



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:54 PM UTC

PDB ID : 1FEL / pdb_00001fel
Title : CRYSTALLOGRAPHIC STUDIES ON COMPLEXES BETWEEN
RETINOIDS AND PLASMA RETINOL-BINDING PROTEIN
Authors : Zanotti, G.; Marcello, M.; Malpeli, G.; Sartori, G.; Berni, R.
Deposited on : 1994-08-29
Resolution : 1.80 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

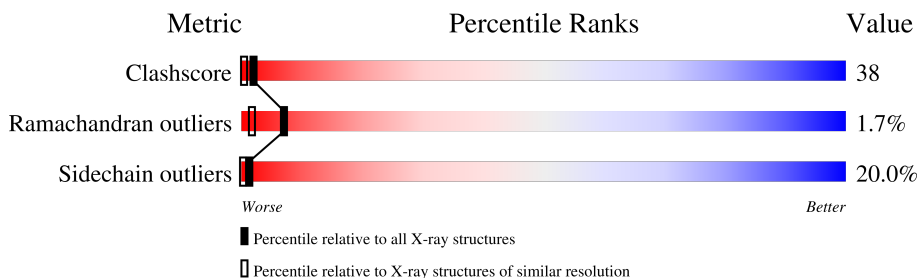
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 Å.

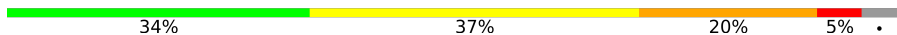
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	183	

2 Entry composition [i](#)

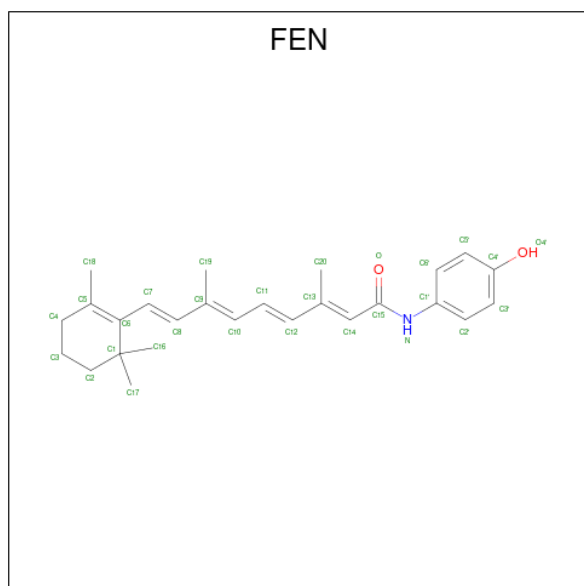
There are 3 unique types of molecules in this entry. The entry contains 1603 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 RETINOL BINDING PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	175	1411	889	246	266	10	0	0	1

- Molecule 2 is N-(4-HYDROXYPHENYL)ALL-TRANS RETINAMIDE (CCD ID: FEN) (formula: C₂₆H₃₃NO₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	29	26	1	2	0	0

- Molecule 3 is water.

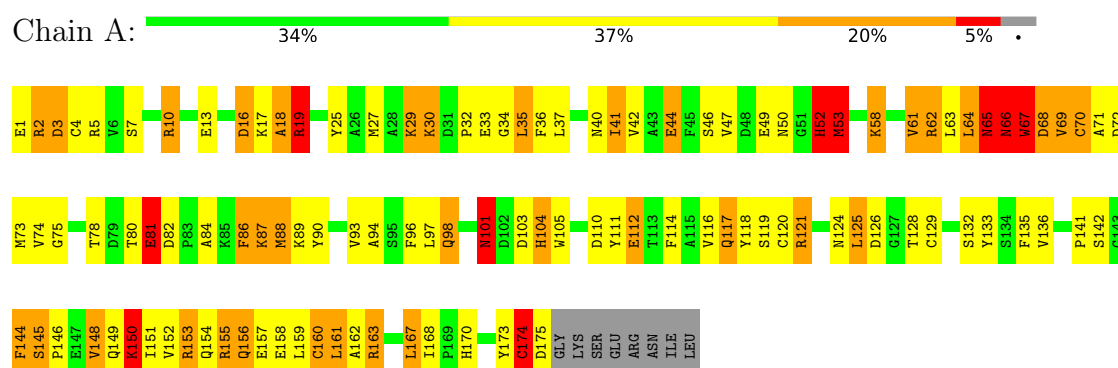
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	163	Total	O	0	0
			163	163		

