



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:51 AM GMT

PDB ID : 2EJ2  
Title : Crystal Structure of T.th.HB8 Branched-Chain Amino Acid Aminotransferase  
Complexed with N-(5'-Phosphopyridoxyl)-L-Glutamate  
Authors : Goto, M.  
Deposited on : 2007-03-14  
Resolution : 2.00 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  
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

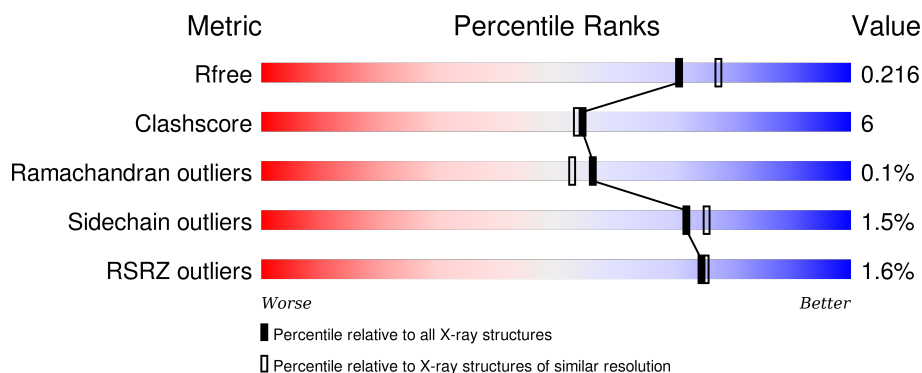
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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))
$R_{free}$	91344	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

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. 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	308	<div> <div>%</div> <div> <div></div> <div>81%</div> <div>13%</div> <div>5%</div> </div> </div>
1	B	308	<div> <div>2%</div> <div> <div></div> <div>85%</div> <div>14%</div> <div>..</div> </div> </div>
1	C	308	<div> <div>2%</div> <div> <div></div> <div>84%</div> <div>12%</div> <div>.</div> </div> </div>
1	D	308	<div> <div>2%</div> <div> <div></div> <div>85%</div> <div>12%</div> <div>..</div> </div> </div>
1	E	308	<div> <div>%</div> <div> <div></div> <div>84%</div> <div>11%</div> <div>..</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	F	308	

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	PPE	A	3413	-	-	-	X
2	PPE	B	3913	-	-	-	X
2	PPE	C	1413	-	-	-	X
2	PPE	D	1913	-	-	-	X
2	PPE	E	2413	-	-	-	X
2	PPE	F	2913	-	-	-	X
3	MPD	A	1415	-	-	-	X
3	MPD	F	2914	-	-	-	X

## 2 Entry composition [i](#)

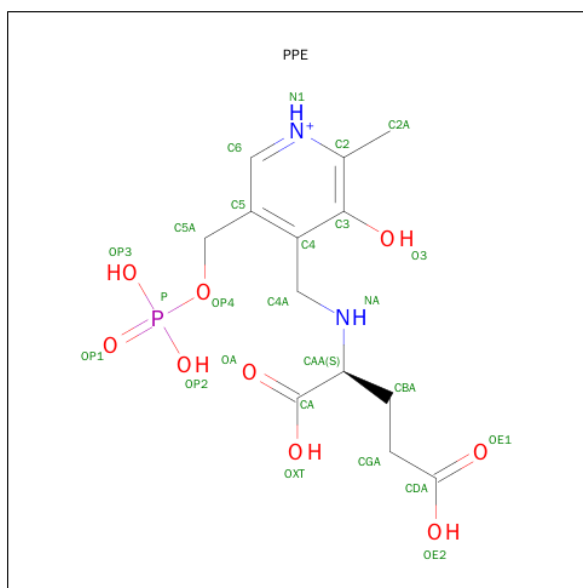
There are 4 unique types of molecules in this entry. The entry contains 15270 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Branched-chain amino acid aminotransferase.

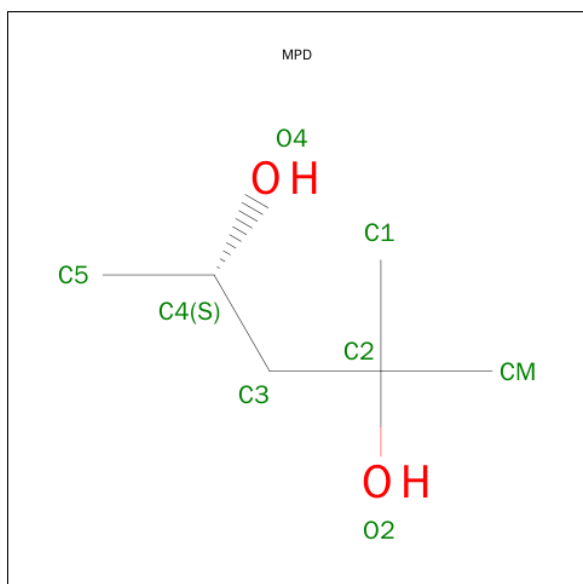
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	294	Total	C	N	O	S	0	0	0
			2282	1460	397	415	10			
1	B	305	Total	C	N	O	S	0	0	0
			2369	1514	412	433	10			
1	C	297	Total	C	N	O	S	0	0	0
			2299	1470	399	420	10			
1	D	301	Total	C	N	O	S	0	0	0
			2326	1489	405	422	10			
1	E	298	Total	C	N	O	S	0	0	0
			2288	1464	396	418	10			
1	F	298	Total	C	N	O	S	0	0	0
			2304	1474	401	419	10			

