



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:47 AM GMT

PDB ID : 3FZN
Title : Intermediate analogue in benzoylformate decarboxylase
Authors : Bruning, M.; Berheide, M.; Meyer, D.; Golbik, R.; Bartunik, H.; Liese, A.; Tittmann, K.
Deposited on : 2009-01-26
Resolution : 1.62 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
<http://wwpdb.org/validation/2016/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 : 1.7 (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

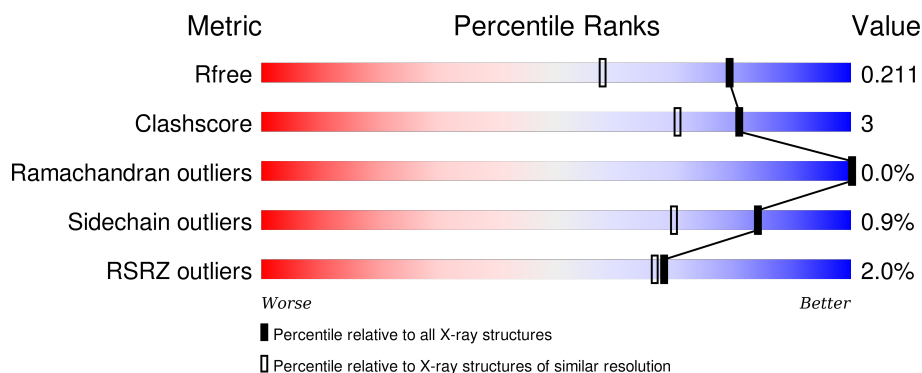
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.62 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	3202 (1.64-1.60)
Clashscore	102246	3500 (1.64-1.60)
Ramachandran outliers	100387	3411 (1.64-1.60)
Sidechain outliers	100360	3410 (1.64-1.60)
RSRZ outliers	91569	3207 (1.64-1.60)

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. 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	534	 2% 93% 5% 2%
1	B	534	 1% 94% 5% 0%
1	C	534	 2% 91% 6% 1%
1	D	534	 3% 93% 5% 0%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	CL	A	709	-	-	X	-
4	CL	B	703	-	-	X	-
4	CL	C	711	-	-	X	-
5	PO4	A	712	-	-	-	X
5	PO4	C	713	-	-	-	X
5	PO4	C	714	-	-	-	X
6	PEG	C	716[A]	-	-	-	X
6	PEG	C	716[B]	-	-	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 18507 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 Benzoylformate decarboxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	523	Total	C	N	O	S	0	18	0
			4013	2546	686	759	22			
1	B	523	Total	C	N	O	S	3	17	0
			4014	2545	689	758	22			
1	C	523	Total	C	N	O	S	0	21	0
			4033	2561	688	762	22			
1	D	523	Total	C	N	O	S	0	18	0
			4010	2544	686	758	22			

There are 24 discrepancies between the modelled and reference sequences:

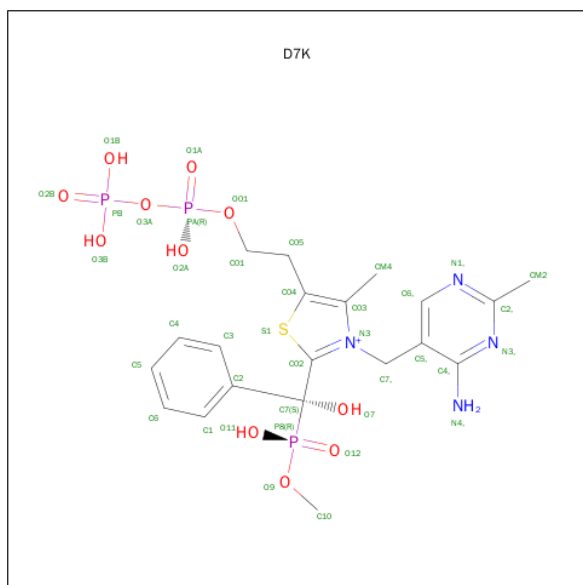
Chain	Residue	Modelled	Actual	Comment	Reference
A	529	HIS	-	EXPRESSION TAG	UNP P20906
A	530	HIS	-	EXPRESSION TAG	UNP P20906
A	531	HIS	-	EXPRESSION TAG	UNP P20906
A	532	HIS	-	EXPRESSION TAG	UNP P20906
A	533	HIS	-	EXPRESSION TAG	UNP P20906
A	534	HIS	-	EXPRESSION TAG	UNP P20906
B	529	HIS	-	EXPRESSION TAG	UNP P20906
B	530	HIS	-	EXPRESSION TAG	UNP P20906
B	531	HIS	-	EXPRESSION TAG	UNP P20906
B	532	HIS	-	EXPRESSION TAG	UNP P20906
B	533	HIS	-	EXPRESSION TAG	UNP P20906
B	534	HIS	-	EXPRESSION TAG	UNP P20906
C	529	HIS	-	EXPRESSION TAG	UNP P20906
C	530	HIS	-	EXPRESSION TAG	UNP P20906
C	531	HIS	-	EXPRESSION TAG	UNP P20906
C	532	HIS	-	EXPRESSION TAG	UNP P20906
C	533	HIS	-	EXPRESSION TAG	UNP P20906
C	534	HIS	-	EXPRESSION TAG	UNP P20906
D	529	HIS	-	EXPRESSION TAG	UNP P20906
D	530	HIS	-	EXPRESSION TAG	UNP P20906
D	531	HIS	-	EXPRESSION TAG	UNP P20906

