Full wwPDB X-ray Structure Validation Report (i)

Aug 7, 2023 – 02:41 PM EDT

PDB ID	:	1OZH
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	:	2.00 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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

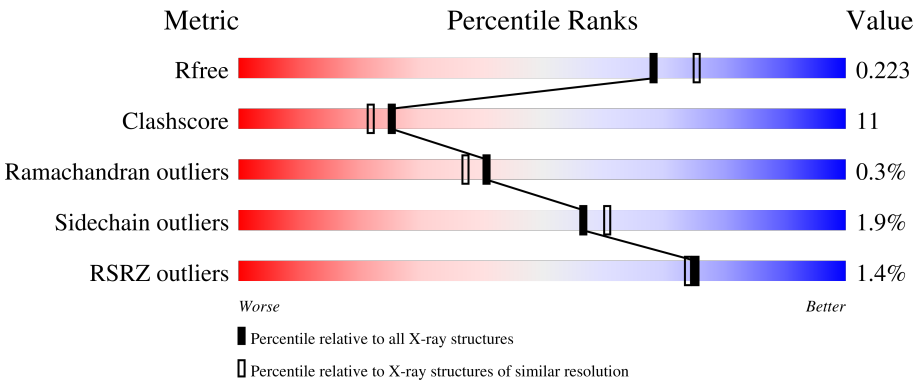
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

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 >=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 <=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	.% 76% 19% • •
1	B	566	.% 75% 21% • •
1	C	566	2% 76% 19% • •
1	D	566	.% 76% 18% • 5%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 17798 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	545	4094	2587	717	771	19	0	1	0
1	B	545	4066	2571	710	767	18	0	1	0
1	C	543	4070	2572	711	769	18	0	0	0
1	D	538	4038	2555	705	761	17	0	0	0

There are 28 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
C	560	GLU	-	expression tag	UNP P27696
C	561	HIS	-	expression tag	UNP P27696
C	562	HIS	-	expression tag	UNP P27696
C	563	HIS	-	expression tag	UNP P27696
C	564	HIS	-	expression tag	UNP P27696
C	565	HIS	-	expression tag	UNP P27696
C	566	HIS	-	expression tag	UNP P27696

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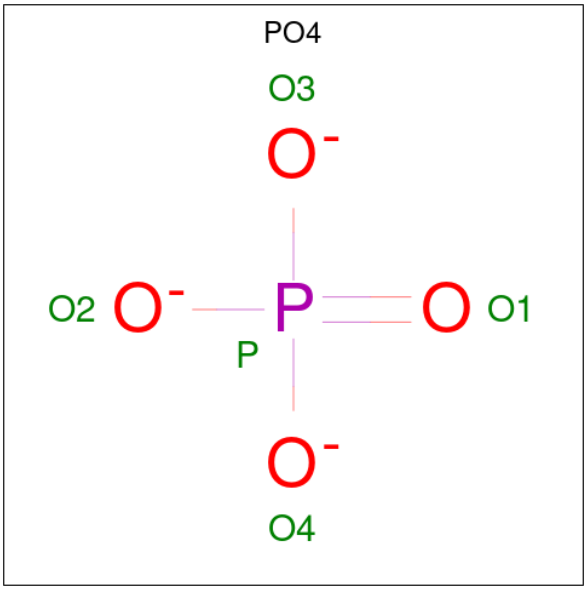
Chain	Residue	Modelled	Actual	Comment	Reference
D	560	GLU	-	expression tag	UNP P27696
D	561	HIS	-	expression tag	UNP P27696
D	562	HIS	-	expression tag	UNP P27696
D	563	HIS	-	expression tag	UNP P27696
D	564	HIS	-	expression tag	UNP P27696
D	565	HIS	-	expression tag	UNP P27696
D	566	HIS	-	expression tag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

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



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

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

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

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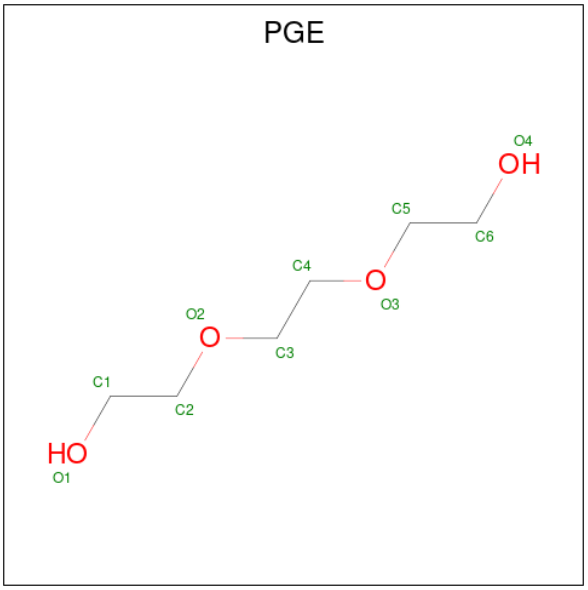
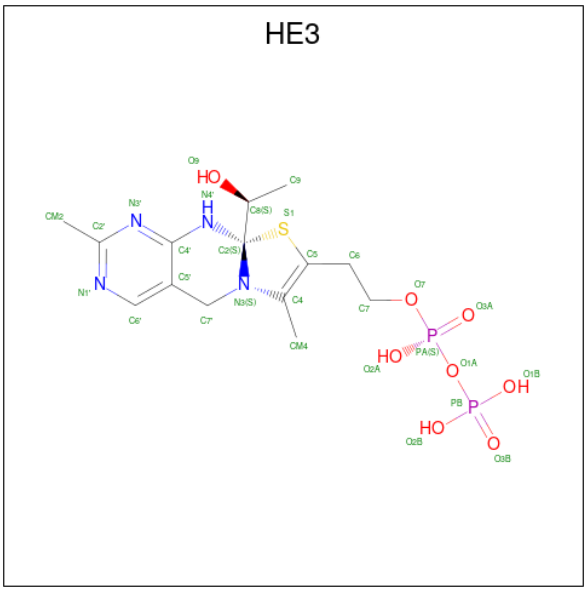
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total Mg 1 1	0	0
3	C	1	Total Mg 1 1	0	0
3	D	1	Total Mg 1 1	0	0

- Molecule 4 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



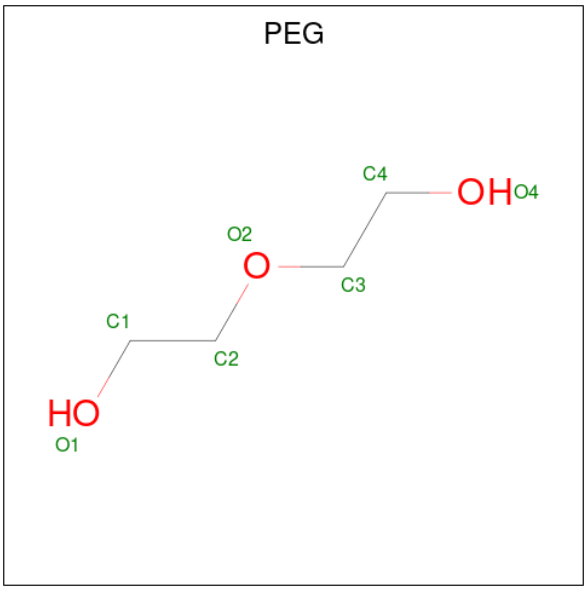
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 10 6 4	0	0
4	A	1	Total C O 10 6 4	0	0

- Molecule 5 is 2-HYDROXYETHYL DIHYDROTHIACHROME DIPHOSPHATE (three-letter code: HE3) (formula: $C_{14}H_{22}N_4O_8P_2S$).



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

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



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

- Molecule 7 is water.

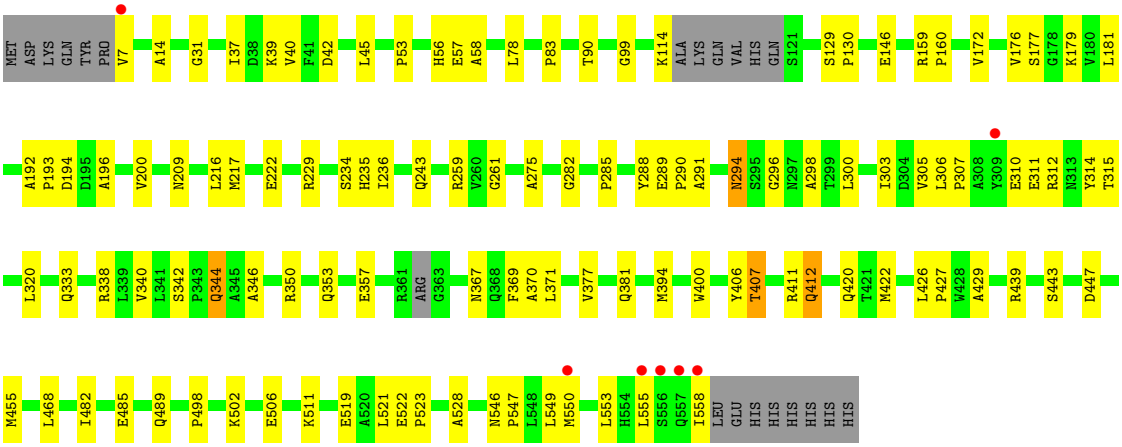
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
7	A	318	318	318	0	0
7	B	352	352	352	0	0
7	C	352	352	352	0	0
7	D	313	313	313	0	0

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.