- Molecule 2 is 4-[(1,3-DICARBOXY-PROPYLAMINO)-METHYL]-3-HYDROXY-2-METHYL-5-PHOSPHONOXYMETHYL-PYRIDINIUM (three-letter code: PPE) (formula:  $C_{13}H_{20}N_2O_9P$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			25	13	2	9	1		
2	B	1	Total	C	N	O	P	0	0
			25	13	2	9	1		
2	C	1	Total	C	N	O	P	0	0
			25	13	2	9	1		
2	D	1	Total	C	N	O	P	0	0
			25	13	2	9	1		
2	E	1	Total	C	N	O	P	0	0
			25	13	2	9	1		
2	F	1	Total	C	N	O	P	0	0
			25	13	2	9	1		

- Molecule 3 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula:  $C_6H_{14}O_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			8	6	2		
3	F	1	Total	C	O	0	0
			8	6	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	208	Total	O	0	0
			208	208		

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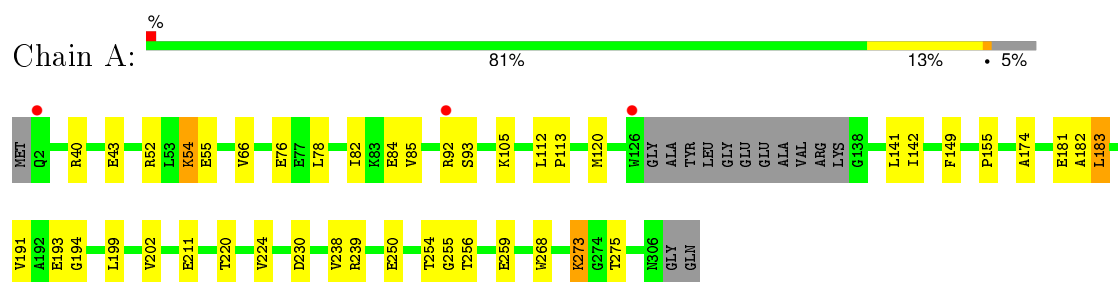
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	205	Total 205	O 205	0	0
4	C	207	Total 207	O 207	0	0
4	D	213	Total 213	O 213	0	0
4	E	190	Total 190	O 190	0	0
4	F	213	Total 213	O 213	0	0

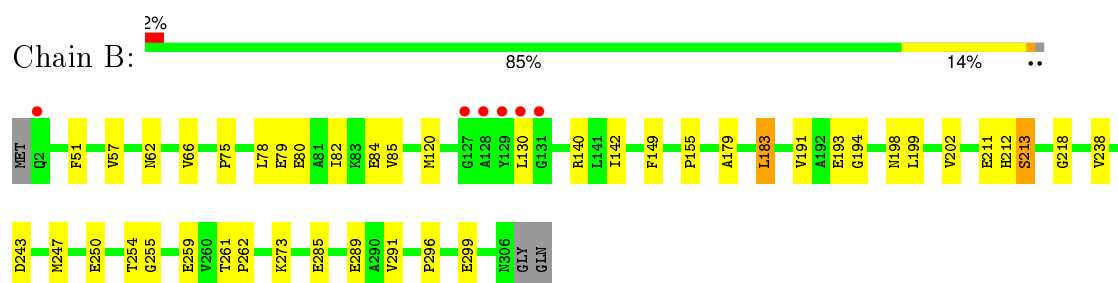
### 3 Residue-property plots

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

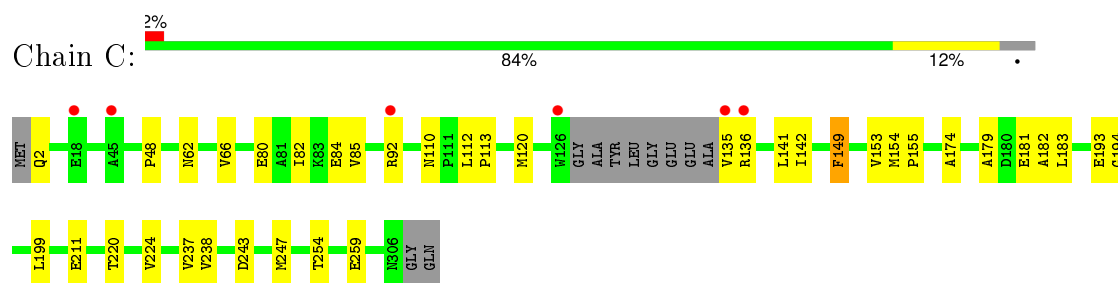
- Molecule 1: Branched-chain amino acid aminotransferase



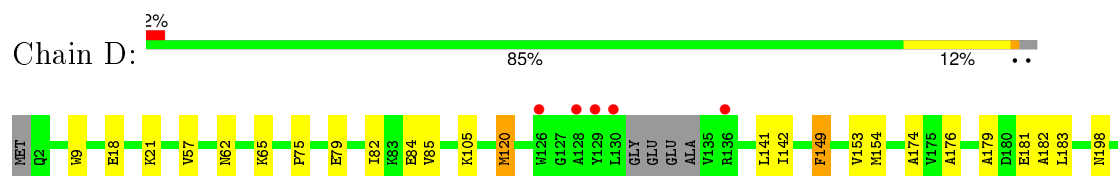
- Molecule 1: Branched-chain amino acid aminotransferase



