



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 17, 2021 – 01:57 AM EDT

PDB ID : 1P6C  
Title : crystal structure of phosphotriesterase triple mutant H254G/H257W/L303T complexed with diisopropylmethylphosphonate  
Authors : Hill, C.M.; Li, W.; Thoden, J.B.; Holden, H.M.; Raushel, F.M.  
Deposited on : 2003-04-29  
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

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.23.2  
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) : 2.23.2

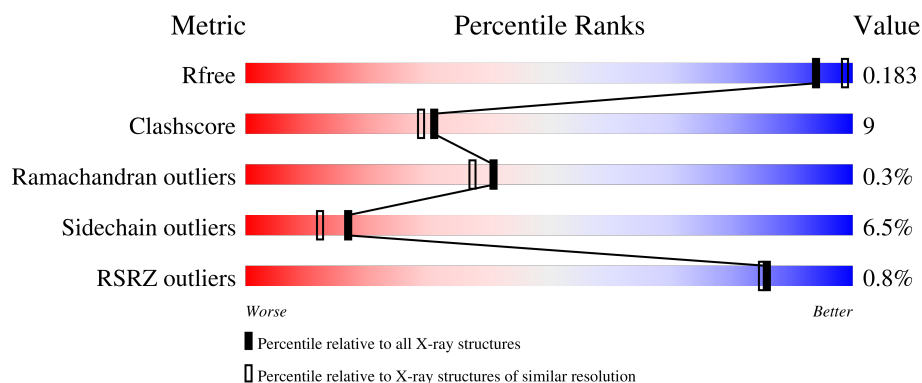
# 1 Overall quality at a glance

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))
$R_{free}$	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (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 of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	336	<div> <div></div> <div>70%</div> <div>25%</div> <div>..</div> </div>
1	B	336	<div> <div></div> <div>65%</div> <div>30%</div> <div>..</div> </div>

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	DII	B	8	-	-	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5431 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 Parathion hydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	331	Total	C	N	O	S	0	0	0
			2526	1598	448	473	7			
1	B	330	Total	C	N	O	S	0	2	0
			2526	1598	447	474	7			

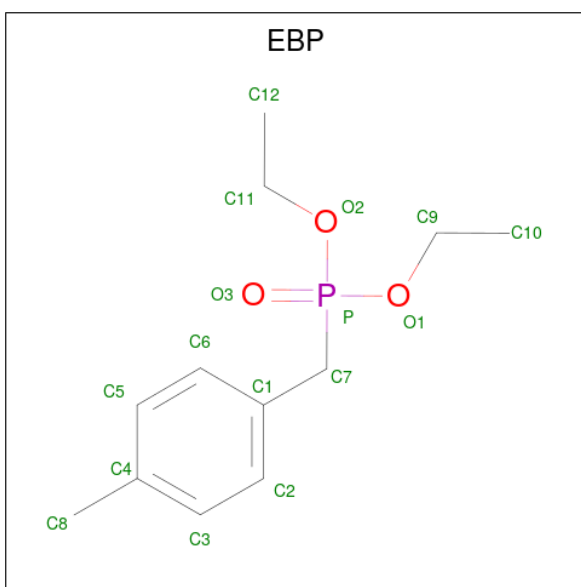
There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	254	GLY	HIS	engineered mutation	UNP P0A433
A	257	TRP	HIS	engineered mutation	UNP P0A433
A	303	THR	LEU	engineered mutation	UNP P0A433
B	254	GLY	HIS	engineered mutation	UNP P0A433
B	257	TRP	HIS	engineered mutation	UNP P0A433
B	303	THR	LEU	engineered mutation	UNP P0A433

