



Full wwPDB X-ray Structure Validation Report ⓘ

May 18, 2020 – 09:14 pm BST

PDB ID : 2EJ0
Title : Crystal Structure of T.th.HB8 Branched-Chain Amino Acid Aminotransferase
with Pyridoxamine 5'-phosphate
Authors : Goto, M.
Deposited on : 2007-03-14
Resolution : 1.60 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The 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 : 2.11
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) : 2.11

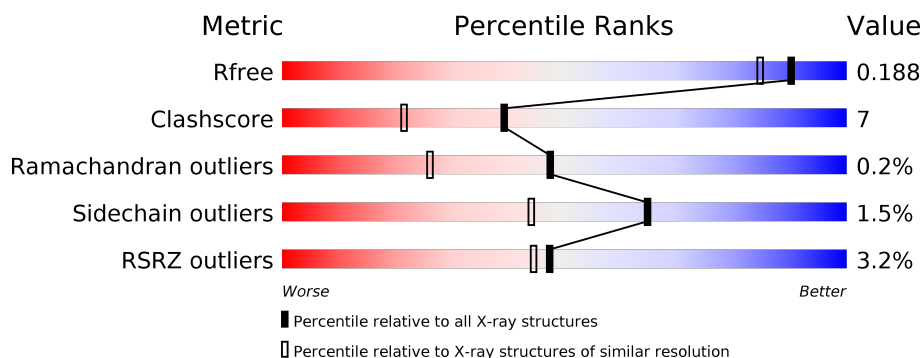
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.60 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3398 (1.60-1.60)
Clashscore	141614	3665 (1.60-1.60)
Ramachandran outliers	138981	3564 (1.60-1.60)
Sidechain outliers	138945	3563 (1.60-1.60)
RSRZ outliers	127900	3321 (1.60-1.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria 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	308	<div> <div>3%</div> <div> <div></div> <div>79%</div> <div>17%</div> <div>• •</div> </div> </div>
1	B	308	<div> <div>3%</div> <div> <div></div> <div>88%</div> <div>11%</div> <div>•</div> </div> </div>
1	C	308	<div> <div>4%</div> <div> <div></div> <div>83%</div> <div>13%</div> <div>• •</div> </div> </div>
1	D	308	<div> <div>3%</div> <div> <div></div> <div>84%</div> <div>13%</div> <div>• •</div> </div> </div>
1	E	308	<div> <div>4%</div> <div> <div></div> <div>81%</div> <div>13%</div> <div>• 5%</div> </div> </div>
1	F	308	<div> <div>3%</div> <div> <div></div> <div>82%</div> <div>14%</div> <div>• •</div> </div> </div>

2 Entry composition [i](#)

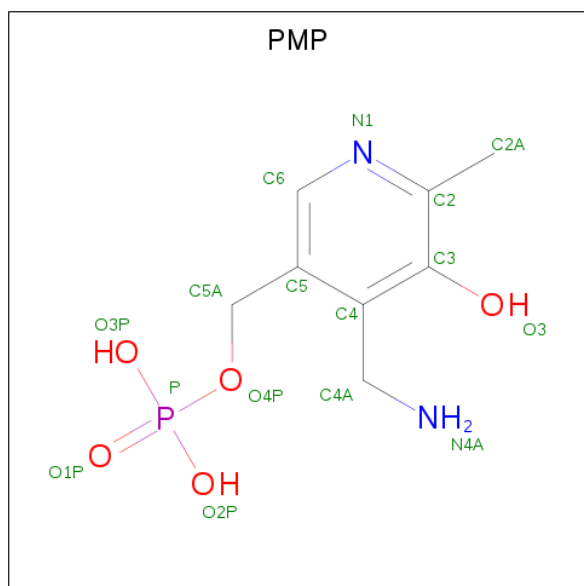
There are 4 unique types of molecules in this entry. The entry contains 15706 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

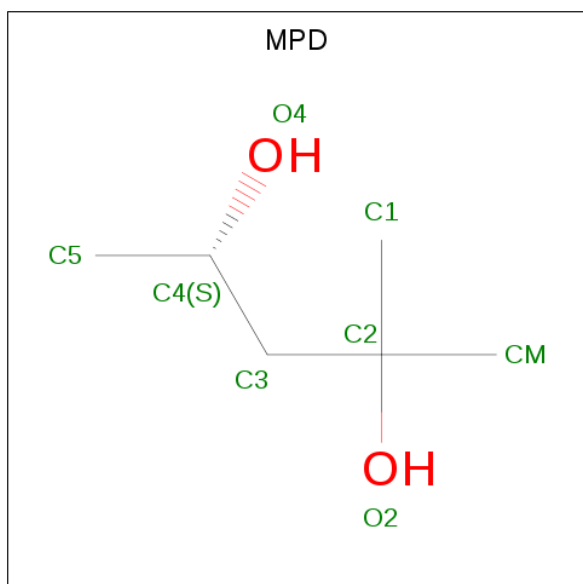
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	297	Total	C	N	O	S	0	0	0
			2311	1478	401	422	10			
1	B	305	Total	C	N	O	S	0	0	0
			2377	1519	413	435	10			
1	C	297	Total	C	N	O	S	0	0	0
			2311	1478	401	422	10			
1	D	301	Total	C	N	O	S	0	0	0
			2350	1504	409	427	10			
1	E	294	Total	C	N	O	S	0	0	0
			2294	1467	398	419	10			
1	F	300	Total	C	N	O	S	0	0	0
			2326	1487	404	425	10			