- Molecule 1: Branched-chain amino acid aminotransferase

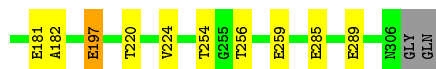
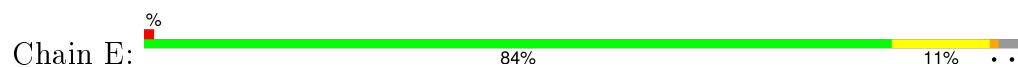


- Molecule 1: Branched-chain amino acid aminotransferase

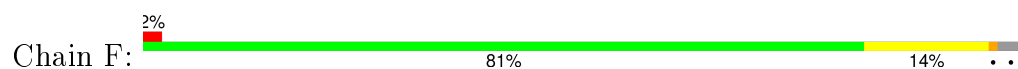




- Molecule 1: Branched-chain amino acid aminotransferase



- Molecule 1: Branched-chain amino acid aminotransferase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	117.02Å 144.22Å 147.04Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.97 – 2.00 20.10 – 2.00	Depositor EDS
% Data completeness (in resolution range)	96.7 (19.97-2.00) 96.9 (20.10-2.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.26 (at 2.01Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.190 , 0.216 0.190 , 0.216	Depositor DCC
$R_{free}$ test set	16164 reflections (9.96%)	DCC
Wilson B-factor (Å <sup>2</sup> )	21.3	Xtriage
Anisotropy	0.325	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 60.8	EDS
Estimated twinning fraction	0.018 for -h,l,k	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtriage
Outliers	0 of 162358 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	15270	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.68% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: MPD, PPE

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	0.32	0/2334	0.60	0/3169
1	B	0.31	0/2423	0.61	0/3289
1	C	0.31	0/2351	0.61	0/3194
1	D	0.31	0/2379	0.61	0/3232
1	E	0.32	0/2340	0.61	0/3181
1	F	0.32	0/2356	0.61	0/3200
All	All	0.32	0/14183	0.61	0/19265

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	2282	0	2264	35	0
1	B	2369	0	2352	26	0
1	C	2299	0	2270	27	0
1	D	2326	0	2299	24	0
1	E	2288	0	2247	30	0
1	F	2304	0	2282	37	0
2	A	25	0	15	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	25	0	15	0	0
2	C	25	0	15	0	0
2	D	25	0	15	0	0
2	E	25	0	15	0	0
2	F	25	0	15	0	0
3	A	8	0	14	1	0
3	F	8	0	14	2	0
4	A	208	0	0	2	0
4	B	205	0	0	1	0
4	C	207	0	0	2	0
4	D	213	0	0	5	0
4	E	190	0	0	1	0
4	F	213	0	0	5	0
All	All	15270	0	13832	178	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 6.