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: RETINOL BINDING PROTEIN



4 Data and refinement statistics

Xtriage (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, α , β , γ	46.63Å 49.26Å 76.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	9.00 – 1.80	Depositor
% Data completeness (in resolution range)	(Not available) (9.00-1.80)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	TNT	Depositor
R, R_{free}	0.204 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	1603	wwPDB-VP
Average B, all atoms (Å ²)	33.0	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: FEN

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	1.34	3/1445 (0.2%)	2.43	84/1952 (4.3%)

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
1	A	1	0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	82	ASP	CA-C	-7.70	1.46	1.52
1	A	174	CYS	C-N	-6.93	1.23	1.33
1	A	70	CYS	CA-C	-5.16	1.46	1.53

All (84) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	160	CYS	CB-CA-C	13.67	131.14	111.73
1	A	81	GLU	CA-C-N	-11.08	107.72	122.56
1	A	81	GLU	C-N-CA	-11.08	107.72	122.56
1	A	65	ASN	CA-CB-CG	10.30	122.91	112.60
1	A	19	ARG	N-CA-C	-9.65	101.50	113.28
1	A	155	ARG	NE-CZ-NH1	9.07	130.57	121.50
1	A	144	PHE	CB-CA-C	-8.64	91.32	109.38
1	A	68	ASP	CA-CB-CG	-8.48	104.12	112.60
1	A	49	GLU	N-CA-CB	8.23	123.04	110.28
1	A	142	SER	N-CA-C	-8.20	103.06	113.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	119	SER	N-CA-CB	8.07	125.74	111.13
1	A	133	TYR	N-CA-CB	7.92	125.31	111.13
1	A	155	ARG	CD-NE-CZ	7.67	135.13	124.40
1	A	3	ASP	N-CA-CB	-7.55	98.94	110.04
1	A	3	ASP	CA-CB-CG	7.49	120.09	112.60
1	A	16	ASP	CA-CB-CG	7.49	120.08	112.60
1	A	154	GLN	O-C-N	-7.48	114.19	122.12
1	A	32	PRO	CB-CA-C	-7.40	99.35	111.56
1	A	7	SER	CA-C-N	-7.34	110.43	122.54
1	A	7	SER	C-N-CA	-7.34	110.43	122.54
1	A	64	LEU	N-CA-CB	7.25	122.75	110.49
1	A	66	ASN	CB-CA-C	-6.98	102.13	111.63
1	A	159	LEU	CA-C-O	6.93	127.46	119.35
1	A	116	VAL	N-CA-CB	6.92	120.64	111.64
1	A	86	PHE	CA-C-N	6.91	132.93	123.11
1	A	86	PHE	C-N-CA	6.91	132.93	123.11
1	A	135	PHE	CA-C-O	-6.52	113.74	121.11
1	A	170	HIS	ND1-CG-CD2	6.51	112.61	106.10
1	A	121	ARG	CD-NE-CZ	6.49	133.48	124.40
