



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:43 AM UTC

PDB ID : 1XO2 / pdb_00001xo2
Title : Crystal structure of a human cyclin-dependent kinase 6 complex with a flavonol inhibitor, fisetin
Authors : Lu, H.S.; Chang, D.J.; Baratte, B.; Meijer, L.; Schulze-Gahmen, U.
Deposited on : 2004-10-05
Resolution : 2.90 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)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

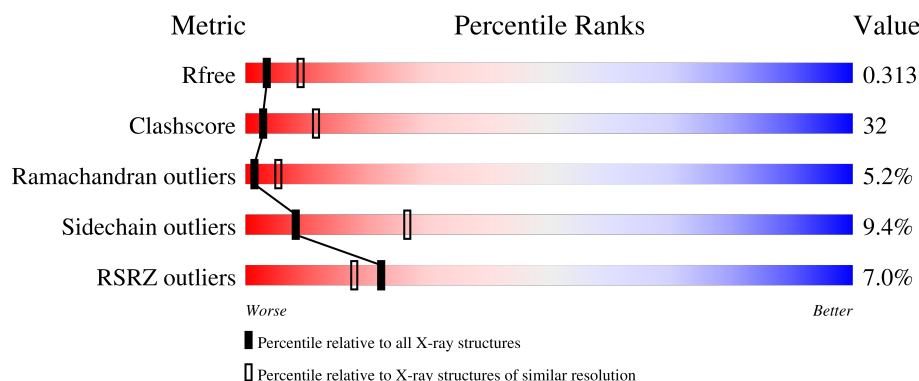
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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}	180053	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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 $\leq 5\%$. 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	254	
2	B	308	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 4172 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.

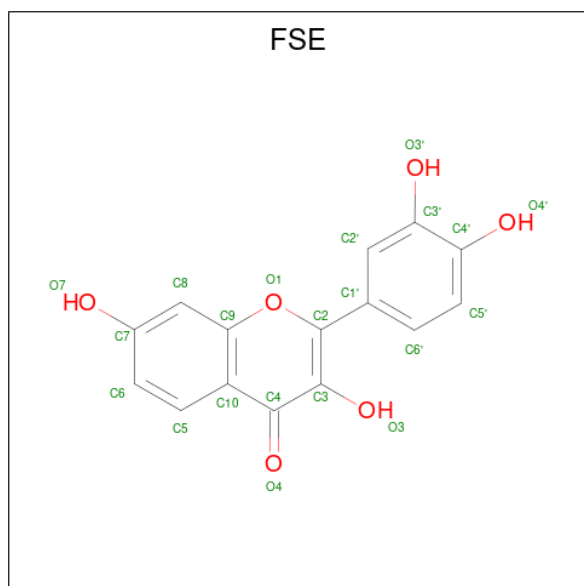
- Molecule 1 is a protein called Cyclin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	243	1911	1227	309	364	11	0	0	0

- Molecule 2 is a protein called Cell division protein kinase 6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	289	2240	1439	381	411	9	0	0	0

- Molecule 3 is 3,7,3',4'-TETRAHYDROXYFLAVONE (CCD ID: FSE) (formula: C₁₅H₁₀O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
3	B	1	21	15	6	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	66.16Å 66.16Å 448.60Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.90 20.00 – 2.90	Depositor EDS
% Data completeness (in resolution range)	91.4 (20.00-2.90) 90.6 (20.00-2.90)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.91 (at 2.81Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.260 , 0.313 0.258 , 0.313	Depositor DCC
R_{free} test set	1046 reflections (7.38%)	wwPDB-VP
Wilson B-factor (Å ²)	53.8	Xtriage
Anisotropy	0.017	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 51.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	4172	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.59% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.51	0/1942	1.06	10/2641 (0.4%)
2	B	0.50	0/2288	1.04	13/3108 (0.4%)
All	All	0.50	0/4230	1.05	23/5749 (0.4%)

There are no bond length outliers.

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	251	ARG	N-CA-C	-10.09	100.96	113.38
2	B	179	VAL	N-CA-C	9.95	121.61	107.88
1	A	147	THR	N-CA-C	9.87	121.80	111.14
2	B	245	ARG	N-CA-C	-9.83	101.29	113.38
1	A	75	LEU	N-CA-C	-7.20	104.62	113.41
1	A	109	ARG	N-CA-C	7.19	121.90	113.20
2	B	73	HIS	CA-C-N	7.16	126.42	118.97
2	B	73	HIS	C-N-CA	7.16	126.42	118.97
1	A	85	CYS	N-CA-C	-6.78	105.29	113.97
1	A	108	ILE	N-CA-C	6.54	116.69	110.74
2	B	252	GLN	N-CA-C	-6.50	104.04	112.23
1	A	131	GLU	N-CA-C	-6.15	104.84	112.90
1	A	167	GLU	N-CA-C	6.02	118.61	111.33
2	B	250	PRO	N-CA-CB	5.90	109.44	103.25
1	A	23	VAL	N-CA-C	-5.87	103.57	111.44
2	B	75	ASN	N-CA-C	5.85	120.11	113.15
1	A	111	VAL	N-CA-C	5.77	115.96	110.42
2	B	303	LEU	N-CA-C	-5.55	101.08	109.85
2	B	179	VAL	CB-CA-C	-5.47	104.19	111.80
2	B	30	ALA	N-CA-C	5.28	117.01	109.14
2	B	297	HIS	CA-C-N	5.28	125.59	119.47
2	B	297	HIS	C-N-CA	5.28	125.59	119.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	155	PHE	N-CA-C	5.13	118.79	112.54

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1911	0	1970	109	0
2	B	2240	0	2190	175	0
3	B	21	0	9	1	0
All	All	4172	0	4169	271	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 32.