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Chain	Residue	Modelled	Actual	Comment	Reference
D	532	HIS	-	EXPRESSION TAG	UNP P20906
D	533	HIS	-	EXPRESSION TAG	UNP P20906
D	534	HIS	-	EXPRESSION TAG	UNP P20906

- Molecule 2 is 3-[(4-AMINO-2-METHYLPYRIMIDIN-5-YL)METHYL]-2-{(S)-HYDROXY[(R)-HYDROXY(METHOXY)PHOSPHORYL]PHENYLMETHYL}-5-(2-{[(R)-HYDROXY(PHOSPHONOOXY)PHOSPHORYL]OXY}ETHYL)-4-METHYL-1,3-THIAZOL-3-IUM (three-letter code: D7K) (formula: C₂₀H₂₈N₄O₁₁P₃S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total 39	C 20	N 4	O 11	P 3	S 1	0	0
2	B	1	Total 39	C 20	N 4	O 11	P 3	S 1	0	0
2	C	1	Total 39	C 20	N 4	O 11	P 3	S 1	0	0
2	D	1	Total 39	C 20	N 4	O 11	P 3	S 1	0	0

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total Mg 1 1	0	0
3	A	1	Total Mg 1 1	0	0

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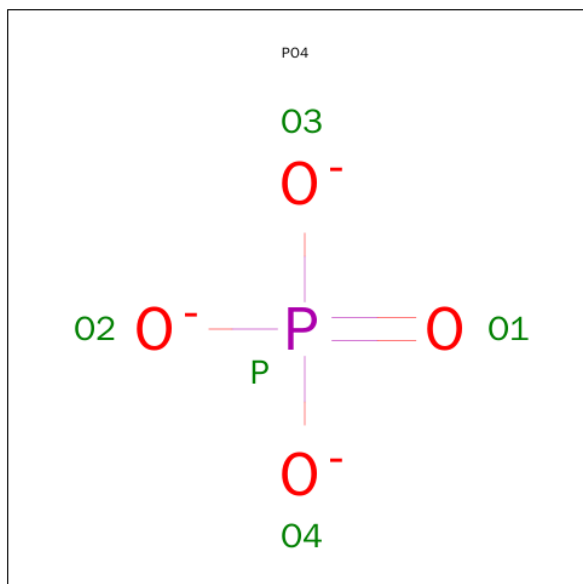
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	1	Total	Mg	0	0
			1	1		
3	C	1	Total	Mg	0	0
			1	1		

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

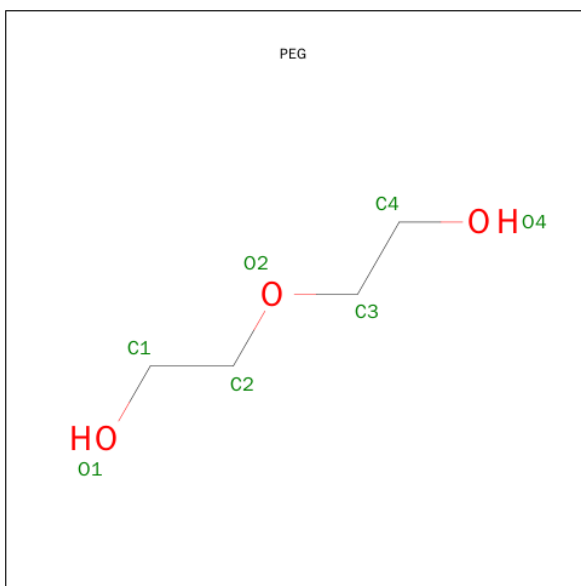
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	4	Total	Cl	0	0
			4	4		
4	A	4	Total	Cl	0	0
			4	4		
4	D	1	Total	Cl	0	0
			1	1		
4	C	2	Total	Cl	0	0
			2	2		

- Molecule 5 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	P	0	0
			5	4	1		
5	C	1	Total	O	P	0	0
			5	4	1		
5	C	1	Total	O	P	0	0
			5	4	1		

- Molecule 6 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	C	1	Total	C	O	0	0
			7	4	3		
6	C	1	Total	C	O	0	1
			14	8	6		
6	D	1	Total	C	O	0	1
			14	8	6		