- Molecule 2 is 4'-DEOXY-4'-AMINOPYRIDOXAL-5'-PHOSPHATE (three-letter code: PMP) (formula: $C_8H_{13}N_2O_5P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			16	8	2	5	1		
2	B	1	Total	C	N	O	P	0	0
			16	8	2	5	1		
2	C	1	Total	C	N	O	P	0	0
			16	8	2	5	1		
2	D	1	Total	C	N	O	P	0	0
			16	8	2	5	1		
2	E	1	Total	C	N	O	P	0	0
			16	8	2	5	1		
2	F	1	Total	C	N	O	P	0	0
			16	8	2	5	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	A	1	Total	C	O	0	0
			8	6	2		
3	B	1	Total	C	O	0	0
			8	6	2		
3	C	1	Total	C	O	0	0
			8	6	2		
3	D	1	Total	C	O	0	0
			8	6	2		

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

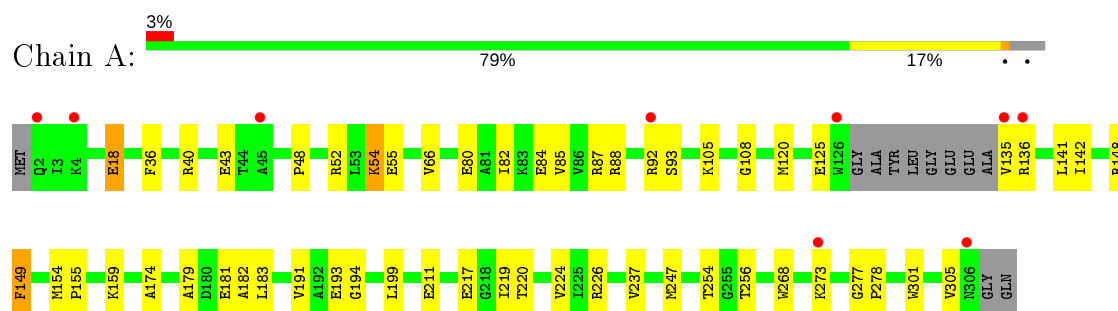
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	254	Total	O	0	0
			254	254		
4	B	269	Total	O	0	0
			269	269		
4	C	264	Total	O	0	0
			264	264		
4	D	280	Total	O	0	0
			280	280		
4	E	248	Total	O	0	0
			248	248		
4	F	262	Total	O	0	0
			262	262		

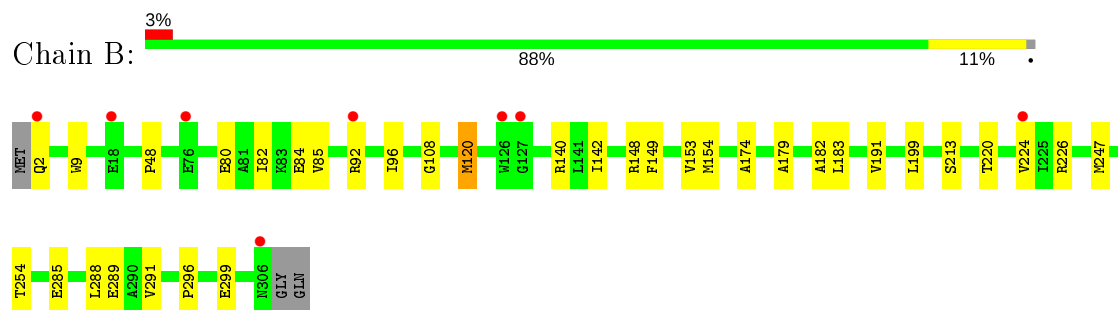
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

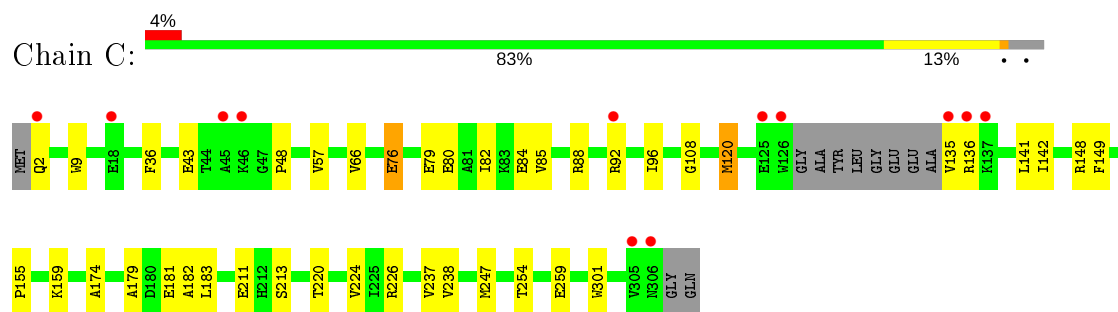
- Molecule 1: Branched-chain amino acid aminotransferase



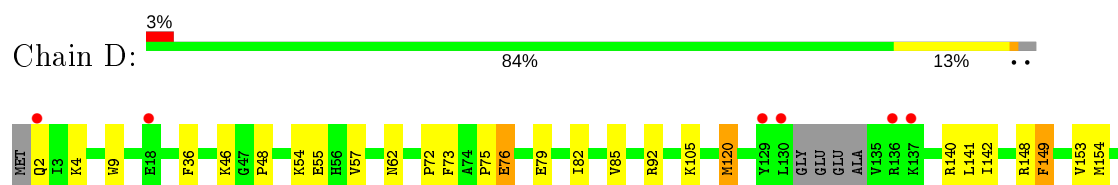
- Molecule 1: Branched-chain amino acid aminotransferase