All (271) 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)
2:B:179:VAL:O	2:B:180:VAL:HG13	1.57	1.04
2:B:181:VAL:O	2:B:186:ARG:HG3	1.70	0.90
2:B:87:ARG:HH21	2:B:93:LYS:HD2	1.39	0.87
1:A:14:ASP:HA	1:A:19:LYS:HE2	1.60	0.84
1:A:187:GLN:HG2	1:A:245:ALA:HA	1.59	0.82
2:B:103:GLN:HE22	2:B:108:TYR:HB2	1.42	0.82
2:B:125:MET:HB2	2:B:212:MET:HE1	1.62	0.81
1:A:166:PRO:HG2	1:A:169:LEU:HD12	1.62	0.81
1:A:66:PHE:CD2	1:A:114:MET:HE1	2.16	0.80
1:A:44:GLN:HE22	1:A:89:GLY:H	1.28	0.79
2:B:34:LYS:HD2	2:B:35:ASN:OD1	1.83	0.78
2:B:51:GLU:O	2:B:51:GLU:HG2	1.86	0.75
2:B:35:ASN:HB2	2:B:38:ARG:HB2	1.69	0.75
1:A:19:LYS:CD	1:A:157:ILE:HG21	2.18	0.73
2:B:49:THR:HG23	2:B:91:GLU:HA	1.71	0.73
1:A:30:ARG:HE	2:B:67:HIS:CE1	2.06	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:216:LYS:HG2	2:B:220:ARG:HH12	1.55	0.72
2:B:147:LYS:HE2	2:B:150:ASN:ND2	2.05	0.72
2:B:192:LEU:HD21	2:B:228:LEU:HD11	1.71	0.71
1:A:90:THR:OG1	1:A:93:THR:HB	1.91	0.71
1:A:169:LEU:O	1:A:172:GLN:HG3	1.91	0.70
1:A:28:LYS:O	1:A:32:LEU:HD23	1.91	0.70
1:A:20:ASP:H	1:A:21:PRO:CD	2.04	0.69
2:B:126:MET:HG3	2:B:209:PHE:CD1	2.28	0.68
1:A:30:ARG:HE	2:B:67:HIS:HE1	1.40	0.68
1:A:18:MET:SD	2:B:170:TYR:HD2	2.17	0.68
2:B:210:ALA:HB2	2:B:277:LEU:HD11	1.76	0.67
1:A:44:GLN:NE2	1:A:89:GLY:H	1.92	0.67
1:A:129:ASN:HD22	2:B:51:GLU:HG3	1.60	0.67
2:B:202:LEU:HD13	2:B:289:ILE:O	1.94	0.67
1:A:163:LEU:HD22	1:A:220:TYR:HB3	1.77	0.67
2:B:128:GLN:NE2	2:B:159:ILE:H	1.93	0.66
2:B:102:ASP:C	2:B:103:GLN:HG3	2.19	0.66
1:A:44:GLN:HE22	1:A:89:GLY:N	1.93	0.66
1:A:18:MET:HE2	1:A:19:LYS:HB3	1.78	0.65
1:A:223:ASP:O	1:A:227:ILE:HG12	1.95	0.65
1:A:16:THR:O	1:A:20:ASP:HB2	1.96	0.65
2:B:107:THR:O	2:B:111:LYS:HG3	1.97	0.65
2:B:58:THR:HG21	2:B:94:LEU:HD13	1.80	0.64
1:A:19:LYS:HD2	1:A:157:ILE:HG21	1.79	0.63
2:B:62:VAL:HG21	2:B:96:LEU:HD11	1.78	0.63
2:B:216:LYS:CG	2:B:220:ARG:HH22	2.12	0.63
2:B:184:TRP:CD1	2:B:221:GLY:H	2.17	0.63
2:B:128:GLN:HE22	2:B:158:GLN:HG3	1.64	0.63
1:A:19:LYS:HD3	1:A:157:ILE:HG21	1.81	0.62
1:A:31:GLU:OE1	1:A:195:PRO:HG2	1.99	0.62
2:B:154:THR:HG23	2:B:158:GLN:O	1.98	0.62
2:B:73:HIS:CE1	2:B:75:ASN:HB2	2.34	0.62
2:B:35:ASN:O	2:B:36:GLY:C	2.43	0.62
2:B:78:ARG:HA	2:B:78:ARG:NE	2.14	0.62
2:B:73:HIS:HE1	2:B:75:ASN:HB2	1.65	0.62
2:B:269:ILE:HG23	2:B:274:LYS:HB3	1.82	0.62
1:A:166:PRO:HG2	1:A:169:LEU:CD1	2.28	0.61
2:B:13:TYR:HD1	2:B:42:LEU:HD11	1.65	0.61