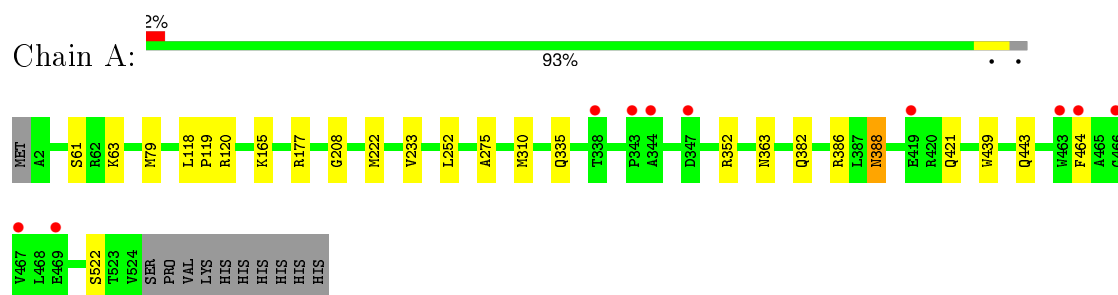
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	556	Total	O	0	0
			556	556		
7	B	560	Total	O	0	0
			560	560		
7	C	554	Total	O	0	0
			554	554		
7	D	546	Total	O	0	0
			546	546		

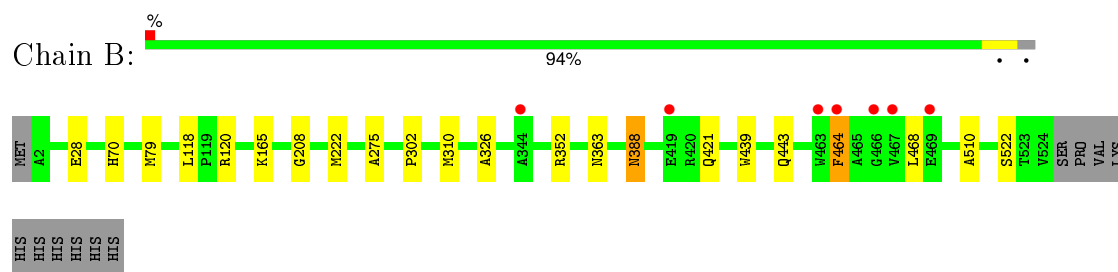
3 Residue-property plots [i](#)

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

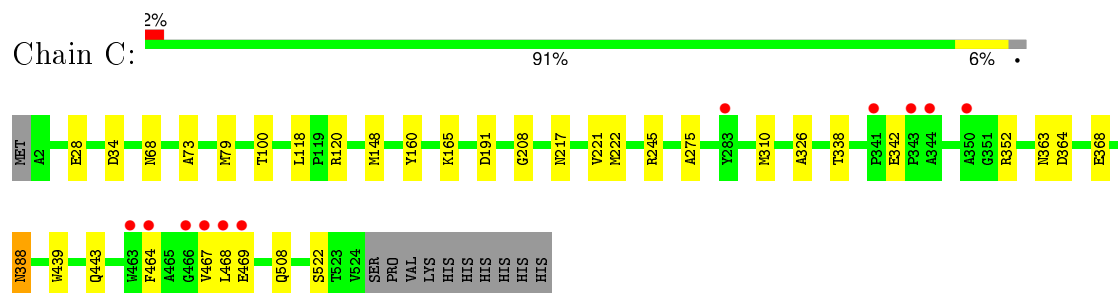
- Molecule 1: Benzoylformate decarboxylase



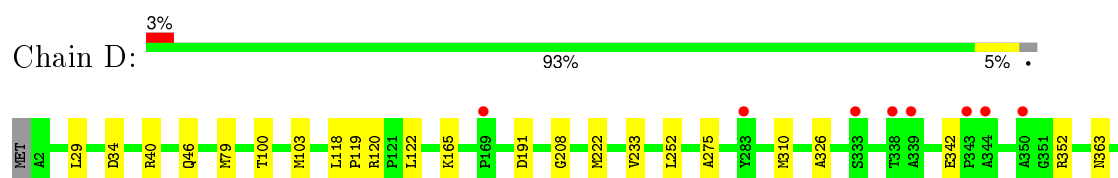
- Molecule 1: Benzoylformate decarboxylase

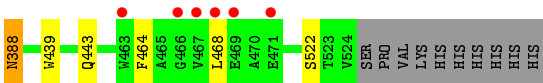


- Molecule 1: Benzoylformate decarboxylase



- Molecule 1: Benzoylformate decarboxylase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	71.51Å 93.34Å 94.53Å 63.46° 72.82° 73.21°	Depositor
Resolution (Å)	19.96 – 1.62 19.93 – 1.62	Depositor EDS
% Data completeness (in resolution range)	93.0 (19.96-1.62) 79.5 (19.93-1.62)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.25 (at 1.62Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.170 , 0.203 0.178 , 0.211	Depositor DCC
R_{free} test set	12259 reflections (5.32%)	DCC
Wilson B-factor (Å ²)	19.0	Xtriage
Anisotropy	0.190	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 72.9	EDS
Estimated twinning fraction	0.339 for -h,-l,-k	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Outliers	0 of 242588 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	18507	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.75% 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, 0.375 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: D7K, MG, PEG, PO4, CL

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.75	0/4167	0.68	1/5694 (0.0%)
1	B	0.73	0/4165	0.69	0/5689
1	C	0.70	0/4194	0.69	0/5729
1	D	0.71	0/4162	0.67	0/5685
All	All	0.72	0/16688	0.68	1/22797 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	1	0

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	177	ARG	NE-CZ-NH2	-5.19	117.70	120.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	C	469	GLU	CA