All (178) 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:183:LEU:HD11	1:A:191:VAL:HG13	1.57	0.85
1:E:220:THR:O	1:E:224:VAL:HG23	1.84	0.77
1:A:52:ARG:HA	1:A:54:LYS:HE2	1.65	0.77
1:B:183:LEU:HD11	1:B:191:VAL:HG13	1.66	0.76
1:B:183:LEU:HD13	1:B:199:LEU:HD11	1.69	0.74
1:A:54:LYS:HD3	1:A:54:LYS:H	1.53	0.74
1:A:183:LEU:HD13	1:A:199:LEU:HD11	1.70	0.72
1:F:220:THR:O	1:F:224:VAL:HG23	1.92	0.69
1:A:220:THR:O	1:A:224:VAL:HG23	1.93	0.68
1:A:54:LYS:HD3	1:A:54:LYS:N	2.10	0.66
1:D:82:ILE:O	1:D:85:VAL:HG12	1.96	0.65
1:D:84:GLU:HG2	4:D:2037:HOH:O	1.96	0.65
1:F:54:LYS:HD3	1:F:55:GLU:H	1.61	0.64
1:E:141:LEU:HD22	1:E:181:GLU:HB3	1.78	0.64
1:A:82:ILE:O	1:A:85:VAL:HG12	1.97	0.64
1:F:54:LYS:NZ	1:F:55:GLU:HG2	2.12	0.64
1:E:82:ILE:O	1:E:85:VAL:HG12	1.98	0.63
1:C:220:THR:O	1:C:224:VAL:HG23	1.99	0.63
1:B:285:GLU:O	1:B:289:GLU:HG3	1.97	0.63
1:C:193:GLU:HA	1:C:199:LEU:HD23	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:82:ILE:O	1:C:85:VAL:HG12	1.99	0.62
1:C:80:GLU:O	1:C:84:GLU:HG3	2.00	0.62
1:B:243:ASP:O	1:B:247:MET:HG2	2.00	0.62
1:A:52:ARG:CA	1:A:54:LYS:HE2	2.30	0.62
1:C:224:VAL:HG21	1:C:254:THR:HG21	1.82	0.61
1:D:57:VAL:HG21	1:D:79:GLU:HG2	1.83	0.61
1:F:82:ILE:O	1:F:85:VAL:HG12	2.01	0.61
1:E:54:LYS:N	1:E:54:LYS:HD3	2.17	0.60
1:F:52:ARG:HA	1:F:54:LYS:HE3	1.82	0.60
1:A:183:LEU:HD13	1:A:199:LEU:CD1	2.30	0.60
1:D:285:GLU:O	1:D:289:GLU:HG3	2.02	0.60
1:B:82:ILE:O	1:B:85:VAL:HG12	2.01	0.60
1:A:43:GLU:HG2	1:A:92:ARG:HB3	1.82	0.60
1:B:80:GLU:O	1:B:84:GLU:HG3	2.01	0.59
1:B:183:LEU:HD13	1:B:199:LEU:CD1	2.33	0.59
1:F:54:LYS:HZ3	1:F:55:GLU:HG2	1.67	0.59
1:D:174:ALA:HB2	1:D:182:ALA:HB2	1.84	0.58
1:F:88:ARG:HH11	1:F:88:ARG:HG3	1.67	0.58
1:A:141:LEU:CD2	1:A:181:GLU:HB3	2.34	0.58
1:D:75:PRO:O	1:D:79:GLU:HG3	2.03	0.58
1:C:141:LEU:HD22	1:C:181:GLU:HB3	1.86	0.58
1:F:40:ARG:HG3	1:F:256:THR:CG2	2.34	0.57
1:A:43:GLU:HG3	1:A:93:SER:OG	2.06	0.56
1:E:54:LYS:H	1:E:54:LYS:HD3	1.69	0.56
3:F:2914:MPD:H53	4:F:2975:HOH:O	2.05	0.56
1:E:224:VAL:HG21	1:E:254:THR:HG21	1.86	0.56
1:A:54:LYS:HE3	1:A:55:GLU:HG2	1.88	0.55
1:B:273:LYS:HG2	4:B:3964:HOH:O	2.07	0.55
1:B:57:VAL:HG21	1:B:79:GLU:HG2	1.89	0.54
1:C:141:LEU:CD2	1:C:181:GLU:HB3	2.37	0.54
1:D:220:THR:O	1:D:224:VAL:HG23	2.07	0.54
1:C:135:VAL:HG13	1:C:136:ARG:H	1.73	0.54
1:C:135:VAL:HG13	1:C:136:ARG:N	2.23	0.53
1:A:112:LEU:HB2	1:A:113:PRO:HD3	1.91	0.53
1:A:66:VAL:HG11	1:A:155:PRO:CB	2.39	0.53
1:F:174:ALA:HB2	1:F:182:ALA:HB2	1.91	0.52
1:F:2:GLN:HG2	1:F:3:ILE:N	2.25	0.52
1:C:110:ASN:OD1	1:F:172:MET:HG2	2.10	0.52
1:F:43:GLU:OE2	1:F:92:ARG:NE	2.33	0.51
1:C:174:ALA:HB2	1:C:182:ALA:HB2	1.92	0.51
1:F:40:ARG:HG3	1:F:256:THR:HG22	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:66:VAL:HG11	1:F:155:PRO:CB	2.41	0.51
1:A:193:GLU:HG3	1:A:194:GLY:O	2.11	0.51
1:A:54:LYS:HG2	1:A:55:GLU:N	2.26	0.51
4:D:1924:HOH:O	1:F:247:MET:HE1	2.11	0.51
1:B:51:PHE:CD1	1:B:291:VAL:HG12	2.46	0.51
1:A:40:ARG:HG3	1:A:256:THR:HG22	1.92	0.51
1:F:126:TRP:HH2	1:F:257:ALA:HB1	1.76	0.51
1:D:105:LYS:HE3	4:D:2029:HOH:O	2.10	0.50
1:F:141:LEU:CD2	1:F:181:GLU:HB3	2.42	0.50
1:B:202:VAL:HB	1:B:250:GLU:HB2	1.92	0.50
1:D:141:LEU:CD2	1:D:181:GLU:HB3	2.42	0.49
1:E:181:GLU:HG3	1:E:182:ALA:N	2.27	0.49
1:C:48:PRO:HG3	1:C:92:ARG:HA	1.93	0.49
1:E:141:LEU:CD2	1:E:181:GLU:HB3	2.42	0.49
1:E:54:LYS:H	1:E:54:LYS:CD	2.26	0.48
1:F:254:THR:HA	1:F:259:GLU:O	2.14	0.48
1:E:54:LYS:NZ	1:E:55:GLU:HG2	2.29	0.48
1:B:130:LEU:N	1:B:130:LEU:HD12	2.28	0.48
1:F:224:VAL:HG21	1:F:254:THR:HG21	1.96	0.47
1:C:2:GLN:HG3	4:F:3032:HOH:O	2.14	0.47
1:C:224:VAL:HG21	1:C:254:THR:CG2	2.43	0.47
1:F:87:ARG:HG3	1:F:305:VAL:CG1	2.44	0.47
1:D:211:GLU:HG3	1:D:238:VAL:C	2.34	0.47
1:E:140:ARG:HG3	1:E:140:ARG:HH11	1.78	0.47
1:A:224:VAL:HG21	1:A:254:THR:HG21	1.96	0.47
1:A:84:GLU:HG2	4:A:3538:HOH:O	2.15	0.47
1:C:211:GLU:HG3	1:C:238:VAL:C	2.35	0.46
1:B:254:THR:HA	1:B:259:GLU:O	2.15	0.46
1:D:105:LYS:HG3	4:D:1993:HOH:O	2.15	0.46
1:A:76:GLU:H	1:A:76:GLU:CD	2.19	0.46
1:C:254:THR:HA	1:C:259:GLU:O	2.15	0.46
1:A:254:THR:HA	1:A:259:GLU:O	2.17	0.45
