Full wwPDB X-ray Structure Validation Report ⓘ

Oct 10, 2023 – 10:28 PM EDT

PDB ID	:	7JOZ
Title	:	Crystal structure of dopamine D1 receptor in complex with G protein and a non-catechol agonist
Authors	:	Sun, B.; Feng, D.; Chu, M.L.; Fish, I.; Kelm, S.; Lebon, F.; Lovera, S.; Valade, A.; Wood, M.; Ceska, T.; Kobilka, T.S.; Sands, Z.; Kobilka, B.K.
Deposited on	:	2020-08-07
Resolution	:	3.80 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:

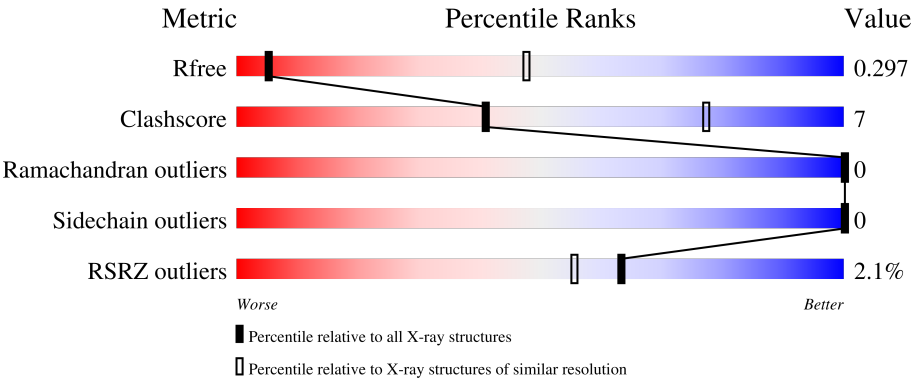
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 3.80 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))
R_{free}	130704	1212 (4.00-3.60)
Clashscore	141614	1288 (4.00-3.60)
Ramachandran outliers	138981	1243 (4.00-3.60)
Sidechain outliers	138945	1237 (4.00-3.60)
RSRZ outliers	127900	1121 (4.00-3.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	380	2% 81% 8% 11%
2	B	350	2% 79% 18%
3	G	71	% 76% 20%
4	N	160	69% 11% 20%

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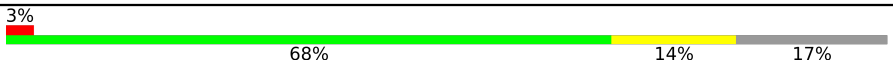
Mol	Chain	Length	Quality of chain
5	R	540	

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 9159 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 Guanine nucleotide-binding protein G(s) subunit alpha isoforms short.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	338	Total	C	N	O	S	0	0	0
			2299	1448	422	422	7			

- Molecule 2 is a protein called Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	340	Total	C	N	O	S	0	0	0
			2446	1517	431	480	18			

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-9	MET	-	expression tag	UNP P62873
B	-8	HIS	-	expression tag	UNP P62873
B	-7	HIS	-	expression tag	UNP P62873
B	-6	HIS	-	expression tag	UNP P62873
B	-5	HIS	-	expression tag	UNP P62873
B	-4	HIS	-	expression tag	UNP P62873
B	-3	HIS	-	expression tag	UNP P62873
B	-2	GLY	-	expression tag	UNP P62873
B	-1	SER	-	expression tag	UNP P62873
B	0	SER	-	expression tag	UNP P62873
B	1	GLY	-	expression tag	UNP P62873

- Molecule 3 is a protein called Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	57	Total	C	N	O	S	0	0	0
			373	233	63	75	2			

- Molecule 4 is a protein called Nanobody 35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	N	128	Total	C	N	O	S	0	0	0
			920	575	158	181	6			

- Molecule 5 is a protein called Endolysin,D(1A) dopamine receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	R	446	Total	C	N	O	S	0	0	0
			3078	1991	519	551	17			

