



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 7, 2023 – 06:20 PM EDT

PDB ID : 1OZG  
Title : The crystal structure of *Klebsiella pneumoniae* acetolactate synthase with enzyme-bound cofactor and with an unusual intermediate  
Authors : Pang, S.S.; Duggleby, R.G.; Schowen, R.L.; Guddat, L.W.  
Deposited on : 2003-04-09  
Resolution : 2.30 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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 : 2.35  
buster-report : 1.1.7 (2018)  
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) : 2.35

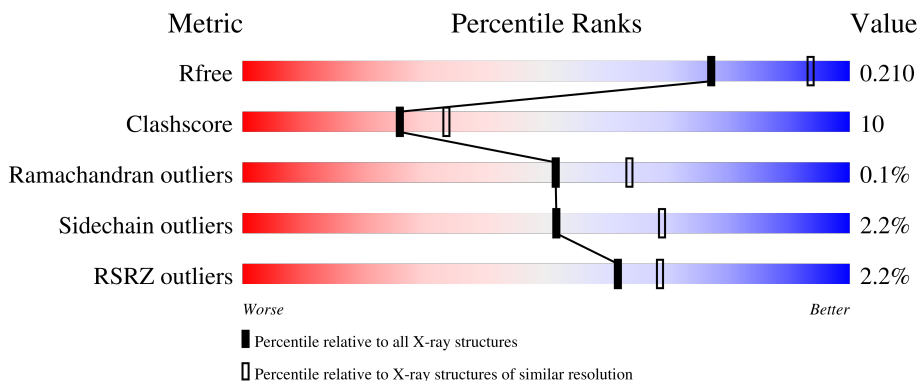
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

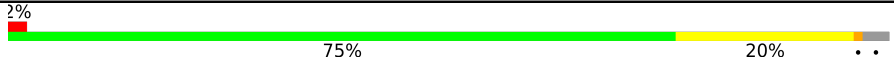

The reported resolution of this entry is 2.30 Å.

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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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	566	 2% 75% 20% ..
1	B	566	 2% 77% 18% ..

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 8994 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 Acetolactate synthase, catabolic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	549	4146	2615	735	778	18	0	0	0
1	B	545	4110	2600	720	772	18	0	0	0

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	560	GLU	-	expression tag	UNP P27696
A	561	HIS	-	expression tag	UNP P27696
A	562	HIS	-	expression tag	UNP P27696
A	563	HIS	-	expression tag	UNP P27696
A	564	HIS	-	expression tag	UNP P27696
A	565	HIS	-	expression tag	UNP P27696
A	566	HIS	-	expression tag	UNP P27696
B	560	GLU	-	expression tag	UNP P27696
B	561	HIS	-	expression tag	UNP P27696
B	562	HIS	-	expression tag	UNP P27696
B	563	HIS	-	expression tag	UNP P27696
B	564	HIS	-	expression tag	UNP P27696
B	565	HIS	-	expression tag	UNP P27696
B	566	HIS	-	expression tag	UNP P27696

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).

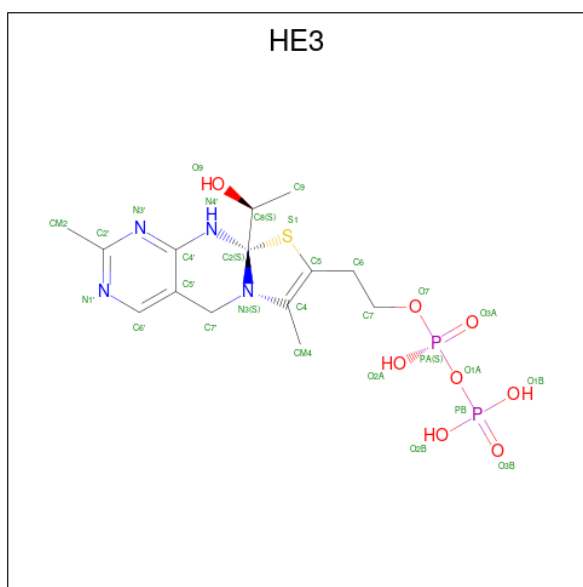


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O P 5 4 1	0	0
2	B	1	Total O P 5 4 1	0	0

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

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

- Molecule 4 is 2-HYDROXYETHYL DIHYDROTHIACHROME DIPHOSPHATE (three-letter code: HE3) (formula: C<sub>14</sub>H<sub>22</sub>N<sub>4</sub>O<sub>8</sub>P<sub>2</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
4	A	1	Total	C	N	O	P	S	0	0
			29	14	4	8	2	1		
4	B	1	Total	C	N	O	P	S	0	0
			29	14	4	8	2	1		

- Molecule 5 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula:  $C_4H_{10}O_3$ ).



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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 7 4 3	0	0
5	A	1	Total C O 7 4 3	0	0
5	A	1	Total C O 7 4 3	0	0
5	A	1	Total C O 7 4 3	0	0
5	B	1	Total C O 7 4 3	0	0
5	B	1	Total C O 7 4 3	0	0