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

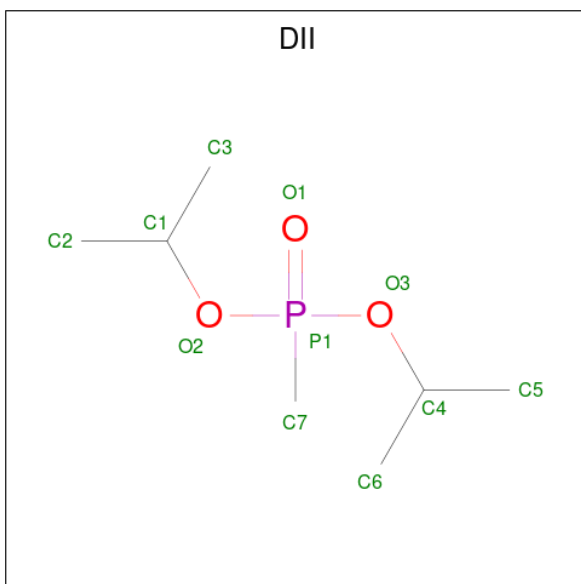
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Zn	0	0
			2	2		
2	B	2	Total	Zn	0	0
			2	2		

- Molecule 3 is DIETHYL 4-METHYLBENZYLPHOSPHONATE (three-letter code: EBP) (formula: C<sub>12</sub>H<sub>19</sub>O<sub>3</sub>P).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	P	0	0
			16	12	3	1		
3	B	1	Total	C	O	P	0	0
			16	12	3	1		

- Molecule 4 is METHYLPHOSPHONIC ACID DIISOPROPYL ESTER (three-letter code: DII) (formula:  $C_7H_{17}O_3P$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O	P	0	0
			11	7	3	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	O	P	0	0
			11	7	3	1		

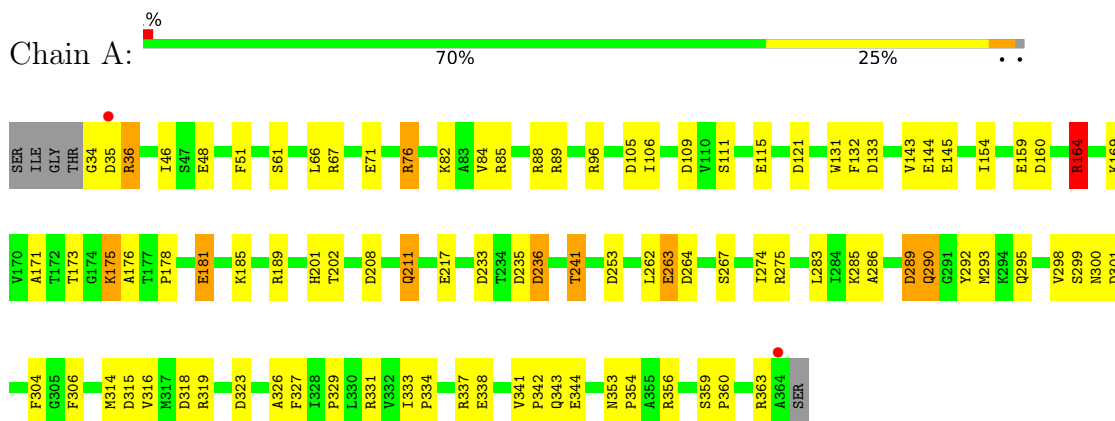
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	163	Total	O	0	0
			163	163		
5	B	158	Total	O	0	0
			158	158		

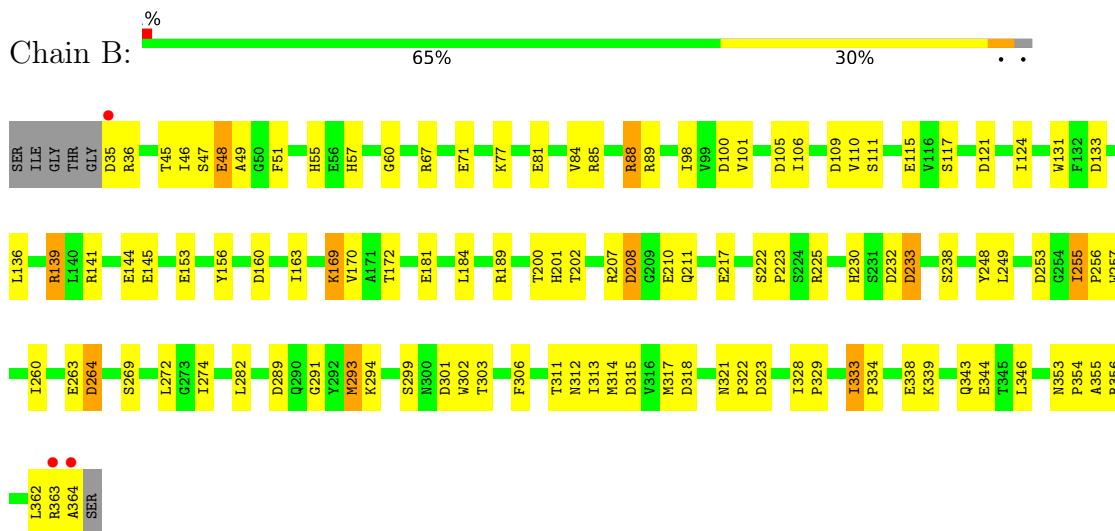
### 3 Residue-property plots [i](#)

