HOH:O	2.18	0.44
1:A:388:CYS:SG	1:A:396:ARG:HD2	2.58	0.43
1:B:152:ALA:HA	1:B:153:PRO:HA	1.83	0.43
1:C:11:LEU:HB3	1:D:101:GLN:HB2	1.99	0.43
1:E:60:ASP:HB2	1:E:313:ILE:HD11	2.01	0.43
1:A:238:ASP:HA	1:A:264:THR:OG1	2.17	0.43
1:D:264:THR:HG22	1:D:278:VAL:HG22	2.00	0.43
1:A:341:VAL:HG21	1:A:419:LEU:HB3	2.01	0.43
1:B:246:ARG:HG3	1:B:353:MET:HB2	2.01	0.43
1:D:152:ALA:HA	1:D:153:PRO:HA	1.82	0.43
1:D:297:TYR:CE2	1:E:274:PRO:HA	2.54	0.43
1:C:240:VAL:O	1:C:267:LLP:HB3	2.19	0.43
1:A:287:ALA:HB3	1:A:288:PRO:HD3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:377:ARG:CZ	1:E:421:ASP:HA	2.49	0.43
1:B:238:ASP:HA	1:B:264:THR:OG1	2.19	0.43
1:C:148:THR:HG22	1:C:150:LYS:H	1.84	0.43
1:C:51:VAL:HG22	1:C:267:LLP:HA	2.01	0.43
1:D:17:GLY:N	3:D:621:HOH:O	2.49	0.43
1:F:363:THR:HG23	1:F:365:GLU:H	1.82	0.43
1:C:330:LEU:HD12	1:C:412:MET:HE1	2.01	0.42
1:E:413:LYS:NZ	1:E:417:ASP:OD2	2.52	0.42
1:A:148:THR:O	1:A:155:LYS:NZ	2.51	0.42
1:E:66:GLU:O	1:E:70:GLN:HG2	2.18	0.42
1:F:148:THR:HG22	1:F:150:LYS:H	1.84	0.42
1:F:283:ASN:HA	3:F:519:HOH:O	2.18	0.42
1:F:228:CYS:HA	1:F:233:ILE:HB	2.01	0.42
1:E:171:PRO:HG2	1:E:220:LEU:HD22	2.02	0.42
1:F:118:VAL:HG21	1:F:147:LEU:HD11	2.01	0.42
1:A:152:ALA:HA	1:A:153:PRO:HA	1.80	0.42
1:D:367:SER:OG	1:D:370:ILE:HG13	2.19	0.42
1:C:213:PHE:HZ	1:C:398:LEU:HD21	1.84	0.42
1:B:36:ASP:OD1	1:B:40:ASN:N	2.52	0.41
1:D:321:GLU:HG3	3:D:656:HOH:O	2.19	0.41
1:F:152:ALA:HA	1:F:153:PRO:HA	1.87	0.41
1:F:97:PRO:O	1:F:260:PRO:HD2	2.20	0.41
1:C:238:ASP:HA	1:C:264:THR:OG1	2.20	0.41
1:E:213:PHE:HZ	1:E:398:LEU:HD21	1.85	0.41
1:F:287:ALA:HB3	1:F:288:PRO:HD3	2.02	0.41
1:F:314:ILE:HG12	1:F:319:LEU:HD12	2.02	0.41
1:C:151:VAL:HA	1:C:155:LYS:HD3	2.01	0.41
1:D:188:ARG:CZ	1:F:169:PRO:HG3	2.51	0.41
1:B:142:TYR:HB3	3:C:510:HOH:O	2.20	0.41
1:D:342:PRO:HB2	1:D:361:PRO:HB3	2.03	0.40
1:E:377:ARG:HH22	1:E:421:ASP:CG	2.24	0.40
1:E:248:GLY:O	1:E:320:CYS:HB3	2.22	0.40
1:B:132:ALA:O	1:B:167:HIS:HA	2.21	0.40
1:E:152:ALA:HA	1:E:153:PRO:HA	1.83	0.40
1:A:244:PHE:HE2	1:A:265:MET:HB3	1.86	0.40
1:C:212:GLY:O	1:C:348:ARG:HD2	2.22	0.40
1:C:35:LYS:HG2	1:C:41:GLU:HG2	2.03	0.40
1:E:79:ILE:HG22	1:E:80:VAL:HG23	2.03	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	417/421 (99%)	398 (95%)	17 (4%)	2 (0%)	29	52
1	B	417/421 (99%)	395 (95%)	21 (5%)	1 (0%)	47	71
1	C	417/421 (99%)	397 (95%)	17 (4%)	3 (1%)	22	44
1	D	417/421 (99%)	401 (96%)	13 (3%)	3 (1%)	22	44
1	E	417/421 (99%)	399 (96%)	17 (4%)	1 (0%)	47	71
1	F	417/421 (99%)	398 (95%)	18 (4%)	1 (0%)	47	71
All	All	2502/2526 (99%)	2388 (95%)	103 (4%)	11 (0%)	34	58