- Molecule 1: Branched-chain amino acid aminotransferase

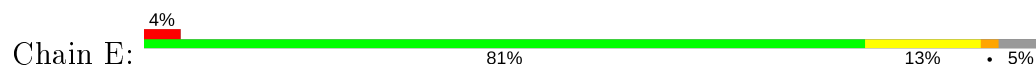


- Molecule 1: Branched-chain amino acid aminotransferase

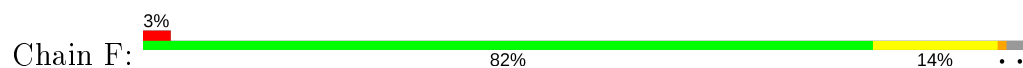




- Molecule 1: Branched-chain amino acid aminotransferase



- 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, α , β , γ	115.88Å 143.69Å 146.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.84 – 1.60 19.90 – 1.60	Depositor EDS
% Data completeness (in resolution range)	99.0 (19.84-1.60) 99.2 (19.90-1.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.28 (at 1.60Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.179 , 0.194 0.173 , 0.188	Depositor DCC
R_{free} test set	31793 reflections (10.01%)	wwPDB-VP
Wilson B-factor (Å ²)	14.1	Xtriage
Anisotropy	0.238	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 60.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.022 for -h,l,k	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	15706	wwPDB-VP
Average B, all atoms (Å ²)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.44% 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: MPD, PMP

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	0.29	0/2363	0.62	1/3207 (0.0%)
1	B	0.29	0/2431	0.61	0/3298
1	C	0.29	0/2363	0.62	1/3207 (0.0%)
1	D	0.29	0/2403	0.62	0/3259
1	E	0.30	0/2346	0.62	0/3183
1	F	0.30	0/2378	0.62	0/3228
All	All	0.29	0/14284	0.62	2/19382 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	108	GLY	N-CA-C	-5.13	100.28	113.10
1	C	108	GLY	N-CA-C	-5.12	100.29	113.10

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	2311	0	2296	48	0
1	B	2377	0	2367	23	0
1	C	2311	0	2296	29	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	2350	0	2346	29	0
1	E	2294	0	2283	38	0
1	F	2326	0	2305	35	0
2	A	16	0	11	0	0
2	B	16	0	11	0	0
2	C	16	0	11	0	0
2	D	16	0	11	0	0
2	E	16	0	11	0	0
2	F	16	0	11	0	0
3	A	16	0	28	6	0
3	B	8	0	14	0	0
3	C	8	0	14	0	0
3	D	16	0	28	4	0
3	E	8	0	14	4	0
3	F	8	0	14	2	0
4	A	254	0	0	7	0
4	B	269	0	0	4	0
4	C	264	0	0	4	0
4	D	280	0	0	3	0
4	E	248	0	0	2	0
4	F	262	0	0	8	0
All	All	15706	0	14071	208	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 7.