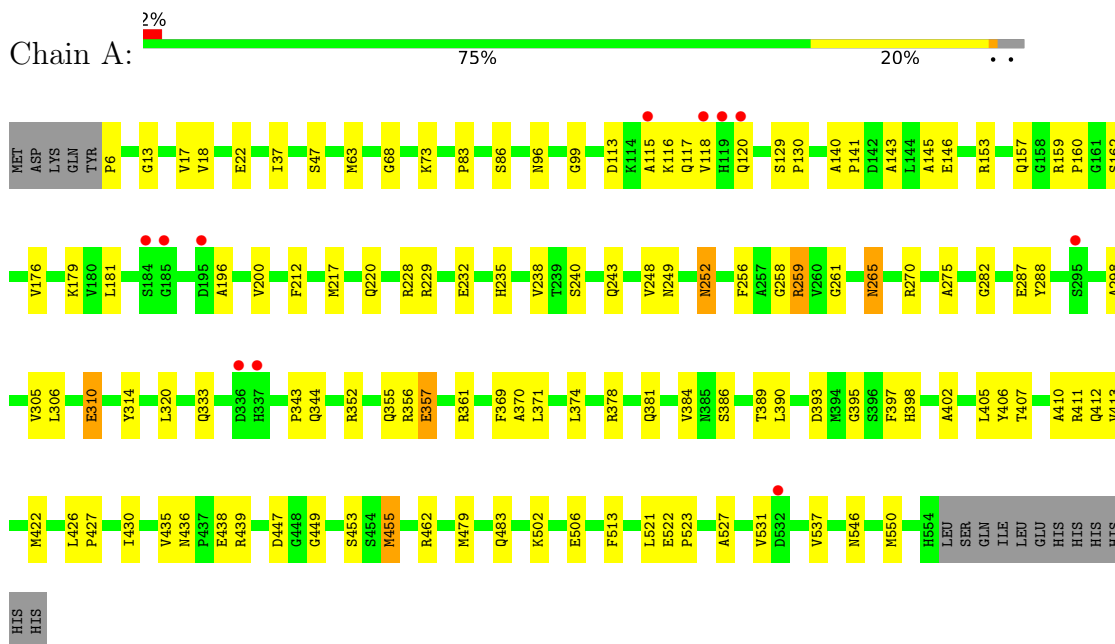
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	326	Total O 326 326	0	0
6	B	286	Total O 286 286	0	0

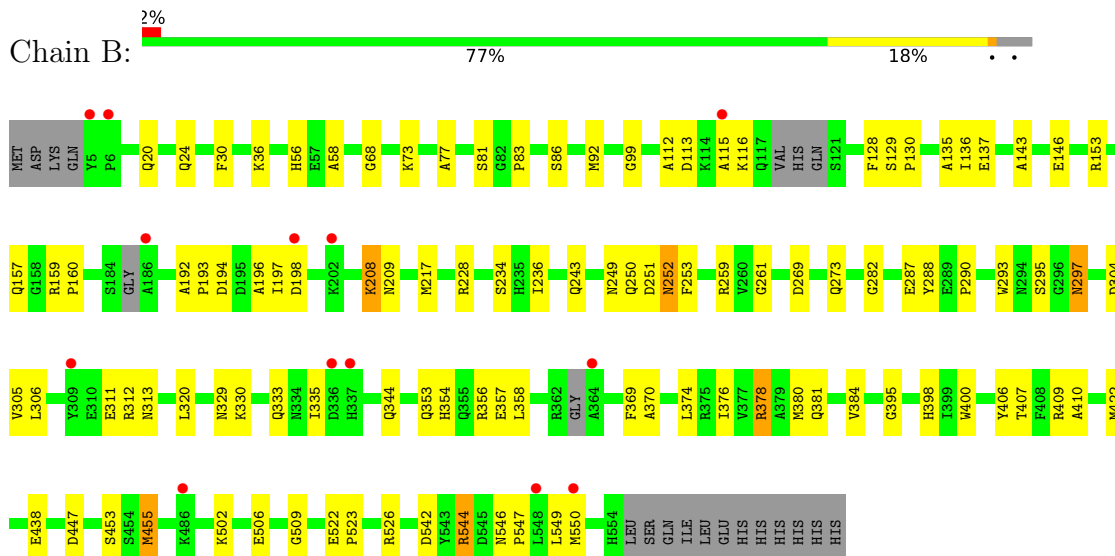
### 3 Residue-property plots [i](#)

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: Acetolactate synthase, catabolic



- Molecule 1: Acetolactate synthase, catabolic



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	117.49Å 160.56Å 129.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	100.00 – 2.30 38.05 – 2.20	Depositor EDS
% Data completeness (in resolution range)	87.9 (100.00-2.30) 81.0 (38.05-2.20)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.94 (at 2.20Å)	Xtrriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.162 , 0.214 0.158 , 0.210	Depositor DCC
$R_{free}$ test set	4836 reflections (9.64%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	19.1	Xtrriage
Anisotropy	0.560	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 59.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	8994	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	26.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.44% 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: HE3, MG, PO4, PEG

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	0.31	0/4227	0.57	0/5752
1	B	0.30	0/4188	0.57	0/5696
All	All	0.31	0/8415	0.57	0/11448

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	4146	0	4127	96	0
1	B	4110	0	4090	83	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	29	0	18	0	0
4	B	29	0	19	1	0
5	A	42	0	60	6	0
5	B	14	0	20	1	0
6	A	326	0	0	9	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	286	0	0	7	0
All	All	8994	0	8334	175	1

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 10.