2:B:80:PHE:HB2	2:B:97:VAL:HG22	1.83	0.60
2:B:82:VAL:HG22	2:B:96:LEU:HD12	1.83	0.60
2:B:128:GLN:NE2	2:B:158:GLN:HG3	2.17	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:148:PRO:HG2	2:B:211:GLU:OE2	2.01	0.60
1:A:33:LEU:C	1:A:35:PRO:HD3	2.28	0.59
1:A:116:VAL:HG13	1:A:132:LEU:HD12	1.85	0.59
1:A:120:THR:C	1:A:122:LEU:N	2.59	0.59
2:B:216:LYS:HB2	2:B:216:LYS:NZ	2.17	0.59
2:B:181:VAL:HB	2:B:186:ARG:CG	2.33	0.59
1:A:20:ASP:H	1:A:21:PRO:HD3	1.66	0.58
1:A:14:ASP:HA	1:A:19:LYS:CE	2.33	0.58
1:A:120:THR:HA	1:A:127:PHE:CE2	2.39	0.58
2:B:44:ARG:HB3	2:B:95:THR:OG1	2.02	0.58
1:A:167:GLU:HG3	1:A:170:TRP:CZ2	2.38	0.58
2:B:171:SER:O	2:B:174:MET:HB3	2.04	0.58
2:B:239:GLY:C	2:B:241:GLU:H	2.11	0.57
2:B:178:SER:O	2:B:179:VAL:HG22	2.04	0.57
2:B:192:LEU:O	2:B:193:GLN:HB2	2.05	0.57
2:B:178:SER:C	2:B:179:VAL:CG2	2.78	0.57
2:B:252:GLN:C	2:B:254:PHE:N	2.61	0.57
2:B:78:ARG:HA	2:B:78:ARG:CZ	2.35	0.57
2:B:126:MET:SD	2:B:209:PHE:HB2	2.45	0.57
2:B:210:ALA:HB2	2:B:277:LEU:CD1	2.34	0.57
1:A:250:ASP:OD2	1:A:252:GLU:HB2	2.06	0.56
2:B:181:VAL:O	2:B:183:LEU:N	2.38	0.56
1:A:187:GLN:HB2	1:A:245:ALA:HB1	1.87	0.56
1:A:138:ASP:HA	1:A:141:GLU:OE1	2.06	0.56
2:B:122:ILE:HD13	2:B:213:PHE:CE1	2.41	0.56
2:B:35:ASN:HB2	2:B:38:ARG:CB	2.36	0.55
2:B:81:ASP:HB3	2:B:97:VAL:CG1	2.37	0.55
2:B:108:TYR:HA	2:B:111:LYS:HD2	1.88	0.55
2:B:147:LYS:HE2	2:B:150:ASN:HD21	1.70	0.55
1:A:218:THR:HG22	1:A:218:THR:O	2.05	0.55
1:A:209:THR:O	1:A:210:ASP:HB2	2.05	0.55
1:A:18:MET:SD	2:B:170:TYR:CD2	3.00	0.55
1:A:157:ILE:HB	1:A:158:PRO:HD3	1.87	0.55
1:A:115:THR:H	1:A:118:LYS:HD2	1.73	0.54
2:B:213:PHE:CZ	2:B:269:ILE:HG13	2.42	0.54
1:A:98:GLY:O	1:A:102:VAL:HG23	2.07	0.54
1:A:120:THR:C	1:A:122:LEU:H	2.15	0.54
1:A:215:ARG:O	1:A:216:PRO:C	2.51	0.54
1:A:148:GLU:HG3	1:A:149:ALA:N	2.22	0.54
1:A:167:GLU:HA	1:A:170:TRP:CD1	2.42	0.54
1:A:26:ASN:HB3	2:B:139:HIS:CD2	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:181:VAL:HB	2:B:186:ARG:HG2	1.88	0.54
1:A:62:LEU:HD11	1:A:122:LEU:HD23	1.90	0.54
1:A:111:VAL:HG23	2:B:177:THR:HG23	1.88	0.54
2:B:181:VAL:O	2:B:182:THR:C	2.50	0.54
2:B:216:LYS:CD	2:B:220:ARG:HH22	2.20	0.54
2:B:152:LEU:HB2	2:B:160:LYS:HB2	1.89	0.53
2:B:184:TRP:CD1	2:B:220:ARG:HA	2.43	0.53
1:A:15:SER:OG	2:B:198:THR:HG23	2.08	0.53
1:A:208:GLU:C	1:A:210:ASP:H	2.15	0.53
1:A:30:ARG:HD3	2:B:139:HIS:CD2	2.44	0.53