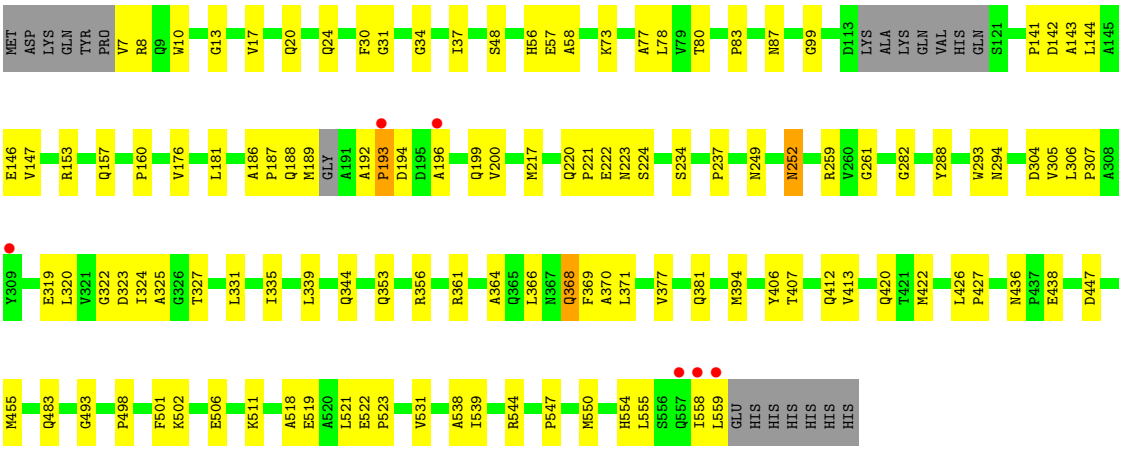
• Molecule 1: Acetolactate synthase, catabolic

Chain A:



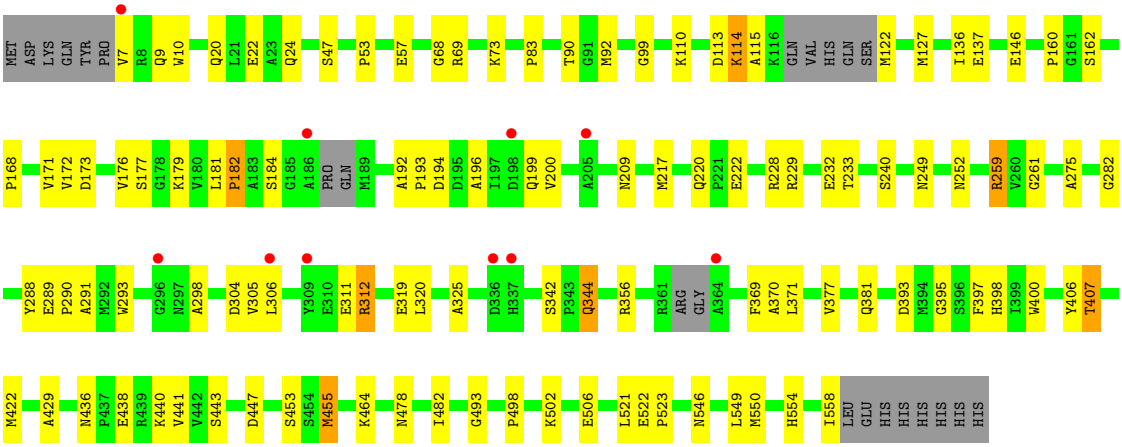
• Molecule 1: Acetolactate synthase, catabolic

Chain B:



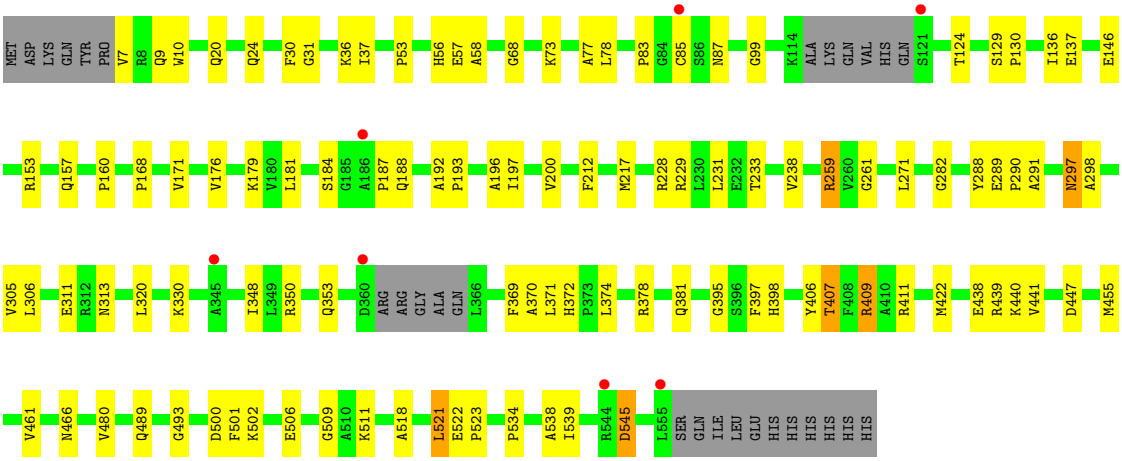
• Molecule 1: Acetolactate synthase, catabolic

Chain C:



- Molecule 1: Acetolactate synthase, catabolic

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	86.32Å 92.81Å 97.42Å 67.97° 63.48° 67.68°	Depositor
Resolution (Å)	100.00 – 2.00 83.17 – 2.00	Depositor EDS
% Data completeness (in resolution range)	91.0 (100.00-2.00) 91.1 (83.17-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.03	Depositor
$< I/\sigma(I) >$ [1]	3.69 (at 2.00Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.191 , 0.228 0.188 , 0.223	Depositor DCC
R_{free} test set	15316 reflections (9.99%)	wwPDB-VP
Wilson B-factor (Å^2)	25.5	Xtriage
Anisotropy	0.146	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 60.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	17798	wwPDB-VP
Average B, all atoms (Å^2)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.39% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: PEG, PGE, MG, PO4, HE3

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	0.30	0/4175	0.58	0/5682
1	B	0.30	0/4146	0.58	0/5649
1	C	0.31	0/4144	0.59	1/5639 (0.0%)
1	D	0.30	0/4115	0.57	0/5601
All	All	0.30	0/16580	0.58	1/22571 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	182	PRO	N-CA-CB	5.52	109.92	103.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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	4094	0	4062	94	0
1	B	4066	0	4006	95	0
1	C	4070	0	4027	85	0
1	D	4038	0	4010	86	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	5	0	0	0	0
2	D	5	0	0	1	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	20	0	28	3	0
5	A	29	0	19	3	0
5	B	29	0	19	3	0
5	C	29	0	19	3	0
5	D	29	0	19	3	0
6	A	7	0	10	1	0
6	B	14	0	20	2	0
6	C	7	0	10	1	0
6	D	7	0	10	2	0
7	A	318	0	0	7	0
7	B	352	0	0	10	0
7	C	352	0	0	8	0
7	D	313	0	0	6	0
All	All	17798	0	16259	350	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 11.

