Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2023 – 11:06 AM EDT

PDB ID	:	1PJ8
Title	:	Structure of a ternary complex of proteinase K, mercury and a substrate-analogue hexapeptide at 2.2 A resolution
Authors	:	Saxena, A.K.; Singh, T.P.; Peters, K.; Fittkau, S.; Visanji, M.; Wilson, K.S.; Betzel, C.
Deposited on	:	2003-06-02
Resolution	:	2.20 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 ⓘ 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 ⓘ) were used in the production of this report:

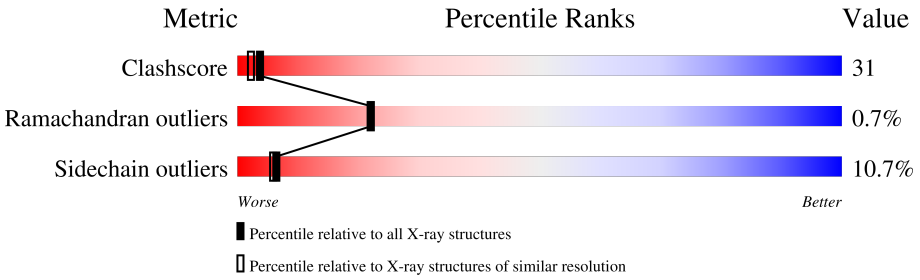
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 2.20 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	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)

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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	279	68% 26% 5% •
2	I	7	43% 14% 43%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 2239 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 Proteinase K.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	279	Total	C	N	O	S	0	0	0
			2015	1240	352	413	10			

- Molecule 2 is a protein called 6-residue peptide (N-Ac-PAPFPA-NH2).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	I	7	Total	C	N	O	0	0	1
			43	30	7	6			

- Molecule 3 is MERCURY (II) ION (three-letter code: HG) (formula: Hg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Hg	0	0
			2	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	177	Total	O	0	0
			177	177		
4	I	2	Total	O	0	0
			2	2		

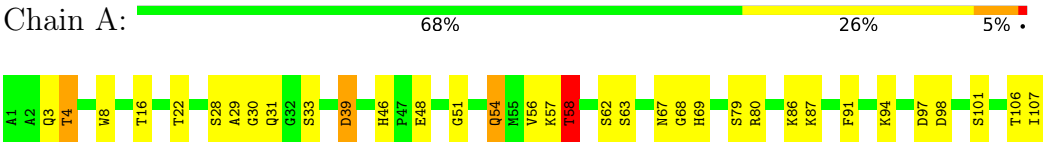
3 Residue-property plots (i)

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.

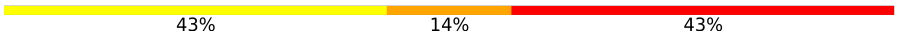
• Molecule 1: Proteinase K

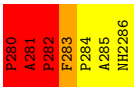
Chain A:



• Molecule 2: 6-residue peptide (N-Ac-PAPFPA-NH2)

Chain I:





4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	68.28Å 68.28Å 107.87Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.20	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-2.20)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.170 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2239	wwPDB-VP
Average B, all atoms (Å^2)	14.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: HG, NH2

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	0.77	0/2054	1.23	20/2793 (0.7%)
2	I	1.28	1/44 (2.3%)	2.27	4/58 (6.9%)
All	All	0.78	1/2098 (0.0%)	1.26	24/2851 (0.8%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	I	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	281	ALA	CA-CB	-5.80	1.40	1.52