1	A	173	TYR	N-CA-C	6.46	117.98	111.07
1	A	41	ILE	N-CA-CB	-6.44	103.26	110.99
1	A	67	TRP	CB-CA-C	-6.40	98.97	109.53
1	A	156	GLN	CA-C-O	6.35	127.48	120.82
1	A	160	CYS	CA-CB-SG	-6.34	99.81	114.40
1	A	167	LEU	CA-C-O	-6.32	114.08	121.16
1	A	150	LYS	CA-C-O	6.31	127.23	120.10
1	A	136	VAL	N-CA-CB	6.28	119.38	111.46
1	A	98	GLN	CA-C-O	-6.26	114.31	121.19
1	A	163	ARG	CA-C-N	-6.25	112.86	122.60
1	A	163	ARG	C-N-CA	-6.25	112.86	122.60
1	A	52	HIS	CA-CB-CG	-6.22	107.58	113.80
1	A	69	VAL	O-C-N	-6.21	116.40	122.92
1	A	161	LEU	CA-C-O	6.10	125.99	119.34
1	A	103	ASP	CA-C-O	-6.07	114.94	121.56
1	A	103	ASP	N-CA-C	-6.07	101.94	110.50
1	A	49	GLU	N-CA-C	6.06	118.85	111.82
1	A	136	VAL	N-CA-C	-6.04	99.03	107.80
1	A	53	MET	N-CA-CB	5.99	120.62	110.49
1	A	88	MET	N-CA-C	5.91	118.15	108.52
1	A	72	ASP	N-CA-C	-5.90	97.56	107.99
1	A	67	TRP	N-CA-CB	5.83	119.68	110.23
1	A	70	CYS	CB-CA-C	-5.78	102.27	111.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	44	GLU	CA-CB-CG	-5.63	102.83	114.10
1	A	84	ALA	N-CA-CB	-5.62	102.39	110.65
1	A	174	CYS	N-CA-CB	5.58	119.98	110.50
1	A	101	ASN	N-CA-CB	-5.53	101.47	110.59
1	A	124	ASN	N-CA-C	-5.49	103.14	110.55
1	A	112	GLU	N-CA-C	5.49	120.25	113.50
1	A	67	TRP	CA-CB-CG	5.46	123.97	113.60
1	A	117	GLN	N-CA-CB	-5.43	102.48	110.85
1	A	145	SER	N-CA-CB	-5.39	100.77	110.37
1	A	42	VAL	CB-CA-C	-5.34	101.84	110.28
1	A	40	ASN	CA-C-N	-5.30	116.26	122.93
1	A	40	ASN	C-N-CA	-5.30	116.26	122.93
1	A	30	LYS	N-CA-C	-5.27	99.82	108.41
1	A	104	HIS	CA-C-O	-5.25	113.39	120.47
1	A	81	GLU	CA-CB-CG	5.25	124.59	114.10
1	A	62	ARG	CA-C-N	-5.22	112.87	120.75
1	A	62	ARG	C-N-CA	-5.22	112.87	120.75
1	A	78	THR	CA-CB-CG2	-5.20	101.65	110.50
1	A	81	GLU	N-CA-CB	5.16	117.96	110.47
1	A	62	ARG	CA-CB-CG	-5.16	103.78	114.10
1	A	67	TRP	N-CA-C	-5.12	101.36	109.96
1	A	18	ALA	N-CA-C	5.10	119.21	112.89
1	A	69	VAL	CB-CA-C	5.08	118.45	111.34
1	A	34	GLY	O-C-N	5.08	127.78	122.86
1	A	126	ASP	N-CA-CB	5.06	118.17	110.44
1	A	128	THR	CA-C-N	-5.05	115.13	122.65
1	A	128	THR	C-N-CA	-5.05	115.13	122.65
1	A	42	VAL	CA-C-N	-5.02	114.38	122.81
1	A	42	VAL	C-N-CA	-5.02	114.38	122.81
1	A	114	PHE	CA-C-O	5.02	126.75	121.33
1	A	141	PRO	O-C-N	-5.01	115.87	122.64
1	A	18	ALA	N-CA-CB	5.01	118.57	110.40