All (350) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:368:GLN:H	1:B:368:GLN:HE21	1.05	0.99
1:A:344:GLN:H	1:A:344:GLN:NE2	1.67	0.93
1:C:482:ILE:HD12	1:C:550:MET:HG3	1.53	0.91
1:D:371:LEU:HD21	1:D:518:ALA:HA	1.59	0.84
1:A:7:VAL:HA	1:A:179:LYS:HB3	1.59	0.82
1:D:212:PHE:HB2	1:D:238:VAL:HG12	1.61	0.82
1:D:371:LEU:HD13	1:D:521:LEU:HD22	1.60	0.81
1:B:371:LEU:HD21	1:B:518:ALA:HA	1.61	0.81
1:B:305:VAL:HG23	1:B:306:LEU:HG	1.61	0.80
1:C:344:GLN:H	1:C:344:GLN:NE2	1.81	0.79
1:C:196:ALA:HB1	1:C:320:LEU:HD22	1.65	0.78
1:B:56:HIS:HD2	1:B:58:ALA:H	1.31	0.78
1:C:371:LEU:HD23	1:C:521:LEU:HD22	1.66	0.77
1:B:305:VAL:HG12	7:B:1579:HOH:O	1.84	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:200:VAL:HG21	1:A:320:LEU:HD11	1.67	0.75
1:B:249:ASN:H	1:B:252:ASN:HD21	1.35	0.75
1:A:344:GLN:H	1:A:344:GLN:HE21	1.34	0.73
1:A:56:HIS:HD2	1:A:58:ALA:H	1.34	0.73
1:A:371:LEU:HD23	1:A:521:LEU:HD22	1.70	0.73
1:D:200:VAL:HG21	1:D:320:LEU:HD11	1.70	0.72
1:C:344:GLN:H	1:C:344:GLN:HE21	1.38	0.70
1:B:371:LEU:HD13	1:B:521:LEU:HD22	1.72	0.70
1:B:221:PRO:HG2	1:B:222:GLU:OE2	1.93	0.69
1:A:371:LEU:CD2	1:A:521:LEU:HD22	2.23	0.68
1:C:498:PRO:HG2	6:D:1430:PEG:H11	1.74	0.68
1:A:340:VAL:HG22	7:A:1502:HOH:O	1.94	0.68
1:D:406:TYR:CE1	1:D:407:THR:HG23	2.29	0.68
1:D:196:ALA:HB1	1:D:320:LEU:HD22	1.76	0.67
1:C:478:ASN:HD21	1:C:546:ASN:HD22	1.42	0.67
1:B:220:GLN:NE2	7:B:1557:HOH:O	2.28	0.67
1:D:7:VAL:HA	1:D:179:LYS:HB3	1.77	0.66
1:A:371:LEU:H	1:A:371:LEU:HD12	1.60	0.65
1:D:229:ARG:O	1:D:233:THR:HG23	1.95	0.65
1:B:200:VAL:HG21	1:B:320:LEU:HD11	1.77	0.65
1:C:192:ALA:HB1	1:C:193:PRO:HD2	1.77	0.65
1:D:369:PHE:HA	1:D:370:ALA:C	2.15	0.65
1:D:372:HIS:HD2	1:D:374:LEU:H	1.45	0.65
1:A:377:VAL:O	1:A:381:GLN:HG3	1.96	0.64
1:B:377:VAL:O	1:B:381:GLN:HG3	1.98	0.64
1:A:369:PHE:HA	1:A:370:ALA:C	2.17	0.64
4:A:1403:PGE:H4	7:A:1543:HOH:O	1.97	0.64
1:A:311:GLU:HG2	1:A:312:ARG:N	2.13	0.64
1:C:99:GLY:O	1:C:160:PRO:HB2	1.98	0.64
1:B:519:GLU:H	1:B:519:GLU:CD	2.01	0.63
1:B:361:ARG:HG2	1:B:364:ALA:HB2	1.81	0.63
1:C:199:GLN:HB3	7:C:1764:HOH:O	1.97	0.63
1:A:311:GLU:HG2	1:A:312:ARG:H	1.64	0.62
1:D:261:GLY:HA2	1:D:288:TYR:CE1	2.35	0.62
1:B:193:PRO:HB2	1:B:196:ALA:HB3	1.81	0.61
1:B:426:LEU:HB3	1:B:427:PRO:HD3	1.83	0.61
1:C:371:LEU:CD2	1:C:521:LEU:HD22	2.30	0.60
1:B:394:MET:HE3	1:B:420:GLN:HA	1.83	0.60
1:B:555:LEU:O	1:B:559:LEU:HD13	2.01	0.60
1:B:436:ASN:HB3	1:B:438:GLU:OE2	2.00	0.60
1:C:377:VAL:O	1:C:381:GLN:HG3	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:193:PRO:HG2	1:A:196:ALA:CB	2.31	0.60
1:B:369:PHE:HA	1:B:370:ALA:C	2.22	0.59
1:C:369:PHE:HA	1:C:370:ALA:C	2.21	0.59
1:A:261:GLY:HA2	1:A:288:TYR:CE1	2.37	0.59
1:B:368:GLN:H	1:B:368:GLN:NE2	1.88	0.59
1:B:73:LYS:HE3	7:B:1437:HOH:O	2.01	0.59
1:C:228:ARG:O	1:C:232:GLU:HG3	2.02	0.59
1:A:546:ASN:O	1:A:550[A]:MET:HG2	2.02	0.59
1:C:554:HIS:O	1:C:558:ILE:HG12	2.02	0.59
1:B:8:ARG:HD3	1:B:10:TRP:CZ2	2.37	0.59
1:A:193:PRO:HG2	1:A:196:ALA:HB3	1.83	0.59
1:B:222:GLU:O	1:B:325:ALA:HB2	2.03	0.59
1:A:411:ARG:NH1	1:A:439:ARG:HD2	2.18	0.58
1:D:372:HIS:CD2	1:D:374:LEU:H	2.21	0.58
1:A:426:LEU:HB3	1:A:427:PRO:HD3	1.85	0.58
1:D:56:HIS:HD2	1:D:58:ALA:H	1.51	0.58
5:A:1406:HE3:N1'	1:B:57:GLU:OE2	2.36	0.58
5:C:1423:HE3:HM23	1:D:83:PRO:HB2	1.83	0.58
1:A:235:HIS:ND1	1:A:338:ARG:HD3	2.18	0.58
1:D:511:LYS:HD2	7:D:1538:HOH:O	2.03	0.58
1:B:502:LYS:O	1:B:506:GLU:HG3	2.04	0.57
1:A:511:LYS:HA	1:A:511:LYS:HE2	1.87	0.57
1:B:261:GLY:HA2	1:B:288:TYR:CE1	2.39	0.57
1:C:200:VAL:HG21	1:C:320:LEU:HD11	1.87	0.56
1:D:502:LYS:O	1:D:506:GLU:HG3	2.05	0.56
1:A:371:LEU:HD12	1:A:371:LEU:N	2.20	0.56
1:B:331:LEU:O	1:B:335:ILE:HG13	2.07	0.55
1:D:36:LYS:HE2	7:D:1679:HOH:O	2.06	0.55
1:D:350:ARG:O	1:D:353:GLN:HB3	2.06	0.55
1:B:30:PHE:O	1:B:77:ALA:HA	2.06	0.55
1:A:307:PRO:HB3	1:D:187:PRO:HG2	1.88	0.55
1:C:229:ARG:O	1:C:233:THR:HG23	2.07	0.55
1:D:297:ASN:HD22	1:D:298:ALA:N	2.04	0.55
1:B:237:PRO:HD3	1:B:339:LEU:HD23	1.89	0.55
1:B:406:TYR:CE1	1:B:407:THR:HG23	2.42	0.55
1:C:146:GLU:HA	1:C:181:LEU:HD12	1.90	0.54
1:D:440:LYS:HE3	1:D:466:ASN:ND2	2.22	0.54
1:C:422:MET:HG2	5:C:1423:HE3:HM22	1.90	0.54
1:D:197:ILE:HD13	1:D:330:LYS:HB2	1.88	0.54
1:B:522:GLU:HB2	1:B:523:PRO:HD3	1.88	0.54
1:B:249:ASN:H	1:B:252:ASN:ND2	2.04	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:356:ARG:HD3	7:C:1666:HOH:O	2.07	0.54
1:A:305:VAL:HG23	1:A:306:LEU:HG	1.90	0.54
1:A:217:MET:HB2	1:A:282:GLY:HA3	1.88	0.54
1:A:216:LEU:HB2	1:A:243:GLN:OE1	2.08	0.54
1:D:522:GLU:HB2	1:D:523:PRO:HD3	1.89	0.54
5:A:1406:HE3:HM23	1:B:83:PRO:HB2	1.89	0.53
1:D:371:LEU:HD12	1:D:539:ILE:HG23	1.90	0.53
1:A:57:GLU:OE2	5:B:1413:HE3:N1'	2.42	0.53
1:D:197:ILE:HD12	1:D:330:LYS:HE2	1.91	0.53
1:B:153:ARG:NH2	7:B:1665:HOH:O	2.31	0.53
1:A:468:LEU:HD13	1:A:528:ALA:HB1	1.90	0.53
1:C:113:ASP:C	1:C:115:ALA:H	2.12	0.53
1:C:478:ASN:HD21	1:C:546:ASN:ND2	2.05	0.53
1:A:114:LYS:HD2	7:A:1678:HOH:O	2.09	0.53
1:A:511:LYS:HE2	1:A:511:LYS:CA	2.38	0.53
1:A:83:PRO:HB2	5:B:1413:HE3:HM23	1.91	0.53
1:C:406:TYR:CE1	1:C:407:THR:HG23	2.44	0.53
1:D:136:ILE:HG12	1:D:137:GLU:N	2.24	0.53
1:B:37:ILE:HG13	1:B:37:ILE:O	2.08	0.53
1:A:315:THR:HG21	1:D:181:LEU:HD22	1.90	0.52
1:A:381:GLN:HE22	1:A:407:THR:CB	2.22	0.52
1:D:440:LYS:HG3	1:D:441:VAL:N	2.25	0.52
1:D:289:GLU:HG2	1:D:291:ALA:HB3	1.92	0.52
1:B:249:ASN:O	1:B:252:ASN:ND2	2.43	0.52
1:C:172:VAL:HG23	1:C:173:ASP:OD1	2.10	0.52
1:A:159:ARG:HG2	1:A:306:LEU:HD12	1.92	0.52
1:C:83:PRO:HB2	5:D:1433:HE3:HM23	1.90	0.52
1:A:411:ARG:HH11	1:A:439:ARG:HD2	1.73	0.52
4:A:1402:PGE:H6	7:A:1573:HOH:O	2.08	0.52
1:B:196:ALA:O	1:B:199:GLN:HB3	2.09	0.52
1:C:193:PRO:HG2	1:C:196:ALA:HB2	1.92	0.52
1:B:146:GLU:HA	1:B:181:LEU:HD22	1.92	0.51
1:A:346:ALA:O	1:A:350:ARG:HG3	2.10	0.51
1:A:482:ILE:HD12	1:A:550[A]:MET:HG3	1.92	0.51
1:A:261:GLY:HA2	1:A:288:TYR:CD1	2.46	0.51
1:B:143:ALA:O	1:B:147:VAL:HG23	2.11	0.51
1:B:335:ILE:HA	7:B:1564:HOH:O	2.10	0.51
1:D:9:GLN:HG3	7:D:1703:HOH:O	2.11	0.51
1:D:545:ASP:HB2	7:D:1665:HOH:O	2.10	0.51
1:C:193:PRO:HG2	1:C:196:ALA:CB	2.41	0.51
1:A:99:GLY:O	1:A:160:PRO:HB2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:146:GLU:HA	1:A:181:LEU:HD12	1.93	0.51
1:D:439:ARG:HG2	1:D:439:ARG:HH11	1.76	0.51
1:C:57:GLU:OE2	5:D:1433:HE3:N1'	2.44	0.50
1:C:182:PRO:HA	7:C:1556:HOH:O	2.10	0.50
1:D:217:MET:HB2	1:D:282:GLY:HA3	1.93	0.50
1:D:10:TRP:HB2	1:D:176:VAL:CG1	2.42	0.50
1:B:193:PRO:HB2	1:B:196:ALA:CB	2.40	0.50
1:B:554:HIS:O	1:B:558:ILE:HG13	2.11	0.50
1:D:157:GLN:OE1	1:D:187:PRO:HD3	2.11	0.50
1:A:429:ALA:HB2	1:A:443:SER:HB3	1.93	0.50
1:B:412:GLN:HG2	1:B:413:VAL:N	2.27	0.50
1:B:422:MET:HG2	5:B:1413:HE3:HM22	1.93	0.50
1:C:217:MET:HB2	1:C:282:GLY:HA3	1.92	0.50
1:A:56:HIS:CD2	1:A:58:ALA:H	2.23	0.50
1:B:48:SER:HB3	7:B:1629:HOH:O	2.10	0.50
1:C:464:LYS:HD3	7:C:1598:HOH:O	2.11	0.50
1:C:371:LEU:N	1:C:371:LEU:HD12	2.27	0.50
1:C:546:ASN:O	1:C:550:MET:HG2	2.12	0.50
4:A:1403:PGE:H2	7:A:1723:HOH:O	2.10	0.49
1:B:8:ARG:HH11	1:B:8:ARG:HG2	1.75	0.49
1:B:99:GLY:O	1:B:160:PRO:HB2	2.11	0.49
1:D:297:ASN:HD22	1:D:297:ASN:N	2.09	0.49
1:A:14:ALA:HB2	1:A:172:VAL:CG1	2.42	0.49
1:D:20:GLN:O	1:D:24:GLN:HG2	2.13	0.49
1:A:502:LYS:O	1:A:506:GLU:HG3	2.12	0.49
1:B:153:ARG:HD3	7:B:1515:HOH:O	2.13	0.49
1:C:9:GLN:NE2	1:C:177:SER:HB3	2.28	0.49
1:B:406:TYR:CE1	1:B:407:THR:CG2	2.95	0.49
1:C:22:GLU:OE2	1:C:47:SER:HB2	2.13	0.49
1:B:192:ALA:HB1	1:B:193:PRO:CD	2.43	0.48
1:D:438:GLU:H	1:D:438:GLU:CD	2.17	0.48
1:D:146:GLU:HA	1:D:181:LEU:HD12	1.94	0.48
1:B:319:GLU:O	1:B:320:LEU:HD23	2.12	0.48
1:A:229:ARG:HH22	1:A:333:GLN:HG2	1.77	0.48
1:B:252:ASN:C	1:B:252:ASN:HD22	2.17	0.48
1:C:502:LYS:O	1:C:506:GLU:HG3	2.13	0.48
5:C:1423:HE3:N1'	1:D:57:GLU:OE2	2.47	0.48