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	4013	0	3974	26	0
1	B	4014	0	3984	26	0
1	C	4033	0	4004	40	2
1	D	4010	0	3977	30	0
2	A	39	0	24	1	0
2	B	39	0	24	1	0
2	C	39	0	24	0	0
2	D	39	0	24	3	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	4	0	0	5	0
4	B	4	0	0	3	0
4	C	2	0	0	4	0
4	D	1	0	0	0	0
5	A	5	0	0	0	0
5	C	10	0	0	0	0
6	C	21	0	30	2	0
6	D	14	0	20	1	0
7	A	556	0	0	4	2
7	B	560	0	0	4	0
7	C	554	0	0	12	0
7	D	546	0	0	5	0
All	All	18507	0	16085	108	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (108) 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:D:191[B]:ASP:OD2	7:D:3088:HOH:O	1.55	1.20
1:A:79[A]:MET:HE1	1:B:79[A]:MET:HE1	1.18	1.16
1:C:222[A]:MET:CE	7:C:3176:HOH:O	1.92	1.15

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:222[A]:MET:HE1	7:C:3176:HOH:O	1.50	1.09
1:A:222[A]:MET:HE1	7:A:3115:HOH:O	0.92	1.08
1:D:34[B]:ASP:OD1	7:D:2569:HOH:O	1.72	1.07
4:B:703:CL:CL	7:B:2859:HOH:O	2.11	1.04
1:A:79[A]:MET:HE1	1:B:79[A]:MET:CE	1.90	1.00
1:D:222[A]:MET:HE2	1:D:326:ALA:HB1	1.46	0.97
1:C:100[B]:THR:HG23	1:C:160:TYR:CZ	2.02	0.93
1:C:79[A]:MET:SD	1:D:79[A]:MET:HE2	2.09	0.91
1:A:79[A]:MET:CE	1:B:79[A]:MET:SD	2.59	0.91
1:A:79[A]:MET:CE	1:B:79[A]:MET:HE1	2.01	0.89
1:C:191[B]:ASP:OD2	7:C:1591:HOH:O	1.89	0.88
1:B:421:GLN:NE2	7:B:2859:HOH:O	2.08	0.86
1:A:79[A]:MET:CE	1:B:79[A]:MET:CE	2.52	0.86
1:A:222[A]:MET:CE	7:A:3115:HOH:O	1.66	0.84
1:A:79[A]:MET:HE2	1:B:79[A]:MET:SD	2.18	0.84
6:C:716[B]:PEG:O1	7:C:3178:HOH:O	1.96	0.83
1:D:233[B]:VAL:HG13	1:D:252:LEU:HA	1.64	0.77
1:D:222[A]:MET:HE2	1:D:326:ALA:CB	2.16	0.76
1:C:467:VAL:HG12	7:C:2949:HOH:O	1.85	0.76
1:C:79[A]:MET:HE2	1:D:79[A]:MET:SD	2.29	0.73
1:C:34:ASP:OD1	7:C:2577:HOH:O	2.09	0.69
1:A:382:GLN:HE21	1:A:386:ARG:HE	1.39	0.69
1:A:79[A]:MET:SD	1:B:79[A]:MET:CE	2.81	0.69
1:C:73:ALA:HB2	7:D:2967:HOH:O	1.92	0.69
1:C:79[A]:MET:SD	1:D:79[A]:MET:CE	2.81	0.68
1:C:79[A]:MET:CE	1:D:79[A]:MET:SD	2.83	0.67
1:D:191[A]:ASP:OD2	7:D:2945:HOH:O	2.13	0.67
1:A:165:LYS:NZ	7:A:2238:HOH:O	2.27	0.66
4:B:708:CL:CL	7:B:2838:HOH:O	2.51	0.65
1:B:222[A]:MET:HE2	1:B:326:ALA:HB1	1.79	0.65
1:C:464[B]:PHE:CD2	1:D:29:LEU:HD12	2.33	0.63
1:C:79[A]:MET:CE	1:D:79[A]:MET:CE	2.78	0.61
1:C:439:TRP:CZ2	1:C:443:GLN:HG3	2.36	0.61
1:C:464[B]:PHE:HD2	1:D:29:LEU:HD12	1.65	0.60
1:A:79[A]:MET:SD	1:B:79[A]:MET:HE2	2.42	0.59
1:C:100[B]:THR:CG2	1:C:160:TYR:CZ	2.81	0.59
1:D:165:LYS:NZ	7:D:2349:HOH:O	2.34	0.59
1:D:363:ASN:ND2	1:D:388:ASN:H	2.01	0.59
1:C:100[B]:THR:HG23	1:C:160:TYR:CE2	2.37	0.58
1:B:28:GLU:OE1	1:B:70:HIS:HD2	1.87	0.57
1:C:222[A]:MET:HE2	7:C:3176:HOH:O	1.79	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:79[A]:MET:HE1	1:D:79[A]:MET:HE1	1.87	0.56
1:C:508[A]:GLN:NE2	7:C:3197:HOH:O	2.36	0.56
1:C:165:LYS:NZ	7:C:1674:HOH:O	2.37	0.56
1:D:439:TRP:CZ2	1:D:443:GLN:HG3	2.42	0.55
