



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 16, 2023 – 08:30 PM EDT

PDB ID : 1IRI  
Title : Crystal structure of human autocrine motility factor complexed with an inhibitor  
Authors : Tanaka, N.; Haga, A.; Uemura, H.; Akiyama, H.; Funasaka, T.; Nagase, H.; Raz, A.; Nakamura, K.T.  
Deposited on : 2001-10-08  
Resolution : 2.40 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)  
Xtrriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

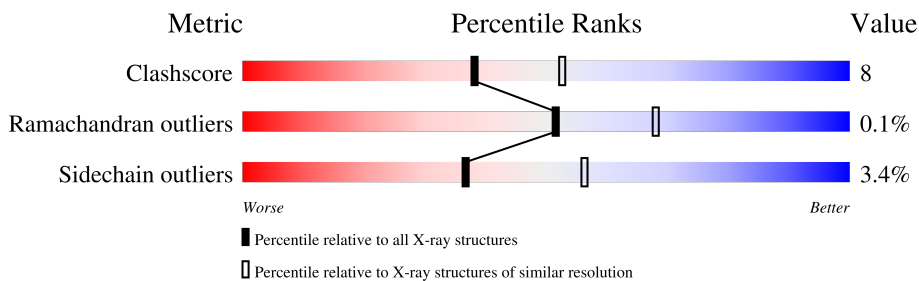
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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))
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)

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  $\leq 5\%$ .

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	558	
1	B	558	
1	C	558	
1	D	558	

## 2 Entry composition [i](#)

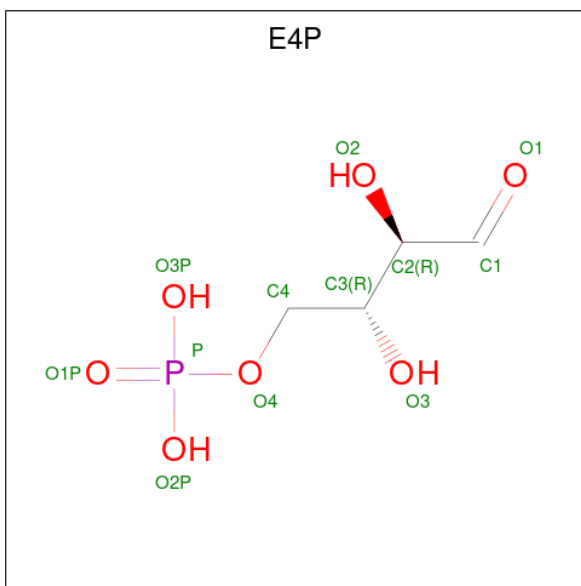
There are 3 unique types of molecules in this entry. The entry contains 18264 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 autocrine motility factor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	557	Total 4445	C 2832	N 783	O 811	S 19	0	0	0
1	B	557	Total 4445	C 2832	N 783	O 811	S 19	0	0	0
1	C	557	Total 4445	C 2832	N 783	O 811	S 19	0	0	0
1	D	557	Total 4445	C 2832	N 783	O 811	S 19	0	0	0

- Molecule 2 is ERYTHROSE-4-PHOSPHATE (three-letter code: E4P) (formula: C<sub>4</sub>H<sub>9</sub>O<sub>7</sub>P).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	P		
2	A	1	Total 13	C 4	O 8	P 1	0	1
2	B	1	Total 13	C 4	O 8	P 1	0	1

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	C	1	Total	C	O	P	0	1
			13	4	8	1		
2	D	1	Total	C	O	P	0	1
			13	4	8	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	128	Total	O	0	0
			128	128		
3	B	121	Total	O	0	0
			121	121		
3	C	109	Total	O	0	0
			109	109		
3	D	74	Total	O	0	0
			74	74		

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

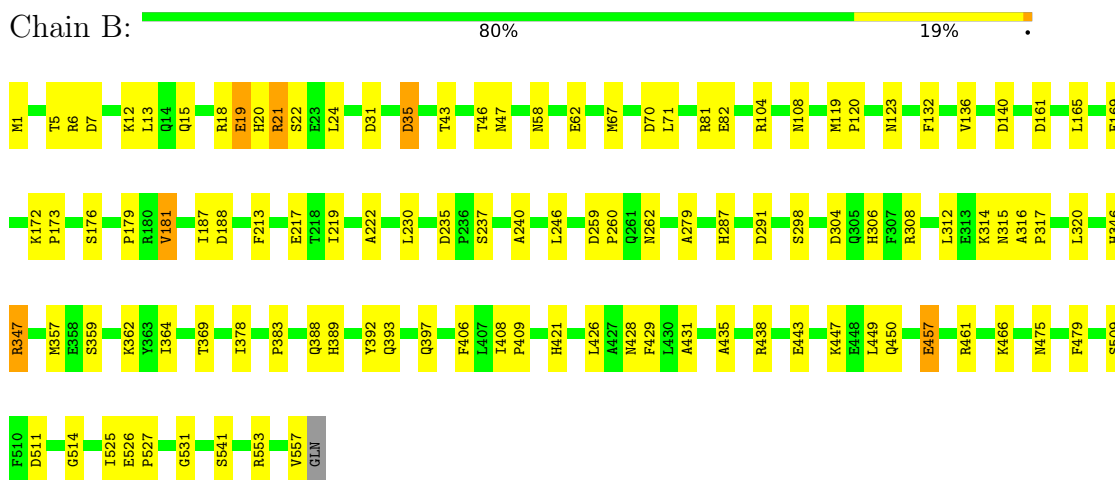
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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.