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	80	ARG	NE-CZ-NH1	-16.75	111.92	120.30
1	A	185	ARG	NE-CZ-NH2	16.03	128.31	120.30
1	A	80	ARG	NE-CZ-NH2	15.50	128.05	120.30
1	A	185	ARG	NE-CZ-NH1	-13.34	113.63	120.30
1	A	97	ASP	CB-CG-OD2	8.05	125.55	118.30
1	A	224	SER	N-CA-CB	7.88	122.32	110.50
1	A	98	ASP	CB-CG-OD2	7.46	125.02	118.30
1	A	39	ASP	CB-CG-OD2	7.14	124.73	118.30
1	A	133	LEU	CA-CB-CG	6.22	129.60	115.30
2	I	282	PRO	N-CA-C	6.15	128.08	112.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	260	ASP	CB-CG-OD2	6.11	123.80	118.30
2	I	283	PHE	CA-CB-CG	6.06	128.44	113.90
1	A	112	ASP	CB-CG-OD2	5.98	123.68	118.30
1	A	121	ARG	NE-CZ-NH2	-5.88	117.36	120.30
2	I	280	PRO	CB-CA-C	-5.71	97.72	112.00
1	A	165	ASP	CB-CG-OD2	5.63	123.36	118.30
1	A	225	MET	CG-SD-CE	5.50	108.99	100.20
1	A	58	THR	CB-CA-C	-5.49	96.79	111.60
1	A	161	ASN	CB-CA-C	-5.45	99.50	110.40
1	A	187	ASP	CB-CG-OD2	5.35	123.11	118.30
1	A	4	THR	N-CA-CB	-5.30	100.22	110.30
1	A	80	ARG	CD-NE-CZ	5.29	131.00	123.60
1	A	117	ASP	CB-CG-OD2	5.26	123.03	118.30
2	I	281	ALA	N-CA-C	5.21	125.05	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	I	280	PRO	Peptide
2	I	281	ALA	Mainchain

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	2015	0	1911	117	0
2	I	43	0	40	68	0
3	A	2	0	0	0	0
4	A	177	0	0	9	0
4	I	2	0	0	3	0
All	All	2239	0	1951	125	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 31.