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	49	GLU	CA

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1411	0	1339	105	0
2	A	29	0	32	13	0
3	A	163	0	0	18	0
All	All	1603	0	1371	107	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 38.

All (107) 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:150:LYS:HE2	1:A:151:ILE:HG13	1.37	1.04
1:A:144:PHE:HB3	1:A:148:VAL:HG13	1.42	0.98
1:A:71:ALA:HB1	1:A:73:MET:HE3	1.49	0.94
1:A:150:LYS:HE2	1:A:151:ILE:CG1	2.03	0.89
1:A:73:MET:HE2	1:A:97:LEU:HD13	1.56	0.88
1:A:63:LEU:HD13	1:A:67:TRP:HB2	1.56	0.88
1:A:73:MET:CE	1:A:97:LEU:HD13	2.04	0.87
1:A:94:ALA:HB1	1:A:96:PHE:CE1	2.09	0.87
1:A:144:PHE:HB3	1:A:148:VAL:CG1	2.04	0.86
1:A:63:LEU:HD13	1:A:67:TRP:CB	2.05	0.86
1:A:36:PHE:HA	2:A:184:FEN:H203	1.57	0.85
1:A:71:ALA:HB1	1:A:73:MET:CE	2.06	0.85
1:A:58:LYS:NZ	1:A:175:ASP:N	2.29	0.80
1:A:13:GLU:HB2	3:A:319:HOH:O	1.82	0.80
1:A:112:GLU:HG3	3:A:322:HOH:O	1.83	0.77
1:A:120:CYS:HG	1:A:129:CYS:HG	1.33	0.76
1:A:61:VAL:HG11	2:A:184:FEN:N	2.02	0.74
1:A:27:MET:HB2	3:A:193:HOH:O	1.88	0.73
1:A:58:LYS:HD2	3:A:238:HOH:O	1.89	0.72
1:A:35:LEU:HB2	3:A:220:HOH:O	1.88	0.71
1:A:63:LEU:HD12	1:A:63:LEU:N	2.06	0.71
1:A:63:LEU:HA	2:A:184:FEN:C3'	2.20	0.71
1:A:53:MET:N	3:A:314:HOH:O	2.24	0.70
1:A:58:LYS:HZ1	1:A:175:ASP:N	1.89	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:LEU:O	1:A:66:ASN:N	2.22	0.68
1:A:70:CYS:HB3	1:A:174:CYS:SG	2.33	0.68
1:A:73:MET:HE1	1:A:97:LEU:HD22	1.75	0.68
1:A:63:LEU:HD12	1:A:63:LEU:H	1.59	0.67
1:A:41:ILE:HA	1:A:58:LYS:O	1.94	0.67
1:A:61:VAL:HG11	2:A:184:FEN:HN	1.58	0.67
1:A:73:MET:HE1	1:A:97:LEU:HB3	1.79	0.64
1:A:150:LYS:HA	1:A:153:ARG:HG2	1.79	0.64
1:A:129:CYS:SG	1:A:132:SER:HB3	2.38	0.64
1:A:63:LEU:HD13	1:A:67:TRP:HB3	1.78	0.64
1:A:150:LYS:O	1:A:153:ARG:HG3	1.97	0.64
1:A:145:SER:OG	1:A:148:VAL:HG12	1.99	0.62
1:A:17:LYS:HG3	3:A:344:HOH:O	2.00	0.62
1:A:150:LYS:HA	1:A:153:ARG:CG	2.29	0.62
1:A:71:ALA:CB	1:A:73:MET:HE3	2.27	0.62
1:A:37:LEU:HD23	1:A:61:VAL:HG22	1.82	0.62
1:A:63:LEU:HA	2:A:184:FEN:H3'	1.83	0.60
1:A:125:LEU:HD13	3:A:298:HOH:O	2.00	0.60
1:A:64:LEU:H	2:A:184:FEN:H3'	1.65	0.60
1:A:89:LYS:NZ	3:A:241:HOH:O	2.35	0.60
1:A:47:VAL:HG23	1:A:52:HIS:O	2.04	0.57
1:A:81:GLU:HG2	1:A:81:GLU:O	2.02	0.57
1:A:73:MET:HE1	1:A:97:LEU:HD13	1.83	0.57
1:A:61:VAL:CG1	2:A:184:FEN:HN	2.18	0.57
1:A:80:THR:HB	3:A:280:HOH:O	2.04	0.56
1:A:152:VAL:O	1:A:156:GLN:HG3	2.05	0.56
1:A:150:LYS:CE	1:A:151:ILE:HG13	2.25	0.56