Note EDS was not executed.

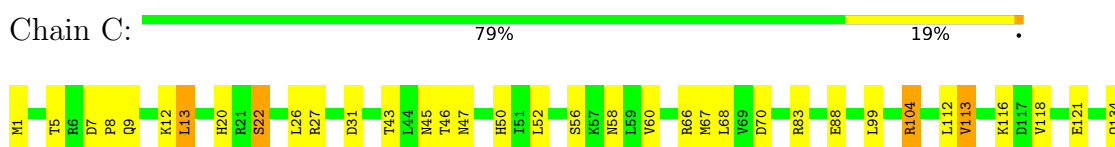
- Molecule 1: autocrine motility factor

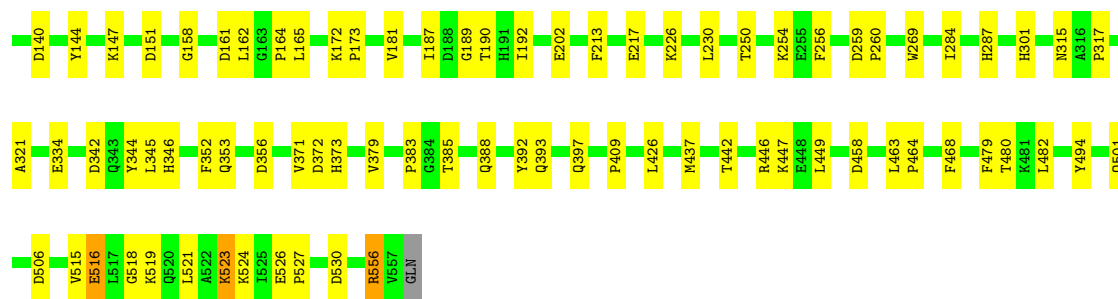


- Molecule 1: autocrine motility factor



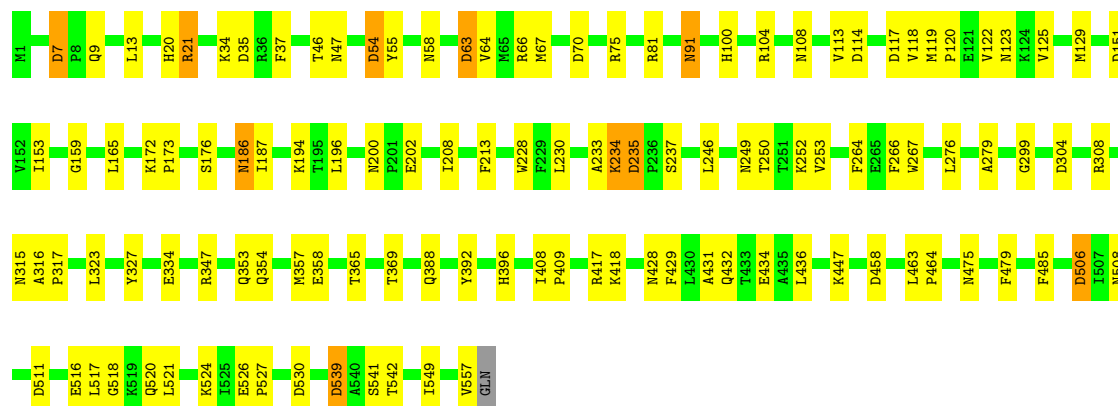
- Molecule 1: autocrine motility factor





- Molecule 1: autocrine motility factor

Chain D: 79% 19%



## 4 Data and refinement statistics

Xtrriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	80.65Å 107.77Å 270.35Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 2.40	Depositor
% Data completeness (in resolution range)	(Not available) (25.00-2.40)	Depositor
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.193 , 0.241	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	18264	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	31.0	wwPDB-VP

## 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: E4P

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	0.64	0/4553	0.84	13/6164 (0.2%)
1	B	0.64	0/4553	0.83	8/6164 (0.1%)
1	C	0.63	0/4553	0.82	9/6164 (0.1%)
1	D	0.58	0/4553	0.81	13/6164 (0.2%)
All	All	0.62	0/18212	0.82	43/24656 (0.2%)

There are no bond length outliers.