1:D:226:ARG:HD3	1:D:301:TRP:CZ2	2.51	0.45
1:B:78:LEU:O	1:B:82:ILE:HG13	2.16	0.45
1:F:273:LYS:HG2	4:F:3046:HOH:O	2.17	0.45
1:A:230:ASP:HB3	3:A:1415:MPD:H53	1.99	0.45
1:C:84:GLU:HG2	4:C:1555:HOH:O	2.16	0.45
1:A:268:TRP:CD1	1:D:176:ALA:HB1	2.51	0.45
1:F:226:ARG:HD3	1:F:301:TRP:CZ2	2.51	0.45
1:B:211:GLU:HG3	1:B:238:VAL:C	2.37	0.44
1:D:153:VAL:HG12	1:D:154:MET:HG2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:9:TRP:O	1:F:120:MET:HA	2.17	0.44
1:A:105:LYS:HE3	4:A:3550:HOH:O	2.17	0.44
1:A:239:ARG:HG3	4:C:1497:HOH:O	2.16	0.44
1:D:18:GLU:O	1:D:21:LYS:HE2	2.17	0.44
1:E:153:VAL:HG12	1:E:154:MET:HG2	1.98	0.44
1:C:112:LEU:HB2	1:C:113:PRO:HD3	2.00	0.44
1:F:112:LEU:HB2	1:F:113:PRO:HD3	1.99	0.44
1:C:62:ASN:HD22	1:C:62:ASN:HA	1.64	0.44
1:E:197:GLU:HB2	1:E:254:THR:O	2.17	0.44
1:E:54:LYS:HZ3	1:E:55:GLU:HG2	1.83	0.44
1:F:84:GLU:OE1	1:F:88:ARG:NH1	2.51	0.44
1:A:52:ARG:CB	1:A:54:LYS:HE2	2.48	0.44
1:C:66:VAL:HG11	1:C:155:PRO:CB	2.48	0.44
1:E:224:VAL:HG21	1:E:254:THR:CG2	2.48	0.43
1:A:211:GLU:HG3	1:A:238:VAL:C	2.39	0.43
1:E:18:GLU:O	1:E:21:LYS:HE2	2.18	0.43
1:E:48:PRO:HG3	1:E:92:ARG:HA	2.00	0.43
1:D:149:PHE:CG	1:D:154:MET:HB2	2.54	0.43
1:F:183:LEU:HD23	1:F:183:LEU:C	2.39	0.43
1:A:202:VAL:HB	1:A:250:GLU:HB2	2.00	0.43
1:B:62:ASN:HD22	1:B:62:ASN:HA	1.66	0.43
1:E:40:ARG:HG3	1:E:256:THR:HG22	1.99	0.43
1:C:211:GLU:HG2	1:C:237:VAL:HG12	2.01	0.43
1:C:153:VAL:HG12	1:C:154:MET:HG2	1.99	0.43
1:F:54:LYS:CD	1:F:54:LYS:N	2.82	0.43
1:E:148:ARG:HA	1:E:148:ARG:HD2	1.89	0.43
1:A:273:LYS:HG3	1:A:275:THR:H	1.84	0.43
1:E:134:ALA:O	1:E:138:GLY:N	2.51	0.42
1:F:230:ASP:HB3	3:F:2914:MPD:H51	2.01	0.42
1:F:190:TYR:CD2	1:F:239:ARG:HG2	2.55	0.42
1:F:82:ILE:HG23	1:F:96:ILE:HG21	2.01	0.42
1:C:193:GLU:HG3	1:C:194:GLY:O	2.20	0.42
1:E:9:TRP:O	1:E:120:MET:HA	2.20	0.42
1:E:83:LYS:O	1:E:87:ARG:HG2	2.18	0.42
1:D:62:ASN:HD22	1:D:62:ASN:HA	1.64	0.42
1:F:142:ILE:HG13	1:F:179:ALA:HB2	2.02	0.42
1:F:125:GLU:HG2	4:F:2984:HOH:O	2.19	0.42
1:D:198:ASN:OD1	1:D:218:GLY:HA3	2.20	0.42
1:B:193:GLU:HG3	1:B:194:GLY:O	2.19	0.42
1:C:183:LEU:HD23	1:C:183:LEU:C	2.39	0.42
1:D:142:ILE:HG13	1:D:179:ALA:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:9:TRP:O	1:D:120:MET:HA	2.20	0.42
1:A:142:ILE:HD11	1:A:268:TRP:CZ2	2.55	0.42
1:E:84:GLU:O	1:E:88:ARG:HG3	2.20	0.42
1:D:250:GLU:CD	1:D:277:GLY:HA3	2.40	0.42
1:E:254:THR:HA	1:E:259:GLU:O	2.20	0.42
1:B:66:VAL:HG11	1:B:155:PRO:CB	2.50	0.42
1:D:65:LYS:NZ	4:D:2060:HOH:O	2.52	0.41
1:A:255:GLY:O	1:A:259:GLU:N	2.51	0.41
1:F:54:LYS:HD2	1:F:54:LYS:H	1.85	0.41
1:E:174:ALA:HB2	1:E:182:ALA:HB2	2.01	0.41
1:B:255:GLY:O	1:B:259:GLU:N	2.51	0.41
1:D:183:LEU:HD23	1:D:183:LEU:C	2.41	0.41
1:F:54:LYS:CD	1:F:54:LYS:H	2.34	0.41
1:F:141:LEU:HD22	1:F:181:GLU:HB3	2.01	0.41
1:C:149:PHE:CG	1:C:154:MET:HB2	2.56	0.41
1:E:2:GLN:N	4:E:2597:HOH:O	2.54	0.41
1:B:75:PRO:O	1:B:79:GLU:HG3	2.20	0.41
1:B:296:PRO:HA	1:B:299:GLU:HG2	2.01	0.41
1:A:174:ALA:HB2	1:A:182:ALA:HB2	2.02	0.41
1:B:142:ILE:HG13	1:B:179:ALA:HB2	2.01	0.41
1:D:254:THR:HA	1:D:259:GLU:O	2.19	0.41
1:F:197:GLU:HB2	1:F:254:THR:O	2.21	0.41
1:E:62:ASN:HA	1:E:62:ASN:HD22	1.64	0.41
1:E:36:PHE:CE1	1:E:159:LYS:HE2	2.56	0.41
1:B:140:ARG:HH11	1:B:140:ARG:HG3	1.86	0.41
1:C:142:ILE:HG13	1:C:179:ALA:HB2	2.03	0.40
1:B:212:HIS:O	1:B:213:SER:C	2.59	0.40
1:A:224:VAL:HG21	1:A:254:THR:CG2	2.50	0.40
1:B:261:THR:HA	1:B:262:PRO:HD3	1.96	0.40
1:E:54:LYS:N	1:E:54:LYS:CD	2.83	0.40
1:A:40:ARG:HG3	1:A:256:THR:CG2	2.52	0.40
1:E:285:GLU:OE1	1:E:289:GLU:OE2	2.39	0.40
1:B:198:ASN:OD1	1:B:218:GLY:HA3	2.21	0.40
1:C:243:ASP:O	1:C:247:MET:HG3	2.22	0.40
1:F:105:LYS:HE3	4:F:3024:HOH:O	2.20	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	290/308 (94%)	281 (97%)	9 (3%)	0	100	100
1	B	303/308 (98%)	295 (97%)	7 (2%)	1 (0%)	46	41
1	C	293/308 (95%)	284 (97%)	9 (3%)	0	100	100
1	D	297/308 (96%)	289 (97%)	8 (3%)	0	100	100
1	E	294/308 (96%)	283 (96%)	11 (4%)	0	100	100
1	F	294/308 (96%)	286 (97%)	8 (3%)	0	100	100
All	All	1771/1848 (96%)	1718 (97%)	52 (3%)	1 (0%)	56	53