1:C:371:LEU:HD12	1:C:371:LEU:H	1.79	0.48
1:B:293:TRP:CZ3	1:B:294:ASN:HB2	2.49	0.48
1:B:511:LYS:HD2	1:B:531:VAL:CG1	2.43	0.48
1:D:409:ARG:HG3	7:D:1514:HOH:O	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:344:GLN:NE2	1:A:344:GLN:N	2.50	0.48
1:B:142:ASP:HB3	1:C:312:ARG:HH21	1.78	0.48
1:A:340:VAL:HG23	1:A:340:VAL:O	2.13	0.48
1:A:485:GLU:OE2	1:A:489:GLN:HA	2.14	0.48
1:B:550:MET:HE3	1:B:550:MET:O	2.14	0.48
1:D:10:TRP:HB2	1:D:176:VAL:HG12	1.95	0.48
1:D:395:GLY:O	1:D:398:HIS:HB3	2.14	0.48
1:B:220:GLN:HG3	1:B:222:GLU:OE1	2.14	0.47
1:D:297:ASN:HD22	1:D:298:ALA:H	1.62	0.47
1:A:522:GLU:HB2	1:A:523:PRO:HD3	1.95	0.47
1:C:90:THR:OG1	1:D:87:ASN:ND2	2.47	0.47
1:A:90:THR:OG1	1:B:87:ASN:ND2	2.47	0.47
1:A:129:SER:HB2	1:A:130:PRO:HD3	1.95	0.47
7:C:1504:HOH:O	1:D:480:VAL:HG13	2.15	0.47
1:D:99:GLY:O	1:D:160:PRO:HB2	2.14	0.47
1:B:192:ALA:HB1	1:B:193:PRO:HD2	1.96	0.47
1:C:522:GLU:HB2	1:C:523:PRO:HD3	1.96	0.47
1:D:193:PRO:HG2	1:D:196:ALA:CB	2.45	0.47
1:A:371:LEU:H	1:A:371:LEU:CD1	2.27	0.47
1:B:20:GLN:O	1:B:24:GLN:HG2	2.15	0.47
1:B:189:MET:HG2	1:B:322:GLY:HA2	1.97	0.47
1:A:235:HIS:CE1	1:A:338:ARG:HD3	2.50	0.47
1:A:243:GLN:HG3	7:A:1471:HOH:O	2.15	0.47
6:C:1420:PEG:H12	1:D:500:ASP:HB2	1.96	0.47
1:B:56:HIS:CD2	1:B:58:ALA:H	2.21	0.47
1:D:371:LEU:HD12	1:D:539:ILE:CG2	2.44	0.47
1:D:168:PRO:HB2	1:D:171:VAL:HG23	1.97	0.46
1:D:193:PRO:HG2	1:D:196:ALA:HB2	1.96	0.46
1:B:141:PRO:HB2	1:B:176:VAL:HG12	1.96	0.46
1:A:406:TYR:CE1	1:A:407:THR:HG23	2.51	0.46
1:D:290:PRO:HB2	1:D:313:ASN:HB2	1.97	0.46
1:A:37:ILE:HG13	1:A:37:ILE:O	2.15	0.46
1:D:231:LEU:HD21	1:D:238:VAL:HG11	1.98	0.46
1:A:40:VAL:HG23	1:A:172:VAL:HG11	1.97	0.46
1:A:159:ARG:NH1	1:A:217:MET:HG2	2.31	0.46
1:D:85:CYS:SG	1:D:124:THR:HG21	2.55	0.46
1:D:271:LEU:HD23	1:D:348:ILE:HD12	1.96	0.46
1:B:34:GLY:HA3	1:B:80:THR:HB	1.98	0.46
1:C:440:LYS:HG3	1:C:441:VAL:N	2.30	0.46
1:D:509:GLY:HA3	6:D:1430:PEG:H22	1.98	0.46
1:A:422:MET:HG2	5:A:1406:HE3:HM22	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:550[B]:MET:HG3	1:A:553:LEU:HD12	1.98	0.45
1:C:7:VAL:HA	1:C:179:LYS:CB	2.46	0.45
1:C:217:MET:HB2	1:C:282:GLY:CA	2.46	0.45
1:C:305:VAL:HG23	1:C:306:LEU:HG	1.98	0.45
1:A:394:MET:HE3	1:A:420:GLN:HA	1.98	0.45
1:C:240:SER:O	1:C:259:ARG:HA	2.17	0.45
1:D:378:ARG:HD2	7:D:1621:HOH:O	2.16	0.45
1:C:436:ASN:HB3	1:C:438:GLU:OE2	2.16	0.45
1:D:129:SER:HB2	1:D:130:PRO:HD3	1.98	0.45
1:A:289:GLU:HG3	1:A:291:ALA:HB3	1.98	0.45
1:B:187:PRO:HG3	1:C:319:GLU:OE1	2.17	0.45
1:C:478:ASN:ND2	1:C:546:ASN:ND2	2.64	0.45
1:D:153:ARG:NH2	1:D:184:SER:OG	2.50	0.45
1:A:275:ALA:O	1:A:298:ALA:HB2	2.17	0.45
1:A:300:LEU:HD21	1:A:314:TYR:CE1	2.52	0.45
1:D:30:PHE:O	1:D:77:ALA:HA	2.16	0.45
1:A:312:ARG:HA	1:D:181:LEU:HD21	1.98	0.45
1:A:498:PRO:HG2	6:B:1410:PEG:H11	1.99	0.45
1:B:371:LEU:HD12	1:B:539:ILE:CG2	2.47	0.45
1:C:176:VAL:HG22	1:C:177:SER:N	2.31	0.45
1:C:20:GLN:O	1:C:24:GLN:HG2	2.17	0.44
1:D:31:GLY:HA3	1:D:78:LEU:O	2.18	0.44
1:D:461:VAL:HA	1:D:534:PRO:HG2	1.99	0.44
1:C:222:GLU:O	1:C:325:ALA:HB2	2.17	0.44
1:B:344:GLN:HG3	7:B:1739:HOH:O	2.17	0.44
1:C:10:TRP:HB2	1:C:176:VAL:CG1	2.47	0.44
1:C:493:GLY:HA2	1:D:53:PRO:HG3	2.00	0.44
1:D:231:LEU:CD2	1:D:238:VAL:HG11	2.48	0.44
1:B:192:ALA:HB3	1:B:327:THR:HG23	2.00	0.44
1:B:438:GLU:CD	1:B:438:GLU:H	2.21	0.44
1:B:220:GLN:HG2	7:B:1574:HOH:O	2.17	0.44
1:C:289:GLU:HG2	1:C:291:ALA:HB3	2.00	0.44
1:A:159:ARG:HG2	1:A:306:LEU:CD1	2.48	0.44
1:A:234:SER:HB2	1:A:236:ILE:HG13	2.00	0.44
1:A:381:GLN:NE2	1:A:407:THR:HB	2.32	0.44
1:B:234:SER:HB3	1:B:335:ILE:HD13	2.00	0.44
1:B:511:LYS:HD2	1:B:531:VAL:CG2	2.48	0.43
1:C:395:GLY:O	1:C:398:HIS:HB3	2.18	0.43
1:B:371:LEU:HD12	1:B:539:ILE:HG23	2.01	0.43
1:D:372:HIS:HD2	1:D:374:LEU:N	2.13	0.43
1:B:157:GLN:OE1	1:B:186:ALA:HA	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:69:ARG:HD3	7:C:1673:HOH:O	2.18	0.43
1:C:122:MET:HG2	1:C:127:MET:HE2	2.00	0.43
1:C:482:ILE:HD12	1:C:550:MET:CG	2.38	0.43
1:A:353:GLN:NE2	6:A:1401:PEG:H41	2.33	0.43
1:C:209:ASN:HD21	1:C:342:SER:CB	2.30	0.43
1:C:220:GLN:HA	1:C:220:GLN:NE2	2.33	0.43
1:C:290:PRO:HA	1:C:293:TRP:NE1	2.34	0.43
1:C:464:LYS:HD2	7:C:1730:HOH:O	2.18	0.43
1:A:367:ASN:HD21	1:A:519:GLU:CD	2.21	0.43
1:A:381:GLN:NE2	1:A:407:THR:CB	2.82	0.43
1:A:229:ARG:HH22	1:A:333:GLN:CG	2.31	0.43
1:D:305:VAL:HG23	1:D:306:LEU:HG	2.00	0.43
1:A:412:GLN:HE21	1:A:412:GLN:HB3	1.53	0.43
1:B:34:GLY:HA3	1:B:80:THR:CB	2.49	0.43
1:D:411:ARG:HG3	1:D:411:ARG:HH11	1.83	0.43
1:B:356:ARG:HG3	1:B:406:TYR:CE1	2.53	0.42
1:D:37:ILE:O	1:D:37:ILE:HG13	2.19	0.42
1:A:209:ASN:ND2	1:A:342:SER:OG	2.48	0.42
1:B:143:ALA:O	1:B:146:GLU:HG2	2.19	0.42
1:B:366:LEU:HA	1:B:368:GLN:HE22	1.84	0.42
1:A:294:ASN:ND2	1:A:296:GLY:H	2.17	0.42
1:A:344:GLN:HE21	1:A:344:GLN:N	2.08	0.42
1:C:68:GLY:HA2	1:C:73:LYS:O	2.20	0.42
1:A:315:THR:CG2	1:D:181:LEU:HD22	2.50	0.42
1:C:53:PRO:HG3	1:D:493:GLY:HA2	2.00	0.42
1:C:249:ASN:ND2	1:C:252:ASN:ND2	2.68	0.42
1:A:53:PRO:HG3	1:B:493:GLY:HA2	2.02	0.42
1:C:381:GLN:HE22	1:C:407:THR:CB	2.32	0.42
1:D:261:GLY:HA2	1:D:288:TYR:CD1	2.54	0.42
1:B:188:GLN:HB3	1:C:193:PRO:HG3	2.01	0.42
1:B:498:PRO:HG2	6:B:1400:PEG:H11	2.01	0.42
1:C:400:TRP:CD2	1:C:549:LEU:HD22	2.55	0.42
1:D:259:ARG:HH21	2:D:1431:PO4:P	2.42	0.42
1:D:395:GLY:HA3	1:D:397:PHE:CE2	2.54	0.42
1:A:511:LYS:HE2	1:A:511:LYS:N	2.35	0.42
1:A:555:LEU:HA	1:A:558:ILE:HB	2.02	0.42
1:B:223:ASN:OD1	1:B:324:ILE:HB	2.20	0.42
1:D:297:ASN:N	1:D:297:ASN:ND2	2.68	0.42
1:D:381:GLN:HE22	1:D:407:THR:CB	2.32	0.42
1:B:224:SER:HB3	7:B:1561:HOH:O	2.19	0.41
1:D:289:GLU:HA	1:D:290:PRO:HD3	1.94	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:282:GLY:HA2	1:B:304:ASP:OD1	2.20	0.41
1:A:546:ASN:N	1:A:547:PRO:CD	2.84	0.41
1:C:168:PRO:HB2	1:C:171:VAL:HG23	2.03	0.41
1:D:422:MET:HG2	5:D:1433:HE3:HM22	2.00	0.41
1:A:39:LYS:HA	1:A:39:LYS:HD2	1.91	0.41
1:B:13:GLY:O	1:B:144:LEU:HD21	2.21	0.41
1:C:289:GLU:HA	1:C:290:PRO:HD3	1.90	0.41
1:A:193:PRO:HD3	1:D:188:GLN:O	2.21	0.41
1:A:400:TRP:CD2	1:A:549:LEU:HD22	2.55	0.41
1:A:482:ILE:HD12	1:A:550[A]:MET:SD	2.61	0.41
1:C:261:GLY:HA2	1:C:288:TYR:CE1	2.56	0.41
1:C:381:GLN:NE2	1:C:407:THR:HB	2.35	0.41
1:C:438:GLU:CD	1:C:438:GLU:H	2.23	0.41
1:C:114:LYS:HG2	1:C:114:LYS:O	2.20	0.41
1:B:519:GLU:CD	1:B:519:GLU:N	2.73	0.41
1:C:393:ASP:HB3	1:C:397:PHE:HZ	1.85	0.41
1:B:217:MET:HB2	1:B:282:GLY:HA3	2.03	0.41
1:B:544:ARG:O	1:B:547:PRO:HD2	2.21	0.41
1:C:220:GLN:HA	1:C:220:GLN:HE21	1.86	0.41
1:C:407:THR:HG21	7:C:1627:HOH:O	2.20	0.41
1:D:192:ALA:HB1	1:D:193:PRO:HD2	2.01	0.41
1:A:192:ALA:HB1	1:A:193:PRO:HD2	2.03	0.41
1:B:31:GLY:HA3	1:B:78:LEU:O	2.21	0.41
1:C:92:MET:CE	1:C:162:SER:HB2	2.51	0.41
1:C:275:ALA:O	1:C:298:ALA:HB2	2.21	0.41
1:D:501:PHE:HB2	1:D:538:ALA:HB2	2.02	0.41
1:A:31:GLY:HA3	1:A:78:LEU:O	2.21	0.41
1:D:68:GLY:HA2	1:D:73:LYS:O	2.21	0.41
1:A:176:VAL:HG22	1:A:177:SER:N	2.37	0.40
1:B:8:ARG:HG2	1:B:8:ARG:NH1	2.36	0.40
1:B:306:LEU:HB3	1:B:307:PRO:HD2	2.02	0.40
1:C:110:LYS:HB2	1:C:113:ASP:OD2	2.22	0.40
1:C:136:ILE:HG12	1:C:137:GLU:N	2.36	0.40
1:C:429:ALA:HB2	1:C:443:SER:HB3	2.03	0.40
1:D:228:ARG:HH11	1:D:228:ARG:HG3	1.87	0.40
1:C:282:GLY:HA2	1:C:304:ASP:OD1	2.21	0.40
1:A:285:PRO:HB3	1:A:290:PRO:HG2	2.02	0.40
1:B:13:GLY:O	1:B:17:VAL:HG23	2.21	0.40
1:A:42:ASP:O	1:A:45:LEU:HB2	2.21	0.40
1:A:303:ILE:HG12	1:A:320:LEU:HD12	2.02	0.40
7:A:1486:HOH:O	1:B:483:GLN:HB2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:453:SER:HA	1:C:455:MET:SD	2.61	0.40
1:D:489:GLN:NE2	1:D:489:GLN:HA	2.36	0.40
1:A:217:MET:HB2	1:A:282:GLY:CA	2.51	0.40
1:A:353:GLN:O	1:A:357:GLU:HG3	2.20	0.40
1:B:7:VAL:O	1:B:8:ARG:HB2	2.21	0.40
1:B:501:PHE:HB2	1:B:538:ALA:HB2	2.04	0.40
1:C:381:GLN:NE2	1:C:407:THR:CB	2.85	0.40
1:D:7:VAL:CA	1:D:179:LYS:HB3	2.49	0.40