All (208) 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:183:LEU:HD13	1:B:199:LEU:HD11	1.56	0.88
1:B:183:LEU:HD11	1:B:191:VAL:HG13	1.64	0.79
1:A:183:LEU:HD13	1:A:199:LEU:HD11	1.62	0.78
1:A:54:LYS:HE3	1:A:55:GLU:HG2	1.66	0.77
1:A:52:ARG:HA	1:A:54:LYS:HE2	1.70	0.74
1:A:18:GLU:CD	1:A:18:GLU:H	1.94	0.70
1:E:219:ILE:HG12	3:E:2414:MPD:H13	1.74	0.70
1:A:183:LEU:HD11	1:A:191:VAL:HG13	1.75	0.68
1:A:219:ILE:HG12	3:A:3414:MPD:H13	1.76	0.67
1:A:43:GLU:HG2	1:A:92:ARG:HB3	1.75	0.67
1:A:55:GLU:OE2	3:A:3414:MPD:H12	1.95	0.66
1:E:247:MET:HE2	4:F:2989:HOH:O	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:220:THR:O	1:B:224:VAL:HG23	1.97	0.65
1:A:54:LYS:N	1:A:54:LYS:HD3	2.12	0.65
1:E:142:ILE:HD11	1:E:268:TRP:CZ2	2.32	0.64
1:A:247:MET:HE2	4:B:3985:HOH:O	1.98	0.64
1:D:76:GLU:H	1:D:76:GLU:CD	1.98	0.64
1:D:285:GLU:O	1:D:289:GLU:HG3	1.99	0.63
1:E:220:THR:O	1:E:224:VAL:HG23	1.99	0.63
1:A:43:GLU:HG3	1:A:93:SER:OG	1.98	0.62
1:C:220:THR:O	1:C:224:VAL:HG23	2.00	0.62
1:E:148:ARG:CZ	1:E:193:GLU:OE2	2.49	0.61
1:F:87:ARG:HG3	1:F:305:VAL:CG1	2.29	0.61
1:A:220:THR:O	1:A:224:VAL:HG23	2.01	0.61
1:D:55:GLU:OE1	3:D:1915:MPD:H12	2.01	0.61
1:F:148:ARG:CZ	1:F:193:GLU:OE1	2.49	0.61
1:A:54:LYS:H	1:A:54:LYS:HD3	1.64	0.60
1:F:197:GLU:HG3	1:F:253:MET:SD	2.41	0.60
3:D:1915:MPD:H11	4:D:1995:HOH:O	2.01	0.60
1:C:82:ILE:O	1:C:85:VAL:HG12	2.02	0.60
1:F:220:THR:O	1:F:224:VAL:HG23	2.01	0.60
1:E:48:PRO:HG3	1:E:92:ARG:HA	1.83	0.59
1:A:52:ARG:CA	1:A:54:LYS:HE2	2.33	0.59
1:D:82:ILE:O	1:D:85:VAL:HG12	2.02	0.59
1:B:285:GLU:O	1:B:289:GLU:HG3	2.01	0.59
1:E:55:GLU:OE2	3:E:2414:MPD:H12	2.03	0.59
1:B:80:GLU:O	1:B:84:GLU:HG3	2.02	0.59
1:A:142:ILE:HD11	1:A:268:TRP:CZ2	2.37	0.59
1:F:82:ILE:O	1:F:85:VAL:HG12	2.03	0.58
1:F:54:LYS:H	1:F:54:LYS:HD3	1.69	0.58
1:C:76:GLU:H	1:C:76:GLU:CD	2.05	0.57
1:F:54:LYS:N	1:F:54:LYS:HD3	2.20	0.57
1:A:82:ILE:O	1:A:85:VAL:HG12	2.04	0.57
1:F:54:LYS:CD	1:F:54:LYS:H	2.18	0.57
3:E:2414:MPD:H11	4:E:2459:HOH:O	2.04	0.56
1:E:76:GLU:CD	1:E:76:GLU:H	2.07	0.56
1:C:80:GLU:O	1:C:84:GLU:HG3	2.05	0.56
1:B:82:ILE:O	1:B:85:VAL:HG12	2.06	0.56
1:F:2:GLN:HG2	1:F:3:ILE:N	2.21	0.56
1:E:224:VAL:HG21	1:E:254:THR:HG21	1.86	0.56
1:D:48:PRO:HG3	1:D:92:ARG:HA	1.89	0.55
1:E:211:GLU:HG2	1:E:237:VAL:HG12	1.89	0.55
1:A:87:ARG:HG3	1:A:305:VAL:CG1	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:84:GLU:HB3	1:A:88:ARG:NH1	2.21	0.55
1:D:174:ALA:HB2	1:D:182:ALA:HB2	1.88	0.55
1:C:48:PRO:HG3	1:C:92:ARG:HA	1.88	0.55
1:A:141:LEU:CD2	1:A:181:GLU:HB3	2.37	0.55
1:F:141:LEU:CD2	1:F:181:GLU:HB3	2.37	0.55
1:C:226:ARG:HD3	1:C:301:TRP:CZ2	2.42	0.55
1:A:125:GLU:HG2	4:A:3627:HOH:O	2.05	0.54
1:B:183:LEU:HD13	1:B:199:LEU:CD1	2.32	0.54
1:B:226:ARG:HH11	1:B:226:ARG:HG2	1.71	0.54
3:F:2914:MPD:H53	4:F:2981:HOH:O	2.08	0.54
3:A:2415:MPD:H53	4:A:3479:HOH:O	2.07	0.54
1:A:80:GLU:O	1:A:84:GLU:HG3	2.08	0.53
1:C:135:VAL:HG13	1:C:136:ARG:N	2.24	0.53
1:D:219:ILE:HG12	3:D:1915:MPD:H13	1.89	0.53
3:A:3414:MPD:H11	4:A:3473:HOH:O	2.07	0.53
1:E:82:ILE:O	1:E:85:VAL:HG12	2.08	0.53
1:F:88:ARG:HG3	1:F:88:ARG:HH11	1.73	0.52
1:C:84:GLU:HB3	1:C:88:ARG:NH1	2.24	0.52
1:D:224:VAL:HG21	1:D:254:THR:HG21	1.92	0.51