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

#### • Molecule 1: Parathion hydrolase



#### • Molecule 1: Parathion hydrolase



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	130.40Å 91.90Å 69.70Å 90.00° 90.90° 90.00°	Depositor
Resolution (Å)	30.00 – 2.00 15.18 – 2.00	Depositor EDS
% Data completeness (in resolution range)	85.3 (30.00-2.00) 85.0 (15.18-2.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.00 (at 2.00Å)	Xtriage
Refinement program	TNT	Depositor
R, $R_{free}$	0.181 , 0.246 0.183 , 0.183	Depositor DCC
$R_{free}$ test set	4728 reflections (9.98%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	21.7	Xtriage
Anisotropy	0.501	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 108.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.156 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	5431	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.21% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: KCX, DII, EBP, ZN

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	0.90	10/2561 (0.4%)	1.40	38/3478 (1.1%)
1	B	0.91	13/2569 (0.5%)	1.39	44/3489 (1.3%)
All	All	0.90	23/5130 (0.4%)	1.40	82/6967 (1.2%)

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	338	GLU	CD-OE2	8.15	1.34	1.25
1	A	338	GLU	CD-OE2	7.19	1.33	1.25
1	B	81	GLU	CD-OE2	7.04	1.33	1.25
1	B	181	GLU	CD-OE2	6.46	1.32	1.25
1	B	344	GLU	CD-OE2	6.38	1.32	1.25
1	A	48	GLU	CD-OE2	6.09	1.32	1.25
1	A	115	GLU	CD-OE2	6.01	1.32	1.25
1	B	115	GLU	CD-OE2	5.93	1.32	1.25
1	B	153	GLU	CD-OE2	5.89	1.32	1.25
1	B	144	GLU	CD-OE2	5.86	1.32	1.25
1	A	263	GLU	CD-OE2	5.85	1.32	1.25
1	B	263	GLU	CD-OE2	5.82	1.32	1.25
1	B	210	GLU	CD-OE2	5.82	1.32	1.25
1	A	71	GLU	CD-OE2	5.82	1.32	1.25
1	B	71	GLU	CD-OE2	5.77	1.31	1.25
1	B	48	GLU	CD-OE2	5.74	1.31	1.25
1	B	217	GLU	CD-OE2	5.62	1.31	1.25
1	A	344	GLU	CD-OE2	5.55	1.31	1.25
1	A	144	GLU	CD-OE2	5.49	1.31	1.25
1	B	145	GLU	CD-OE2	5.36	1.31	1.25
1	A	181	GLU	CD-OE2	5.26	1.31	1.25
1	A	217	GLU	CD-OE2	5.15	1.31	1.25
1	A	145	GLU	CD-OE2	5.13	1.31	1.25