1:A:73:MET:CE	1:A:97:LEU:HD22	2.35	0.55
1:A:13:GLU:H	1:A:13:GLU:CD	2.15	0.55
1:A:86:PHE:O	1:A:104:HIS:N	2.35	0.55
1:A:70:CYS:HB3	1:A:174:CYS:HB3	1.89	0.54
1:A:129:CYS:O	3:A:223:HOH:O	2.17	0.54
1:A:64:LEU:N	2:A:184:FEN:H3'	2.23	0.54
1:A:63:LEU:HB2	1:A:67:TRP:HB2	1.90	0.54
1:A:36:PHE:HA	2:A:184:FEN:C20	2.34	0.53
1:A:16:ASP:OD2	1:A:19:ARG:HD2	2.08	0.53
1:A:71:ALA:HB1	1:A:73:MET:HE2	1.90	0.52
1:A:4:CYS:SG	1:A:160:CYS:CB	2.98	0.52
1:A:110:ASP:C	1:A:112:GLU:H	2.17	0.52
2:A:184:FEN:H181	2:A:184:FEN:C8	2.41	0.51
1:A:88:MET:HE1	2:A:184:FEN:H7	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:37:LEU:HD23	1:A:61:VAL:CG2	2.40	0.51
1:A:65:ASN:HD21	1:A:67:TRP:CG	2.28	0.51
1:A:145:SER:O	1:A:149:GLN:HG3	2.10	0.51
1:A:63:LEU:O	1:A:64:LEU:C	2.54	0.50
1:A:35:LEU:HD13	1:A:35:LEU:N	2.26	0.50
1:A:29:LYS:HB3	1:A:168:ILE:HD11	1.94	0.50
1:A:30:LYS:HD3	1:A:30:LYS:C	2.36	0.50
1:A:63:LEU:N	1:A:67:TRP:O	2.44	0.50
1:A:125:LEU:HA	3:A:298:HOH:O	2.11	0.50
1:A:88:MET:HE1	2:A:184:FEN:C7	2.43	0.49
2:A:184:FEN:H181	2:A:184:FEN:H8	1.95	0.49
1:A:2:ARG:HB2	3:A:199:HOH:O	2.13	0.48
1:A:75:GLY:HA2	1:A:89:LYS:O	2.14	0.48
1:A:64:LEU:HD12	1:A:64:LEU:O	2.14	0.47
1:A:94:ALA:HA	3:A:197:HOH:O	2.15	0.47
1:A:58:LYS:CE	1:A:175:ASP:N	2.77	0.47
1:A:90:TYR:OH	1:A:98:GLN:NE2	2.47	0.47
1:A:3:ASP:OD2	1:A:5:ARG:NH2	2.33	0.47
1:A:63:LEU:N	1:A:63:LEU:CD1	2.78	0.46
1:A:25:TYR:HE2	3:A:207:HOH:O	1.98	0.46
1:A:18:ALA:HB2	1:A:47:VAL:HG11	1.97	0.46
1:A:87:LYS:HA	1:A:87:LYS:HE3	1.98	0.46
1:A:50:ASN:ND2	3:A:235:HOH:O	2.37	0.45
1:A:88:MET:O	1:A:101:ASN:HA	2.17	0.45
1:A:10:ARG:HG2	3:A:272:HOH:O	2.16	0.45
1:A:70:CYS:HB3	1:A:174:CYS:CB	2.46	0.45
1:A:58:LYS:HZ2	1:A:175:ASP:N	2.15	0.44
1:A:74:VAL:O	1:A:90:TYR:HA	2.17	0.44
1:A:145:SER:HB2	1:A:146:PRO:HD2	1.99	0.44
1:A:150:LYS:C	1:A:153:ARG:HG3	2.43	0.43
1:A:117:GLN:HG2	1:A:118:TYR:N	2.34	0.43
1:A:63:LEU:H	1:A:63:LEU:CD1	2.28	0.42
1:A:87:LYS:HE2	3:A:321:HOH:O	2.19	0.42
1:A:105:TRP:N	1:A:105:TRP:CD1	2.83	0.42
1:A:13:GLU:CD	1:A:13:GLU:N	2.77	0.41
1:A:58:LYS:HE3	1:A:175:ASP:N	2.35	0.41
1:A:161:LEU:HA	1:A:161:LEU:HD23	1.86	0.41
1:A:63:LEU:C	1:A:65:ASN:N	2.75	0.41
1:A:150:LYS:HE2	1:A:151:ILE:HG12	1.96	0.41
1:A:62:ARG:HH11	1:A:62:ARG:HD3	1.74	0.41
1:A:157:GLU:HA	1:A:162:ALA:HB2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:37:LEU:HD23	1:A:37:LEU:HA	1.92	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	173/183 (94%)	161 (93%)	9 (5%)	3 (2%)	7 2