1:F:65:LYS:HD2	4:F:3102:HOH:O	2.10	0.51
1:E:54:LYS:H	1:E:54:LYS:CD	2.23	0.51
1:E:226:ARG:HD3	1:E:301:TRP:CZ2	2.46	0.51
1:A:48:PRO:HG3	1:A:92:ARG:HA	1.93	0.51
1:C:135:VAL:HG13	1:C:136:ARG:H	1.74	0.51
1:F:183:LEU:HD23	1:F:183:LEU:C	2.32	0.50
1:D:54:LYS:HG2	1:D:79:GLU:OE2	2.12	0.50
1:F:226:ARG:HD3	1:F:301:TRP:CZ2	2.46	0.50
1:A:142:ILE:HG13	1:A:179:ALA:HB2	1.93	0.50
1:A:54:LYS:HG2	1:A:55:GLU:N	2.27	0.50
1:C:141:LEU:CD2	1:C:181:GLU:HB3	2.41	0.50
1:C:211:GLU:HG2	1:C:237:VAL:HG12	1.93	0.50
1:D:220:THR:O	1:D:224:VAL:HG23	2.11	0.50
1:A:224:VAL:HG21	1:A:254:THR:HG21	1.93	0.50
1:E:217:GLU:OE2	3:E:2414:MPD:H51	2.12	0.50
1:D:141:LEU:CD2	1:D:181:GLU:HB3	2.42	0.49
1:A:52:ARG:CB	1:A:54:LYS:HE2	2.42	0.49
1:E:197:GLU:HG3	1:E:253:MET:SD	2.52	0.49
1:E:141:LEU:CD2	1:E:181:GLU:HB3	2.43	0.49
1:E:211:GLU:HG3	1:E:238:VAL:C	2.32	0.48
1:A:226:ARG:HD3	1:A:301:TRP:CZ2	2.48	0.48
1:B:2:GLN:HG3	4:D:2084:HOH:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:54:LYS:HD3	1:E:54:LYS:N	2.29	0.48
1:C:148:ARG:CZ	4:C:5618:HOH:O	2.61	0.48
1:C:183:LEU:HD23	1:C:183:LEU:C	2.34	0.48
1:C:84:GLU:HB3	1:C:88:ARG:HH11	1.77	0.48
1:C:82:ILE:HG23	1:C:96:ILE:HG21	1.95	0.48
1:A:36:PHE:CE1	1:A:159:LYS:HE2	2.49	0.47
1:A:183:LEU:CD1	1:A:199:LEU:HD11	2.38	0.47
1:F:230:ASP:HB3	3:F:2914:MPD:H51	1.97	0.47
1:A:88:ARG:HG3	1:A:88:ARG:HH11	1.80	0.47
1:E:183:LEU:C	1:E:183:LEU:HD23	2.34	0.47
1:F:190:TYR:CD2	1:F:239:ARG:HG2	2.50	0.47
1:F:141:LEU:HD22	1:F:181:GLU:HB3	1.97	0.47
1:A:84:GLU:HB3	1:A:88:ARG:HH11	1.79	0.47
1:E:9:TRP:O	1:E:120:MET:HA	2.15	0.47
1:D:105:LYS:HE3	4:D:2072:HOH:O	2.14	0.47
1:D:148:ARG:CZ	1:D:193:GLU:OE1	2.62	0.47
1:D:226:ARG:HD3	1:D:301:TRP:CZ2	2.49	0.47
1:D:75:PRO:O	1:D:79:GLU:HG3	2.15	0.47
1:A:183:LEU:HD13	1:A:199:LEU:CD1	2.38	0.46
1:A:247:MET:HE1	4:B:3964:HOH:O	2.15	0.46
1:A:40:ARG:HG3	1:A:256:THR:HG22	1.96	0.46
1:D:57:VAL:HG21	1:D:79:GLU:HG2	1.97	0.46
1:C:174:ALA:HB2	1:C:182:ALA:HB2	1.97	0.46
1:E:174:ALA:HB2	1:E:182:ALA:HB2	1.96	0.46
1:C:2:GLN:HG3	4:F:2986:HOH:O	2.15	0.46
1:C:66:VAL:HG11	1:C:155:PRO:CB	2.45	0.46
1:E:66:VAL:HG11	1:E:155:PRO:CB	2.46	0.46
1:A:273:LYS:HZ1	1:A:278:PRO:HD3	1.81	0.46
1:A:54:LYS:HE3	1:A:55:GLU:CG	2.42	0.46
1:F:40:ARG:HG3	1:F:256:THR:HG22	1.98	0.45
1:D:183:LEU:HD23	1:D:183:LEU:C	2.37	0.45
1:E:54:LYS:HD3	1:E:54:LYS:H	1.80	0.45
3:A:3414:MPD:H53	4:A:3506:HOH:O	2.17	0.45
1:C:211:GLU:HG3	1:C:238:VAL:C	2.37	0.45
1:F:54:LYS:CD	1:F:54:LYS:N	2.79	0.45
1:A:105:LYS:HE3	4:A:3523:HOH:O	2.17	0.45
1:D:76:GLU:N	1:D:76:GLU:CD	2.69	0.45
1:A:135:VAL:HG13	1:A:136:ARG:N	2.32	0.44
1:E:92:ARG:HH11	1:E:92:ARG:HG3	1.82	0.44
1:B:9:TRP:O	1:B:120:MET:HA	2.17	0.44
1:E:247:MET:CE	4:F:2989:HOH:O	2.59	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:224:VAL:HG21	1:F:254:THR:HG21	1.98	0.44
1:B:142:ILE:HG13	1:B:179:ALA:HB2	1.99	0.44
1:D:153:VAL:HG12	1:D:154:MET:HG2	1.99	0.44
1:B:108:GLY:HA2	3:D:1914:MPD:H12	1.99	0.44
1:E:247:MET:HG2	4:F:3161:HOH:O	2.18	0.44
1:F:76:GLU:H	1:F:76:GLU:CD	2.21	0.44
1:A:273:LYS:NZ	1:A:277:GLY:HA2	2.33	0.44
1:F:174:ALA:HB2	1:F:182:ALA:HB2	2.00	0.44
1:A:66:VAL:HG11	1:A:155:PRO:CB	2.48	0.44