1:A:79[A]:MET:HE1	1:B:79[A]:MET:SD	2.39	0.55
1:A:335[B]:GLN:HG3	7:A:2784:HOH:O	2.06	0.55
1:B:222[A]:MET:HE2	1:B:326:ALA:C	2.28	0.54
1:C:79[A]:MET:HE1	1:D:79[A]:MET:CE	2.37	0.54
1:A:439:TRP:CZ2	1:A:443:GLN:HG3	2.44	0.53
1:B:165:LYS:NZ	7:B:1530:HOH:O	2.42	0.52
1:C:100[B]:THR:HG23	1:C:160:TYR:CE1	2.45	0.52
1:C:100[B]:THR:CG2	1:C:160:TYR:CE1	2.93	0.52
1:C:120:ARG:O	4:C:711:CL:CL	2.65	0.51
1:D:464:PHE:CD1	2:D:603:D7K:C10	2.94	0.51
1:C:363:ASN:ND2	1:C:388:ASN:H	2.10	0.50
4:C:711:CL:CL	1:D:120:ARG:O	2.67	0.50
2:A:601:D7K:O9	2:A:601:D7K:H1	2.13	0.48
1:C:364:ASP:OD1	7:C:2597:HOH:O	2.20	0.48
1:A:363:ASN:ND2	1:A:388:ASN:H	2.11	0.48
1:A:233[B]:VAL:HG12	1:A:252:LEU:HA	1.96	0.48
1:A:233[B]:VAL:CG1	1:A:252:LEU:HA	2.43	0.48
1:C:352:ARG:CZ	1:C:522[B]:SER:OG	2.62	0.48
4:C:711:CL:CL	1:D:118:LEU:O	2.69	0.48
1:C:221:VAL:HG21	6:C:716[B]:PEG:H22	1.94	0.47
1:A:118:LEU:O	4:A:709:CL:CL	2.68	0.47
2:B:602:D7K:H1	2:B:602:D7K:O9	2.15	0.47
4:A:709:CL:CL	1:B:120:ARG:O	2.69	0.47
1:C:464[B]:PHE:HD2	1:D:29:LEU:CD1	2.28	0.47
1:A:208:GLY:HA3	1:A:275:ALA:HB2	1.97	0.47
1:A:120:ARG:O	4:A:709:CL:CL	2.70	0.46
1:C:118:LEU:O	4:C:711:CL:CL	2.70	0.46
1:B:222[A]:MET:HE2	1:B:326:ALA:CB	2.44	0.46
1:B:363:ASN:ND2	1:B:388:ASN:H	2.13	0.46
1:B:464:PHE:O	1:B:468:LEU:HD13	2.16	0.46
1:D:208:GLY:HA3	1:D:275:ALA:HB2	1.98	0.45
1:B:352:ARG:CZ	1:B:522[B]:SER:OG	2.65	0.45
4:A:709:CL:CL	1:B:118:LEU:O	2.72	0.44
1:B:352:ARG:NH1	1:B:522[B]:SER:OG	2.51	0.44
1:D:352:ARG:NH1	1:D:522[B]:SER:OG	2.51	0.44
1:B:439:TRP:CZ2	1:B:443:GLN:HG3	2.53	0.44
1:B:208:GLY:HA3	1:B:275:ALA:HB2	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:510:ALA:O	4:B:703:CL:CL	2.73	0.44
1:D:464:PHE:CE1	2:D:603:D7K:H10B	2.54	0.43
1:D:40:ARG:HB3	6:D:718[B]:PEG:H21	1.99	0.43
1:C:439:TRP:CH2	1:C:443:GLN:HG3	2.53	0.43
1:B:28:GLU:OE1	1:B:70:HIS:CD2	2.69	0.43
1:C:222[A]:MET:CE	1:C:326:ALA:HB1	2.49	0.43
2:D:603:D7K:O9	2:D:603:D7K:H1	2.19	0.42
1:C:245[B]:ARG:HD2	7:C:2939:HOH:O	2.18	0.42
1:D:439:TRP:CE2	1:D:443:GLN:HG3	2.54	0.42
1:D:100:THR:CG2	1:D:103[B]:MET:HG3	2.49	0.42
1:B:302:PRO:O	1:C:148:MET:HE1	2.20	0.42
1:C:208:GLY:HA3	1:C:275:ALA:HB2	2.02	0.42
1:A:61[B]:SER:OG	1:A:63:LYS:HG2	2.20	0.42
1:D:79[B]:MET:CE	1:D:122:LEU:HD12	2.50	0.42
1:A:352:ARG:NH1	1:A:522[B]:SER:OG	2.52	0.41
1:D:79[B]:MET:SD	1:D:119:PRO:HA	2.60	0.41
1:C:222[A]:MET:HE2	1:C:326:ALA:HB1	2.02	0.41
1:C:468:LEU:HA	7:C:2949:HOH:O	2.20	0.41
1:A:382:GLN:NE2	1:A:386:ARG:HE	2.12	0.41
1:C:464[B]:PHE:CZ	1:C:468:LEU:HD11	2.55	0.41
1:C:28:GLU:HB3	1:C:68:ASN:HD21	1.86	0.41
1:A:421:GLN:NE2	4:A:710:CL:CL	2.90	0.41
1:A:79[B]:MET:SD	1:A:119:PRO:HA	2.62	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:368[A]:GLU:OE2	7:A:2784:HOH:O[1_465]	1.71	0.49
1:C:338[A]:THR:OG1	7:A:2494:HOH:O[1_565]	2.19	0.01