All (175) 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:115:ALA:HB1	1:A:120:GLN:HB3	1.43	0.97
1:A:356:ARG:HH22	5:A:691:PEG:H11	1.39	0.86
1:A:352:ARG:HA	1:A:355:GLN:HE21	1.41	0.86
1:A:115:ALA:HA	1:A:118:VAL:HG22	1.60	0.84
1:A:270:ARG:HD2	6:A:986:HOH:O	1.84	0.76
1:B:249:ASN:HB3	6:B:850:HOH:O	1.86	0.76
1:A:371:LEU:HD23	1:A:521:LEU:HD22	1.68	0.75
1:B:159:ARG:HG2	6:B:961:HOH:O	1.84	0.75
1:A:113:ASP:OD2	1:A:115:ALA:HB3	1.86	0.75
1:B:406:TYR:CE1	1:B:407:THR:HG23	2.24	0.72
1:A:406:TYR:CE1	1:A:407:THR:HG23	2.25	0.70
1:B:502:LYS:O	1:B:506:GLU:HG3	1.92	0.69
1:A:143:ALA:HB2	1:B:116:LYS:HE2	1.75	0.68
1:B:243:GLN:NE2	1:B:287:GLU:HG2	2.10	0.67
1:B:153:ARG:HG2	1:B:157:GLN:HE22	1.60	0.66
1:A:243:GLN:NE2	1:A:287:GLU:HG2	2.12	0.65
1:B:208:LYS:HD2	1:B:209:ASN:N	2.13	0.64
1:B:353:GLN:O	1:B:357:GLU:HG3	1.98	0.64
1:A:389:THR:HG23	1:A:412:GLN:HG3	1.80	0.63
1:A:200:VAL:HG21	1:A:320:LEU:HD11	1.79	0.63
1:A:371:LEU:CD2	1:A:521:LEU:HD22	2.28	0.63
1:A:426:LEU:HB3	1:A:427:PRO:HD3	1.80	0.63
1:A:305:VAL:HG23	1:A:306:LEU:HG	1.81	0.63
1:A:361:ARG:HG3	1:A:374:LEU:HD23	1.80	0.63
1:A:275:ALA:O	1:A:298:ALA:HB2	1.99	0.63
1:A:115:ALA:HA	1:A:118:VAL:CG2	2.29	0.62
1:A:113:ASP:O	1:A:116:LYS:HB2	1.99	0.62
1:A:217:MET:HB2	1:A:282:GLY:HA3	1.82	0.62
1:B:509:GLY:HA3	5:B:701:PEG:H42	1.81	0.62
1:A:159:ARG:HG2	6:A:928:HOH:O	2.00	0.61
1:B:153:ARG:HG2	1:B:157:GLN:NE2	2.14	0.61
1:B:311:GLU:HG2	1:B:312:ARG:H	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:436:ASN:HB3	1:A:438:GLU:OE2	2.01	0.61
1:B:234:SER:HB3	1:B:335:ILE:HD13	1.82	0.60
1:B:196:ALA:HB1	1:B:320:LEU:CD2	2.30	0.59
1:A:378:ARG:HD2	6:A:884:HOH:O	2.02	0.59
1:B:261:GLY:HA2	1:B:288:TYR:CE1	2.38	0.58
1:A:261:GLY:HA2	1:A:288:TYR:CE1	2.38	0.58
1:B:395:GLY:O	1:B:398:HIS:HB3	2.03	0.58
1:B:250:GLN:HG2	1:B:356:ARG:NH1	2.19	0.58
1:B:354:HIS:O	1:B:358:LEU:HG	2.04	0.57
1:B:546:ASN:O	1:B:550:MET:HG2	2.04	0.57
1:A:361:ARG:HH11	1:A:361:ARG:HG2	1.69	0.57
1:B:438:GLU:H	1:B:438:GLU:CD	2.07	0.57
1:A:369:PHE:HA	1:A:370:ALA:C	2.25	0.56
1:A:248:VAL:HG13	1:A:252:ASN:HD21	1.70	0.56
1:B:297:ASN:C	1:B:297:ASN:HD22	2.09	0.56
1:B:406:TYR:CD1	1:B:407:THR:HG23	2.41	0.56
1:B:369:PHE:HA	1:B:370:ALA:C	2.26	0.55
1:B:153:ARG:NH1	1:B:157:GLN:HE22	2.04	0.55
1:B:135:ALA:O	1:B:136:ILE:HD13	2.07	0.55
1:A:371:LEU:HD12	1:A:371:LEU:N	2.23	0.54
1:B:378:ARG:NE	6:B:972:HOH:O	2.39	0.54
1:A:343:PRO:HG2	1:A:344:GLN:NE2	2.22	0.53
1:B:311:GLU:HG2	1:B:312:ARG:N	2.22	0.53
1:A:390:LEU:HB3	1:A:413:VAL:HG22	1.90	0.53
1:A:22:GLU:OE2	1:A:47:SER:HB2	2.09	0.53
1:B:542:ASP:OD1	1:B:544:ARG:HB2	2.08	0.53
1:A:37:ILE:O	1:A:37:ILE:HG13	2.09	0.52
1:A:462:ARG:HD2	6:A:744:HOH:O	2.08	0.52
1:B:252:ASN:HD22	1:B:253:PHE:N	2.07	0.52
1:A:196:ALA:HB1	1:A:320:LEU:CD2	2.40	0.52
1:B:409:ARG:HD2	6:B:974:HOH:O	2.09	0.52
1:A:217:MET:HB2	1:A:282:GLY:CA	2.40	0.52
1:B:282:GLY:HA2	1:B:304:ASP:OD1	2.10	0.51
1:B:344:GLN:N	1:B:344:GLN:OE1	2.43	0.51
1:B:381:GLN:NE2	1:B:407:THR:OG1	2.43	0.51
1:A:63:MET:HE3	1:A:430:ILE:HG21	1.91	0.51
1:B:522:GLU:HB2	1:B:523:PRO:HD3	1.92	0.51
1:A:252:ASN:C	1:A:252:ASN:HD22	2.15	0.51
1:A:232:GLU:HG3	6:A:807:HOH:O	2.10	0.50
1:A:356:ARG:NH2	5:A:691:PEG:H11	2.18	0.50
1:A:352:ARG:HA	1:A:355:GLN:NE2	2.17	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:249:ASN:H	1:A:252:ASN:HD21	1.60	0.50
1:B:290:PRO:HA	1:B:293:TRP:NE1	2.26	0.50
1:B:99:GLY:O	1:B:160:PRO:HB2	2.10	0.50
1:A:145:ALA:HB3	6:A:792:HOH:O	2.11	0.50
1:A:228:ARG:HH11	5:A:695:PEG:H22	1.77	0.50
1:A:352:ARG:O	1:A:355:GLN:HG2	2.12	0.50
1:B:159:ARG:NH2	1:B:282:GLY:O	2.45	0.49
1:A:228:ARG:NH1	5:A:695:PEG:H41	2.27	0.49
1:A:117:GLN:HE22	1:B:143:ALA:HB3	1.77	0.49
1:A:386:SER:O	1:A:411:ARG:HB2	2.13	0.49
1:A:371:LEU:HD12	1:A:371:LEU:H	1.76	0.49
1:B:136:ILE:HG22	1:B:137:GLU:N	2.28	0.49
1:A:422:MET:HE2	1:A:449:GLY:HA2	1.94	0.49