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	188	ASP	CB-CG-OD2	7.76	125.28	118.30
1	A	140	ASP	CB-CG-OD2	6.70	124.33	118.30
1	B	31	ASP	CB-CG-OD2	6.66	124.29	118.30
1	B	35	ASP	CB-CG-OD2	6.56	124.21	118.30
1	A	511	ASP	CB-CG-OD2	6.47	124.13	118.30
1	C	356	ASP	CB-CG-OD2	6.44	124.10	118.30
1	B	140	ASP	CB-CG-OD2	6.40	124.06	118.30
1	A	114	ASP	CB-CG-OD2	6.26	123.93	118.30
1	A	127	ASP	CB-CG-OD2	6.21	123.89	118.30
1	B	304	ASP	CB-CG-OD2	6.20	123.88	118.30
1	C	70	ASP	CB-CG-OD2	6.08	123.78	118.30
1	A	506	ASP	CB-CG-OD2	6.02	123.72	118.30
1	D	70	ASP	CB-CG-OD2	6.01	123.71	118.30
1	D	54	ASP	CB-CG-OD2	6.01	123.71	118.30
1	A	54	ASP	CB-CG-OD2	5.98	123.68	118.30
1	D	63	ASP	CB-CG-OD2	5.98	123.68	118.30
1	A	31	ASP	CB-CG-OD2	5.88	123.59	118.30
1	C	31	ASP	CB-CG-OD2	5.87	123.58	118.30
1	D	539	ASP	CB-CG-OD2	5.79	123.51	118.30
1	D	117	ASP	CB-CG-OD2	5.77	123.50	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	114	ASP	CB-CG-OD2	5.77	123.49	118.30
1	C	530	ASP	CB-CG-OD2	5.72	123.45	118.30
1	C	161	ASP	CB-CG-OD2	5.71	123.44	118.30
1	D	7	ASP	CB-CG-OD2	5.70	123.43	118.30
1	D	304	ASP	CB-CG-OD2	5.69	123.42	118.30
1	A	161	ASP	CB-CG-OD2	5.68	123.41	118.30
1	B	70	ASP	CB-CG-OD2	5.66	123.40	118.30
1	D	530	ASP	CB-CG-OD2	5.56	123.31	118.30
1	D	151	ASP	CB-CG-OD2	5.53	123.27	118.30
1	A	7	ASP	CB-CG-OD2	5.49	123.24	118.30
1	D	506	ASP	CB-CG-OD2	5.43	123.18	118.30
1	A	372	ASP	CB-CG-OD2	5.41	123.17	118.30
1	A	291	ASP	CB-CG-OD2	5.38	123.14	118.30
1	C	506	ASP	CB-CG-OD2	5.27	123.04	118.30
1	A	458	ASP	CB-CG-OD2	5.20	122.98	118.30
1	B	235	ASP	CB-CG-OD2	5.20	122.98	118.30
1	D	511	ASP	CB-CG-OD2	5.19	122.97	118.30
1	C	151	ASP	CB-CG-OD2	5.15	122.93	118.30
1	A	63	ASP	CB-CG-OD2	5.11	122.90	118.30
1	C	458	ASP	CB-CG-OD2	5.07	122.86	118.30
1	B	7	ASP	CB-CG-OD2	5.06	122.85	118.30
1	C	140	ASP	CB-CG-OD2	5.00	122.80	118.30
1	D	458	ASP	CB-CG-OD2	5.00	122.80	118.30

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	4445	0	4404	57	0
1	B	4445	0	4404	80	0
1	C	4445	0	4404	73	0
1	D	4445	0	4404	81	0
2	A	13	0	2	1	0
2	B	13	0	2	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	13	0	2	0	0
2	D	13	0	2	0	0
3	A	128	0	0	1	0
3	B	121	0	0	5	0
3	C	109	0	0	3	0
3	D	74	0	0	2	0
All	All	18264	0	17624	268	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 8.