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	213	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	229/241 (95%)	223 (97%)	6 (3%)	54	54
1	B	237/241 (98%)	234 (99%)	3 (1%)	76	79
1	C	230/241 (95%)	228 (99%)	2 (1%)	84	88
1	D	231/241 (96%)	229 (99%)	2 (1%)	84	88
1	E	226/241 (94%)	222 (98%)	4 (2%)	66	69
1	F	230/241 (95%)	226 (98%)	4 (2%)	68	71

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	1383/1446 (96%)	1362 (98%)	21 (2%)	72	75

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	54	LYS
1	A	78	LEU
1	A	120	MET
1	A	149	PHE
1	A	183	LEU
1	A	273	LYS
1	B	120	MET
1	B	149	PHE
1	B	183	LEU
1	C	120	MET
1	C	149	PHE
1	D	120	MET
1	D	149	PHE
1	E	54	LYS
1	E	120	MET
1	E	149	PHE
1	E	197	GLU
1	F	54	LYS
1	F	120	MET
1	F	149	PHE
1	F	197	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	62	ASN
1	A	306	ASN
1	B	62	ASN
1	C	62	ASN
1	D	62	ASN
1	E	62	ASN
1	E	236	GLN
1	E	306	ASN
1	F	62	ASN

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

8 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$
3	MPD	A	1415	-	6,7,7	0.56	0	7,10,10	1.10	0
2	PPE	A	3413	-	19,25,25	3.41	7 (36%)	23,35,35	4.09	13 (56%)
2	PPE	B	3913	-	19,25,25	3.32	7 (36%)	23,35,35	4.04	12 (52%)
2	PPE	C	1413	-	19,25,25	3.36	7 (36%)	23,35,35	4.14	10 (43%)
2	PPE	D	1913	-	19,25,25	3.29	8 (42%)	23,35,35	4.02	12 (52%)
2	PPE	E	2413	-	19,25,25	3.43	7 (36%)	23,35,35	4.13	11 (47%)
2	PPE	F	2913	-	19,25,25	3.42	8 (42%)	23,35,35	4.15	12 (52%)
3	MPD	F	2914	-	6,7,7	0.53	0	7,10,10	1.09	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
3	MPD	A	1415	-	-	0/5/5/5	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PPE	A	3413	-	-	0/14/20/20	0/1/1/1
2	PPE	B	3913	-	-	0/14/20/20	0/1/1/1
2	PPE	C	1413	-	-	0/14/20/20	0/1/1/1
2	PPE	D	1913	-	-	0/14/20/20	0/1/1/1
2	PPE	E	2413	-	-	0/14/20/20	0/1/1/1
2	PPE	F	2913	-	-	0/14/20/20	0/1/1/1
3	MPD	F	2914	-	-	0/5/5/5	0/0/0/0