1:B:174:ALA:HB2	1:B:182:ALA:HB2	1.99	0.43
1:F:273:LYS:HG2	4:F:3025:HOH:O	2.16	0.43
1:B:288:LEU:HA	1:B:291:VAL:HG22	2.00	0.43
1:D:36:PHE:CE1	1:D:159:LYS:HE2	2.53	0.43
1:E:87:ARG:HD3	1:E:305:VAL:CG1	2.49	0.43
1:D:141:LEU:HD22	1:D:181:GLU:HB3	2.00	0.43
1:E:224:VAL:HG21	1:E:254:THR:CG2	2.48	0.43
4:A:3540:HOH:O	1:C:247:MET:HG2	2.18	0.43
1:E:40:ARG:HG3	1:E:256:THR:HG22	1.99	0.43
1:B:140:ARG:NH1	4:B:4052:HOH:O	2.52	0.43
1:C:224:VAL:HG21	1:C:254:THR:HG21	2.00	0.43
1:F:36:PHE:CE1	1:F:159:LYS:HE2	2.54	0.43
1:F:52:ARG:HA	1:F:54:LYS:HE3	2.01	0.43
1:F:140:ARG:HG3	1:F:140:ARG:HH11	1.83	0.43
1:F:9:TRP:O	1:F:120:MET:HA	2.18	0.43
1:B:148:ARG:HD2	1:B:148:ARG:HA	1.79	0.43
1:C:148:ARG:HD2	1:C:148:ARG:HA	1.82	0.43
1:E:105:LYS:HE3	4:E:2609:HOH:O	2.18	0.43
1:A:193:GLU:HG3	1:A:194:GLY:O	2.19	0.42
1:B:226:ARG:NH1	4:B:4084:HOH:O	2.50	0.42
1:C:36:PHE:CE1	1:C:159:LYS:HE2	2.54	0.42
1:C:254:THR:HA	1:C:259:GLU:O	2.19	0.42
1:E:148:ARG:CZ	1:E:149:PHE:CE1	3.02	0.42
1:F:48:PRO:HG3	1:F:92:ARG:HA	2.01	0.42
1:B:224:VAL:HG21	1:B:254:THR:HG21	2.01	0.42
1:D:149:PHE:CG	1:D:154:MET:HB2	2.54	0.42
4:C:5630:HOH:O	1:E:177:ALA:HA	2.19	0.42
1:A:148:ARG:HA	1:A:148:ARG:HD2	1.86	0.42
1:B:48:PRO:HG3	1:B:92:ARG:HA	2.00	0.42
1:C:57:VAL:HG21	1:C:79:GLU:HG2	2.01	0.42
4:C:5547:HOH:O	1:E:142:ILE:HG23	2.18	0.42
1:F:148:ARG:HG2	1:F:214:VAL:HG23	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:142:ILE:HG13	1:D:179:ALA:HB2	2.00	0.42
1:D:224:VAL:HG21	1:D:254:THR:CG2	2.49	0.42
1:E:54:LYS:HG2	1:E:55:GLU:N	2.34	0.42
1:E:92:ARG:NH1	1:E:92:ARG:HG3	2.35	0.42
1:C:142:ILE:HG13	1:C:179:ALA:HB2	2.01	0.42
1:D:62:ASN:HA	1:D:62:ASN:HD22	1.68	0.42
1:E:69:MET:HG3	1:E:117:ALA:HB2	2.02	0.42
1:A:174:ALA:HB2	1:A:182:ALA:HB2	2.01	0.42
1:A:183:LEU:CD1	1:A:199:LEU:CD1	2.98	0.41
1:A:217:GLU:OE2	3:A:3414:MPD:H51	2.20	0.41
1:B:247:MET:HE2	1:B:247:MET:HB3	1.87	0.41
1:C:148:ARG:NH2	4:C:5502:HOH:O	2.45	0.41
1:E:141:LEU:HD22	1:E:181:GLU:HB3	2.01	0.41
1:F:62:ASN:ND2	4:F:3102:HOH:O	2.53	0.41
1:B:153:VAL:HG12	1:B:154:MET:HG2	2.02	0.41
1:B:296:PRO:HA	1:B:299:GLU:HG2	2.02	0.41
1:C:43:GLU:OE2	1:C:92:ARG:CZ	2.69	0.41
1:E:149:PHE:CG	1:E:154:MET:HB2	2.55	0.41
1:B:82:ILE:HG23	1:B:96:ILE:HG21	2.02	0.41
1:D:9:TRP:O	1:D:120:MET:HA	2.21	0.41
1:F:149:PHE:CG	1:F:154:MET:HB2	2.55	0.41
1:D:72:PRO:HG2	1:D:73:PHE:CE1	2.56	0.41
1:D:2:GLN:OE1	1:D:4:LYS:HE2	2.20	0.41
1:F:135:VAL:HG13	1:F:136:ARG:N	2.36	0.41
1:A:148:ARG:NE	4:A:3584:HOH:O	2.51	0.40
1:F:140:ARG:NH2	1:F:178:GLY:O	2.53	0.40
1:A:211:GLU:HG2	1:A:237:VAL:HG12	2.04	0.40
1:A:149:PHE:CG	1:A:154:MET:HB2	2.57	0.40
1:D:140:ARG:HG3	1:D:140:ARG:HH11	1.87	0.40
1:F:149:PHE:HA	1:F:150:PRO:HD3	1.97	0.40
1:C:9:TRP:O	1:C:120:MET:HA	2.20	0.40
1:F:197:GLU:HG3	1:F:253:MET:HB3	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	293/308 (95%)	285 (97%)	8 (3%)	0	100	100
1	B	303/308 (98%)	294 (97%)	8 (3%)	1 (0%)	41	21
1	C	293/308 (95%)	285 (97%)	7 (2%)	1 (0%)	41	21
1	D	297/308 (96%)	289 (97%)	8 (3%)	0	100	100
1	E	290/308 (94%)	282 (97%)	7 (2%)	1 (0%)	41	21
1	F	296/308 (96%)	289 (98%)	7 (2%)	0	100	100
All	All	1772/1848 (96%)	1724 (97%)	45 (2%)	3 (0%)	47	26