All (268) 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:C:524:LYS:HB3	1:C:524:LYS:NZ	1.68	1.08
1:C:344:TYR:OH	1:D:194:LYS:NZ	1.94	1.00
1:C:524:LYS:HB3	1:C:524:LYS:HZ2	1.26	0.96
1:B:108:ASN:ND2	1:B:123:ASN:HD21	1.67	0.93
1:C:426:LEU:HD22	1:D:549:ILE:HD13	1.48	0.92
1:D:408:ILE:HG13	1:D:409:PRO:HD2	1.50	0.92
1:C:9:GLN:OE1	1:C:12:LYS:HE2	1.70	0.91
1:C:9:GLN:OE1	1:C:12:LYS:CE	2.19	0.91
1:C:9:GLN:OE1	1:C:12:LYS:NZ	2.05	0.90
1:C:144:TYR:OH	1:C:202:GLU:OE1	1.92	0.87
1:A:393:GLN:HE22	1:B:514:GLY:H	1.18	0.85
1:B:108:ASN:HD21	1:B:123:ASN:HD21	1.29	0.81
1:A:388:GLN:HE22	1:A:428:ASN:HB3	1.48	0.78
1:B:306:HIS:HE1	1:B:316:ALA:H	1.30	0.76
1:B:19:GLU:OE1	1:B:20:HIS:CE1	2.40	0.75
1:C:393:GLN:HE22	1:C:397:GLN:HE21	1.33	0.73
1:B:19:GLU:OE1	1:B:20:HIS:CD2	2.41	0.73
1:B:19:GLU:CD	1:B:20:HIS:CD2	2.62	0.72
1:B:291:ASP:HB2	3:B:692:HOH:O	1.89	0.72
1:D:91:ASN:ND2	1:D:508:ASN:HD21	1.88	0.72
1:A:306:HIS:HE1	1:A:316:ALA:H	1.38	0.72
1:B:82:GLU:OE1	1:B:308:ARG:NH2	2.22	0.70
1:A:224:THR:OG1	1:B:421:HIS:HE1	1.76	0.69
1:A:226:LYS:NZ	1:A:256:PHE:O	2.25	0.69
1:D:526:GLU:HB2	1:D:527:PRO:CD	2.24	0.69
1:B:388:GLN:HE22	1:B:428:ASN:HB3	1.59	0.68
1:C:46:THR:O	1:C:47:ASN:HB2	1.92	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:396:HIS:CD2	1:D:436:LEU:HD23	2.29	0.68
1:A:57:LYS:NZ	1:A:433:THR:OG1	2.27	0.67
1:D:557:VAL:HG23	1:D:557:VAL:O	1.94	0.67
1:B:19:GLU:OE1	1:B:20:HIS:NE2	2.28	0.66
1:C:524:LYS:HB3	1:C:524:LYS:HZ3	1.57	0.66
1:D:316:ALA:HB3	1:D:317:PRO:HD3	1.76	0.66
1:D:186:ASN:HD22	1:D:187:ILE:N	1.94	0.65
1:D:526:GLU:HB2	1:D:527:PRO:HD3	1.78	0.65
1:C:226:LYS:NZ	1:C:256:PHE:O	2.29	0.65
1:B:438:ARG:NE	3:B:679:HOH:O	2.05	0.64
1:C:371:VAL:HG13	1:C:373:HIS:H	1.62	0.63
1:D:108:ASN:ND2	1:D:123:ASN:HD21	1.97	0.63
1:B:531:GLY:O	1:B:553:ARG:NH1	2.32	0.63
1:B:108:ASN:ND2	1:B:123:ASN:ND2	2.46	0.62
1:B:393:GLN:HE22	1:B:397:GLN:HE21	1.46	0.61
1:A:393:GLN:HE22	1:B:514:GLY:N	1.95	0.61
1:D:108:ASN:HD21	1:D:123:ASN:HD21	1.47	0.61
1:D:517:LEU:O	1:D:521:LEU:HG	2.00	0.61
1:C:426:LEU:HD22	1:D:549:ILE:CD1	2.27	0.61
1:B:511:ASP:OD1	3:B:635:HOH:O	2.16	0.61
1:D:7:ASP:OD1	1:D:9:GLN:N	2.34	0.61
1:A:525:ILE:HD12	1:B:431:ALA:HB2	1.82	0.60
1:A:172:LYS:N	1:A:173:PRO:CD	2.64	0.59
1:C:556:ARG:HH11	1:C:556:ARG:HG2	1.67	0.59
1:D:316:ALA:HB3	1:D:317:PRO:CD	2.32	0.59
1:B:46:THR:O	1:B:47:ASN:HB2	2.03	0.59
1:B:408:ILE:HD13	1:B:426:LEU:HD23	1.84	0.59
1:C:43:THR:HG22	1:C:52:LEU:HD13	1.84	0.59
1:C:353:GLN:HG3	1:C:379:VAL:O	2.02	0.58
1:D:186:ASN:HD22	1:D:187:ILE:H	1.50	0.58
1:D:20:HIS:O	1:D:21:ARG:C	2.41	0.58
1:C:250:THR:HG22	1:C:254:LYS:HE3	1.86	0.57
1:D:46:THR:O	1:D:47:ASN:HB2	2.04	0.57
1:B:19:GLU:OE2	1:B:20:HIS:NE2	2.38	0.57
1:D:557:VAL:O	1:D:557:VAL:CG2	2.53	0.57
1:D:408:ILE:HG22	1:D:429:PHE:CZ	2.40	0.56
1:A:301:HIS:CE1	1:A:305:GLN:NE2	2.73	0.56
1:B:259:ASP:OD1	1:B:260:PRO:HD2	2.06	0.56
1:A:315:ASN:ND2	1:A:317:PRO:HD2	2.21	0.56
1:B:19:GLU:CD	1:B:20:HIS:NE2	2.59	0.56