All (82) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	164	ARG	NE-CZ-NH1	11.98	126.29	120.30
1	A	236	ASP	CB-CG-OD2	-11.52	107.94	118.30
1	A	76	ARG	NE-CZ-NH2	-9.22	115.69	120.30
1	B	301	ASP	CB-CG-OD1	9.17	126.56	118.30
1	A	235	ASP	CB-CG-OD2	-8.81	110.37	118.30
1	A	236	ASP	CB-CG-OD1	8.66	126.09	118.30
1	B	139	ARG	NE-CZ-NH1	8.53	124.56	120.30
1	A	253	ASP	CB-CG-OD2	-8.44	110.71	118.30
1	A	301	ASP	CB-CG-OD1	8.39	125.85	118.30
1	A	105	ASP	CB-CG-OD2	-8.35	110.78	118.30
1	B	109	ASP	CB-CG-OD1	8.31	125.78	118.30
1	A	318	ASP	CB-CG-OD2	-8.07	111.03	118.30
1	A	301	ASP	CB-CG-OD2	-7.89	111.20	118.30
1	A	289	ASP	CB-CG-OD2	-7.74	111.33	118.30
1	A	356	ARG	NE-CZ-NH1	7.70	124.15	120.30
1	B	141	ARG	NE-CZ-NH1	7.56	124.08	120.30
1	A	76	ARG	NE-CZ-NH1	7.45	124.03	120.30
1	B	225	ARG	NE-CZ-NH2	-7.38	116.61	120.30
1	B	232	ASP	CB-CG-OD2	-7.37	111.67	118.30
1	B	233	ASP	CB-CG-OD2	-7.32	111.71	118.30
1	B	318	ASP	CB-CG-OD2	-7.28	111.75	118.30
1	A	121	ASP	CB-CG-OD2	-7.25	111.77	118.30
1	A	121	ASP	CB-CG-OD1	7.16	124.74	118.30
1	A	164	ARG	NE-CZ-NH2	-7.07	116.77	120.30
1	A	323	ASP	CB-CG-OD2	-7.04	111.96	118.30
1	B	318	ASP	CB-CG-OD1	6.99	124.59	118.30
1	A	253	ASP	CB-CG-OD1	6.97	124.57	118.30
1	B	208	ASP	CB-CG-OD2	-6.89	112.10	118.30
1	B	233	ASP	CB-CG-OD1	6.79	124.41	118.30
1	A	67	ARG	NE-CZ-NH2	-6.72	116.94	120.30
1	B	100	ASP	CB-CG-OD1	6.71	124.34	118.30
1	B	232	ASP	CB-CG-OD1	6.46	124.11	118.30
1	B	225	ARG	NE-CZ-NH1	6.44	123.52	120.30
1	B	264	ASP	CB-CG-OD2	-6.44	112.50	118.30
1	A	160	ASP	CB-CG-OD1	6.43	124.09	118.30
1	B	315	ASP	CB-CG-OD1	6.37	124.03	118.30
1	A	363	ARG	NE-CZ-NH2	-6.36	117.12	120.30
1	B	139	ARG	NE-CZ-NH2	-6.34	117.13	120.30
1	B	89	ARG	NE-CZ-NH2	-6.25	117.17	120.30
1	B	289	ASP	CB-CG-OD1	6.18	123.87	118.30
1	B	189	ARG	NE-CZ-NH2	-6.17	117.21	120.30
1	A	36	ARG	NE-CZ-NH1	6.17	123.39	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	109	ASP	CB-CG-OD2	-6.15	112.77	118.30
1	A	289	ASP	CB-CG-OD1	6.14	123.83	118.30
1	A	319	ARG	NE-CZ-NH1	6.14	123.37	120.30
1	B	121	ASP	CB-CG-OD2	-6.12	112.79	118.30
1	B	85	ARG	NE-CZ-NH1	6.12	123.36	120.30
1	B	315	ASP	CB-CG-OD2	-6.12	112.79	118.30
1	B	189	ARG	NE-CZ-NH1	6.07	123.33	120.30
1	B	88	ARG	NE-CZ-NH2	-6.06	117.27	120.30
1	A	89	ARG	NE-CZ-NH1	6.02	123.31	120.30
1	A	160	ASP	CB-CG-OD2	-6.00	112.90	118.30
1	B	301	ASP	CB-CG-OD2	-5.99	112.91	118.30
1	B	289	ASP	CB-CG-OD2	-5.99	112.91	118.30
1	A	318	ASP	CB-CG-OD1	5.96	123.67	118.30
1	B	85	ARG	NE-CZ-NH2	-5.76	117.42	120.30
1	B	160	ASP	CB-CG-OD2	-5.75	113.12	118.30
1	B	323	ASP	CB-CG-OD2	-5.71	113.16	118.30
1	B	105	ASP	CB-CG-OD2	-5.71	113.17	118.30
1	B	172	THR	N-CA-CB	5.69	121.10	110.30
1	B	160	ASP	CB-CG-OD1	5.65	123.38	118.30
1	A	264	ASP	CB-CG-OD1	5.64	123.38	118.30
1	B	121	ASP	CB-CG-OD1	5.63	123.37	118.30
1	B	100	ASP	CB-CG-OD2	-5.52	113.33	118.30
1	A	315	ASP	CB-CG-OD2	-5.51	113.34	118.30
1	A	323	ASP	CB-CG-OD1	5.43	123.19	118.30
1	A	233	ASP	CB-CG-OD2	-5.43	113.41	118.30
1	A	133	ASP	CB-CG-OD1	5.41	123.17	118.30
1	A	85	ARG	NE-CZ-NH2	-5.39	117.61	120.30
1	B	88	ARG	NE-CZ-NH1	5.32	122.96	120.30
1	B	133	ASP	CB-CG-OD1	5.31	123.08	118.30
1	B	253	ASP	CB-CG-OD1	5.31	123.08	118.30
1	B	207	ARG	NE-CZ-NH2	-5.27	117.67	120.30
1	B	49	ALA	CB-CA-C	5.21	117.92	110.10
1	B	36	ARG	NE-CZ-NH1	5.19	122.89	120.30
1	B	208	ASP	CB-CG-OD1	5.15	122.94	118.30
1	A	35	ASP	CB-CG-OD1	5.14	122.92	118.30
1	B	264	ASP	CB-CG-OD1	5.12	122.91	118.30
1	A	109	ASP	CB-CG-OD1	5.12	122.91	118.30
1	A	66	LEU	CB-CA-C	5.11	119.90	110.20
1	A	61	SER	N-CA-CB	-5.05	102.92	110.50
1	A	35	ASP	CB-CG-OD2	-5.05	113.75	118.30