All (125) 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:223:THR:N	2:I:281:ALA:HB3	1.60	1.14
1:A:69:HIS:HB2	2:I:283:PHE:HB2	1.23	1.11
1:A:69:HIS:CB	2:I:283:PHE:HB2	1.80	1.10
1:A:69:HIS:CG	2:I:283:PHE:HB2	1.88	1.09
1:A:221:SER:N	2:I:284:PRO:HG2	1.66	1.09
1:A:224:SER:HB2	2:I:281:ALA:O	1.54	1.08
1:A:69:HIS:CG	2:I:283:PHE:CB	2.37	1.06
2:I:281:ALA:HB1	2:I:282:PRO:HD2	1.36	1.05
1:A:224:SER:H	2:I:281:ALA:CA	1.68	1.05
1:A:67:ASN:ND2	2:I:283:PHE:CE2	2.25	1.05
1:A:221:SER:H	2:I:284:PRO:HG2	0.93	1.04
1:A:230:VAL:HB	4:A:359:HOH:O	1.63	0.97
1:A:54:GLN:NE2	1:A:91:PHE:CE2	2.34	0.95
1:A:223:THR:H	2:I:281:ALA:HB3	1.24	0.94
1:A:58:THR:HG21	1:A:62:SER:O	1.66	0.94
1:A:221:SER:H	2:I:284:PRO:CG	1.81	0.94
1:A:54:GLN:HE22	1:A:91:PHE:HE2	1.11	0.93
1:A:180:VAL:HG21	1:A:230:VAL:HG21	1.48	0.91
1:A:224:SER:HB2	2:I:281:ALA:C	1.90	0.91
1:A:261:LEU:H	1:A:270:ASN:HD21	1.17	0.91
1:A:69:HIS:CD2	2:I:283:PHE:CB	2.54	0.90
1:A:67:ASN:HD21	2:I:283:PHE:HE2	1.10	0.90
1:A:69:HIS:CD2	2:I:283:PHE:CA	2.56	0.88
1:A:223:THR:H	2:I:281:ALA:CB	1.86	0.88
1:A:69:HIS:CG	2:I:283:PHE:HB3	2.08	0.87
1:A:223:THR:N	2:I:281:ALA:CB	2.36	0.87
1:A:54:GLN:NE2	1:A:91:PHE:HE2	1.70	0.87
1:A:158:ALA:HB3	2:I:280:PRO:HA	1.56	0.86
1:A:69:HIS:CD2	2:I:283:PHE:HA	2.11	0.85
1:A:158:ALA:CB	2:I:280:PRO:HA	2.14	0.78
1:A:161:ASN:OD1	1:A:192:PHE:CD1	2.37	0.78
1:A:224:SER:CB	2:I:281:ALA:C	2.52	0.77
1:A:224:SER:CB	2:I:281:ALA:O	2.31	0.77
1:A:161:ASN:ND2	2:I:282:PRO:CD	2.48	0.76
1:A:69:HIS:CD2	2:I:283:PHE:HB3	2.21	0.76
1:A:160:GLY:HA2	2:I:280:PRO:O	1.83	0.76
1:A:207:SER:HB2	4:A:376:HOH:O	1.86	0.74
1:A:224:SER:H	2:I:281:ALA:N	1.89	0.71
1:A:223:THR:CA	2:I:281:ALA:HB3	2.21	0.71
1:A:180:VAL:CG2	1:A:230:VAL:HG21	2.21	0.70
1:A:221:SER:CA	2:I:284:PRO:HG2	2.22	0.69
1:A:224:SER:H	2:I:281:ALA:CB	2.05	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:224:SER:N	2:I:281:ALA:N	2.40	0.69
2:I:281:ALA:HB1	2:I:282:PRO:CD	2.19	0.69
1:A:224:SER:N	2:I:281:ALA:CA	2.50	0.69
1:A:58:THR:CG2	1:A:94:LYS:HD3	2.23	0.68
1:A:185:ARG:HH21	1:A:185:ARG:HB3	1.60	0.66
1:A:224:SER:CA	2:I:281:ALA:H	2.09	0.66
1:A:207:SER:HB2	2:I:286:NH2:N	2.12	0.65
1:A:133:LEU:HA	2:I:280:PRO:HB3	1.78	0.65
1:A:161:ASN:ND2	2:I:282:PRO:HD2	2.11	0.65
1:A:224:SER:OG	2:I:281:ALA:N	2.29	0.64
1:A:132:SER:HB3	1:A:224:SER:HB3	1.78	0.64
1:A:69:HIS:HD2	2:I:283:PHE:HA	1.59	0.63
1:A:164:ALA:H	1:A:194:ASN:ND2	1.96	0.63
2:I:281:ALA:CB	2:I:282:PRO:HD2	2.13	0.63
1:A:263:ASN:HB2	4:A:379:HOH:O	1.98	0.63
1:A:30:GLY:C	1:A:239:THR:HG21	2.18	0.63
1:A:69:HIS:HB2	2:I:283:PHE:CB	2.16	0.63
1:A:160:GLY:HA2	2:I:280:PRO:N	2.14	0.63
1:A:115:ALA:O	1:A:118:LYS:HE3	1.99	0.63
1:A:250:ARG:HB2	4:A:467:HOH:O	2.00	0.62
1:A:67:ASN:OD1	2:I:283:PHE:CD2	2.52	0.62
2:I:281:ALA:CB	2:I:282:PRO:CD	2.75	0.62
1:A:161:ASN:OD1	1:A:192:PHE:HD1	1.81	0.61
1:A:125:LYS:HG3	1:A:239:THR:HB	1.83	0.61
2:I:280:PRO:O	2:I:281:ALA:HB2	2.00	0.61
1:A:224:SER:N	2:I:281:ALA:H	1.99	0.60
1:A:28:SER:O	1:A:31:GLN:HG2	2.01	0.60
1:A:162:ASN:H	1:A:194:ASN:ND2	2.00	0.59
1:A:54:GLN:NE2	1:A:91:PHE:CD2	2.71	0.59
1:A:250:ARG:CB	4:A:467:HOH:O	2.51	0.58
1:A:3:GLN:HE22	1:A:86:LYS:HZ1	1.50	0.57
1:A:221:SER:HB2	2:I:284:PRO:CG	2.34	0.57
1:A:182:ALA:HB2	1:A:223:THR:HA	1.86	0.57
1:A:207:SER:HA	2:I:286:NH2:N	2.18	0.57