There are 55 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	956	ASP	-	expression tag	UNP D9IEF7
R	957	TYR	-	expression tag	UNP D9IEF7
R	958	LYS	-	expression tag	UNP D9IEF7
R	959	ASP	-	expression tag	UNP D9IEF7
R	960	ASP	-	expression tag	UNP D9IEF7
R	961	ASP	-	expression tag	UNP D9IEF7
R	962	ASP	-	expression tag	UNP D9IEF7
R	963	ALA	-	expression tag	UNP D9IEF7
R	964	ALA	-	expression tag	UNP D9IEF7
R	965	ALA	-	expression tag	UNP D9IEF7
R	966	GLY	-	expression tag	UNP D9IEF7
R	967	GLN	-	expression tag	UNP D9IEF7
R	968	PRO	-	expression tag	UNP D9IEF7
R	969	GLY	-	expression tag	UNP D9IEF7
R	970	ASN	-	expression tag	UNP D9IEF7
R	971	GLY	-	expression tag	UNP D9IEF7
R	972	SER	-	expression tag	UNP D9IEF7
R	973	ALA	-	expression tag	UNP D9IEF7
R	974	PHE	-	expression tag	UNP D9IEF7
R	975	LEU	-	expression tag	UNP D9IEF7
R	976	LEU	-	expression tag	UNP D9IEF7
R	977	ALA	-	expression tag	UNP D9IEF7
R	978	PRO	-	expression tag	UNP D9IEF7
R	979	ASN	-	expression tag	UNP D9IEF7
R	980	ARG	-	expression tag	UNP D9IEF7
R	981	SER	-	expression tag	UNP D9IEF7
R	982	HIS	-	expression tag	UNP D9IEF7
R	983	ALA	-	expression tag	UNP D9IEF7
R	984	PRO	-	expression tag	UNP D9IEF7

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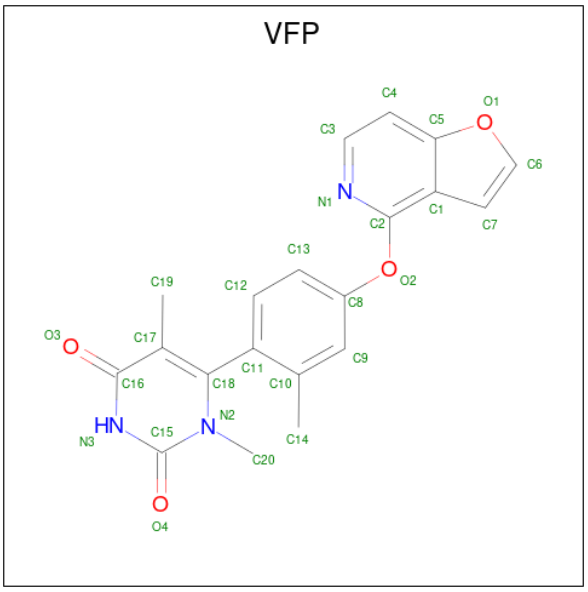
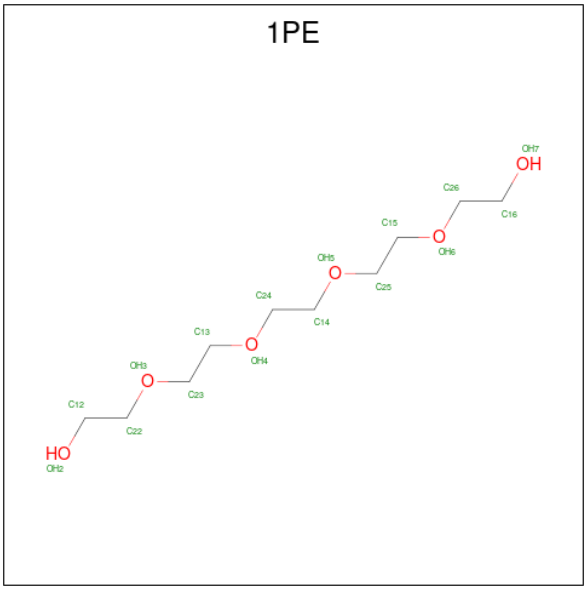
Chain	Residue	Modelled	Actual	Comment	Reference
R	985	GLY	-	expression tag	UNP D9IEF7
R	986	GLY	-	expression tag	UNP D9IEF7
R	987	GLY	-	expression tag	UNP D9IEF7
R	988	GLY	-	expression tag	UNP D9IEF7
R	989	SER	-	expression tag	UNP D9IEF7
R	990	LEU	-	expression tag	UNP D9IEF7
R	991	GLU	-	expression tag	UNP D9IEF7
R	992	VAL	-	expression tag	UNP D9IEF7
R	993	LEU	-	expression tag	UNP D9IEF7
R	994	PHE	-	expression tag	UNP D9IEF7
R	995	GLN	-	expression tag	UNP D9IEF7
R	996	GLY	-	expression tag	UNP D9IEF7
R	997	PRO	-	expression tag	UNP D9IEF7
R	998	GLY	-	expression tag	UNP D9IEF7
R	999	GLY	-	expression tag	UNP D9IEF7
R	1000	GLY	-	expression tag	UNP D9IEF7
R	1001	SER	-	expression tag	UNP D9IEF7
R	1054	THR	CYS	conflict	UNP D9IEF7
R	1097	ALA	CYS	conflict	UNP D9IEF7
R	1162	ALA	-	linker	UNP D9IEF7
R	348	HIS	-	expression tag	UNP P21728
R	349	HIS	-	expression tag	UNP P21728
R	350	HIS	-	expression tag	UNP P21728
R	351	HIS	-	expression tag	UNP P21728
R	352	HIS	-	expression tag	UNP P21728
R	353	HIS	-	expression tag	UNP P21728