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	76	ALA
1	D	76	ALA
1	F	76	ALA
1	B	76	ALA
1	C	76	ALA
1	C	266	ALA
1	D	266	ALA
1	E	76	ALA
1	D	128	PRO
1	C	128	PRO
1	A	128	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	319/320 (100%)	318 (100%)	1 (0%)	92	97
1	B	319/320 (100%)	318 (100%)	1 (0%)	92	97
1	C	319/320 (100%)	318 (100%)	1 (0%)	92	97
1	D	319/320 (100%)	318 (100%)	1 (0%)	92	97
1	E	319/320 (100%)	317 (99%)	2 (1%)	86	94
1	F	319/320 (100%)	318 (100%)	1 (0%)	92	97
All	All	1914/1920 (100%)	1907 (100%)	7 (0%)	91	96

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	82	TYR
1	B	82	TYR
1	C	82	TYR
1	D	82	TYR
1	E	82	TYR
1	E	376	GLN
1	F	82	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

6 non-standard protein/DNA/RNA residues 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
1	LLP	D	267	1	23,24,25	2.71	5 (21%)	25,32,34	1.73	6 (24%)
1	LLP	B	267	1	23,24,25	2.66	5 (21%)	25,32,34	1.30	4 (16%)
1	LLP	C	267	1	23,24,25	2.54	5 (21%)	25,32,34	1.72	6 (24%)
1	LLP	E	267	1	23,24,25	2.64	6 (26%)	25,32,34	1.73	5 (20%)
1	LLP	A	267	1	23,24,25	2.63	6 (26%)	25,32,34	1.62	6 (24%)
1	LLP	F	267	1	23,24,25	2.78	8 (34%)	25,32,34	1.53	5 (20%)

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
1	LLP	D	267	1	-	9/16/17/19	0/1/1/1
1	LLP	B	267	1	-	7/16/17/19	0/1/1/1
1	LLP	C	267	1	-	6/16/17/19	0/1/1/1
1	LLP	E	267	1	-	6/16/17/19	0/1/1/1
1	LLP	A	267	1	-	10/16/17/19	0/1/1/1
1	LLP	F	267	1	-	8/16/17/19	0/1/1/1

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	267	LLP	C4-C4'	8.60	1.63	1.46
1	B	267	LLP	C4-C4'	8.40	1.62	1.46
1	E	267	LLP	C4-C4'	8.30	1.62	1.46
1	D	267	LLP	C4-C4'	8.25	1.62	1.46
1	C	267	LLP	C4-C4'	8.00	1.61	1.46
1	A	267	LLP	C4-C4'	7.95	1.61	1.46
1	B	267	LLP	C4'-NZ	5.75	1.46	1.27
1	A	267	LLP	C4'-NZ	5.54	1.45	1.27
1	E	267	LLP	C4'-NZ	5.47	1.45	1.27
1	D	267	LLP	C4'-NZ	5.46	1.45	1.27
1	C	267	LLP	C4'-NZ	5.44	1.45	1.27
1	F	267	LLP	C4'-NZ	5.25	1.44	1.27
1	A	267	LLP	C4-C5	-4.25	1.36	1.42
1	D	267	LLP	C4-C5	-4.22	1.36	1.42
1	F	267	LLP	C4-C5	-3.92	1.37	1.42
1	C	267	LLP	C2'-C2	3.83	1.56	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	267	LLP	C4-C5	-3.77	1.37	1.42
1	E	267	LLP	C2'-C2	3.74	1.56	1.50
1	F	267	LLP	C2'-C2	3.71	1.56	1.50
1	E	267	LLP	C6-N1	3.70	1.42	1.34
1	D	267	LLP	C2'-C2	3.68	1.56	1.50
1	F	267	LLP	C6-N1	3.46	1.41	1.34
1	A	267	LLP	C2'-C2	3.42	1.56	1.50
1	A	267	LLP	C6-N1	3.33	1.41	1.34
1	D	267	LLP	C6-N1	3.29	1.41	1.34
1	B	267	LLP	C2'-C2	3.16	1.55	1.50
1	C	267	LLP	C4-C5	-2.99	1.38	1.42
1	C	267	LLP	C6-N1	2.83	1.40	1.34
1	B	267	LLP	C6-N1	2.82	1.40	1.34
1	E	267	LLP	C4-C5	-2.53	1.38	1.42
1	A	267	LLP	C4-C3	-2.42	1.37	1.40
1	F	267	LLP	C4-C3	-2.33	1.37	1.40
1	E	267	LLP	C5'-C5	2.33	1.57	1.50
1	F	267	LLP	C3-C2	2.33	1.43	1.40
1	F	267	LLP	C6-C5	2.00	1.41	1.37