2:B:149:GLN:HE21	2:B:149:GLN:HA	1.74	0.53
1:A:189:ASN:O	1:A:192:LEU:HD13	2.08	0.52
2:B:62:VAL:CG2	2:B:96:LEU:HD11	2.40	0.52
2:B:178:SER:C	2:B:179:VAL:HG22	2.34	0.52
2:B:214:ARG:HD2	2:B:265:PHE:O	2.09	0.52
2:B:232:LEU:C	2:B:234:VAL:H	2.18	0.52
2:B:133:LEU:HD22	2:B:205:VAL:HG21	1.92	0.52
2:B:208:ILE:O	2:B:212:MET:HG3	2.10	0.52
2:B:128:GLN:HE22	2:B:158:GLN:HA	1.75	0.51
2:B:44:ARG:HA	2:B:95:THR:HA	1.92	0.51
1:A:20:ASP:N	1:A:21:PRO:HD3	2.24	0.51
2:B:35:ASN:CG	2:B:38:ARG:HD2	2.35	0.51
2:B:232:LEU:CD2	2:B:238:PRO:HD3	2.41	0.51
1:A:120:THR:O	1:A:122:LEU:N	2.43	0.51
2:B:98:PHE:CE2	3:B:309:FSE:H5'	2.45	0.51
2:B:216:LYS:HD3	2:B:220:ARG:NH2	2.26	0.51
2:B:21:GLU:HB2	2:B:26:LYS:HA	1.92	0.51
1:A:54:ILE:HG12	1:A:253:ILE:HG22	1.93	0.50
1:A:208:GLU:O	1:A:210:ASP:N	2.33	0.50
1:A:148:GLU:HG3	1:A:149:ALA:H	1.77	0.50
1:A:217:TRP:CZ2	1:A:239:LYS:HE2	2.46	0.50
1:A:197:LEU:HD23	1:A:228:LEU:HD13	1.92	0.50
2:B:32:ASP:OD2	2:B:34:LYS:HB3	2.12	0.50
2:B:50:GLY:O	2:B:51:GLU:HB2	2.12	0.50
2:B:216:LYS:HB2	2:B:216:LYS:HZ2	1.77	0.50
2:B:239:GLY:O	2:B:241:GLU:N	2.45	0.50
2:B:47:VAL:CG2	2:B:94:LEU:HB2	2.41	0.50
2:B:81:ASP:HB3	2:B:97:VAL:HG13	1.94	0.50
2:B:198:THR:N	2:B:199:PRO:CD	2.76	0.49
2:B:68:LEU:O	2:B:69:GLU:C	2.54	0.49
1:A:28:LYS:O	1:A:31:GLU:HB3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:70:LYS:HD2	1:A:178:SER:OG	2.13	0.49
2:B:103:GLN:NE2	2:B:108:TYR:HB2	2.21	0.49
1:A:208:GLU:HG3	1:A:217:TRP:CZ3	2.48	0.49
1:A:214:CYS:O	1:A:215:ARG:C	2.54	0.49
2:B:232:LEU:O	2:B:234:VAL:N	2.46	0.49
1:A:157:ILE:O	1:A:158:PRO:C	2.54	0.48
2:B:199:PRO:HA	2:B:202:LEU:HD12	1.94	0.48
2:B:269:ILE:HD13	2:B:274:LYS:HA	1.95	0.48
1:A:111:VAL:O	1:A:113:PRO:HD3	2.14	0.48
2:B:181:VAL:O	2:B:186:ARG:CG	2.52	0.48
2:B:19:ILE:HG12	2:B:27:VAL:O	2.13	0.48
2:B:232:LEU:C	2:B:234:VAL:N	2.69	0.48
2:B:252:GLN:O	2:B:254:PHE:N	2.47	0.48
2:B:16:VAL:O	2:B:17:ALA:HB2	2.13	0.48
2:B:216:LYS:HG3	2:B:220:ARG:HH22	1.78	0.48
2:B:239:GLY:C	2:B:241:GLU:N	2.71	0.48
2:B:232:LEU:HD22	2:B:238:PRO:HD3	1.95	0.48
1:A:156:LEU:HD21	1:A:177:ALA:HB1	1.96	0.48
1:A:215:ARG:H	1:A:215:ARG:HD3	1.79	0.48
1:A:78:SER:OG	1:A:82:ARG:NH2	2.43	0.47
1:A:217:TRP:CD1	1:A:217:TRP:C	2.91	0.47
2:B:252:GLN:C	2:B:254:PHE:H	2.21	0.47
1:A:83:TYR:CE1	1:A:139:ILE:HA	2.50	0.47
2:B:144:ARG:NH1	2:B:168:ARG:HD3	2.29	0.47
2:B:304:GLU:O	2:B:305:ARG:C	2.58	0.47
2:B:21:GLU:CB	2:B:26:LYS:HA	2.45	0.47