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	539/534 (101%)	532 (99%)	7 (1%)	0	100	100
1	B	539/534 (101%)	533 (99%)	6 (1%)	0	100	100
1	C	542/534 (102%)	537 (99%)	4 (1%)	1 (0%)	52	27
1	D	538/534 (101%)	530 (98%)	8 (2%)	0	100	100
All	All	2158/2136 (101%)	2132 (99%)	25 (1%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	469	GLU

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	427/420 (102%)	424 (99%)	3 (1%)	88	77
1	B	427/420 (102%)	424 (99%)	3 (1%)	88	77
1	C	430/420 (102%)	426 (99%)	4 (1%)	84	70
1	D	427/420 (102%)	422 (99%)	5 (1%)	78	59
All	All	1711/1680 (102%)	1696 (99%)	15 (1%)	84	70

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	310	MET
1	A	388	ASN
1	A	464	PHE
1	B	310	MET
1	B	388	ASN
1	B	464	PHE
1	C	217	ASN
1	C	310	MET

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Mol	Chain	Res	Type
1	C	342	GLU
1	C	388	ASN
1	D	46	GLN
1	D	310	MET
1	D	342	GLU
1	D	388	ASN
1	D	468	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	68	ASN
1	A	363	ASN
1	A	382	GLN
1	A	388	ASN
1	A	445	ASN
1	B	68	ASN
1	B	70	HIS
1	B	363	ASN
1	B	388	ASN
1	B	391	ASN
1	B	421	GLN
1	C	68	ASN
1	C	363	ASN
1	C	388	ASN
1	C	421	GLN
1	C	443	GLN
1	D	68	ASN
1	D	363	ASN
1	D	382	GLN
1	D	388	ASN
1	D	421	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 27 ligands modelled in this entry, 15 are monoatomic - leaving 12 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	D7K	A	601	3	33,41,41	3.10	8 (24%)	41,63,63	1.68	12 (29%)
5	PO4	A	712	-	4,4,4	0.39	0	6,6,6	0.27	0
2	D7K	B	602	3	33,41,41	2.86	10 (30%)	41,63,63	1.85	13 (31%)
2	D7K	C	604	3	33,41,41	3.11	7 (21%)	41,63,63	1.76	10 (24%)
5	PO4	C	713	-	4,4,4	0.51	0	6,6,6	0.28	0
5	PO4	C	714	-	4,4,4	0.30	0	6,6,6	0.26	0
6	PEG	C	715	-	6,6,6	0.40	0	5,5,5	0.62	0
6	PEG	C	716[A]	-	6,6,6	0.47	0	5,5,5	0.30	0
6	PEG	C	716[B]	-	6,6,6	0.50	0	5,5,5	0.23	0
2	D7K	D	603	3	33,41,41	2.81	9 (27%)	41,63,63	1.75	11 (26%)
6	PEG	D	718[A]	-	6,6,6	0.44	0	5,5,5	0.27	0
6	PEG	D	718[B]	-	6,6,6	0.49	0	5,5,5	0.24	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	D7K	A	601	3	-	0/31/41/41	0/3/3/3
5	PO4	A	712	-	-	0/0/0/0	0/0/0/0
2	D7K	B	602	3	-	0/31/41/41	0/3/3/3
2	D7K	C	604	3	-	0/31/41/41	0/3/3/3
5	PO4	C	713	-	-	0/0/0/0	0/0/0/0
5	PO4	C	714	-	-	0/0/0/0	0/0/0/0
6	PEG	C	715	-	-	0/4/4/4	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	PEG	C	716[A]	-	-	0/4/4/4	0/0/0/0
6	PEG	C	716[B]	-	-	0/4/4/4	0/0/0/0
2	D7K	D	603	3	-	0/31/41/41	0/3/3/3
6	PEG	D	718[A]	-	-	0/4/4/4	0/0/0/0
6	PEG	D	718[B]	-	-	0/4/4/4	0/0/0/0