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	267	LLP	C4-C4'-NZ	-4.38	104.21	124.31
1	A	267	LLP	C4-C4'-NZ	-4.28	104.65	124.31
1	E	267	LLP	OP4-C5'-C5	4.23	117.41	109.35
1	D	267	LLP	C4-C4'-NZ	-3.86	106.58	124.31
1	E	267	LLP	C4-C4'-NZ	-3.82	106.75	124.31
1	B	267	LLP	C4-C4'-NZ	-3.59	107.81	124.31
1	D	267	LLP	OP4-C5'-C5	3.44	115.91	109.35
1	D	267	LLP	C5-C6-N1	-3.14	118.59	123.82
1	F	267	LLP	C4-C4'-NZ	-3.13	109.95	124.31
1	D	267	LLP	C2'-C2-C3	-3.02	117.16	120.89
1	A	267	LLP	OP4-C5'-C5	2.93	114.93	109.35
1	B	267	LLP	C2'-C2-C3	-2.73	117.51	120.89
1	C	267	LLP	C2'-C2-N1	2.72	122.99	117.67
1	F	267	LLP	C5-C6-N1	-2.68	119.35	123.82
1	A	267	LLP	C2'-C2-N1	2.66	122.88	117.67
1	D	267	LLP	C2'-C2-N1	2.62	122.78	117.67
1	F	267	LLP	CE-NZ-C4'	-2.62	110.87	118.90
1	C	267	LLP	C2'-C2-C3	-2.61	117.66	120.89
1	A	267	LLP	C5-C6-N1	-2.57	119.53	123.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	267	LLP	C2'-C2-C3	-2.56	117.73	120.89
1	E	267	LLP	C2'-C2-N1	2.52	122.59	117.67
1	C	267	LLP	OP4-C5'-C5	2.50	114.11	109.35
1	C	267	LLP	C3-C4-C4'	-2.49	115.78	120.41
1	F	267	LLP	OP4-C5'-C5	2.40	113.93	109.35
1	E	267	LLP	C4-C3-C2	2.33	121.63	120.19
1	E	267	LLP	C2'-C2-C3	-2.33	118.01	120.89
1	D	267	LLP	C3-C4-C5	2.28	120.01	118.26
1	B	267	LLP	C5-C6-N1	-2.26	120.05	123.82
1	A	267	LLP	C2'-C2-C3	-2.25	118.11	120.89
1	C	267	LLP	C5-C6-N1	-2.21	120.13	123.82
1	B	267	LLP	C2'-C2-N1	2.09	121.75	117.67
1	A	267	LLP	C3-C4-C5	2.05	119.84	118.26

There are no chirality outliers.

All (46) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	D	267	LLP	C4-C4'-NZ-CE
1	D	267	LLP	C5'-OP4-P-OP1
1	D	267	LLP	C5'-OP4-P-OP2
1	D	267	LLP	C5'-OP4-P-OP3
1	D	267	LLP	O-C-CA-CB
1	B	267	LLP	C4-C4'-NZ-CE
1	B	267	LLP	O-C-CA-CB
1	B	267	LLP	CG-CD-CE-NZ
1	C	267	LLP	C4-C4'-NZ-CE
1	C	267	LLP	C-CA-CB-CG
1	C	267	LLP	O-C-CA-CB
1	E	267	LLP	C4-C4'-NZ-CE
1	E	267	LLP	C5'-OP4-P-OP2
1	E	267	LLP	O-C-CA-CB
1	A	267	LLP	C5'-OP4-P-OP1
1	A	267	LLP	C5'-OP4-P-OP2
1	A	267	LLP	C5'-OP4-P-OP3
1	A	267	LLP	O-C-CA-CB
1	A	267	LLP	CG-CD-CE-NZ
1	F	267	LLP	C4-C4'-NZ-CE
1	F	267	LLP	C5'-OP4-P-OP1
1	F	267	LLP	C5'-OP4-P-OP2
1	F	267	LLP	C5'-OP4-P-OP3
1	F	267	LLP	O-C-CA-CB