There are no symmetry-related clashes.

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	540/566 (95%)	520 (96%)	19 (4%)	1 (0%)	47	44
1	B	540/566 (95%)	513 (95%)	25 (5%)	2 (0%)	34	30
1	C	535/566 (94%)	511 (96%)	22 (4%)	2 (0%)	34	30
1	D	532/566 (94%)	513 (96%)	18 (3%)	1 (0%)	47	44
All	All	2147/2264 (95%)	2057 (96%)	84 (4%)	6 (0%)	41	37

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	184	SER
1	A	310	GLU
1	C	114	LYS
1	D	521	LEU
1	B	323	ASP
1	B	193	PRO

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	425/452 (94%)	416 (98%)	9 (2%)	53	57
1	B	417/452 (92%)	410 (98%)	7 (2%)	60	65
1	C	420/452 (93%)	412 (98%)	8 (2%)	57	61
1	D	419/452 (93%)	411 (98%)	8 (2%)	57	61
All	All	1681/1808 (93%)	1649 (98%)	32 (2%)	57	61

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	194	ASP
1	A	222	GLU
1	A	259	ARG
1	A	294	ASN
1	A	344	GLN
1	A	407	THR
1	A	412	GLN
1	A	447	ASP
1	A	455	MET
1	B	194	ASP
1	B	252	ASN
1	B	259	ARG
1	B	353	GLN
1	B	368	GLN
1	B	447	ASP
1	B	455	MET
1	C	194	ASP
1	C	259	ARG
1	C	311	GLU
1	C	312	ARG
1	C	344	GLN
1	C	407	THR
1	C	447	ASP
1	C	455	MET

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Mol	Chain	Res	Type
1	D	259	ARG
1	D	297	ASN
1	D	311	GLU
1	D	407	THR
1	D	409	ARG
1	D	447	ASP
1	D	455	MET
1	D	545	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	GLN
1	A	56	HIS
1	A	188	GLN
1	A	209	ASN
1	A	273	GLN
1	A	294	ASN
1	A	344	GLN
1	A	353	GLN
1	A	367	ASN
1	A	381	GLN
1	A	412	GLN
1	B	56	HIS
1	B	87	ASN
1	B	209	ASN
1	B	220	GLN
1	B	252	ASN
1	B	297	ASN
1	B	329	ASN
1	B	368	GLN
1	B	381	GLN
1	C	9	GLN
1	C	24	GLN
1	C	87	ASN
1	C	150	ASN
1	C	199	GLN
1	C	209	ASN
1	C	220	GLN
1	C	297	ASN
1	C	329	ASN
1	C	344	GLN

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Mol	Chain	Res	Type
1	C	381	GLN
1	C	478	ASN
1	D	24	GLN
1	D	56	HIS
1	D	87	ASN
1	D	199	GLN
1	D	297	ASN
1	D	372	HIS
1	D	381	GLN
1	D	475	ASN
1	D	489	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 19 ligands modelled in this entry, 4 are monoatomic - leaving 15 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	PO4	D	1431	-	4,4,4	1.63	0	6,6,6	0.43	0
5	HE3	A	1406	3	22,31,31	4.32	15 (68%)	26,49,49	3.22	14 (53%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	HE3	D	1433	3	22,31,31	4.34	15 (68%)	26,49,49	3.19	13 (50%)
6	PEG	B	1400	-	6,6,6	0.60	0	5,5,5	1.53	1 (20%)
4	PGE	A	1402	-	9,9,9	0.72	0	8,8,8	1.33	0
6	PEG	C	1420	-	6,6,6	0.48	0	5,5,5	1.49	1 (20%)
2	PO4	B	1411	-	4,4,4	1.61	0	6,6,6	0.40	0
5	HE3	B	1413	3	22,31,31	4.24	15 (68%)	26,49,49	3.25	13 (50%)
4	PGE	A	1403	-	9,9,9	0.69	0	8,8,8	1.32	1 (12%)
5	HE3	C	1423	3	22,31,31	4.26	15 (68%)	26,49,49	3.18	12 (46%)
6	PEG	D	1430	-	6,6,6	0.54	0	5,5,5	1.53	1 (20%)
6	PEG	A	1401	-	6,6,6	0.59	0	5,5,5	1.57	1 (20%)
6	PEG	B	1410	-	6,6,6	0.54	0	5,5,5	1.50	1 (20%)
2	PO4	A	1404	-	4,4,4	1.61	0	6,6,6	0.41	0
2	PO4	C	1421	-	4,4,4	1.56	0	6,6,6	0.42	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	HE3	A	1406	3	-	4/13/47/47	0/3/3/3
6	PEG	B	1400	-	-	0/4/4/4	-
5	HE3	D	1433	3	-	4/13/47/47	0/3/3/3
4	PGE	A	1402	-	-	2/7/7/7	-
6	PEG	C	1420	-	-	0/4/4/4	-
5	HE3	B	1413	3	-	4/13/47/47	0/3/3/3
4	PGE	A	1403	-	-	2/7/7/7	-
5	HE3	C	1423	3	-	4/13/47/47	0/3/3/3
6	PEG	D	1430	-	-	1/4/4/4	-
6	PEG	A	1401	-	-	1/4/4/4	-
6	PEG	B	1410	-	-	1/4/4/4	-