1:C:524:LYS:NZ	1:C:524:LYS:CB	2.51	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:75:ARG:NH2	1:D:506:ASP:HB2	2.20	0.56
1:D:408:ILE:CG1	1:D:409:PRO:HD2	2.29	0.56
1:B:19:GLU:OE1	1:B:20:HIS:CG	2.58	0.55
1:D:63:ASP:OD1	1:D:66:ARG:NH2	2.39	0.55
1:B:12:LYS:HD2	1:B:67:MET:SD	2.46	0.55
1:C:521:LEU:HD13	1:D:434:GLU:OE2	2.07	0.54
1:A:408:ILE:HG12	1:A:409:PRO:HD2	1.90	0.54
1:C:172:LYS:N	1:C:173:PRO:CD	2.70	0.54
1:C:172:LYS:HD3	1:C:287:HIS:HE1	1.72	0.54
1:A:231:GLN:O	1:A:234:LYS:HE2	2.08	0.54
1:B:457:GLU:HB2	1:B:461:ARG:NH2	2.22	0.54
1:A:20:HIS:O	1:A:21:ARG:C	2.46	0.54
1:D:249:ASN:O	1:D:253:VAL:HG23	2.09	0.53
1:C:371:VAL:CG1	1:C:373:HIS:H	2.21	0.53
1:C:468:PHE:CE2	1:D:517:LEU:HD22	2.44	0.53
1:B:443:GLU:OE1	1:B:447:LYS:NZ	2.36	0.52
1:A:408:ILE:CG1	1:A:409:PRO:HD2	2.39	0.52
2:A:601[B]:E4P:H1	1:B:389:HIS:HB3	1.91	0.52
1:A:171:LEU:C	1:A:173:PRO:HD2	2.30	0.52
1:C:56:SER:OG	1:D:541:SER:HB2	2.08	0.52
1:A:139:GLY:O	1:A:142:LYS:NZ	2.39	0.52
1:C:346:HIS:HA	1:C:383:PRO:HG3	1.91	0.52
1:B:108:ASN:HD21	1:B:123:ASN:ND2	2.03	0.52
1:C:259:ASP:OD1	1:C:260:PRO:HD2	2.10	0.51
1:D:396:HIS:HE1	1:D:432:GLN:OE1	1.92	0.51
1:A:315:ASN:HD22	1:A:317:PRO:HD2	1.75	0.51
1:D:81:ARG:HD2	1:D:308:ARG:HA	1.92	0.51
1:C:342:ASP:OD2	1:C:344:TYR:HB2	2.11	0.51
1:C:442:THR:O	1:C:446:ARG:N	2.25	0.51
1:D:125:VAL:O	1:D:129:MET:HG3	2.11	0.51
1:B:362:LYS:NZ	1:B:511:ASP:O	2.38	0.50
1:D:353:GLN:O	1:D:357:MET:HB2	2.11	0.50
1:D:234:LYS:O	1:D:235:ASP:HB2	2.11	0.50
1:A:187:ILE:HB	1:A:217:GLU:HG3	1.94	0.50
1:C:371:VAL:CG1	1:C:373:HIS:O	2.59	0.50
1:D:539:ASP:OD2	1:D:542:THR:OG1	2.29	0.50
1:D:388:GLN:HE22	1:D:428:ASN:HB3	1.77	0.50
1:B:306:HIS:CE1	1:B:316:ALA:H	2.21	0.49
1:C:112:LEU:HA	1:C:116:LYS:O	2.12	0.49
1:B:19:GLU:HB2	3:B:693:HOH:O	2.11	0.49
1:C:385:THR:O	1:C:388:GLN:HB2	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:246:LEU:HD13	1:B:279:ALA:O	2.13	0.49
1:A:13:LEU:HD11	1:A:68:LEU:HD23	1.95	0.49
1:A:187:ILE:O	1:B:421:HIS:HD2	1.96	0.49
1:B:58:ASN:OD1	1:B:475:ASN:ND2	2.46	0.49
1:C:518:GLY:O	1:C:521:LEU:N	2.45	0.49
1:D:119:MET:N	1:D:120:PRO:CD	2.74	0.49
1:C:99:LEU:HB2	1:C:269:TRP:CE3	2.48	0.49
1:B:181:VAL:HG22	1:B:287:HIS:CD2	2.48	0.48
1:B:132:PHE:O	1:B:136:VAL:HG23	2.12	0.48
1:D:165:LEU:HD23	1:D:165:LEU:C	2.33	0.48
1:A:352:PHE:CZ	1:A:494:TYR:HB2	2.48	0.48
1:A:499:PHE:HD1	1:A:510:PHE:HZ	1.62	0.48
1:B:315:ASN:OD1	1:B:317:PRO:HD2	2.14	0.48
1:B:406:PHE:HB3	1:B:429:PHE:CE1	2.49	0.48
1:A:57:LYS:HE3	1:B:541:SER:OG	2.13	0.48
1:B:1:MET:HB3	1:B:6:ARG:HG3	1.96	0.47
1:D:517:LEU:HG	1:D:521:LEU:HD21	1.96	0.47
1:A:521:LEU:HB2	1:B:431:ALA:HB1	1.97	0.47
1:B:526:GLU:HB2	1:B:527:PRO:CD	2.44	0.47
1:C:26:LEU:HD13	1:C:437:MET:HG2	1.97	0.47
1:C:12:LYS:HE3	1:C:67:MET:HG2	1.97	0.47
1:D:276:LEU:C	1:D:276:LEU:HD12	2.34	0.47
1:A:99:LEU:HB2	1:A:269:TRP:CE3	2.50	0.47
1:C:162:LEU:HD12	3:C:700:HOH:O	2.14	0.47
1:A:316:ALA:HB3	1:A:317:PRO:HD3	1.97	0.46
1:D:91:ASN:C	1:D:91:ASN:HD22	2.18	0.46
1:B:449:LEU:HD21	1:B:466:LYS:HE3	1.97	0.46