All (44) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	2913	PPE	P-OP1	-2.22	1.43	1.51
2	B	3913	PPE	P-OP1	-2.19	1.44	1.51
2	D	1913	PPE	P-OP1	-2.02	1.44	1.51
2	D	1913	PPE	CBA-CAA	2.20	1.56	1.53
2	A	3413	PPE	C6-C5	2.28	1.42	1.37
2	F	2913	PPE	C6-C5	2.32	1.42	1.37
2	B	3913	PPE	CAA-NA	2.34	1.51	1.47
2	D	1913	PPE	C6-C5	2.36	1.42	1.37
2	C	1413	PPE	C6-C5	2.36	1.42	1.37
2	E	2413	PPE	C6-C5	2.39	1.42	1.37
2	A	3413	PPE	CBA-CAA	2.39	1.56	1.53
2	B	3913	PPE	C6-C5	2.44	1.43	1.37
2	C	1413	PPE	CBA-CAA	2.53	1.56	1.53
2	D	1913	PPE	CAA-NA	2.54	1.51	1.47
2	A	3413	PPE	CAA-NA	2.67	1.51	1.47
2	F	2913	PPE	C6-N1	2.76	1.40	1.34
2	C	1413	PPE	C6-N1	2.78	1.40	1.34
2	D	1913	PPE	C6-N1	2.91	1.40	1.34
2	A	3413	PPE	C6-N1	3.01	1.40	1.34
2	C	1413	PPE	CAA-NA	3.08	1.52	1.47
2	B	3913	PPE	C6-N1	3.08	1.41	1.34
2	E	2413	PPE	C6-N1	3.16	1.41	1.34
2	E	2413	PPE	CAA-NA	3.23	1.52	1.47
2	F	2913	PPE	CAA-NA	3.25	1.53	1.47
2	F	2913	PPE	CBA-CAA	3.54	1.58	1.53
2	E	2413	PPE	CBA-CAA	3.72	1.58	1.53
2	F	2913	PPE	C2-N1	3.78	1.42	1.34
2	C	1413	PPE	C2-N1	3.85	1.42	1.34
2	B	3913	PPE	C2-N1	3.89	1.42	1.34
2	A	3413	PPE	C2-N1	3.92	1.42	1.34
2	D	1913	PPE	C2-N1	3.97	1.42	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	2413	PPE	C2-N1	4.00	1.42	1.34
2	B	3913	PPE	C5-C4	4.66	1.47	1.40
2	A	3413	PPE	C5-C4	4.95	1.47	1.40
2	D	1913	PPE	C5-C4	4.97	1.47	1.40
2	C	1413	PPE	C5-C4	5.09	1.47	1.40
2	E	2413	PPE	C5-C4	5.44	1.48	1.40
2	F	2913	PPE	C5-C4	5.53	1.48	1.40
2	E	2413	PPE	C3-C2	10.95	1.48	1.40
2	F	2913	PPE	C3-C2	11.10	1.48	1.40
2	D	1913	PPE	C3-C2	11.20	1.48	1.40
2	C	1413	PPE	C3-C2	11.32	1.48	1.40
2	B	3913	PPE	C3-C2	11.52	1.48	1.40
2	A	3413	PPE	C3-C2	11.79	1.48	1.40