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	213	SER
1	C	213	SER
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	233/241 (97%)	229 (98%)	4 (2%)	60	38
1	B	239/241 (99%)	237 (99%)	2 (1%)	81	70
1	C	233/241 (97%)	230 (99%)	3 (1%)	69	50
1	D	237/241 (98%)	233 (98%)	4 (2%)	60	38
1	E	232/241 (96%)	227 (98%)	5 (2%)	52	27
1	F	233/241 (97%)	230 (99%)	3 (1%)	69	50
All	All	1407/1446 (97%)	1386 (98%)	21 (2%)	65	44

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

Mol	Chain	Res	Type
1	A	18	GLU
1	A	54	LYS
1	A	120	MET
1	A	149	PHE
1	B	120	MET
1	B	149	PHE
1	C	76	GLU
1	C	120	MET
1	C	149	PHE
1	D	46	LYS
1	D	76	GLU
1	D	120	MET
1	D	149	PHE
1	E	54	LYS
1	E	76	GLU
1	E	120	MET
1	E	149	PHE
1	E	197	GLU
1	F	54	LYS
1	F	120	MET
1	F	149	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	62	ASN
1	A	306	ASN
1	B	62	ASN
1	B	306	ASN
1	C	62	ASN
1	C	306	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 [i](#)

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

14 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	B	3914	-	7,7,7	0.97	0	9,10,10	1.11	0
2	PMP	B	3913	-	16,16,16	1.12	2 (12%)	21,23,23	1.07	2 (9%)
2	PMP	E	2413	-	16,16,16	1.22	3 (18%)	21,23,23	1.01	1 (4%)
3	MPD	C	5414	-	7,7,7	0.94	0	9,10,10	1.09	0
3	MPD	F	2914	-	7,7,7	0.88	0	9,10,10	0.98	0
3	MPD	A	2415	-	7,7,7	0.85	0	9,10,10	0.96	0
3	MPD	D	1915	-	7,7,7	0.85	0	9,10,10	0.95	0
2	PMP	F	2913	-	16,16,16	1.33	3 (18%)	21,23,23	1.14	2 (9%)
2	PMP	A	3413	-	16,16,16	1.05	1 (6%)	21,23,23	1.18	1 (4%)
2	PMP	C	4413	-	16,16,16	1.18	2 (12%)	21,23,23	1.15	2 (9%)
3	MPD	A	3414	-	7,7,7	0.89	0	9,10,10	0.99	0
3	MPD	D	1914	-	7,7,7	0.87	0	9,10,10	1.01	0
2	PMP	D	1913	-	16,16,16	1.18	1 (6%)	21,23,23	1.17	2 (9%)
3	MPD	E	2414	-	7,7,7	0.90	0	9,10,10	0.98	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	B	3914	-	-	2/5/5/5	-
2	PMP	B	3913	-	-	0/8/8/8	0/1/1/1
2	PMP	E	2413	-	-	0/8/8/8	0/1/1/1
3	MPD	C	5414	-	-	2/5/5/5	-
3	MPD	F	2914	-	-	1/5/5/5	-
3	MPD	A	2415	-	-	1/5/5/5	-
3	MPD	D	1915	-	-	1/5/5/5	-
2	PMP	F	2913	-	-	0/8/8/8	0/1/1/1
2	PMP	A	3413	-	-	0/8/8/8	0/1/1/1
2	PMP	C	4413	-	-	0/8/8/8	0/1/1/1
3	MPD	A	3414	-	-	1/5/5/5	-
3	MPD	D	1914	-	-	4/5/5/5	-
2	PMP	D	1913	-	-	0/8/8/8	0/1/1/1
3	MPD	E	2414	-	-	1/5/5/5	-

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	2913	PMP	C2A-C2	2.69	1.54	1.50
2	C	4413	PMP	C3-C2	-2.59	1.38	1.40
2	E	2413	PMP	C2A-C2	2.55	1.54	1.50
2	B	3913	PMP	C4A-C4	2.34	1.59	1.51
2	A	3413	PMP	C4A-C4	2.30	1.59	1.51
2	F	2913	PMP	C4A-C4	2.20	1.58	1.51
2	D	1913	PMP	C4A-C4	2.11	1.58	1.51
2	F	2913	PMP	C3-C2	-2.10	1.38	1.40
2	C	4413	PMP	C4A-C4	2.09	1.58	1.51
2	E	2413	PMP	C3-C2	-2.07	1.38	1.40
2	E	2413	PMP	C4A-C4	2.07	1.58	1.51
2	B	3913	PMP	C3-C2	-2.06	1.38	1.40

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	3413	PMP	C6-C5-C4	3.13	120.33	118.12
2	F	2913	PMP	C6-C5-C4	2.94	120.19	118.12
2	D	1913	PMP	C6-C5-C4	2.81	120.11	118.12
2	B	3913	PMP	C6-C5-C4	2.59	119.95	118.12
2	C	4413	PMP	C6-C5-C4	2.56	119.93	118.12
2	C	4413	PMP	O2P-P-O4P	-2.40	100.34	106.73
2	E	2413	PMP	C6-C5-C4	2.32	119.76	118.12
2	B	3913	PMP	C5-C6-N1	-2.17	120.20	123.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	2913	PMP	O3P-P-O1P	2.15	119.08	110.68
2	D	1913	PMP	O2P-P-O4P	-2.05	101.29	106.73