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	2526	0	2543	44	0
1	B	2526	0	2542	46	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	16	0	19	2	0
3	B	16	0	19	2	0
4	A	11	0	17	1	0
4	B	11	0	17	1	0
5	A	163	0	0	7	0
5	B	158	0	0	3	0
All	All	5431	0	5157	93	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 9.

All (93) 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:176:ALA:H	1:A:211:GLN:HE22	1.31	0.78
1:B:110:VAL:HG13	1:B:163:ILE:HD12	1.68	0.73
1:A:82:LYS:HE2	1:A:304:PHE:O	1.91	0.71
1:B:333:ILE:HB	1:B:334:PRO:HD3	1.77	0.66
4:A:7:DII:H62	4:A:7:DII:H72	1.77	0.65
1:A:36:ARG:NH2	5:A:479:HOH:O	2.29	0.65
1:B:363:ARG:HG2	1:B:364:ALA:N	2.12	0.65
1:A:176:ALA:H	1:A:211:GLN:NE2	1.95	0.65
1:B:328:ILE:HB	1:B:329:PRO:HD3	1.78	0.64
1:A:169:KCX:OQ2	1:A:201:HIS:HB2	1.98	0.63
1:B:139:ARG:HB3	5:B:465:HOH:O	1.98	0.63
1:B:294:LYS:O	1:B:356:ARG:NH2	2.32	0.62
1:A:202:THR:HB	1:A:208:ASP:HB2	1.81	0.62
1:A:46:ILE:HD12	1:A:359:SER:HB3	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:262:LEU:HD21	1:A:316:VAL:HG13	1.82	0.60
1:A:84:VAL:O	1:A:88:ARG:HG3	2.02	0.60
1:B:46:ILE:CG2	1:B:355:ALA:HB1	2.32	0.60
1:B:46:ILE:HG22	1:B:355:ALA:HB1	1.83	0.60
1:A:154:ILE:HG23	5:A:445:HOH:O	2.02	0.59
1:B:333:ILE:CB	1:B:334:PRO:HD3	2.33	0.58
1:A:76:ARG:NH2	5:A:505:HOH:O	2.23	0.57
1:A:164:ARG:NH1	5:A:501:HOH:O	2.38	0.56
1:A:337:ARG:NH1	1:A:343:GLN:H	2.03	0.56
1:B:156:TYR:CG	3:B:6:EBP:H122	2.41	0.55
1:B:257:TRP:CE3	1:B:272:LEU:HD23	2.43	0.53
4:B:8:DII:O2	4:B:8:DII:H62	2.08	0.53
1:B:353:ASN:HB2	1:B:354:PRO:HD3	1.90	0.53
1:B:84:VAL:O	1:B:88:ARG:HG3	2.08	0.52
1:B:170:VAL:HG22	1:B:200:THR:HG22	1.91	0.52
1:B:249:LEU:N	1:B:249:LEU:HD12	2.24	0.52
3:A:5:EBP:H6	3:A:5:EBP:H92	1.92	0.51
1:A:333:ILE:HB	1:A:334:PRO:HD3	1.91	0.50
1:B:202:THR:HB	1:B:208:ASP:HB2	1.94	0.50
1:B:293:MET:HG2	5:B:387:HOH:O	2.12	0.50
1:A:171:ALA:HB2	1:A:201:HIS:HB3	1.93	0.50
1:A:300:ASN:OD1	1:A:327:PHE:HB3	2.11	0.49
1:A:353:ASN:HB2	1:A:354:PRO:HD3	1.94	0.49
1:B:291:GLY:HA2	5:B:387:HOH:O	2.11	0.49
1:A:241:THR:HG22	1:A:292:TYR:CE1	2.48	0.49
3:A:5:EBP:H6	3:A:5:EBP:C9	2.43	0.49
1:A:286:ALA:O	1:A:290:GLN:HG2	2.14	0.48
1:A:241:THR:HG22	1:A:292:TYR:HE1	1.78	0.48
1:B:106:ILE:HG22	1:B:106:ILE:O	2.13	0.47
1:A:111:SER:O	5:A:485:HOH:O	2.20	0.47