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	604	D7K	C7-C2	-8.88	1.42	1.53
2	D	603	D7K	C7-C2	-7.96	1.43	1.53
2	B	602	D7K	C7-C2	-7.24	1.44	1.53
2	A	601	D7K	C7-C2	-6.36	1.45	1.53
2	C	604	D7K	C04-S1	-4.95	1.64	1.74
2	D	603	D7K	C04-S1	-4.82	1.65	1.74
2	A	601	D7K	P8-O11	-3.80	1.48	1.56
2	C	604	D7K	P8-O11	-3.57	1.49	1.56
2	D	603	D7K	P8-O11	-3.23	1.49	1.56
2	B	602	D7K	P8-O11	-2.76	1.50	1.56
2	B	602	D7K	C04-S1	-2.58	1.69	1.74
2	D	603	D7K	CM2-C2,	-2.39	1.42	1.49
2	A	601	D7K	C02-N3	2.04	1.39	1.35
2	C	604	D7K	CM4-C03	2.07	1.54	1.49
2	B	602	D7K	C02-N3	2.09	1.40	1.35
2	B	602	D7K	PB-O3B	2.24	1.62	1.54
2	D	603	D7K	CM4-C03	2.30	1.54	1.49
2	B	602	D7K	C4,-N3,	2.45	1.38	1.35
2	A	601	D7K	C4,-N3,	2.58	1.39	1.35
2	D	603	D7K	PB-O3B	2.69	1.64	1.54
2	B	602	D7K	CM4-C03	2.78	1.55	1.49
2	A	601	D7K	CM4-C03	3.42	1.57	1.49
2	B	602	D7K	P8-O9	4.14	1.62	1.57
2	D	603	D7K	C6,-N1,	4.21	1.43	1.34
2	A	601	D7K	C6,-N1,	4.48	1.44	1.34
2	C	604	D7K	C6,-N1,	4.56	1.44	1.34
2	B	602	D7K	C6,-N1,	5.07	1.45	1.34
2	A	601	D7K	P8-O9	5.44	1.63	1.57
2	D	603	D7K	P8-O9	5.56	1.63	1.57
2	C	604	D7K	P8-O9	7.41	1.65	1.57
2	D	603	D7K	P8-C7	8.66	1.92	1.84
2	C	604	D7K	P8-C7	9.53	1.93	1.84
2	B	602	D7K	P8-C7	10.79	1.94	1.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	D7K	P8-C7	12.85	1.96	1.84

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	604	D7K	N1,-C2,-N3,	-3.72	118.71	125.60
2	B	602	D7K	O9-P8-O12	-3.70	105.22	114.37
2	B	602	D7K	C5,-C4,-N4,	-3.63	116.92	122.25
2	D	603	D7K	C5,-C4,-N4,	-3.59	116.99	122.25
2	B	602	D7K	N1,-C2,-N3,	-3.43	119.26	125.60
2	D	603	D7K	N1,-C2,-N3,	-3.41	119.30	125.60
2	C	604	D7K	O9-P8-O12	-3.29	106.23	114.37
2	A	601	D7K	CM4-C03-C04	-3.15	121.82	128.90
2	A	601	D7K	N1,-C2,-N3,	-3.15	119.77	125.60
2	A	601	D7K	C5,-C4,-N4,	-3.05	117.77	122.25
2	D	603	D7K	PA-O3A-PB	-3.02	122.56	132.67
2	C	604	D7K	PA-O3A-PB	-2.95	122.76	132.67
2	C	604	D7K	CM4-C03-C04	-2.95	122.26	128.90
2	D	603	D7K	CM4-C03-C04	-2.95	122.26	128.90
2	B	602	D7K	CM4-C03-C04	-2.83	122.53	128.90
2	C	604	D7K	C5,-C4,-N4,	-2.77	118.19	122.25
2	A	601	D7K	PA-O3A-PB	-2.66	123.75	132.67
2	B	602	D7K	C5,-C6,-N1,	-2.52	119.49	123.86
2	A	601	D7K	O9-P8-O12	-2.45	108.30	114.37
2	D	603	D7K	O9-P8-O12	-2.41	108.39	114.37
2	B	602	D7K	PA-O3A-PB	-2.31	124.94	132.67
2	A	601	D7K	N4,-C4,-N3,	2.04	119.90	116.95
2	D	603	D7K	N4,-C4,-N3,	2.07	119.95	116.95
2	B	602	D7K	N4,-C4,-N3,	2.22	120.16	116.95
2	A	601	D7K	C05-C04-C03	2.23	129.56	127.56
2	C	604	D7K	C6,-N1,-C2,	2.34	119.85	115.77
2	C	604	D7K	C2,-N3,-C4,	2.35	122.87	118.19
2	A	601	D7K	C6,-N1,-C2,	2.39	119.94	115.77
2	D	603	D7K	CM2-C2,-N3,	2.40	121.29	117.20
2	A	601	D7K	CM2-C2,-N1,	2.53	120.06	117.03
2	A	601	D7K	O11-P8-C7	2.60	111.89	106.07
2	B	602	D7K	O11-P8-O12	2.67	118.12	111.51
2	A	601	D7K	O11-P8-O12	2.84	118.53	111.51
2	B	602	D7K	O11-P8-C7	2.91	112.56	106.07
2	D	603	D7K	C04-C03-N3	2.93	114.65	107.83
2	D	603	D7K	C6,-N1,-C2,	2.96	120.94	115.77
2	B	602	D7K	CM2-C2,-N1,	2.98	120.60	117.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	602	D7K	C5,-C7,-N3	3.02	118.31	113.31
2	D	603	D7K	O11-P8-O12	3.04	119.05	111.51
2	B	602	D7K	C04-C03-N3	3.12	115.07	107.83
2	D	603	D7K	O11-P8-C7	3.23	113.28	106.07
2	A	601	D7K	C04-C03-N3	3.24	115.35	107.83
2	C	604	D7K	C04-C03-N3	3.47	115.89	107.83
2	B	602	D7K	C6,-N1,-C2,	3.52	121.93	115.77
2	C	604	D7K	O11-P8-O12	3.60	120.42	111.51
2	C	604	D7K	CM2-C2,-N1,	3.66	121.42	117.03