1:A:48:GLU:HB3	1:A:79:SER:HB2	1.87	0.56
1:A:46:HIS:HD2	1:A:48:GLU:H	1.53	0.56
1:A:58:THR:HG23	1:A:94:LYS:HD3	1.88	0.56
1:A:224:SER:H	2:I:281:ALA:HB3	1.71	0.55
1:A:221:SER:O	2:I:284:PRO:CG	2.54	0.55
2:I:284:PRO:N	4:I:483:HOH:O	2.40	0.54
1:A:173:SER:O	1:A:175:PRO:HD3	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:227:THR:O	1:A:230:VAL:HG22	2.08	0.53
1:A:126:GLY:HA3	1:A:238:MET:CE	2.39	0.52
1:A:164:ALA:H	1:A:194:ASN:HD22	1.57	0.52
1:A:224:SER:CA	2:I:281:ALA:O	2.58	0.51
1:A:227:THR:O	1:A:230:VAL:CG2	2.59	0.51
1:A:222:GLY:O	1:A:225:MET:HB2	2.12	0.50
1:A:227:THR:HB	1:A:228:PRO:HD3	1.94	0.49
1:A:208:ILE:O	1:A:219:SER:HA	2.11	0.49
2:I:285:ALA:HB1	4:I:486:HOH:O	2.11	0.49
1:A:221:SER:O	2:I:284:PRO:HG2	2.13	0.48
1:A:46:HIS:HE1	1:A:216:SER:O	1.96	0.48
1:A:250:ARG:HG3	4:A:467:HOH:O	2.14	0.48
2:I:284:PRO:CD	4:I:483:HOH:O	2.61	0.47
1:A:33:SER:HB3	1:A:239:THR:HG22	1.97	0.47
1:A:207:SER:CB	4:A:376:HOH:O	2.54	0.46
1:A:225:MET:HE2	1:A:225:MET:HA	1.97	0.46
1:A:161:ASN:HD21	2:I:282:PRO:HD2	1.77	0.46
1:A:186:TYR:O	1:A:187:ASP:HB2	2.15	0.46
1:A:225:MET:O	1:A:229:HIS:HD2	1.99	0.46
1:A:30:GLY:HA2	1:A:239:THR:CG2	2.46	0.46
1:A:68:GLY:HA2	1:A:213:ILE:HG23	1.97	0.45
1:A:212:TRP:NE1	1:A:218:ARG:NH2	2.65	0.44
1:A:224:SER:N	2:I:281:ALA:O	2.50	0.44
1:A:161:ASN:ND2	2:I:282:PRO:HD3	2.32	0.43
1:A:180:VAL:HG21	1:A:230:VAL:CG2	2.34	0.43
1:A:224:SER:H	2:I:281:ALA:C	2.20	0.43
1:A:261:LEU:HD21	1:A:272:LEU:HD22	2.00	0.43
1:A:8:TRP:CH2	1:A:204:PRO:HB3	2.54	0.43
1:A:69:HIS:ND1	2:I:283:PHE:HB3	2.34	0.42
1:A:138:SER:OG	4:A:338:HOH:O	2.22	0.42
1:A:207:SER:CB	2:I:286:NH2:N	2.82	0.42
1:A:160:GLY:CA	2:I:280:PRO:O	2.62	0.42
1:A:161:ASN:ND2	2:I:282:PRO:CG	2.83	0.42
1:A:224:SER:N	2:I:281:ALA:HB3	2.34	0.42
1:A:235:ALA:O	1:A:239:THR:HG23	2.20	0.42
1:A:67:ASN:ND2	2:I:283:PHE:HE2	1.88	0.41
1:A:29:ALA:HB3	1:A:87:LYS:HD2	2.02	0.41
1:A:58:THR:CG2	1:A:63:SER:HA	2.51	0.41
1:A:223:THR:CB	2:I:281:ALA:HB3	2.50	0.41
1:A:30:GLY:HA2	1:A:239:THR:HG23	2.03	0.41
1:A:3:GLN:O	1:A:22:THR:HA	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:51:GLY:HA2	4:A:472:HOH:O	2.21	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	277/279 (99%)	264 (95%)	12 (4%)	1 (0%)	34 37
2	I	3/7 (43%)	2 (67%)	0	1 (33%)	0 0
All	All	280/286 (98%)	266 (95%)	12 (4%)	2 (1%)	22 22

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	I	282	PRO
1	A	39	ASP

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	210/213 (99%)	187 (89%)	23 (11%)	6 5
2	I	4/4 (100%)	4 (100%)	0	100 100
All	All	214/217 (99%)	191 (89%)	23 (11%)	6 6

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	THR
1	A	16	THR
1	A	54	GLN
1	A	56	VAL
1	A	57	LYS
1	A	58	THR
1	A	101	SER
1	A	106	THR
1	A	107	ILE
1	A	120	ASN
1	A	133	LEU
1	A	154	MET
1	A	162	ASN
1	A	185	ARG
1	A	207	SER
1	A	218	ARG
1	A	219	SER
1	A	225	MET
1	A	239	THR
1	A	240	LEU
1	A	250	ARG
1	A	262	SER
1	A	270	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	GLN
1	A	46	HIS
1	A	54	GLN
1	A	69	HIS
1	A	161	ASN
1	A	162	ASN
1	A	168	ASN
1	A	194	ASN
1	A	229	HIS
1	A	257	ASN
1	A	270	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	I	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	I	283:PHE	C	284:PRO	N	5.15

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.