1:D:396:HIS:CD2	1:D:436:LEU:CD2	2.97	0.46
1:B:179:PRO:O	1:B:287:HIS:HD2	1.98	0.46
1:D:323:LEU:HD13	1:D:475:ASN:HD21	1.81	0.46
1:B:165:LEU:C	1:B:165:LEU:HD23	2.36	0.46
1:B:408:ILE:HG13	1:B:409:PRO:HD2	1.97	0.46
1:C:83:ARG:HG2	1:C:88:GLU:OE1	2.16	0.46
1:C:526:GLU:HB2	1:C:527:PRO:CD	2.45	0.46
1:A:449:LEU:HB3	1:A:459:LEU:HD12	1.97	0.46
1:B:169:GLU:OE2	1:B:346:HIS:NE2	2.31	0.46
1:C:165:LEU:C	1:C:165:LEU:HD23	2.35	0.46
1:D:200:ASN:OD1	1:D:202:GLU:HB2	2.16	0.46
1:B:347:ARG:HD2	1:B:347:ARG:HA	1.71	0.46
1:C:409:PRO:HA	1:C:479:PHE:O	2.15	0.46
1:C:164:PRO:HA	1:C:284:ILE:HD11	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:408:ILE:CG1	1:A:409:PRO:CD	2.93	0.46
1:B:259:ASP:OD1	1:B:260:PRO:CD	2.64	0.46
1:D:365:THR:HG23	1:D:369:THR:O	2.16	0.46
1:C:334:GLU:OE2	1:D:334:GLU:HG3	2.16	0.46
1:A:446:ARG:O	1:A:450:GLN:HG2	2.16	0.45
1:A:455:SER:C	1:A:457:GLU:H	2.19	0.45
1:C:518:GLY:O	1:C:519:LYS:C	2.54	0.45
1:A:46:THR:O	1:A:47:ASN:HB2	2.17	0.45
1:A:57:LYS:CE	1:B:541:SER:OG	2.65	0.45
1:B:187:ILE:HB	1:B:217:GLU:CG	2.46	0.45
1:D:37:PHE:HB3	3:D:621:HOH:O	2.16	0.45
1:A:58:ASN:ND2	1:A:327:TYR:OH	2.41	0.45
1:C:158:GLY:HA2	3:C:700:HOH:O	2.17	0.45
1:C:189:GLY:O	1:C:190:THR:C	2.52	0.45
1:D:409:PRO:HA	1:D:479:PHE:O	2.17	0.45
1:B:19:GLU:OE2	1:B:20:HIS:CD2	2.70	0.45
1:D:388:GLN:HA	1:D:392:TYR:CG	2.52	0.45
1:A:463:LEU:HB3	1:A:464:PRO:HD3	1.98	0.45
1:A:519:LYS:O	1:A:520:GLN:C	2.53	0.45
1:C:104:ARG:O	1:C:301:HIS:HB2	2.16	0.45
1:C:315:ASN:OD1	1:C:317:PRO:HD2	2.17	0.45
1:D:113:VAL:HG13	1:D:118:VAL:HG13	1.98	0.45
1:D:408:ILE:HG13	1:D:409:PRO:CD	2.35	0.45
1:B:172:LYS:N	1:B:173:PRO:CD	2.80	0.45
1:A:521:LEU:HD12	1:B:435:ALA:HB2	1.99	0.44
1:B:409:PRO:HA	1:B:479:PHE:O	2.18	0.44
1:C:463:LEU:HB3	1:C:464:PRO:CD	2.47	0.44
1:C:463:LEU:HB3	1:C:464:PRO:HD3	1.98	0.44
1:C:20:HIS:O	1:C:22:SER:N	2.50	0.44
1:D:75:ARG:HH21	1:D:506:ASP:HB2	1.82	0.44
1:B:81:ARG:HD2	1:B:308:ARG:HA	2.00	0.44
1:D:516:GLU:O	1:D:517:LEU:C	2.55	0.44
1:D:518:GLY:HA2	1:D:521:LEU:HD12	1.98	0.44
1:A:465:HIS:CE1	1:B:364:ILE:HG22	2.53	0.44
1:C:345:LEU:HD21	1:C:482:LEU:HD21	1.99	0.44
1:C:352:PHE:CZ	1:C:494:TYR:HB2	2.53	0.44
1:D:208:ILE:HD13	1:D:208:ILE:N	2.32	0.44
1:C:1:MET:HA	1:C:372:ASP:OD2	2.17	0.44
1:A:465:HIS:CE1	1:B:364:ILE:CG2	3.00	0.44
1:A:466:LYS:NZ	3:A:704:HOH:O	2.47	0.44
1:C:523:LYS:HA	1:C:523:LYS:HD2	1.75	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:187:ILE:HB	1:C:217:GLU:HG3	1.99	0.43
1:D:64:VAL:HA	1:D:67:MET:HE3	1.99	0.43
1:D:187:ILE:O	1:D:187:ILE:HG13	2.16	0.43
1:D:316:ALA:CB	1:D:317:PRO:CD	2.96	0.43
1:A:7:ASP:OD2	1:A:9:GLN:HB2	2.18	0.43
1:A:165:LEU:C	1:A:165:LEU:HD23	2.39	0.43
1:C:121:GLU:HA	1:C:121:GLU:OE2	2.19	0.43
1:A:455:SER:C	1:A:457:GLU:N	2.72	0.43
1:D:172:LYS:N	1:D:173:PRO:CD	2.81	0.43
1:B:21:ARG:HG3	1:B:22:SER:N	2.33	0.43
1:D:246:LEU:HD13	1:D:279:ALA:O	2.18	0.43
1:B:119:MET:N	1:B:120:PRO:CD	2.81	0.43
1:B:346:HIS:HA	1:B:383:PRO:HG3	2.00	0.43
1:D:54:ASP:C	1:D:54:ASP:OD1	2.57	0.43