All (60) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1406	HE3	C5'-C4'	9.71	1.50	1.41
5	D	1433	HE3	C5'-C4'	9.66	1.50	1.41
5	C	1423	HE3	C5'-C4'	9.44	1.50	1.41
5	B	1413	HE3	C5'-C4'	9.36	1.50	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	1423	HE3	C2'-N1'	7.81	1.46	1.34
5	B	1413	HE3	C2'-N1'	7.74	1.46	1.34
5	B	1413	HE3	C6'-N1'	7.60	1.50	1.34
5	A	1406	HE3	C2'-N1'	7.53	1.46	1.34
5	D	1433	HE3	C2'-N1'	7.45	1.46	1.34
5	D	1433	HE3	C6'-N1'	7.29	1.49	1.34
5	A	1406	HE3	C6'-N1'	7.10	1.49	1.34
5	C	1423	HE3	C6'-N1'	7.07	1.49	1.34
5	D	1433	HE3	C5-C4	6.52	1.49	1.35
5	A	1406	HE3	C5-C4	6.45	1.48	1.35
5	B	1413	HE3	C5-C4	6.32	1.48	1.35
5	C	1423	HE3	C5-C4	6.29	1.48	1.35
5	D	1433	HE3	C4'-N3'	5.56	1.45	1.34
5	A	1406	HE3	C4'-N3'	5.33	1.44	1.34
5	B	1413	HE3	C4'-N3'	5.13	1.44	1.34
5	C	1423	HE3	C4'-N3'	5.06	1.44	1.34
5	D	1433	HE3	C7'-N3	4.64	1.53	1.46
5	A	1406	HE3	C7'-N3	4.57	1.53	1.46
5	C	1423	HE3	C7'-N3	4.51	1.53	1.46
5	D	1433	HE3	C6'-C5'	4.47	1.47	1.37
5	A	1406	HE3	C6'-C5'	4.37	1.46	1.37
5	D	1433	HE3	C2'-N3'	4.37	1.41	1.34
5	C	1423	HE3	C6'-C5'	4.34	1.46	1.37
5	A	1406	HE3	C2'-N3'	4.32	1.41	1.34
5	B	1413	HE3	C6'-C5'	4.31	1.46	1.37
5	B	1413	HE3	C7'-N3	4.31	1.52	1.46
5	C	1423	HE3	C2'-N3'	4.30	1.41	1.34
5	A	1406	HE3	O9-C8	4.10	1.53	1.43
5	B	1413	HE3	C2'-N3'	3.90	1.41	1.34
5	C	1423	HE3	C6-C5	-3.85	1.43	1.50
5	C	1423	HE3	CM4-C4	3.80	1.55	1.49
5	D	1433	HE3	O9-C8	3.79	1.53	1.43
5	A	1406	HE3	CM4-C4	3.77	1.55	1.49
5	A	1406	HE3	C6-C5	-3.74	1.43	1.50
5	D	1433	HE3	CM4-C4	3.71	1.55	1.49
5	B	1413	HE3	O9-C8	3.56	1.52	1.43
5	B	1413	HE3	C6-C5	-3.53	1.44	1.50
5	B	1413	HE3	CM4-C4	3.49	1.54	1.49
5	C	1423	HE3	O9-C8	3.45	1.52	1.43
5	D	1433	HE3	C6-C5	-3.42	1.44	1.50
5	D	1433	HE3	PA-O7	-3.27	1.46	1.59
5	C	1423	HE3	PA-O7	-3.20	1.46	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1406	HE3	PA-O7	-3.13	1.46	1.59
5	B	1413	HE3	PA-O7	-3.07	1.46	1.59
5	D	1433	HE3	PB-O1B	-3.05	1.43	1.54
5	B	1413	HE3	PB-O1B	-3.00	1.43	1.54
5	A	1406	HE3	PB-O1B	-2.84	1.43	1.54
5	C	1423	HE3	PB-O1B	-2.76	1.44	1.54
5	D	1433	HE3	PA-O2A	-2.74	1.42	1.55
5	A	1406	HE3	CM2-C2'	-2.72	1.41	1.49
5	A	1406	HE3	PA-O2A	-2.59	1.43	1.55
5	C	1423	HE3	PA-O2A	-2.56	1.43	1.55
5	B	1413	HE3	PA-O2A	-2.56	1.43	1.55
5	D	1433	HE3	CM2-C2'	-2.54	1.42	1.49
5	C	1423	HE3	CM2-C2'	-2.51	1.42	1.49
5	B	1413	HE3	CM2-C2'	-2.44	1.42	1.49

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	1413	HE3	CM2-C2'-N1'	9.17	127.23	117.14
5	C	1423	HE3	CM2-C2'-N1'	8.87	126.90	117.14
5	D	1433	HE3	CM2-C2'-N1'	8.85	126.87	117.14
5	A	1406	HE3	CM2-C2'-N1'	8.82	126.84	117.14
5	B	1413	HE3	O9-C8-C9	-7.60	91.36	109.02
5	D	1433	HE3	O9-C8-C9	-7.50	91.60	109.02
5	A	1406	HE3	O9-C8-C9	-7.41	91.82	109.02
5	C	1423	HE3	O9-C8-C9	-7.32	92.03	109.02
5	B	1413	HE3	N1'-C2'-N3'	-5.11	116.75	125.54
5	C	1423	HE3	N1'-C2'-N3'	-5.08	116.80	125.54
5	D	1433	HE3	N1'-C2'-N3'	-5.08	116.80	125.54
5	A	1406	HE3	N1'-C2'-N3'	-5.06	116.82	125.54
5	A	1406	HE3	C6'-N1'-C2'	4.98	124.43	115.96
5	D	1433	HE3	C6'-N1'-C2'	4.94	124.37	115.96
5	C	1423	HE3	C6'-N1'-C2'	4.91	124.32	115.96
5	B	1413	HE3	C6'-N1'-C2'	4.72	123.99	115.96
5	A	1406	HE3	PA-O7-C7	3.38	138.22	121.59
5	B	1413	HE3	PA-O7-C7	3.34	138.03	121.59
5	D	1433	HE3	PA-O7-C7	3.29	137.79	121.59
5	A	1406	HE3	O7-C7-C6	3.14	121.46	108.64
5	C	1423	HE3	PA-O7-C7	3.05	136.61	121.59
5	B	1413	HE3	O7-C7-C6	3.03	121.00	108.64
5	C	1423	HE3	O7-C7-C6	3.01	120.93	108.64
5	D	1433	HE3	O7-C7-C6	2.96	120.74	108.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	1406	HE3	C6-C5-C4	-2.94	120.73	128.20
5	C	1423	HE3	C5'-C4'-N3'	2.80	126.79	122.44
5	B	1413	HE3	C5'-C4'-N3'	2.80	126.78	122.44
5	C	1423	HE3	C6-C5-C4	-2.77	121.16	128.20
5	B	1413	HE3	C6-C5-C4	-2.73	121.26	128.20
6	A	1401	PEG	O2-C2-C1	2.73	122.06	110.07
5	A	1406	HE3	C5'-C4'-N3'	2.71	126.66	122.44
5	D	1433	HE3	C5'-C4'-N3'	2.70	126.64	122.44
5	D	1433	HE3	C6-C5-C4	-2.70	121.35	128.20
5	C	1423	HE3	C5'-C6'-N1'	-2.65	119.41	123.82
5	B	1413	HE3	C7'-C5'-C6'	2.63	125.43	120.05
6	B	1410	PEG	O2-C2-C1	2.63	121.62	110.07
6	B	1400	PEG	O2-C2-C1	2.62	121.60	110.07
6	D	1430	PEG	O2-C2-C1	2.62	121.58	110.07
5	C	1423	HE3	C7'-C5'-C6'	2.57	125.30	120.05
5	A	1406	HE3	C7'-C5'-C6'	2.57	125.29	120.05
5	A	1406	HE3	C5'-C6'-N1'	-2.56	119.56	123.82
5	B	1413	HE3	C5'-C6'-N1'	-2.55	119.57	123.82
5	B	1413	HE3	C7-C6-C5	2.54	120.80	112.73
5	D	1433	HE3	C7-C6-C5	2.52	120.72	112.73
5	D	1433	HE3	C7'-C5'-C6'	2.51	125.17	120.05
5	D	1433	HE3	C5'-C6'-N1'	-2.47	119.70	123.82
6	C	1420	PEG	O2-C2-C1	2.42	120.72	110.07
5	A	1406	HE3	C6-C5-S1	2.28	124.09	119.18
5	A	1406	HE3	C7-C6-C5	2.25	119.87	112.73
5	C	1423	HE3	C7-C6-C5	2.23	119.80	112.73
5	D	1433	HE3	C6'-C5'-C4'	-2.16	112.75	115.66
5	B	1413	HE3	C6'-C5'-C4'	-2.12	112.80	115.66
5	C	1423	HE3	C5'-C7'-N3	-2.09	107.92	111.51
5	B	1413	HE3	C6-C5-S1	2.08	123.66	119.18
5	D	1433	HE3	C6-C5-S1	2.08	123.66	119.18
5	A	1406	HE3	C6'-C5'-C4'	-2.06	112.88	115.66
4	A	1403	PGE	C5-O3-C4	2.06	122.19	113.29
5	A	1406	HE3	C5'-C7'-N3	-2.04	108.01	111.51

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1403	PGE	O1-C1-C2-O2
5	A	1406	HE3	PA-O1A-PB-O3B
5	B	1413	HE3	PA-O1A-PB-O3B

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Mol	Chain	Res	Type	Atoms
5	C	1423	HE3	PA-O1A-PB-O3B
5	D	1433	HE3	PA-O1A-PB-O3B
6	A	1401	PEG	C4-C3-O2-C2
5	C	1423	HE3	C6-C7-O7-PA
5	D	1433	HE3	C6-C7-O7-PA
6	D	1430	PEG	C4-C3-O2-C2
6	B	1410	PEG	C4-C3-O2-C2
4	A	1402	PGE	O2-C3-C4-O3
4	A	1403	PGE	O2-C3-C4-O3
5	A	1406	HE3	PA-O1A-PB-O1B
5	A	1406	HE3	PA-O1A-PB-O2B
5	B	1413	HE3	PA-O1A-PB-O1B
5	B	1413	HE3	PA-O1A-PB-O2B
5	C	1423	HE3	PA-O1A-PB-O1B
5	C	1423	HE3	PA-O1A-PB-O2B
5	D	1433	HE3	PA-O1A-PB-O1B
5	D	1433	HE3	PA-O1A-PB-O2B
4	A	1402	PGE	C4-C3-O2-C2
5	A	1406	HE3	C6-C7-O7-PA
5	B	1413	HE3	C6-C7-O7-PA

There are no ring outliers.