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	52	HIS
1	A	53	MET
1	A	111	TYR

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	150/158 (95%)	120 (80%)	30 (20%)	1 0

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	GLU
1	A	2	ARG
1	A	10	ARG
1	A	19	ARG
1	A	29	LYS
1	A	33	GLU
1	A	35	LEU
1	A	44	GLU
1	A	46	SER
1	A	58	LYS
1	A	61	VAL
1	A	65	ASN
1	A	66	ASN
1	A	67	TRP
1	A	68	ASP
1	A	69	VAL
1	A	81	GLU
1	A	87	LYS
1	A	93	VAL
1	A	101	ASN
1	A	121	ARG
1	A	125	LEU
1	A	148	VAL
1	A	150	LYS
1	A	153	ARG
1	A	155	ARG
1	A	158	GLU
1	A	163	ARG
1	A	167	LEU
1	A	174	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	50	ASN
1	A	66	ASN
1	A	98	GLN
1	A	149	GLN
1	A	156	GLN
1	A	170	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

1 ligand is 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	FEN	A	184	-	30,30,30	1.80	6 (20%)	40,41,41	5.00	16 (40%)

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	FEN	A	184	-	-	6/19/36/36	0/2/2/2

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	184	FEN	O-C15	6.15	1.36	1.24
2	A	184	FEN	C14-C13	3.66	1.40	1.35
2	A	184	FEN	C1-C6	2.55	1.57	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	184	FEN	C6'-C5'	2.32	1.42	1.38
2	A	184	FEN	C18-C5	2.24	1.54	1.50
2	A	184	FEN	C19-C9	2.17	1.55	1.50

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	184	FEN	O-C15-C14	-22.16	88.56	124.42
2	A	184	FEN	C14-C15-N	12.04	131.65	112.80
2	A	184	FEN	O-C15-N	11.76	138.59	123.11
2	A	184	FEN	C18-C5-C6	-5.60	118.37	124.48
2	A	184	FEN	C1'-N-C15	-4.94	118.77	128.07
2	A	184	FEN	C16-C1-C6	4.81	117.78	110.24
2	A	184	FEN	C1-C6-C5	-4.32	116.73	122.64
2	A	184	FEN	C4-C5-C6	-4.15	117.09	122.70
2	A	184	FEN	C3-C4-C5	-3.82	107.24	114.06
2	A	184	FEN	C17-C1-C6	-3.68	104.47	110.24
2	A	184	FEN	C2-C3-C4	-3.67	103.21	111.28
2	A	184	FEN	C17-C1-C16	-3.12	99.70	108.63
2	A	184	FEN	C6'-C1'-C2'	-3.06	114.98	119.04
2	A	184	FEN	C16-C1-C2	2.83	119.82	108.95
2	A	184	FEN	C8-C9-C10	-2.76	114.67	119.01
2	A	184	FEN	C3'-C2'-C1'	2.68	123.38	120.30

There are no chirality outliers.

All (6) torsion outliers are listed below:

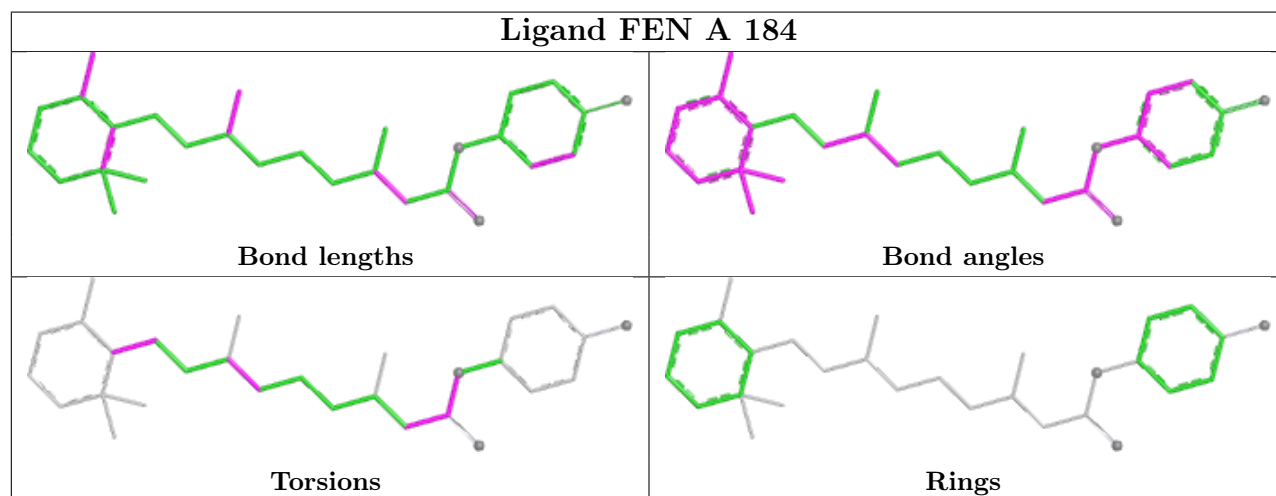
Mol	Chain	Res	Type	Atoms
2	A	184	FEN	C13-C14-C15-O
2	A	184	FEN	C13-C14-C15-N
2	A	184	FEN	C14-C15-N-C1'
2	A	184	FEN	C11-C10-C9-C19
2	A	184	FEN	C5-C6-C7-C8
2	A	184	FEN	O-C15-N-C1'

There are no ring outliers.

1 monomer is involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	184	FEN	13	0

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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.