1:B:302:TRP:CH2	1:B:321:ASN:HB3	2.49	0.47
1:A:341:VAL:HG13	1:A:342:PRO:HD2	1.97	0.47
1:A:159:GLU:HG2	1:B:67:ARG:O	2.14	0.47
1:A:34:GLY:HA2	1:A:360:PRO:O	2.15	0.46
1:A:106:ILE:HD11	1:A:131:TRP:CG	2.51	0.46
1:A:143:VAL:HG12	5:A:387:HOH:O	2.14	0.46
1:B:55:HIS:CE1	1:B:101:VAL:HG21	2.51	0.46
1:A:185:LYS:O	1:A:189:ARG:HG3	2.16	0.46
1:B:136:LEU:HD23	1:B:136:LEU:HA	1.74	0.45
1:B:311:THR:O	1:B:312:ASN:HB2	2.15	0.45
1:B:106:ILE:HD11	1:B:131:TRP:CD1	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:337:ARG:HH11	1:A:343:GLN:HB2	1.81	0.45
1:B:328:ILE:HB	1:B:329:PRO:CD	2.44	0.45
1:B:343:GLN:O	1:B:346:LEU:HB2	2.16	0.45
1:A:175:LYS:HB2	1:A:175:LYS:HE3	1.63	0.45
1:B:156:TYR:CD2	3:B:6:EBP:H122	2.52	0.44
1:A:290:GLN:HG2	1:A:290:GLN:H	1.49	0.44
1:B:333:ILE:HG23	1:B:346:LEU:HD13	2.00	0.44
1:B:314:MET:HE2	1:B:317:MET:HB2	2.00	0.44
1:A:341:VAL:HA	1:A:342:PRO:HD3	1.86	0.44
1:A:337:ARG:HH11	1:A:343:GLN:H	1.66	0.43
1:B:60:GLY:O	1:B:306:PHE:HA	2.19	0.43
1:A:326:ALA:O	1:A:329:PRO:HD2	2.19	0.43
1:A:327:PHE:CE2	1:A:331:ARG:HD3	2.54	0.43
1:B:106:ILE:HD11	1:B:131:TRP:CG	2.54	0.43
1:B:321:ASN:HA	1:B:322:PRO:HD2	1.78	0.43
1:B:45:THR:OG1	1:B:48:GLU:HG3	2.19	0.43
1:B:363:ARG:CG	1:B:364:ALA:N	2.80	0.42
1:B:353:ASN:HB2	1:B:354:PRO:CD	2.49	0.42
1:A:262:LEU:CD2	1:A:316:VAL:HG13	2.48	0.42
1:B:169:KCX:OQ1	1:B:201:HIS:HB2	2.19	0.42
1:B:223:PRO:HB3	1:B:248:TYR:CZ	2.55	0.42
1:A:106:ILE:HD11	1:A:131:TRP:CD1	2.55	0.42
1:A:285:LYS:NZ	1:A:289:ASP:OD2	2.51	0.42
1:B:282:LEU:HD23	1:B:282:LEU:HA	1.93	0.41
1:B:313:ILE:HD12	1:B:313:ILE:HA	1.74	0.41
1:A:275:ARG:HH11	1:A:275:ARG:HD3	1.72	0.41
1:A:285:LYS:O	1:A:286:ALA:C	2.58	0.41
1:A:178:PRO:O	1:A:181:GLU:HB2	2.21	0.41
1:B:333:ILE:N	1:B:334:PRO:CD	2.83	0.41
1:B:57:HIS:O	1:B:303:THR:HA	2.21	0.41
1:A:283:LEU:HD23	1:A:283:LEU:HA	1.94	0.40
1:B:117:SER:HB2	1:B:124:ILE:HD12	2.03	0.40
1:A:181:GLU:O	1:A:185:LYS:HG3	2.21	0.40
1:B:98:ILE:O	1:B:98:ILE:HG13	2.21	0.40
1:B:230:HIS:HB3	1:B:233:ASP:OD2	2.21	0.40
1:B:255:ILE:N	1:B:256:PRO:HD2	2.36	0.40
1:A:96:ARG:HD3	5:A:403:HOH:O	2.21	0.40
1:A:131:TRP:CG	1:A:132:PHE:N	2.89	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	328/336 (98%)	307 (94%)	20 (6%)	1 (0%)	41	37
1	B	329/336 (98%)	311 (94%)	17 (5%)	1 (0%)	41	37
All	All	657/672 (98%)	618 (94%)	37 (6%)	2 (0%)	41	37