1:B:359:SER:O	1:B:509:SER:HA	2.19	0.43
1:C:45:ASN:HB2	1:C:50:HIS:NE2	2.34	0.43
1:D:408:ILE:CG1	1:D:409:PRO:CD	2.96	0.43
1:A:342:ASP:OD2	1:A:344:TYR:HB2	2.19	0.43
1:B:388:GLN:HA	1:B:392:TYR:CG	2.53	0.43
1:C:13:LEU:HD11	1:C:68:LEU:HD23	2.01	0.43
1:C:83:ARG:HG2	1:C:88:GLU:CD	2.39	0.43
1:D:463:LEU:HB3	1:D:464:PRO:HD3	2.00	0.43
1:A:224:THR:HG1	1:B:421:HIS:HE1	1.66	0.43
1:D:408:ILE:HG22	1:D:429:PHE:CE1	2.53	0.43
1:B:62:GLU:HG2	3:B:649:HOH:O	2.19	0.43
1:C:388:GLN:HA	1:C:392:TYR:CG	2.54	0.42
1:C:480:THR:HG21	1:D:557:VAL:HG12	2.00	0.42
1:D:159:GLY:N	1:D:354:GLN:HE22	2.16	0.42
1:D:417:ARG:O	1:D:418:LYS:HB2	2.19	0.42
1:B:13:LEU:CD1	1:B:71:LEU:HD22	2.50	0.42
1:A:200:ASN:OD1	1:A:201:PRO:HD2	2.19	0.42
1:B:230:LEU:HA	1:B:230:LEU:HD23	1.77	0.42
1:D:196:LEU:HD13	1:D:228:TRP:CG	2.55	0.42
1:C:7:ASP:HA	1:C:8:PRO:HD3	1.86	0.42
1:C:192:ILE:HG22	3:C:640:HOH:O	2.19	0.42
1:A:409:PRO:HA	1:A:479:PHE:O	2.18	0.42
1:B:316:ALA:HB3	1:B:317:PRO:HD3	2.00	0.42
1:B:240:ALA:O	1:B:262:ASN:ND2	2.51	0.42
1:C:521:LEU:HB2	1:D:431:ALA:HB1	2.01	0.42
1:D:153:ILE:N	1:D:153:ILE:HD12	2.35	0.42
1:D:230:LEU:HD23	1:D:230:LEU:HA	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:233:ALA:O	1:D:234:LYS:C	2.58	0.42
1:C:321:ALA:HB1	1:C:501:GLN:HG3	2.02	0.41
1:D:396:HIS:HD2	3:D:663:HOH:O	2.02	0.41
1:A:171:LEU:C	1:A:173:PRO:CD	2.89	0.41
1:B:312:LEU:HA	1:B:312:LEU:HD23	1.85	0.41
1:D:165:LEU:CD2	1:D:347:ARG:HG3	2.49	0.41
1:B:15:GLN:HG2	1:B:18:ARG:HH22	1.85	0.41
1:C:515:VAL:CG2	1:C:516:GLU:N	2.83	0.41
1:A:56:SER:OG	1:B:541:SER:HB2	2.20	0.41
1:A:179:PRO:O	1:A:287:HIS:HD2	2.04	0.41
1:C:526:GLU:HB2	1:C:527:PRO:HD3	2.03	0.41
1:B:320:LEU:HA	1:B:320:LEU:HD23	1.78	0.41
1:C:113:VAL:HG12	1:C:118:VAL:CG1	2.50	0.41
1:A:1:MET:HB3	1:A:6:ARG:HE	1.86	0.41
1:A:173:PRO:HG3	1:A:344:TYR:CE1	2.56	0.41
1:A:408:ILE:HA	1:A:409:PRO:HD3	1.84	0.41
1:A:408:ILE:HD13	1:A:426:LEU:HD23	2.02	0.41
1:A:517:LEU:O	1:A:521:LEU:HG	2.20	0.41
1:B:187:ILE:HB	1:B:217:GLU:HG3	2.02	0.41
1:C:393:GLN:HB3	1:D:358:GLU:HA	2.03	0.41
1:D:108:ASN:HD22	1:D:108:ASN:HA	1.67	0.41
1:A:13:LEU:HD11	1:A:68:LEU:CD2	2.50	0.41
1:B:525:ILE:O	1:B:526:GLU:C	2.59	0.41
1:B:20:HIS:O	1:B:21:ARG:C	2.60	0.40
1:C:58:ASN:O	1:C:60:VAL:N	2.49	0.40
1:A:483:THR:HB	1:A:484:PRO:HD2	2.03	0.40
1:D:299:GLY:HA3	1:D:485:PHE:O	2.21	0.40
1:B:357:MET:HE3	1:B:378:ILE:HA	2.03	0.40
1:C:187:ILE:HB	1:C:217:GLU:CG	2.52	0.40
1:C:230:LEU:HD23	1:C:230:LEU:HA	1.87	0.40
1:D:58:ASN:ND2	1:D:327:TYR:OH	2.43	0.40
1:D:122:VAL:HA	1:D:267:TRP:CH2	2.56	0.40
1:B:219:ILE:O	1:B:222:ALA:HB3	2.22	0.40
1:D:55:TYR:HB2	1:D:323:LEU:HD11	2.04	0.40
1:D:234:LYS:O	1:D:235:ASP:CB	2.69	0.40
1:D:246:LEU:HA	1:D:264:PHE:O	2.22	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	555/558 (100%)	530 (96%)	25 (4%)	0	100	100
1	B	555/558 (100%)	534 (96%)	21 (4%)	0	100	100
1	C	555/558 (100%)	523 (94%)	32 (6%)	0	100	100
1	D	555/558 (100%)	525 (95%)	28 (5%)	2 (0%)	34	48
All	All	2220/2232 (100%)	2112 (95%)	106 (5%)	2 (0%)	51	68