2:B:73:HIS:CE1	2:B:75:ASN:H	2.32	0.47
2:B:149:GLN:HE21	2:B:149:GLN:CA	2.27	0.47
1:A:111:VAL:CG2	2:B:177:THR:HG23	2.45	0.46
2:B:118:PRO:HG2	2:B:121:THR:HB	1.97	0.46
1:A:128:THR:C	1:A:130:LEU:H	2.23	0.46
2:B:111:LYS:HD3	2:B:111:LYS:C	2.40	0.46
1:A:82:ARG:O	1:A:85:CYS:HB2	2.16	0.46
2:B:216:LYS:HD3	2:B:220:ARG:HH22	1.81	0.46
2:B:228:LEU:HD13	2:B:254:PHE:CE2	2.49	0.46
1:A:16:THR:HG22	1:A:20:ASP:OD1	2.16	0.46
1:A:10:ARG:HD2	2:B:194:SER:HA	1.98	0.46
1:A:121:TYR:C	1:A:122:LEU:HD12	2.41	0.46
2:B:77:VAL:HG12	2:B:161:LEU:O	2.16	0.46
2:B:81:ASP:C	2:B:97:VAL:HG13	2.40	0.46
1:A:21:PRO:HB2	1:A:22:ARG:H	1.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:80:PHE:CE2	2:B:99:GLU:HA	2.51	0.46
1:A:106:SER:O	1:A:110:THR:HG22	2.15	0.45
2:B:122:ILE:HD13	2:B:213:PHE:CD1	2.51	0.45
1:A:75:LEU:O	1:A:79:ILE:HG13	2.16	0.45
2:B:216:LYS:HG3	2:B:217:PRO:HD2	1.97	0.45
2:B:13:TYR:CD1	2:B:42:LEU:HD11	2.48	0.45
2:B:181:VAL:HB	2:B:186:ARG:HG3	1.97	0.45
2:B:271:GLU:HA	2:B:274:LYS:HG2	1.97	0.45
1:A:167:GLU:HG3	1:A:170:TRP:CE2	2.52	0.45
2:B:13:TYR:CD1	2:B:42:LEU:HD21	2.52	0.45
2:B:56:LEU:HD23	2:B:56:LEU:C	2.42	0.45
2:B:147:LYS:HG2	2:B:150:ASN:HD22	1.82	0.45
2:B:192:LEU:CD2	2:B:228:LEU:HD11	2.44	0.45
1:A:103:LEU:O	1:A:107:LYS:HG3	2.17	0.45
1:A:170:TRP:N	1:A:171:PRO:HD2	2.31	0.44
2:B:82:VAL:HG22	2:B:96:LEU:CD1	2.45	0.44
1:A:250:ASP:O	1:A:253:ILE:HG13	2.17	0.44
2:B:224:ASP:O	2:B:228:LEU:HB2	2.16	0.44
1:A:111:VAL:HG13	1:A:112:LYS:N	2.33	0.44
2:B:47:VAL:HG23	2:B:94:LEU:HB2	1.99	0.44
2:B:128:GLN:HE22	2:B:158:GLN:CG	2.31	0.44
2:B:77:VAL:HG22	2:B:78:ARG:N	2.33	0.44
2:B:297:HIS:HA	2:B:298:PRO:HD3	1.85	0.44
1:A:44:GLN:HE22	1:A:88:GLN:HA	1.82	0.44
1:A:66:PHE:HD2	1:A:114:MET:HE1	1.74	0.44
1:A:187:GLN:HB3	1:A:189:ASN:OD1	2.18	0.44
2:B:108:TYR:C	2:B:110:ASP:H	2.26	0.44
1:A:208:GLU:HG2	1:A:209:THR:N	2.31	0.43
2:B:263:GLU:C	2:B:265:PHE:N	2.75	0.43
2:B:219:PHE:CE1	2:B:231:ILE:HA	2.53	0.43
2:B:266:VAL:O	2:B:268:ASP:N	2.51	0.43
1:A:183:LYS:HE2	1:A:249:TYR:CE2	2.53	0.43
1:A:116:VAL:O	1:A:120:THR:HG23	2.19	0.43
1:A:118:LYS:O	1:A:122:LEU:HD13	2.19	0.43
2:B:47:VAL:HB	2:B:92:THR:OG1	2.19	0.43
2:B:182:THR:HG22	2:B:183:LEU:N	2.32	0.43
1:A:230:PHE:CD1	1:A:234:THR:HG21	2.54	0.43
2:B:126:MET:HE2	2:B:209:PHE:CD2	2.54	0.43
1:A:17:THR:HG21	2:B:290:SER:CB	2.49	0.43
1:A:36:LYS:C	1:A:38:THR:H	2.27	0.43