1:B:228:ARG:HG2	1:B:228:ARG:HH11	1.78	0.49
6:A:771:HOH:O	1:B:115:ALA:HB3	2.14	0.48
1:A:374:LEU:HG	6:A:972:HOH:O	2.14	0.48
1:A:522:GLU:HB2	1:A:523:PRO:HD3	1.95	0.48
1:A:115:ALA:CA	1:A:118:VAL:HG22	2.37	0.48
1:B:192:ALA:HB1	1:B:193:PRO:HD2	1.96	0.48
1:B:378:ARG:HG2	1:B:378:ARG:HH11	1.79	0.48
1:A:343:PRO:HG2	1:A:344:GLN:HE22	1.78	0.48
1:B:295:SER:OG	1:B:297:ASN:ND2	2.46	0.48
1:A:117:GLN:HE22	1:B:143:ALA:CB	2.27	0.48
1:B:83:PRO:HA	1:B:86:SER:OG	2.15	0.47
1:A:228:ARG:HG3	5:A:695:PEG:H41	1.96	0.47
1:B:113:ASP:HA	1:B:116:LYS:CG	2.45	0.47
1:A:99:GLY:O	1:A:160:PRO:HB2	2.15	0.47
1:A:479:MET:O	1:A:483:GLN:HG3	2.14	0.47
1:B:36:LYS:NZ	6:B:910:HOH:O	2.48	0.47
1:B:113:ASP:HA	1:B:116:LYS:HG2	1.94	0.47
1:A:361:ARG:HG3	1:A:374:LEU:CD2	2.45	0.47
1:B:56:HIS:HD2	1:B:58:ALA:H	1.62	0.47
1:B:196:ALA:HB1	1:B:320:LEU:HD22	1.96	0.46
1:B:234:SER:HB2	1:B:236:ILE:HG13	1.96	0.46
1:B:68:GLY:HA2	1:B:73:LYS:O	2.15	0.46
1:B:196:ALA:HB1	1:B:320:LEU:HD21	1.96	0.46
1:A:435:VAL:HG12	1:A:436:ASN:OD1	2.16	0.46
1:A:439:ARG:HH11	1:A:439:ARG:HG2	1.81	0.46
1:A:355:GLN:NE2	6:A:725:HOH:O	2.48	0.46
1:A:395:GLY:O	1:A:398:HIS:HB3	2.15	0.46
1:B:153:ARG:HH11	1:B:157:GLN:HE22	1.62	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:229:ARG:NH2	1:A:333:GLN:HG2	2.31	0.46
1:B:20:GLN:O	1:B:24:GLN:HG2	2.16	0.46
1:B:197:ILE:HD13	1:B:330:LYS:HB2	1.97	0.46
1:B:252:ASN:HD22	1:B:252:ASN:C	2.19	0.46
1:A:502:LYS:O	1:A:506:GLU:HG3	2.16	0.46
1:B:217:MET:HB2	1:B:282:GLY:HA3	1.98	0.46
1:A:527:ALA:O	1:A:531:VAL:HG23	2.17	0.45
1:A:453:SER:HA	1:A:455:MET:SD	2.56	0.45
1:B:422:MET:HG2	4:B:705:HE3:HM22	1.98	0.45
1:B:228:ARG:HG2	1:B:228:ARG:NH1	2.32	0.45
1:B:129:SER:HB2	1:B:130:PRO:HD3	1.99	0.45
1:B:269:ASP:O	1:B:273:GLN:HG3	2.17	0.45
1:B:311:GLU:OE1	1:B:313:ASN:HB2	2.17	0.45
1:A:546:ASN:O	1:A:550:MET:HG2	2.16	0.44
1:B:159:ARG:HD2	6:B:872:HOH:O	2.17	0.44
1:A:357:GLU:OE2	5:A:692:PEG:H41	2.18	0.44
1:A:384:VAL:CG1	1:A:410:ALA:HB2	2.46	0.44
1:A:141:PRO:HB3	1:A:176:VAL:HG12	2.00	0.44
1:A:406:TYR:CE1	1:A:407:THR:CG2	3.00	0.44
1:B:249:ASN:O	1:B:252:ASN:ND2	2.51	0.44
1:A:439:ARG:HG2	1:A:439:ARG:NH1	2.33	0.44
1:A:115:ALA:HB1	1:A:120:GLN:CB	2.30	0.43
1:B:376:ILE:O	1:B:380:MET:HG3	2.17	0.43
1:A:217:MET:HA	1:A:220:GLN:HG2	1.99	0.43
1:A:146:GLU:HA	1:A:181:LEU:HD12	2.00	0.43
1:B:36:LYS:HG3	1:B:81:SER:OG	2.18	0.43
1:B:378:ARG:N	1:B:378:ARG:HD2	2.34	0.43
1:B:400:TRP:CD2	1:B:549:LEU:HD22	2.54	0.43
1:A:256:PHE:CE2	1:A:258:GLY:HA2	2.54	0.43
1:A:6:PRO:C	1:A:179:LYS:HB3	2.39	0.43
1:A:140:ALA:HB2	1:B:112:ALA:O	2.19	0.42
1:A:212:PHE:HB2	1:A:238:VAL:HG22	2.01	0.42
1:A:229:ARG:HH21	1:A:333:GLN:HG2	1.82	0.42
1:A:83:PRO:HA	1:A:86:SER:OG	2.19	0.42
1:A:402:ALA:HA	1:A:405:LEU:HG	2.01	0.42
1:A:513:PHE:HB2	1:A:537:VAL:HG22	2.01	0.42
1:B:329:ASN:O	1:B:333:GLN:HG3	2.19	0.42
1:A:406:TYR:CD1	1:A:407:THR:HG23	2.54	0.42
1:B:153:ARG:HD2	6:B:835:HOH:O	2.19	0.42
1:B:384:VAL:CG1	1:B:410:ALA:HB2	2.50	0.42
1:A:129:SER:HB2	1:A:130:PRO:HD3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:261:GLY:HA2	1:B:288:TYR:CD1	2.55	0.41
1:B:526:ARG:O	1:B:526:ARG:HD3	2.19	0.41
1:B:305:VAL:HG23	1:B:306:LEU:HG	2.02	0.41
1:A:153:ARG:HG2	1:A:157:GLN:NE2	2.35	0.41
1:B:453:SER:HA	1:B:455:MET:SD	2.61	0.41
1:A:381:GLN:NE2	1:A:407:THR:OG1	2.54	0.41
1:A:96:ASN:HB2	1:A:162:SER:OG	2.21	0.41
1:A:265:ASN:H	1:A:265:ASN:HD22	1.68	0.41
1:A:310:GLU:HA	1:A:314:TYR:O	2.21	0.41
1:B:374:LEU:O	1:B:378:ARG:HD3	2.21	0.41
1:A:18:VAL:O	1:A:22:GLU:HG3	2.20	0.41
1:B:208:LYS:HD2	1:B:208:LYS:C	2.40	0.41
1:B:30:PHE:O	1:B:77:ALA:HA	2.22	0.41
1:A:68:GLY:HA2	1:A:73:LYS:O	2.22	0.40
1:B:92:MET:HG3	1:B:128:PHE:HE2	1.86	0.40
1:A:361:ARG:HG2	1:A:361:ARG:NH1	2.34	0.40
1:B:546:ASN:N	1:B:547:PRO:CD	2.84	0.40
1:A:13:GLY:O	1:A:17:VAL:HG23	2.21	0.40
1:A:240:SER:O	1:A:259:ARG:HA	2.20	0.40
1:A:393:ASP:HB3	1:A:397:PHE:HZ	1.86	0.40