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	3914	MPD	C2-C3-C4-C5
3	C	5414	MPD	C2-C3-C4-C5
3	F	2914	MPD	C2-C3-C4-C5
3	A	2415	MPD	C2-C3-C4-C5
3	D	1915	MPD	C2-C3-C4-C5
3	A	3414	MPD	C2-C3-C4-C5
3	D	1914	MPD	C2-C3-C4-C5
3	E	2414	MPD	C2-C3-C4-C5
3	B	3914	MPD	C1-C2-C3-C4
3	C	5414	MPD	C1-C2-C3-C4
3	D	1914	MPD	C1-C2-C3-C4
3	D	1914	MPD	CM-C2-C3-C4
3	D	1914	MPD	O2-C2-C3-C4

There are no ring outliers.

6 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	2914	MPD	2	0
3	A	2415	MPD	1	0
3	D	1915	MPD	3	0
3	A	3414	MPD	5	0
3	D	1914	MPD	1	0
3	E	2414	MPD	4	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2			OWAB(Å ²)	Q < 0.9
1	A	297/308 (96%)	-0.02	9 (3%)	50	48	8, 13, 27, 38	0
1	B	305/308 (99%)	0.03	8 (2%)	56	53	8, 14, 26, 37	0
1	C	297/308 (96%)	0.04	12 (4%)	38	35	8, 13, 27, 44	0
1	D	301/308 (97%)	-0.03	8 (2%)	54	52	8, 14, 25, 35	0
1	E	294/308 (95%)	0.02	11 (3%)	41	39	7, 13, 26, 38	0
1	F	300/308 (97%)	-0.02	10 (3%)	46	43	8, 13, 26, 40	0
All	All	1794/1848 (97%)	0.00	58 (3%)	47	44	7, 14, 26, 44	0

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	135	VAL	10.1
1	C	126	TRP	7.7
1	E	126	TRP	7.4
1	C	136	ARG	7.4
1	F	126	TRP	5.7
1	A	135	VAL	5.3
1	F	134	ALA	5.2
1	B	127	GLY	5.1
1	A	136	ARG	4.8
1	D	2	GLN	4.8
1	F	2	GLN	4.6
1	D	130	LEU	4.4
1	E	92	ARG	4.4
1	C	92	ARG	4.3
1	E	2	GLN	4.0
1	D	129	TYR	3.7
1	C	2	GLN	3.7
1	F	18	GLU	3.7
1	D	18	GLU	3.6

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Mol	Chain	Res	Type	RSRZ
1	C	45	ALA	3.5
1	F	92	ARG	3.4
1	C	137	LYS	3.3
1	F	133	GLU	3.3
1	A	92	ARG	3.2
1	A	126	TRP	3.2
1	B	2	GLN	3.2
1	E	306	ASN	3.1
1	C	18	GLU	3.1
1	C	306	ASN	3.0
1	B	18	GLU	3.0
1	B	76	GLU	2.9
1	A	2	GLN	2.9
1	A	45	ALA	2.7
1	F	135	VAL	2.7
1	F	305	VAL	2.7
1	E	45	ALA	2.6
1	A	273	LYS	2.5
1	D	136	ARG	2.5
1	E	46	LYS	2.5
1	A	306	ASN	2.4
1	A	4	LYS	2.4
1	D	268	TRP	2.4
1	E	140	ARG	2.4
1	E	273	LYS	2.4
1	D	137	LYS	2.3
1	B	306	ASN	2.3
1	E	18	GLU	2.3
1	C	125	GLU	2.3
1	F	306	ASN	2.3
1	B	92	ARG	2.2
1	C	305	VAL	2.2
1	C	46	LYS	2.2
1	B	224	VAL	2.1
1	F	4	LYS	2.1
1	E	305	VAL	2.0
1	B	126	TRP	2.0
1	D	306	ASN	2.0
1	E	224	VAL	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. 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(\AA^2)	Q<0.9
3	MPD	D	1915	8/8	0.46	0.26	22,26,29,31	0
3	MPD	F	2914	8/8	0.66	0.20	22,25,28,30	0
3	MPD	A	3414	8/8	0.67	0.22	16,20,24,26	0
3	MPD	A	2415	8/8	0.72	0.20	23,27,30,31	0
3	MPD	C	5414	8/8	0.75	0.18	19,20,24,25	0
3	MPD	D	1914	8/8	0.78	0.16	41,42,45,45	0
3	MPD	E	2414	8/8	0.78	0.17	15,18,21,22	0
3	MPD	B	3914	8/8	0.87	0.17	24,25,28,28	0
2	PMP	D	1913	16/16	0.96	0.08	10,12,14,16	0
2	PMP	A	3413	16/16	0.96	0.09	10,13,18,19	0
2	PMP	B	3913	16/16	0.97	0.07	10,12,15,15	0
2	PMP	C	4413	16/16	0.97	0.08	9,12,16,18	0
2	PMP	E	2413	16/16	0.97	0.07	10,12,16,19	0
2	PMP	F	2913	16/16	0.98	0.08	11,12,16,19	0

6.5 Other polymers [i](#)

There are no such residues in this entry.