2:B:48:GLN:HA	2:B:91:GLU:HB2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:66:ARG:HD2	2:B:69:GLU:OE2	2.19	0.43
2:B:183:LEU:C	2:B:185:TYR:H	2.25	0.42
1:A:197:LEU:HD23	1:A:197:LEU:HA	1.78	0.42
2:B:110:ASP:C	2:B:112:VAL:H	2.27	0.42
2:B:69:GLU:O	2:B:70:THR:C	2.62	0.42
2:B:37:GLY:O	2:B:38:ARG:C	2.63	0.42
2:B:135:PHE:O	2:B:136:LEU:C	2.62	0.42
2:B:219:PHE:HE1	2:B:234:VAL:HG21	1.84	0.42
2:B:18:GLU:HA	2:B:28:PHE:HA	2.01	0.42
2:B:210:ALA:CB	2:B:218:LEU:HD22	2.49	0.42
2:B:35:ASN:OD1	2:B:38:ARG:HD2	2.20	0.42
1:A:51:ASN:HD22	1:A:51:ASN:HA	1.74	0.42
2:B:180:VAL:O	2:B:181:VAL:HB	2.19	0.42
2:B:166:LEU:CD2	2:B:180:VAL:HG12	2.50	0.42
2:B:303:LEU:C	2:B:305:ARG:N	2.77	0.42
1:A:132:LEU:HD23	1:A:132:LEU:HA	1.81	0.41
2:B:102:ASP:C	2:B:103:GLN:CG	2.90	0.41
1:A:17:THR:HG21	2:B:290:SER:HB3	2.01	0.41
2:B:214:ARG:O	2:B:214:ARG:CG	2.67	0.41
2:B:271:GLU:O	2:B:274:LYS:HG3	2.21	0.41
1:A:216:PRO:O	1:A:217:TRP:C	2.63	0.41
2:B:11:GLN:HG2	2:B:12:GLN:N	2.33	0.41
2:B:168:ARG:CZ	2:B:174:MET:HE2	2.51	0.41
1:A:70:LYS:HD2	1:A:178:SER:CB	2.50	0.41
1:A:73:PHE:O	1:A:77:VAL:HG23	2.19	0.41
1:A:118:LYS:O	1:A:122:LEU:HD22	2.19	0.41
2:B:128:GLN:HB3	2:B:159:ILE:HB	2.01	0.41
1:A:177:ALA:O	1:A:181:ILE:HG13	2.21	0.41
2:B:106:THR:OG1	2:B:148:PRO:HB2	2.21	0.41
2:B:214:ARG:O	2:B:214:ARG:HG2	2.20	0.41
1:A:166:PRO:CG	1:A:169:LEU:HD12	2.43	0.41
1:A:167:GLU:HA	1:A:170:TRP:CG	2.55	0.41
2:B:42:LEU:CD2	2:B:97:VAL:HB	2.51	0.41
2:B:154:THR:HG21	2:B:158:GLN:HB3	2.03	0.41
2:B:166:LEU:HD23	2:B:180:VAL:CG1	2.51	0.41
2:B:179:VAL:O	2:B:180:VAL:CG1	2.47	0.41
2:B:180:VAL:O	2:B:186:ARG:HG2	2.21	0.41
2:B:277:LEU:O	2:B:281:LEU:HG	2.20	0.41
2:B:119:THR:HA	2:B:122:ILE:CG2	2.51	0.41
2:B:263:GLU:O	2:B:265:PHE:N	2.54	0.41
1:A:20:ASP:N	1:A:21:PRO:CD	2.74	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:147:LYS:HG2	2:B:150:ASN:ND2	2.36	0.40
1:A:46:GLU:HG2	1:A:46:GLU:O	2.21	0.40
1:A:192:LEU:HD12	1:A:192:LEU:N	2.37	0.40
1:A:203:LEU:HD12	1:A:203:LEU:HA	1.92	0.40
2:B:126:MET:HE2	2:B:209:PHE:CG	2.56	0.40
2:B:85:VAL:HB	2:B:93:LYS:HG2	2.02	0.40
2:B:303:LEU:O	2:B:304:GLU:C	2.64	0.40
1:A:214:CYS:C	1:A:215:ARG:O	2.63	0.40
2:B:54:MET:HB2	2:B:59:ILE:HD11	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	239/254 (94%)	204 (85%)	27 (11%)	8 (3%)	3	13
2	B	283/308 (92%)	230 (81%)	34 (12%)	19 (7%)	1	3
All	All	522/562 (93%)	434 (83%)	61 (12%)	27 (5%)	1	5