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	236	ASP
1	B	260	ILE

### 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	263/267 (98%)	247 (94%)	16 (6%)	18	14
1	B	265/267 (99%)	245 (92%)	20 (8%)	13	9
All	All	528/534 (99%)	492 (93%)	36 (7%)	17	11

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	51	PHE
1	A	164	ARG
1	A	173	THR
1	A	175	LYS

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Mol	Chain	Res	Type
1	A	211	GLN
1	A	241	THR
1	A	263	GLU
1	A	267	SER
1	A	274	ILE
1	A	290	GLN
1	A	293	MET
1	A	295	GLN
1	A	298	VAL
1	A	299	SER
1	A	306	PHE
1	A	314	MET
1	B	35	ASP
1	B	47	SER
1	B	51	PHE
1	B	77	LYS
1	B	111[A]	SER
1	B	111[B]	SER
1	B	184	LEU
1	B	211	GLN
1	B	222	SER
1	B	238[A]	SER
1	B	238[B]	SER
1	B	255	ILE
1	B	264	ASP
1	B	269	SER
1	B	274	ILE
1	B	293	MET
1	B	299	SER
1	B	333	ILE
1	B	339	LYS
1	B	362	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	211	GLN
1	A	212	GLN
1	B	312	ASN



### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
1	KCX	A	169	1,2	7,11,12	0.38	0	4,12,14	0.30	0
1	KCX	B	169	1,2	7,11,12	0.71	0	4,12,14	1.39	1 (25%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	KCX	A	169	1,2	-	3/7/10/12	-
1	KCX	B	169	1,2	-	2/7/10/12	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	169	KCX	CE-NZ-CX	-2.54	118.65	122.95

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	169	KCX	C-CA-CB-CG
1	B	169	KCX	C-CA-CB-CG