All (70) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1413	PPE	C3-C4-C5	-5.04	113.52	118.82
2	F	2913	PPE	C3-C4-C5	-5.01	113.55	118.82
2	E	2413	PPE	C3-C4-C5	-4.86	113.70	118.82
2	A	3413	PPE	C3-C4-C5	-4.78	113.78	118.82
2	B	3913	PPE	C3-C4-C5	-4.54	114.04	118.82
2	D	1913	PPE	C3-C4-C5	-4.52	114.06	118.82
2	E	2413	PPE	C5-C6-N1	-4.09	116.77	123.86
2	B	3913	PPE	C5-C6-N1	-4.08	116.77	123.86
2	C	1413	PPE	C5-C6-N1	-4.05	116.84	123.86
2	A	3413	PPE	C5-C6-N1	-4.04	116.85	123.86
2	D	1913	PPE	C5-C6-N1	-4.04	116.86	123.86
2	F	2913	PPE	C5-C6-N1	-3.95	117.00	123.86
2	F	2913	PPE	C5A-C5-C6	-3.90	111.90	119.28
2	C	1413	PPE	C5A-C5-C6	-3.89	111.92	119.28
2	F	2913	PPE	C2A-C2-N1	-3.72	109.69	117.95
2	E	2413	PPE	C5A-C5-C6	-3.72	112.24	119.28
2	A	3413	PPE	C2A-C2-N1	-3.71	109.73	117.95
2	D	1913	PPE	C2A-C2-N1	-3.66	109.83	117.95
2	C	1413	PPE	C2A-C2-N1	-3.66	109.83	117.95
2	B	3913	PPE	C2A-C2-N1	-3.64	109.89	117.95
2	E	2413	PPE	C2A-C2-N1	-3.60	109.96	117.95
2	A	3413	PPE	C5A-C5-C6	-3.57	112.52	119.28
2	B	3913	PPE	C5A-C5-C6	-3.49	112.67	119.28
2	D	1913	PPE	C5A-C5-C6	-3.49	112.67	119.28
2	D	1913	PPE	C4A-NA-CAA	-3.39	108.62	113.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	3913	PPE	C4A-NA-CAA	-2.84	109.47	113.81
2	F	2913	PPE	O3-C3-C2	-2.84	112.73	117.66
2	E	2413	PPE	O3-C3-C2	-2.79	112.81	117.66
2	C	1413	PPE	O3-C3-C2	-2.74	112.89	117.66
2	A	3413	PPE	C4A-NA-CAA	-2.69	109.69	113.81
2	D	1913	PPE	O3-C3-C2	-2.69	112.99	117.66
2	A	3413	PPE	O3-C3-C2	-2.64	113.06	117.66
2	B	3913	PPE	O3-C3-C2	-2.57	113.18	117.66
2	B	3913	PPE	C3-C2-N1	-2.33	117.40	120.61
2	A	3413	PPE	C3-C2-N1	-2.24	117.52	120.61
2	E	2413	PPE	C3-C2-N1	-2.23	117.53	120.61
2	D	1913	PPE	C3-C2-N1	-2.22	117.55	120.61
2	C	1413	PPE	C3-C2-N1	-2.20	117.57	120.61
2	F	2913	PPE	C3-C2-N1	-2.16	117.63	120.61
2	D	1913	PPE	CGA-CBA-CAA	2.02	117.09	112.99
2	A	3413	PPE	CGA-CBA-CAA	2.12	117.30	112.99
2	B	3913	PPE	OP2-P-OP1	2.14	117.48	110.58
2	D	1913	PPE	OP2-P-OP1	2.25	117.83	110.58
2	A	3413	PPE	OP4-C5A-C5	2.25	112.72	108.99
2	A	3413	PPE	OP2-P-OP1	2.27	117.88	110.58
2	C	1413	PPE	OP2-P-OP1	2.27	117.89	110.58
2	B	3913	PPE	OP4-C5A-C5	2.27	112.75	108.99
2	F	2913	PPE	OP2-P-OP1	2.35	118.14	110.58
2	E	2413	PPE	OP2-P-OP1	2.38	118.25	110.58
2	F	2913	PPE	OP4-C5A-C5	2.42	112.99	108.99
2	F	2913	PPE	CGA-CBA-CAA	2.44	117.94	112.99
2	E	2413	PPE	CGA-CBA-CAA	3.07	119.23	112.99
2	D	1913	PPE	C4A-C4-C5	8.14	126.96	119.71
2	A	3413	PPE	C4A-C4-C5	8.38	127.18	119.71
2	B	3913	PPE	C4A-C4-C5	8.39	127.19	119.71
2	E	2413	PPE	C4A-C4-C5	9.24	127.94	119.71
2	C	1413	PPE	C4A-C4-C5	9.24	127.95	119.71
2	F	2913	PPE	C4A-C4-C5	9.37	128.06	119.71
2	E	2413	PPE	C2A-C2-C3	9.51	132.51	121.04
2	C	1413	PPE	C2A-C2-C3	9.59	132.60	121.04
2	D	1913	PPE	C2A-C2-C3	9.61	132.62	121.04
2	F	2913	PPE	C2A-C2-C3	9.65	132.68	121.04
2	B	3913	PPE	C2A-C2-C3	9.69	132.72	121.04
2	A	3413	PPE	C2A-C2-C3	9.72	132.75	121.04
2	F	2913	PPE	C6-C5-C4	9.75	125.37	118.09
2	D	1913	PPE	C6-C5-C4	9.78	125.39	118.09
2	E	2413	PPE	C6-C5-C4	9.89	125.47	118.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	3913	PPE	C6-C5-C4	9.90	125.48	118.09
2	A	3413	PPE	C6-C5-C4	10.18	125.69	118.09
2	C	1413	PPE	C6-C5-C4	10.19	125.69	118.09

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1415	MPD	1	0
3	F	2914	MPD	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, 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	294/308 (95%)	-0.37	3 (1%) 84 84	13, 20, 34, 47	0
1	B	305/308 (99%)	-0.25	6 (1%) 68 69	13, 21, 34, 47	0
1	C	297/308 (96%)	-0.26	6 (2%) 68 69	13, 20, 35, 55	0
1	D	301/308 (97%)	-0.29	5 (1%) 73 73	12, 21, 33, 57	0
1	E	298/308 (96%)	-0.26	4 (1%) 79 80	13, 21, 35, 47	0
1	F	298/308 (96%)	-0.32	5 (1%) 73 73	13, 20, 33, 52	0
All	All	1793/1848 (97%)	-0.29	29 (1%) 74 75	12, 21, 34, 57	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	135	VAL	6.2
1	B	127	GLY	6.2
1	D	129	TYR	5.3
1	F	135	VAL	5.0
1	D	130	LEU	4.6
1	C	136	ARG	4.5
1	F	134	ALA	4.2
1	F	126	TRP	4.0
1	C	126	TRP	3.8
1	E	126	TRP	3.8
1	E	135	VAL	3.7
1	C	18	GLU	3.6
1	B	128	ALA	3.2
1	D	126	TRP	3.2
1	D	128	ALA	3.1
1	B	131	GLY	3.0
1	C	92	ARG	2.9
1	A	92	ARG	2.9
1	A	126	TRP	2.8

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Mol	Chain	Res	Type	RSRZ
1	E	45	ALA	2.6
1	D	136	ARG	2.6
1	B	2	GLN	2.5
1	F	2	GLN	2.3
1	C	45	ALA	2.3
1	E	46	LYS	2.1
1	F	136	ARG	2.1
1	B	129	TYR	2.1
1	A	2	GLN	2.0
1	B	130	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	MPD	F	2914	8/8	0.70	0.26	6.71	37,39,42,43	0
3	MPD	A	1415	8/8	0.86	0.19	3.77	43,44,45,46	0
2	PPE	A	3413	25/25	0.92	0.14	3.03	17,20,48,49	0
2	PPE	B	3913	25/25	0.91	0.15	2.89	16,23,54,56	0
2	PPE	E	2413	25/25	0.93	0.14	2.80	16,21,49,50	0
2	PPE	D	1913	25/25	0.94	0.14	2.48	15,21,49,51	0
2	PPE	C	1413	25/25	0.93	0.14	2.37	14,21,48,50	0
2	PPE	F	2913	25/25	0.93	0.13	2.31	17,20,44,47	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.