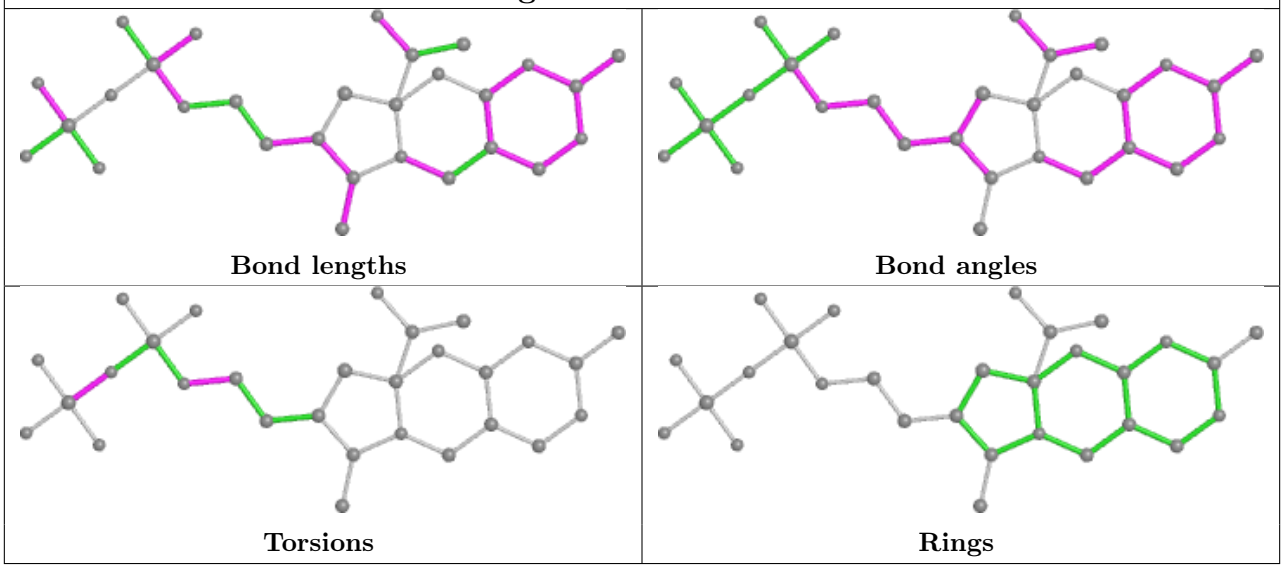
12 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1431	PO4	1	0
5	A	1406	HE3	3	0
5	D	1433	HE3	3	0
6	B	1400	PEG	1	0
4	A	1402	PGE	1	0
6	C	1420	PEG	1	0
5	B	1413	HE3	3	0
4	A	1403	PGE	2	0
5	C	1423	HE3	3	0
6	D	1430	PEG	2	0
6	A	1401	PEG	1	0
6	B	1410	PEG	1	0

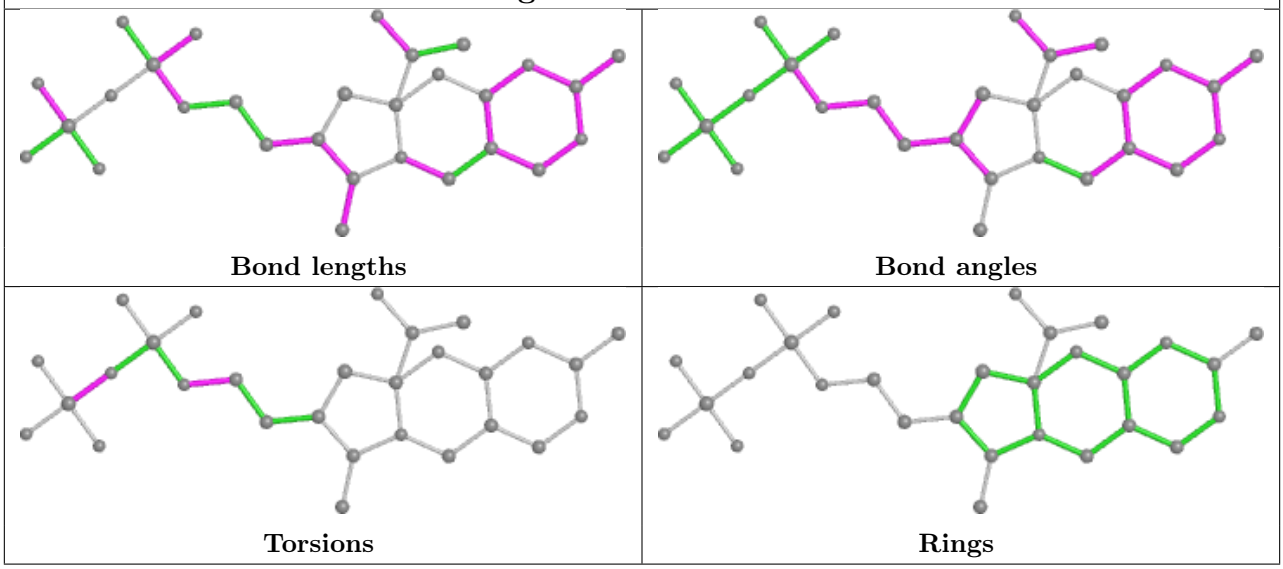
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 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.

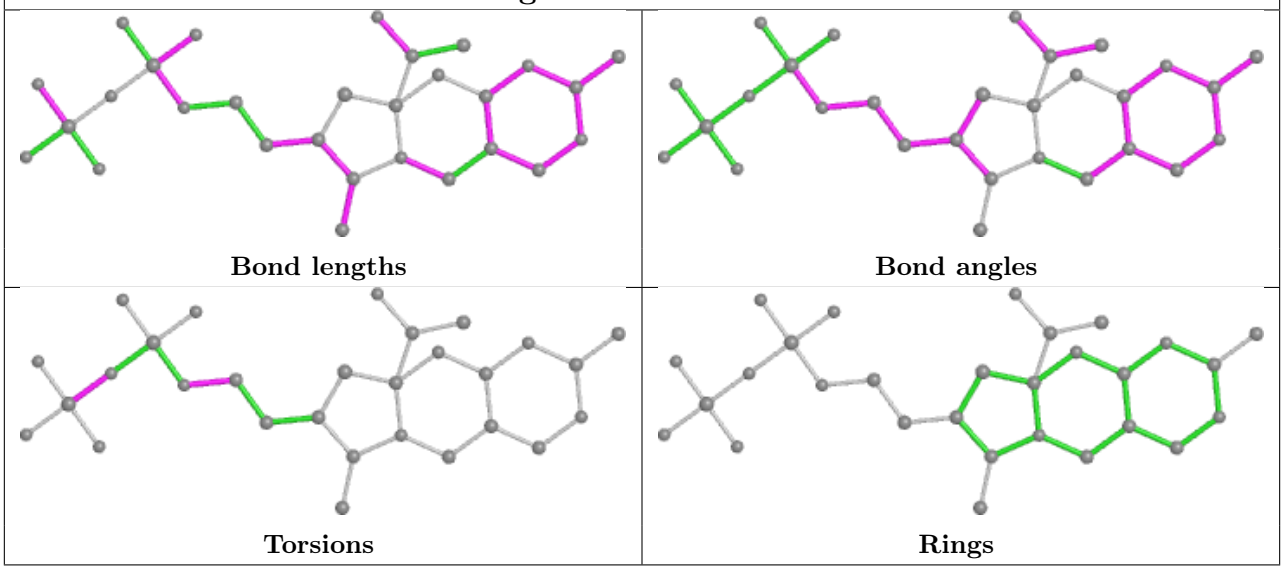
Ligand HE3 A 1406



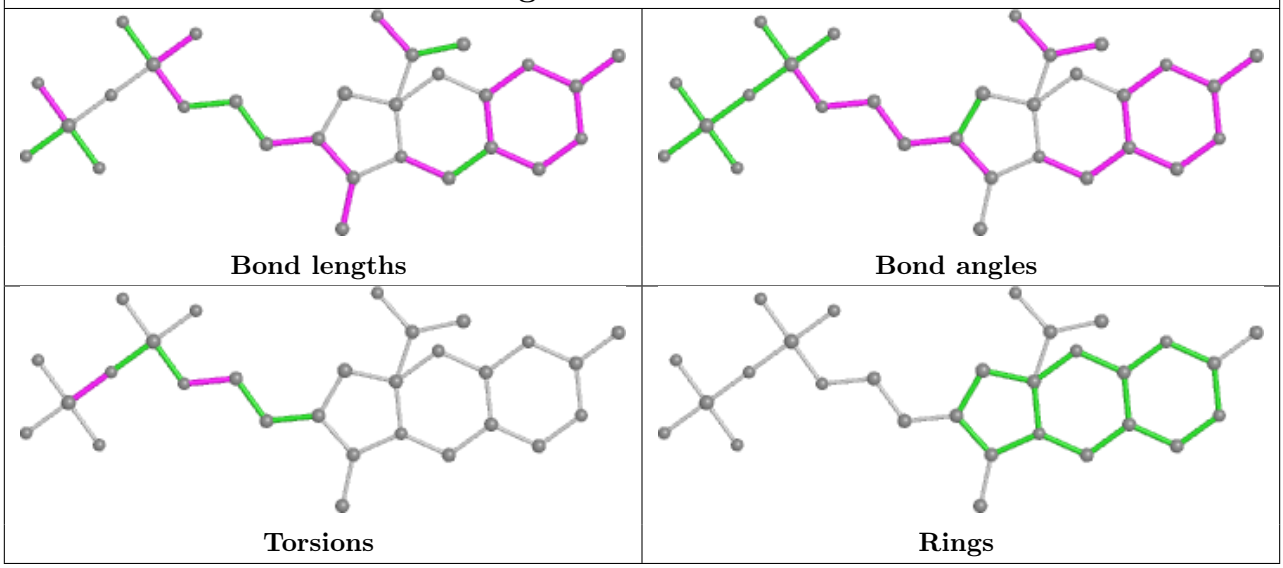
Ligand HE3 D 1433



Ligand HE3 B 1413



Ligand HE3 C 1423



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, 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	545/566 (96%)	-0.18	7 (1%)	77	76	17, 30, 52, 85	1 (0%)
1	B	545/566 (96%)	-0.18	6 (1%)	80	79	16, 29, 58, 86	1 (0%)
1	C	543/566 (95%)	-0.18	10 (1%)	68	66	16, 29, 58, 77	0
1	D	538/566 (95%)	-0.15	7 (1%)	77	76	17, 32, 56, 75	0
All	All	2171/2264 (95%)	-0.17	30 (1%)	75	74	16, 30, 57, 86	2 (0%)