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Mol	Chain	Res	Type	Atoms
1	A	169	KCX	CG-CD-CE-NZ
1	A	169	KCX	CA-CB-CG-CD
1	B	169	KCX	CA-CB-CG-CD

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	169	KCX	1	0
1	B	169	KCX	1	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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$
3	EBP	B	6	-	16,16,16	3.03	5 (31%)	21,21,21	1.43	1 (4%)
4	DII	B	8	-	8,10,10	2.23	2 (25%)	10,14,14	1.13	0
4	DII	A	7	2	8,10,10	2.71	2 (25%)	10,14,14	0.99	1 (10%)
3	EBP	A	5	-	16,16,16	3.02	2 (12%)	21,21,21	1.42	3 (14%)

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	EBP	B	6	-	-	1/13/13/13	0/1/1/1
4	DII	B	8	-	-	5/10/10/10	-
4	DII	A	7	2	-	4/10/10/10	-
3	EBP	A	5	-	-	1/13/13/13	0/1/1/1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	5	EBP	P-C7	-10.99	1.62	1.79
3	B	6	EBP	P-C7	-10.91	1.62	1.79
4	A	7	DII	P1-O1	5.69	1.56	1.47
4	B	8	DII	P1-C7	-4.89	1.64	1.77
4	A	7	DII	P1-C7	-4.84	1.64	1.77
4	B	8	DII	P1-O1	3.59	1.52	1.47
3	B	6	EBP	C3-C2	2.69	1.43	1.38
3	B	6	EBP	C6-C5	2.45	1.43	1.38
3	A	5	EBP	C3-C2	2.45	1.43	1.38
3	B	6	EBP	C6-C1	2.16	1.43	1.38
3	B	6	EBP	C2-C1	2.14	1.43	1.38

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	6	EBP	O3-P-C7	-5.19	102.19	114.19
3	A	5	EBP	O3-P-C7	-4.75	103.21	114.19
3	A	5	EBP	P-C7-C1	-2.28	108.47	113.73
3	A	5	EBP	O2-P-O3	2.21	120.58	114.21
4	A	7	DII	O1-P1-C7	-2.04	107.30	114.83

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	7	DII	C1-O2-P1-C7
4	B	8	DII	C4-O3-P1-O1
4	B	8	DII	C4-O3-P1-O2
3	B	6	EBP	C9-O1-P-C7
4	B	8	DII	C1-O2-P1-O3
4	B	8	DII	C6-C4-O3-P1
4	A	7	DII	C1-O2-P1-O1
4	A	7	DII	C4-O3-P1-C7
4	A	7	DII	C1-O2-P1-O3

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Mol	Chain	Res	Type	Atoms
3	A	5	EBP	C9-O1-P-C7
4	B	8	DII	C5-C4-O3-P1

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	6	EBP	2	0
4	B	8	DII	1	0
4	A	7	DII	1	0
3	A	5	EBP	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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	330/336 (98%)	-0.41	2 (0%) 89 88	13, 27, 61, 100	0
1	B	329/336 (97%)	-0.38	3 (0%) 84 83	13, 26, 59, 97	0
All	All	659/672 (98%)	-0.40	5 (0%) 86 85	13, 27, 61, 100	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	363	ARG	2.5
1	B	35	ASP	2.4
1	B	364	ALA	2.4
1	A	364	ALA	2.4
1	A	35	ASP	2.3

### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
1	KCX	A	169	12/13	0.93	0.12	15,24,29,29	0
1	KCX	B	169	12/13	0.96	0.11	15,20,24,28	0

### 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	DII	A	7	11/11	0.71	0.28	0,44,64,81	0
3	EBP	A	5	16/16	0.73	0.19	0,35,85,88	0
4	DII	B	8	11/11	0.76	0.42	0,32,70,78	0
3	EBP	B	6	16/16	0.96	0.10	17,31,81,90	0
2	ZN	A	401	1/1	0.99	0.02	23,23,23,23	0
2	ZN	A	402	1/1	0.99	0.03	28,28,28,28	0
2	ZN	B	403	1/1	0.99	0.02	23,23,23,23	0
2	ZN	B	404	1/1	0.99	0.03	27,27,27,27	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.