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	20	ASP
1	A	21	PRO
1	A	209	THR
1	A	210	ASP
2	B	36	GLY
2	B	51	GLU
2	B	180	VAL
2	B	182	THR
2	B	183	LEU

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Mol	Chain	Res	Type
1	A	208	GLU
2	B	38	ARG
2	B	119	THR
2	B	181	VAL
2	B	240	GLU
2	B	248	ALA
2	B	267	THR
1	A	121	TYR
2	B	144	ARG
2	B	233	ASP
2	B	238	PRO
1	A	70	LYS
2	B	253	ALA
2	B	264	LYS
1	A	32	LEU
2	B	109	LEU
2	B	250	PRO
2	B	115	PRO

5.3.2 Protein sidechains ⓘ

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	220/234 (94%)	204 (93%)	16 (7%)	13	38
2	B	237/272 (87%)	210 (89%)	27 (11%)	5	18
All	All	457/506 (90%)	414 (91%)	43 (9%)	8	26

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	MET
1	A	22	ARG
1	A	24	LEU
1	A	38	THR
1	A	43	ILE

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Mol	Chain	Res	Type
1	A	47	VAL
1	A	62	LEU
1	A	75	LEU
1	A	92	LYS
1	A	93	THR
1	A	132	LEU
1	A	138	ASP
1	A	147	THR
1	A	172	GLN
1	A	217	TRP
1	A	233	ASN
2	B	18	GLU
2	B	33	LEU
2	B	42	LEU
2	B	56	LEU
2	B	70	THR
2	B	94	LEU
2	B	97	VAL
2	B	103	GLN
2	B	111	LYS
2	B	136	LEU
2	B	149	GLN
2	B	154	THR
2	B	156	SER
2	B	166	LEU
2	B	171	SER
2	B	174	MET
2	B	177	THR
2	B	179	VAL
2	B	188	PRO
2	B	198	THR
2	B	214	ARG
2	B	216	LYS
2	B	220	ARG
2	B	228	LEU
2	B	270	ASP
2	B	274	LYS
2	B	279	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	44	GLN
1	A	51	ASN
1	A	129	ASN
1	A	134	ASN
1	A	172	GLN
1	A	211	ASN
1	A	241	GLN
2	B	11	GLN
2	B	12	GLN
2	B	67	HIS
2	B	103	GLN
2	B	128	GLN
2	B	139	HIS
2	B	149	GLN
2	B	158	GLN
2	B	173	GLN

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
3	FSE	B	309	-	23,23,23	3.82	15 (65%)	34,34,34	1.89	8 (23%)

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
3	FSE	B	309	-	-	0/4/4/4	0/3/3/3

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	309	FSE	C5-C10	7.85	1.51	1.39
3	B	309	FSE	C3-C2	7.60	1.43	1.36
3	B	309	FSE	C2'-C1'	7.21	1.50	1.39
3	B	309	FSE	O1-C9	5.85	1.47	1.38
3	B	309	FSE	O1-C2	4.49	1.43	1.37
3	B	309	FSE	C10-C9	4.26	1.48	1.40
3	B	309	FSE	C8-C9	4.24	1.46	1.38
3	B	309	FSE	C8-C7	4.05	1.45	1.39
3	B	309	FSE	C6-C7	2.88	1.44	1.39
3	B	309	FSE	C5-C6	2.85	1.43	1.38
3	B	309	FSE	C3-C4	2.58	1.52	1.46
3	B	309	FSE	O3'-C3'	2.51	1.41	1.36
3	B	309	FSE	O4-C4	2.45	1.28	1.23
3	B	309	FSE	O3-C3	2.43	1.41	1.33
3	B	309	FSE	C6'-C1'	2.08	1.42	1.39

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	309	FSE	O1-C9-C10	-5.19	116.85	121.57
3	B	309	FSE	C5-C10-C4	4.58	126.78	120.10
3	B	309	FSE	C5-C10-C9	-3.89	113.10	118.21
3	B	309	FSE	C9-O1-C2	3.35	125.80	120.67
3	B	309	FSE	C1'-C2-C3	2.71	132.70	128.44
3	B	309	FSE	O1-C2-C3	-2.64	117.69	120.19
3	B	309	FSE	O1-C9-C8	2.39	119.22	115.83
3	B	309	FSE	C5'-C4'-C3'	2.03	121.83	119.66

There are no chirality outliers.