All (1) 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)
6:A:708:HOH:O	6:A:708:HOH:O[4_556]	2.05	0.15

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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	547/566 (97%)	524 (96%)	22 (4%)	1 (0%)	47 58

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	537/566 (95%)	518 (96%)	19 (4%)	0	100	100
All	All	1084/1132 (96%)	1042 (96%)	41 (4%)	1 (0%)	51	64

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	310	GLU

### 5.3.2 Protein sidechains [i](#)

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	431/452 (95%)	424 (98%)	7 (2%)	62	78
1	B	427/452 (94%)	415 (97%)	12 (3%)	43	60
All	All	858/904 (95%)	839 (98%)	19 (2%)	52	69

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	235	HIS
1	A	252	ASN
1	A	259	ARG
1	A	265	ASN
1	A	357	GLU
1	A	447	ASP
1	A	455	MET
1	B	146	GLU
1	B	194	ASP
1	B	198	ASP
1	B	208	LYS
1	B	251	ASP
1	B	252	ASN
1	B	259	ARG
1	B	297	ASN

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Mol	Chain	Res	Type
1	B	378	ARG
1	B	447	ASP
1	B	455	MET
1	B	544	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	GLN
1	A	157	GLN
1	A	209	ASN
1	A	235	HIS
1	A	243	GLN
1	A	252	ASN
1	A	265	ASN
1	A	355	GLN
1	A	381	GLN
1	A	554	HIS
1	B	9	GLN
1	B	56	HIS
1	B	87	ASN
1	B	157	GLN
1	B	199	GLN
1	B	243	GLN
1	B	252	ASN
1	B	297	ASN
1	B	313	ASN
1	B	381	GLN

### 5.3.3 RNA [i](#)

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 monosaccharides in this entry.