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	D7K	1	0
2	B	602	D7K	1	0
6	C	716[B]	PEG	2	0
2	D	603	D7K	3	0
6	D	718[B]	PEG	1	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	523/534 (97%)	-0.21	10 (1%) 70 68	11, 16, 27, 49	3 (0%)
1	B	523/534 (97%)	-0.24	7 (1%) 79 78	11, 16, 27, 49	5 (0%)
1	C	523/534 (97%)	-0.18	11 (2%) 67 65	11, 16, 30, 72	2 (0%)
1	D	523/534 (97%)	-0.17	14 (2%) 58 55	11, 16, 30, 61	4 (0%)
All	All	2092/2136 (97%)	-0.20	42 (2%) 68 67	11, 16, 29, 72	14 (0%)

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	463[A]	TRP	5.2
1	C	463[A]	TRP	5.1
1	C	344	ALA	5.1
1	C	469	GLU	4.9
1	A	469	GLU	4.6
1	C	350	ALA	4.5
1	C	466	GLY	4.5
1	A	466	GLY	4.3
1	D	344	ALA	3.7
1	D	469	GLU	3.7
1	D	466	GLY	3.5
1	C	464[A]	PHE	3.4
1	A	463[A]	TRP	3.4
1	D	339	ALA	3.2
1	A	464	PHE	3.2
1	D	343	PRO	3.2
1	D	350	ALA	3.1
1	B	469	GLU	3.1
1	D	333	SER	3.1
1	B	466	GLY	3.0
1	A	344	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	283	TYR	2.9
1	B	463[A]	TRP	2.9
1	B	464	PHE	2.7
1	B	467	VAL	2.7
1	D	338	THR	2.6
1	D	467	VAL	2.6
1	C	283	TYR	2.6
1	B	344	ALA	2.6
1	C	341	PRO	2.5
1	A	467	VAL	2.4
1	D	468	LEU	2.3
1	C	467	VAL	2.2
1	A	338[A]	THR	2.2
1	A	343	PRO	2.2
1	A	347	ASP	2.2
1	B	419	GLU	2.1
1	D	471	GLU	2.1
1	C	343	PRO	2.1
1	D	169	PRO	2.1
1	A	419	GLU	2.0
1	C	468	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, 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	LLDF	B-factors(Å ²)	Q<0.9
5	PO4	A	712	5/5	0.93	0.29	10.99	36,47,56,68	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
6	PEG	C	716[B]	7/7	0.84	0.21	8.84	19,35,55,64	7
5	PO4	C	713	5/5	0.85	0.33	7.21	104,106,111,112	0
6	PEG	C	716[A]	7/7	0.84	0.21	2.45	14,22,39,41	7
5	PO4	C	714	5/5	0.90	0.14	2.19	15,19,27,31	5
4	CL	B	708	1/1	0.98	0.10	1.80	23,23,23,23	1
2	D7K	D	603	39/39	0.96	0.09	1.10	11,15,26,28	0
6	PEG	D	718[A]	7/7	0.91	0.14	0.88	26,32,40,40	7
6	PEG	D	718[B]	7/7	0.91	0.14	0.88	18,30,34,34	7
6	PEG	C	715	7/7	0.92	0.11	0.42	34,39,44,53	0
2	D7K	C	604	39/39	0.96	0.09	0.32	11,15,26,36	0
2	D7K	B	602	39/39	0.96	0.08	-0.06	10,14,26,27	0
2	D7K	A	601	39/39	0.96	0.08	-0.15	9,14,26,29	0
4	CL	B	703	1/1	0.99	0.07	-1.01	22,22,22,22	0
3	MG	C	607	1/1	0.99	0.06	-1.09	13,13,13,13	0
4	CL	A	710	1/1	0.98	0.04	-1.83	21,21,21,21	0
4	CL	C	707	1/1	0.98	0.04	-1.94	21,21,21,21	0
3	MG	B	606	1/1	0.99	0.04	-2.17	13,13,13,13	0
4	CL	C	711	1/1	1.00	0.05	-2.28	12,12,12,12	0
3	MG	D	608	1/1	0.99	0.04	-2.84	14,14,14,14	0
4	CL	D	706	1/1	0.99	0.02	-3.35	21,21,21,21	0
3	MG	A	605	1/1	1.00	0.04	-3.68	13,13,13,13	0
4	CL	A	709	1/1	1.00	0.04	-4.04	12,12,12,12	0
4	CL	A	704	1/1	0.99	0.05	-	22,22,22,22	0
4	CL	B	702	1/1	1.00	0.02	-	23,23,23,23	0
4	CL	A	705	1/1	0.99	0.03	-	23,23,23,23	0
4	CL	B	701	1/1	0.99	0.03	-	23,23,23,23	0

6.5 Other polymers ⓘ

There are no such residues in this entry.