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	558	ILE	5.6
1	D	555	LEU	4.7
1	D	186	ALA	4.0
1	A	550[A]	MET	3.7
1	B	557	GLN	3.7
1	A	309	TYR	3.6
1	A	7	VAL	3.6
1	B	559	LEU	3.6
1	A	556	SER	3.2
1	B	309	TYR	3.2
1	A	555	LEU	2.9
1	D	121	SER	2.8
1	C	296	GLY	2.6
1	C	337	HIS	2.6
1	C	309	TYR	2.6
1	D	360	ASP	2.6
1	C	205	ALA	2.5
1	C	7	VAL	2.5
1	B	558	ILE	2.4
1	B	196	ALA	2.4
1	B	193	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	336	ASP	2.3
1	C	186	ALA	2.3
1	C	364	ALA	2.2
1	D	544	ARG	2.1
1	A	557	GLN	2.1
1	D	85	CYS	2.1
1	C	306	LEU	2.0
1	D	345	ALA	2.0
1	C	198	ASP	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	PEG	A	1401	7/7	0.79	0.16	55,55,57,58	0
4	PGE	A	1403	10/10	0.85	0.13	43,46,50,50	0
6	PEG	B	1400	7/7	0.85	0.16	48,50,53,54	0
6	PEG	B	1410	7/7	0.85	0.16	48,49,50,52	0
4	PGE	A	1402	10/10	0.86	0.14	46,49,54,54	0
6	PEG	D	1430	7/7	0.89	0.19	57,58,59,60	0
6	PEG	C	1420	7/7	0.90	0.14	45,46,50,51	0
3	MG	D	1432	1/1	0.93	0.07	32,32,32,32	0
2	PO4	B	1411	5/5	0.94	0.14	28,32,36,43	0
2	PO4	C	1421	5/5	0.94	0.12	29,31,38,40	0
2	PO4	D	1431	5/5	0.96	0.13	57,57,58,58	0
2	PO4	A	1404	5/5	0.97	0.12	31,31,37,40	0
3	MG	A	1405	1/1	0.97	0.07	22,22,22,22	0
5	HE3	B	1413	29/29	0.98	0.10	15,20,23,24	0

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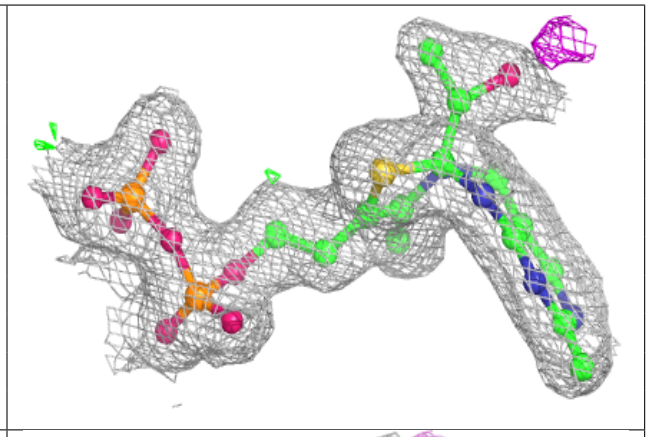
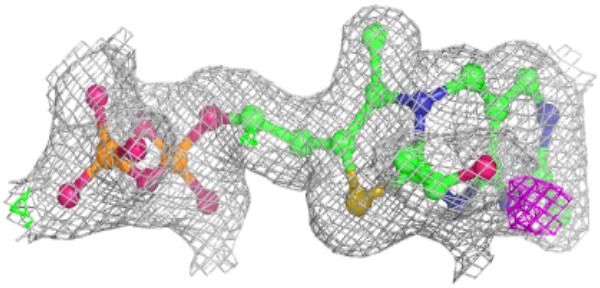
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	HE3	C	1423	29/29	0.98	0.09	16,20,24,25	0
5	HE3	D	1433	29/29	0.98	0.10	23,26,28,30	0
5	HE3	A	1406	29/29	0.98	0.11	19,24,26,27	0
3	MG	B	1412	1/1	0.99	0.04	21,21,21,21	0
3	MG	C	1422	1/1	0.99	0.09	19,19,19,19	0

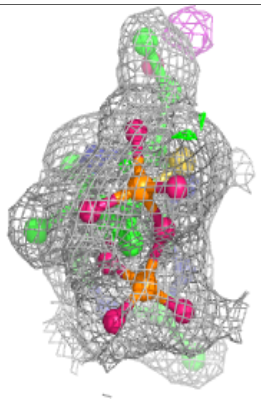
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around HE3 B 1413:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

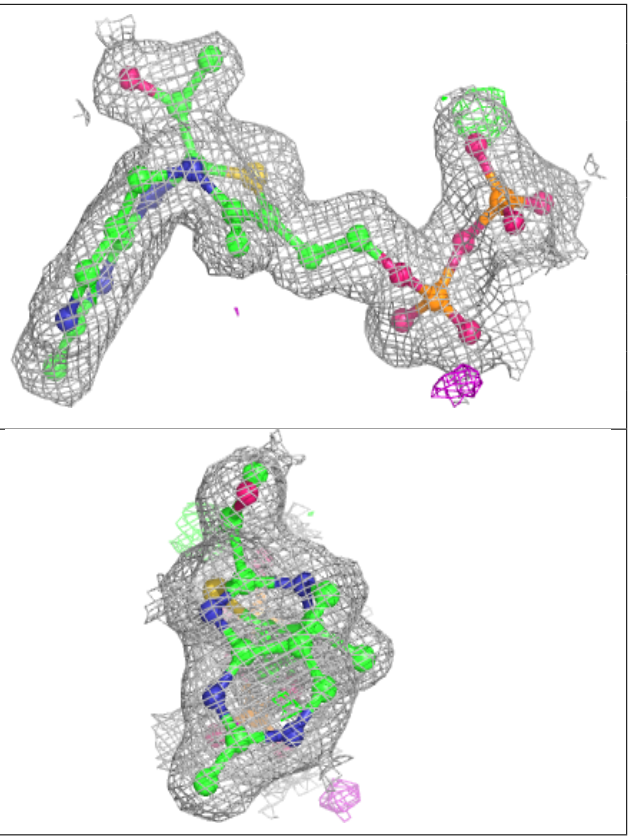






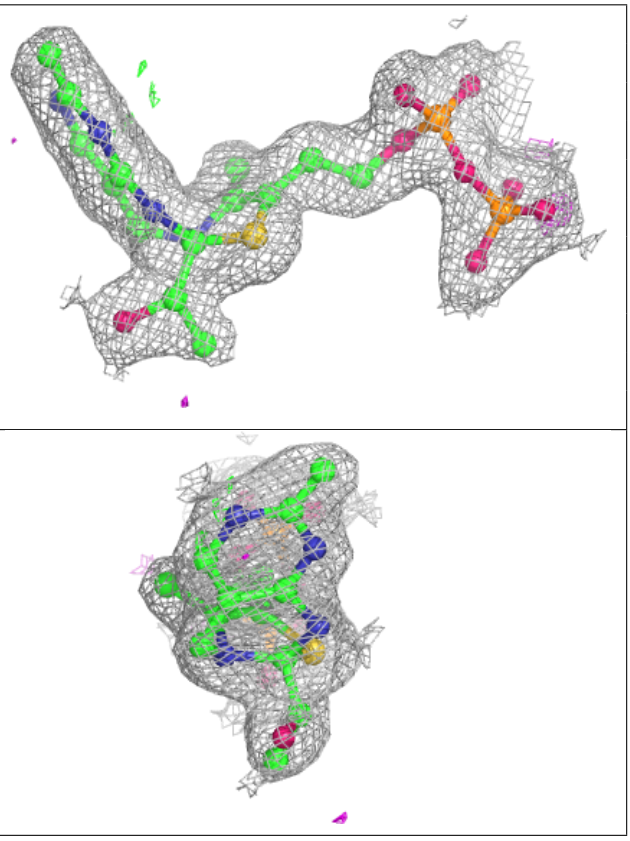
Electron density around HE3 C 1423:

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



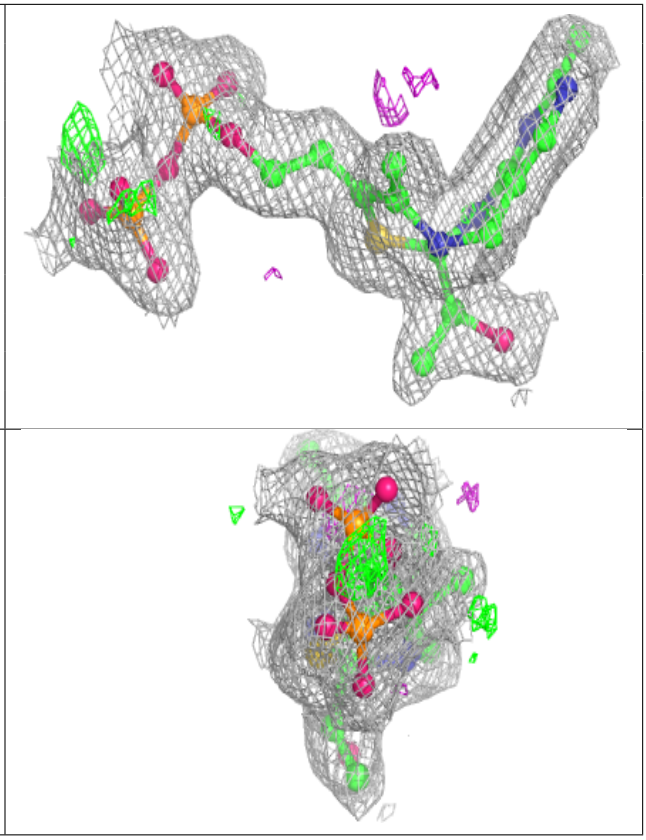
Electron density around HE3 D 1433:

$2mF_o$-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 A 1406:

$2mF_o$-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.