## 5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 2 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
5	PEG	B	702	-	6,6,6	0.74	0	5,5,5	1.64	1 (20%)
5	PEG	A	691	-	6,6,6	0.72	0	5,5,5	1.61	1 (20%)
4	HE3	A	700	3	22,31,31	4.43	15 (68%)	26,49,49	3.22	14 (53%)
4	HE3	B	705	3	22,31,31	4.36	15 (68%)	26,49,49	3.18	12 (46%)
5	PEG	A	692	-	6,6,6	0.70	0	5,5,5	1.64	1 (20%)
5	PEG	A	695	-	6,6,6	0.72	0	5,5,5	1.65	1 (20%)
5	PEG	A	693	-	6,6,6	0.63	0	5,5,5	1.61	1 (20%)
5	PEG	A	696	-	6,6,6	0.67	0	5,5,5	1.63	1 (20%)
5	PEG	B	701	-	6,6,6	0.68	0	5,5,5	1.60	1 (20%)
2	PO4	A	697	-	4,4,4	1.59	0	6,6,6	0.44	0
5	PEG	A	694	-	6,6,6	0.65	0	5,5,5	1.66	1 (20%)
2	PO4	B	703	-	4,4,4	1.63	0	6,6,6	0.43	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
5	PEG	B	702	-	-	1/4/4/4	-
5	PEG	A	691	-	-	2/4/4/4	-
4	HE3	A	700	3	-	4/13/47/47	0/3/3/3
4	HE3	B	705	3	-	3/13/47/47	0/3/3/3
5	PEG	A	692	-	-	1/4/4/4	-
5	PEG	A	695	-	-	1/4/4/4	-
5	PEG	A	693	-	-	0/4/4/4	-
5	PEG	B	701	-	-	2/4/4/4	-
5	PEG	A	694	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	PEG	A	696	-	-	1/4/4/4	-

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	700	HE3	C5'-C4'	9.78	1.50	1.41
4	B	705	HE3	C5'-C4'	9.47	1.50	1.41
4	A	700	HE3	C2'-N1'	8.06	1.47	1.34
4	B	705	HE3	C2'-N1'	8.04	1.47	1.34
4	A	700	HE3	C6'-N1'	7.57	1.50	1.34
4	B	705	HE3	C6'-N1'	7.41	1.50	1.34
4	A	700	HE3	C5-C4	6.48	1.49	1.35
4	B	705	HE3	C5-C4	6.48	1.49	1.35
4	B	705	HE3	C4'-N3'	5.66	1.45	1.34
4	A	700	HE3	C4'-N3'	5.35	1.44	1.34
4	A	700	HE3	C7'-N3	4.96	1.53	1.46
4	A	700	HE3	C6'-C5'	4.76	1.47	1.37
4	B	705	HE3	C2'-N3'	4.74	1.42	1.34
4	B	705	HE3	C6'-C5'	4.73	1.47	1.37
4	A	700	HE3	C2'-N3'	4.35	1.41	1.34
4	B	705	HE3	C7'-N3	4.14	1.52	1.46
4	A	700	HE3	C6-C5	-3.99	1.43	1.50
4	A	700	HE3	O9-C8	3.78	1.53	1.43
4	B	705	HE3	O9-C8	3.76	1.52	1.43
4	B	705	HE3	CM4-C4	3.67	1.55	1.49
4	A	700	HE3	CM4-C4	3.33	1.54	1.49
4	B	705	HE3	PA-O7	-3.30	1.46	1.59
4	A	700	HE3	PA-O7	-3.26	1.46	1.59
4	B	705	HE3	C6-C5	-3.11	1.44	1.50
4	A	700	HE3	PB-O1B	-2.83	1.43	1.54
4	B	705	HE3	PB-O1B	-2.82	1.44	1.54
4	B	705	HE3	PA-O2A	-2.58	1.43	1.55
4	A	700	HE3	PA-O2A	-2.50	1.43	1.55
4	B	705	HE3	CM2-C2'	-2.40	1.42	1.49
4	A	700	HE3	CM2-C2'	-2.35	1.43	1.49

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	700	HE3	CM2-C2'-N1'	8.98	127.02	117.14
4	B	705	HE3	CM2-C2'-N1'	8.79	126.81	117.14
4	A	700	HE3	O9-C8-C9	-7.72	91.10	109.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	705	HE3	O9-C8-C9	-7.45	91.71	109.02
4	B	705	HE3	N1'-C2'-N3'	-5.09	116.78	125.54
4	A	700	HE3	N1'-C2'-N3'	-5.01	116.92	125.54
4	B	705	HE3	C6'-N1'-C2'	4.67	123.92	115.96
4	A	700	HE3	C6'-N1'-C2'	4.65	123.88	115.96
4	A	700	HE3	PA-O7-C7	3.48	138.72	121.59
4	B	705	HE3	PA-O7-C7	3.37	138.16	121.59
4	B	705	HE3	O7-C7-C6	3.09	121.25	108.64
4	A	700	HE3	O7-C7-C6	2.97	120.78	108.64
4	A	700	HE3	C6-C5-C4	-2.86	120.94	128.20
4	B	705	HE3	C7-C6-C5	2.85	121.79	112.73
4	B	705	HE3	C6-C5-C4	-2.85	120.96	128.20
5	A	692	PEG	O2-C2-C1	2.68	121.85	110.07
5	B	702	PEG	O2-C2-C1	2.66	121.77	110.07
5	A	691	PEG	O2-C2-C1	2.65	121.72	110.07
4	A	700	HE3	C5'-C4'-N3'	2.65	126.56	122.44
4	A	700	HE3	C7'-C5'-C6'	2.62	125.40	120.05
5	A	695	PEG	O2-C2-C1	2.60	121.50	110.07
4	B	705	HE3	C5'-C4'-N3'	2.59	126.47	122.44
5	A	694	PEG	O2-C2-C1	2.55	121.27	110.07
5	A	696	PEG	O2-C2-C1	2.54	121.22	110.07
5	B	701	PEG	O2-C2-C1	2.54	121.22	110.07
4	A	700	HE3	C5'-C6'-N1'	-2.52	119.62	123.82
5	A	693	PEG	O2-C2-C1	2.51	121.08	110.07
4	B	705	HE3	C7'-C5'-C6'	2.49	125.13	120.05
4	B	705	HE3	C5'-C6'-N1'	-2.36	119.89	123.82
4	A	700	HE3	C7-C6-C5	2.34	120.16	112.73
4	B	705	HE3	C6-C5-S1	2.27	124.07	119.18
4	A	700	HE3	C6-C5-S1	2.06	123.63	119.18
4	A	700	HE3	C6'-C5'-C4'	-2.01	112.95	115.66
4	A	700	HE3	O2B-PB-O1B	2.00	115.28	107.64