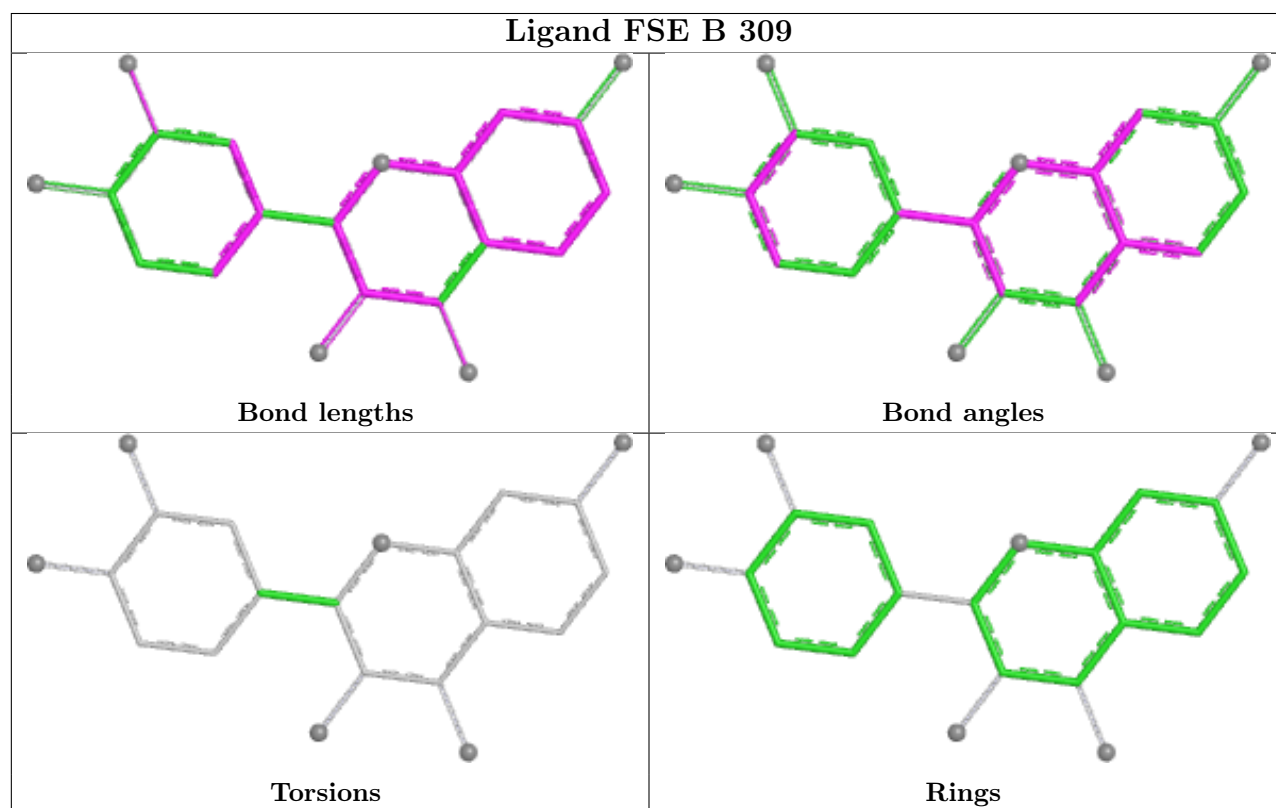
There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	309	FSE	1	0

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



5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	243/254 (95%)	-0.00	8 (3%) 49 40	21, 46, 89, 134	0
2	B	289/308 (93%)	0.54	29 (10%) 12 10	22, 59, 123, 186	0
All	All	532/562 (94%)	0.29	37 (6%) 22 18	21, 53, 114, 186	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	180	VAL	5.0
1	A	37	PHE	4.5
2	B	39	PHE	4.4
2	B	24	TYR	3.8
2	B	36	GLY	3.6
2	B	301	GLN	3.5
1	A	22	ARG	3.5
1	A	129	ASN	3.4
2	B	270	ASP	3.3
2	B	181	VAL	3.3
2	B	255	HIS	3.1
2	B	38	ARG	2.9
2	B	37	GLY	2.9
2	B	47	VAL	2.9
2	B	27	VAL	2.8
1	A	212	THR	2.8
1	A	21	PRO	2.8
1	A	127	PHE	2.7
2	B	267	THR	2.6
2	B	18	GLU	2.6
2	B	253	ALA	2.5
2	B	50	GLY	2.4
2	B	83	CYS	2.4
2	B	268	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
2	B	116	GLY	2.3
2	B	259	ALA	2.3
2	B	269	ILE	2.3
2	B	20	GLY	2.3
2	B	86	SER	2.3
2	B	40	VAL	2.3
2	B	30	ALA	2.2
2	B	263	GLU	2.2
1	A	128	THR	2.1
2	B	254	PHE	2.1
2	B	305	ARG	2.0
1	A	13	ILE	2.0
2	B	25	GLY	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

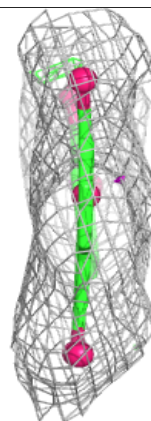
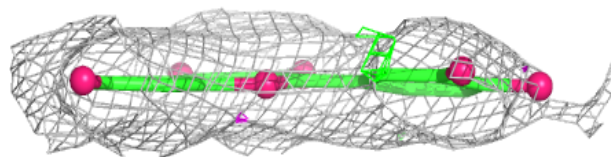
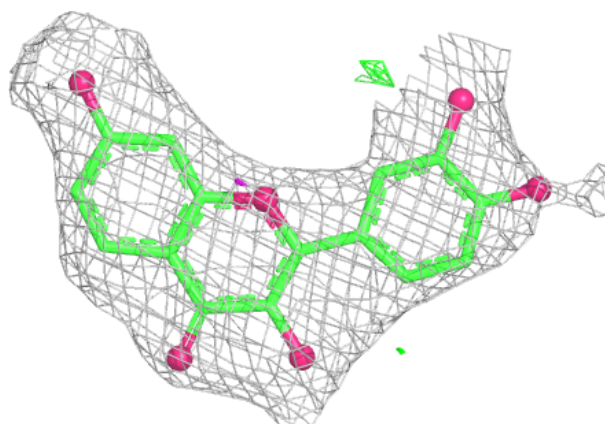
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	FSE	B	309	21/21	0.88	0.08	23,26,29,30	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 FSE B 309:

$2mF_o-DF_c$ (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.