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Mol	Chain	Res	Type	Atoms
1	F	267	LLP	CG-CD-CE-NZ
1	A	267	LLP	C4-C4'-NZ-CE
1	D	267	LLP	CG-CD-CE-NZ
1	E	267	LLP	CG-CD-CE-NZ
1	D	267	LLP	CD-CE-NZ-C4'
1	E	267	LLP	CD-CE-NZ-C4'
1	B	267	LLP	C5'-OP4-P-OP3
1	D	267	LLP	C3-C4-C4'-NZ
1	A	267	LLP	C3-C4-C4'-NZ
1	A	267	LLP	CD-CE-NZ-C4'
1	C	267	LLP	CG-CD-CE-NZ
1	C	267	LLP	CD-CE-NZ-C4'
1	B	267	LLP	C3-C4-C4'-NZ
1	C	267	LLP	C3-C4-C4'-NZ
1	E	267	LLP	C3-C4-C4'-NZ
1	F	267	LLP	C3-C4-C4'-NZ
1	B	267	LLP	CD-CE-NZ-C4'
1	F	267	LLP	CD-CE-NZ-C4'
1	A	267	LLP	C6-C5-C5'-OP4
1	D	267	LLP	C5-C4-C4'-NZ
1	B	267	LLP	C5-C4-C4'-NZ
1	A	267	LLP	C5-C4-C4'-NZ

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C	267	LLP	3	0
1	A	267	LLP	2	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

2 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	PEG	B	501	-	6,6,6	0.47	0	5,5,5	0.25	0
2	PEG	D	501	-	6,6,6	0.47	0	5,5,5	0.69	0

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	PEG	B	501	-	-	1/4/4/4	-
2	PEG	D	501	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	501	PEG	C1-C2-O2-C3
2	D	501	PEG	C1-C2-O2-C3
2	D	501	PEG	O2-C3-C4-O4

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	501	PEG	2	0
2	D	501	PEG	2	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

### 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	419/421 (99%)	-0.43	2 (0%) 91 92	24, 36, 63, 99	0
1	B	419/421 (99%)	-0.48	1 (0%) 95 96	22, 37, 70, 109	0
1	C	419/421 (99%)	-0.37	7 (1%) 70 71	24, 39, 78, 107	0
1	D	419/421 (99%)	-0.46	1 (0%) 95 96	21, 35, 69, 108	0
1	E	419/421 (99%)	-0.47	0 100 100	23, 36, 59, 95	0
1	F	419/421 (99%)	-0.41	2 (0%) 91 92	23, 37, 64, 108	0
All	All	2514/2526 (99%)	-0.44	13 (0%) 91 92	21, 37, 68, 109	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	421	ASP	3.3
1	C	173	ASP	3.0
1	C	174	LEU	2.7
1	F	173	ASP	2.7
1	B	197	LYS	2.6
1	C	321	GLU	2.5
1	F	421	ASP	2.5
1	C	345	ALA	2.3
1	A	421	ASP	2.3
1	C	340	SER	2.2
1	A	362	GLN	2.1
1	C	176	GLY	2.1
1	C	420	SER	2.0

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

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	LLP	C	267	24/25	0.96	0.11	35,38,39,40	0
1	LLP	E	267	24/25	0.96	0.12	34,37,38,39	0
1	LLP	A	267	24/25	0.96	0.12	31,37,39,39	0
1	LLP	B	267	24/25	0.97	0.10	31,34,36,36	0
1	LLP	D	267	24/25	0.97	0.10	30,32,35,36	0
1	LLP	F	267	24/25	0.98	0.10	32,37,38,39	0

### 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	PEG	D	501	7/7	0.87	0.19	66,80,80,80	0
2	PEG	B	501	7/7	0.89	0.25	64,78,81,81	17

### 6.5 Other polymers [i](#)

There are no such residues in this entry.