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	694	PEG	O1-C1-C2-O2
5	A	695	PEG	O1-C1-C2-O2
5	B	701	PEG	O1-C1-C2-O2
5	B	702	PEG	O1-C1-C2-O2
5	A	691	PEG	O1-C1-C2-O2
5	A	696	PEG	O1-C1-C2-O2

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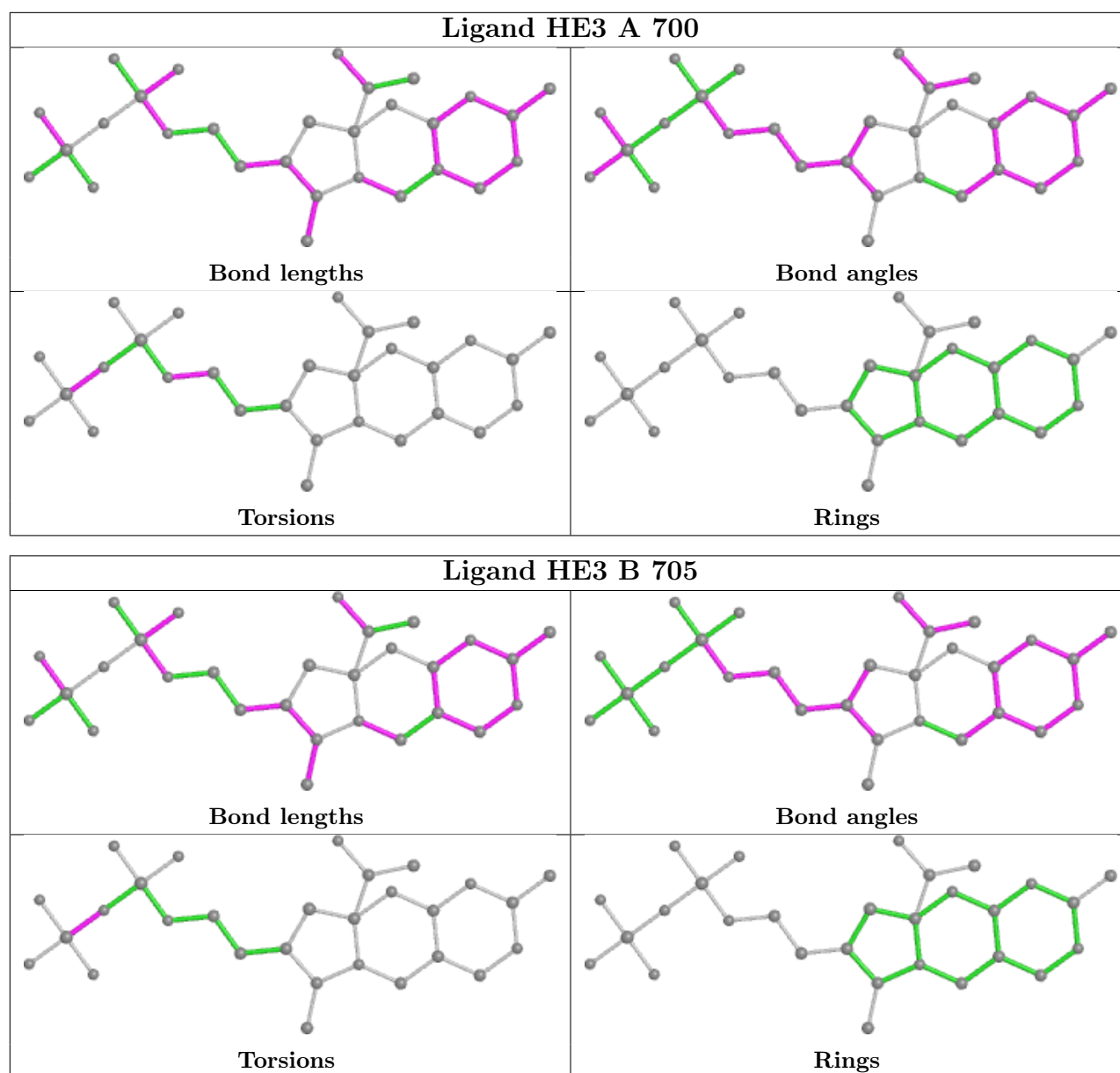
Mol	Chain	Res	Type	Atoms
4	A	700	HE3	PA-O1A-PB-O3B
4	B	705	HE3	PA-O1A-PB-O3B
5	A	691	PEG	C4-C3-O2-C2
5	B	701	PEG	C4-C3-O2-C2
5	A	694	PEG	C4-C3-O2-C2
5	A	692	PEG	C4-C3-O2-C2
4	A	700	HE3	PA-O1A-PB-O1B
4	A	700	HE3	PA-O1A-PB-O2B
4	B	705	HE3	PA-O1A-PB-O1B
4	B	705	HE3	PA-O1A-PB-O2B
4	A	700	HE3	C6-C7-O7-PA

There are no ring outliers.