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	235	ASP
1	D	234	LYS

### 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	476/477 (100%)	464 (98%)	12 (2%)	47	67
1	B	476/477 (100%)	457 (96%)	19 (4%)	31	49
1	C	476/477 (100%)	460 (97%)	16 (3%)	37	56
1	D	476/477 (100%)	458 (96%)	18 (4%)	33	51
All	All	1904/1908 (100%)	1839 (97%)	65 (3%)	37	56

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	LEU
1	A	34	LYS
1	A	100	HIS
1	A	104	ARG
1	A	134	GLN
1	A	213	PHE
1	A	308	ARG
1	A	315	ASN
1	A	449	LEU
1	A	450	GLN
1	A	479	PHE
1	A	524	LYS
1	B	5	THR
1	B	19	GLU
1	B	21	ARG
1	B	24	LEU
1	B	35	ASP
1	B	43	THR
1	B	104	ARG
1	B	161	ASP
1	B	176	SER
1	B	181	VAL
1	B	213	PHE
1	B	237	SER
1	B	298	SER
1	B	314	LYS
1	B	347	ARG
1	B	369	THR
1	B	450	GLN
1	B	457	GLU
1	B	557	VAL
1	C	5	THR
1	C	13	LEU
1	C	22	SER
1	C	27	ARG
1	C	66	ARG
1	C	104	ARG
1	C	113	VAL
1	C	134	GLN
1	C	147	LYS
1	C	181	VAL
1	C	213	PHE
1	C	447	LYS

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Mol	Chain	Res	Type
1	C	449	LEU
1	C	516	GLU
1	C	523	LYS
1	C	556	ARG
1	D	13	LEU
1	D	21	ARG
1	D	34	LYS
1	D	35	ASP
1	D	91	ASN
1	D	100	HIS
1	D	104	ARG
1	D	176	SER
1	D	186	ASN
1	D	213	PHE
1	D	237	SER
1	D	250	THR
1	D	252	LYS
1	D	266	PHE
1	D	315	ASN
1	D	447	LYS
1	D	520	GLN
1	D	524	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (58) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	58	ASN
1	A	134	GLN
1	A	216	GLN
1	A	287	HIS
1	A	292	ASN
1	A	305	GLN
1	A	306	HIS
1	A	315	ASN
1	A	354	GLN
1	A	388	GLN
1	A	393	GLN
1	A	397	GLN
1	A	465	HIS
1	A	475	ASN
1	B	15	GLN
1	B	58	ASN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	86	ASN
1	B	108	ASN
1	B	216	GLN
1	B	287	HIS
1	B	306	HIS
1	B	354	GLN
1	B	388	GLN
1	B	397	GLN
1	B	421	HIS
1	B	428	ASN
1	B	432	GLN
1	B	475	ASN
1	C	20	HIS
1	C	58	ASN
1	C	86	ASN
1	C	123	ASN
1	C	198	GLN
1	C	216	GLN
1	C	261	GLN
1	C	287	HIS
1	C	292	ASN
1	C	354	GLN
1	C	360	ASN
1	C	388	GLN
1	C	397	GLN
1	D	11	GLN
1	D	58	ASN
1	D	86	ASN
1	D	91	ASN
1	D	108	ASN
1	D	186	ASN
1	D	198	GLN
1	D	216	GLN
1	D	292	ASN
1	D	305	GLN
1	D	315	ASN
1	D	354	GLN
1	D	388	GLN
1	D	396	HIS
1	D	450	GLN
1	D	465	HIS
1	D	475	ASN

### 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](#)

8 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	E4P	B	602[B]	-	9,11,11	1.28	1 (11%)	12,15,15	1.21	0
2	E4P	A	601[B]	-	9,11,11	1.17	1 (11%)	12,15,15	1.02	1 (8%)
2	E4P	C	603[B]	-	9,11,11	1.34	1 (11%)	12,15,15	1.19	1 (8%)
2	E4P	A	601[A]	-	9,11,11	1.12	1 (11%)	12,15,15	1.02	1 (8%)
2	E4P	C	603[A]	-	9,11,11	1.33	1 (11%)	12,15,15	1.19	1 (8%)
2	E4P	B	602[A]	-	9,11,11	1.29	1 (11%)	12,15,15	1.21	0
2	E4P	D	604[A]	-	9,11,11	1.10	1 (11%)	12,15,15	1.29	2 (16%)
2	E4P	D	604[B]	-	9,11,11	1.11	1 (11%)	12,15,15	1.29	2 (16%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	E4P	B	602[B]	-	-	0/10/12/12	-
2	E4P	A	601[B]	-	-	0/10/12/12	-
2	E4P	C	603[B]	-	-	0/10/12/12	-
2	E4P	A	601[A]	-	-	0/10/12/12	-
2	E4P	C	603[A]	-	-	0/10/12/12	-
2	E4P	B	602[A]	-	-	0/10/12/12	-
2	E4P	D	604[A]	-	-	0/10/12/12	-
2	E4P	D	604[B]	-	-	0/10/12/12	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	603[A]	E4P	P-O4	-3.11	1.50	1.60
2	C	603[B]	E4P	P-O4	-3.11	1.50	1.60
2	B	602[A]	E4P	P-O4	-3.03	1.50	1.60
2	B	602[B]	E4P	P-O4	-3.03	1.50	1.60
2	D	604[A]	E4P	P-O4	-2.59	1.51	1.60
2	D	604[B]	E4P	P-O4	-2.59	1.51	1.60
2	A	601[A]	E4P	P-O4	-2.38	1.52	1.60
2	A	601[B]	E4P	P-O4	-2.38	1.52	1.60

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601[A]	E4P	C3-C2-C1	-2.21	103.83	110.75
2	A	601[B]	E4P	C3-C2-C1	-2.21	103.83	110.75
2	D	604[A]	E4P	O3P-P-O4	-2.15	101.02	106.73
2	D	604[B]	E4P	O3P-P-O4	-2.15	101.02	106.73
2	D	604[A]	E4P	C3-C2-C1	-2.09	104.19	110.75
2	D	604[B]	E4P	C3-C2-C1	-2.09	104.19	110.75
2	C	603[A]	E4P	O4-C4-C3	2.09	114.94	109.36
2	C	603[B]	E4P	O4-C4-C3	2.09	114.94	109.36

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601[B]	E4P	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

### 6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.