5 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	691	PEG	2	0
4	B	705	HE3	1	0
5	A	692	PEG	1	0
5	A	695	PEG	3	0
5	B	701	PEG	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## 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	549/566 (96%)	-0.52	11 (2%) 65 71	10, 21, 46, 85	0
1	B	545/566 (96%)	-0.40	13 (2%) 59 66	11, 24, 50, 73	0
All	All	1094/1132 (96%)	-0.46	24 (2%) 62 69	10, 22, 49, 85	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	337	HIS	4.7
1	A	120	GLN	4.3
1	B	5	TYR	3.8
1	A	295	SER	3.3
1	B	336	ASP	3.1
1	B	186	ALA	3.0
1	A	184	SER	3.0
1	B	364	ALA	2.9
1	A	115	ALA	2.8
1	B	548	LEU	2.7
1	A	185	GLY	2.7
1	A	195	ASP	2.6
1	A	532	ASP	2.5
1	A	336	ASP	2.5
1	B	115	ALA	2.4
1	A	119	HIS	2.4
1	B	198	ASP	2.3
1	B	6	PRO	2.2
1	B	486	LYS	2.1
1	A	337	HIS	2.1
1	A	118	VAL	2.1
1	B	202	LYS	2.1
1	B	309	TYR	2.1
1	B	550	MET	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 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.

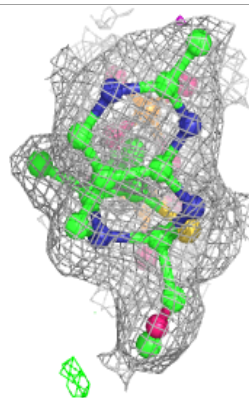
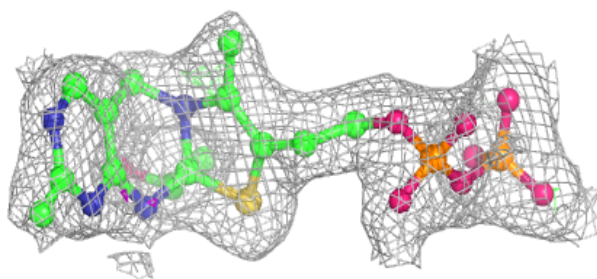
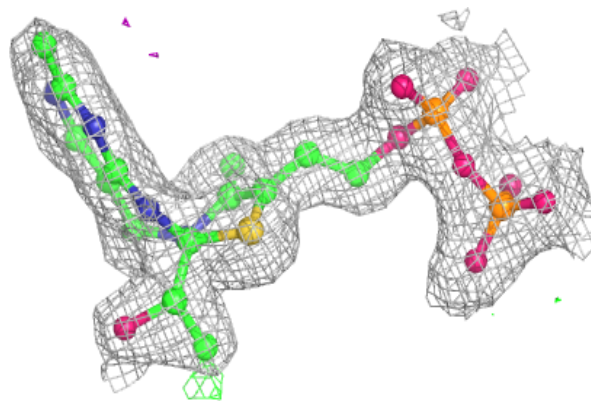
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
5	PEG	A	696	7/7	0.65	0.22	55,56,57,57	0
5	PEG	A	692	7/7	0.83	0.20	51,51,52,55	0
5	PEG	B	702	7/7	0.85	0.20	61,64,67,67	0
5	PEG	B	701	7/7	0.87	0.23	56,57,60,61	0
5	PEG	A	694	7/7	0.88	0.14	41,42,44,45	0
5	PEG	A	693	7/7	0.88	0.18	45,46,48,51	0
5	PEG	A	695	7/7	0.92	0.15	37,39,40,42	0
5	PEG	A	691	7/7	0.92	0.17	33,36,38,39	0
3	MG	A	699	1/1	0.97	0.08	14,14,14,14	0
4	HE3	A	700	29/29	0.98	0.09	8,23,27,32	0
4	HE3	B	705	29/29	0.98	0.11	8,15,19,22	0
2	PO4	B	703	5/5	0.99	0.08	22,24,25,26	0
2	PO4	A	697	5/5	0.99	0.07	12,13,16,17	0
3	MG	B	704	1/1	1.00	0.06	10,10,10,10	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

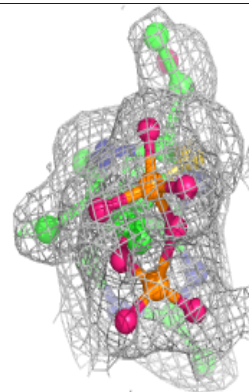
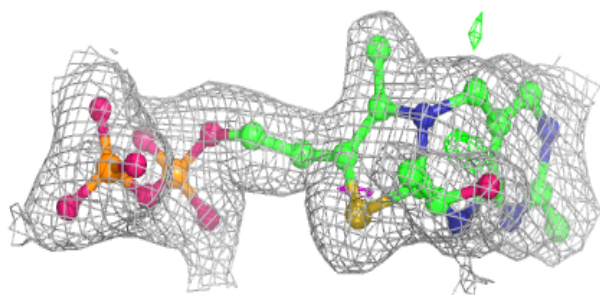
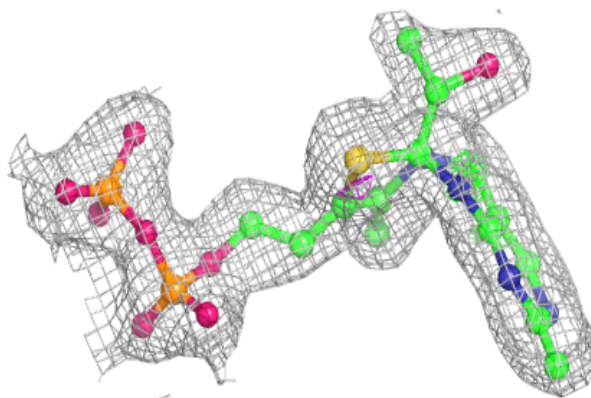


**Electron density around HE3 A 700:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around HE3 B 705:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





## 6.5 Other polymers [i](#)

There are no such residues in this entry.