- Molecule 6 is 6-{4-[(furo[3,2-c]pyridin-4-yl)oxy]-2-methylphenyl}-1,5-dimethylpyrimidine -2,4(1H,3H)-dione (three-letter code: VFP) (formula: $C_{20}H_{17}N_3O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	R	1	Total C N O 27 20 3 4	0	0

- Molecule 7 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: $C_{10}H_{22}O_6$).

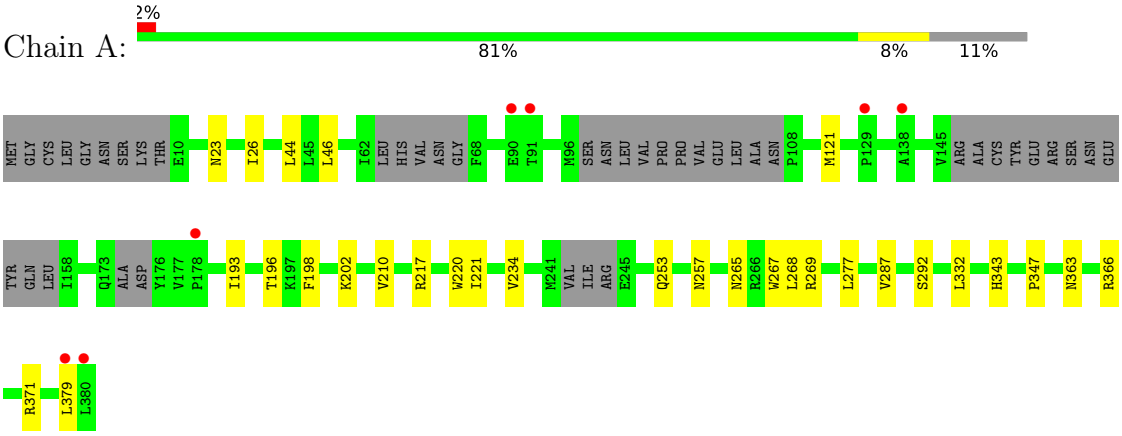


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	R	1	Total C O 16 10 6	0	0

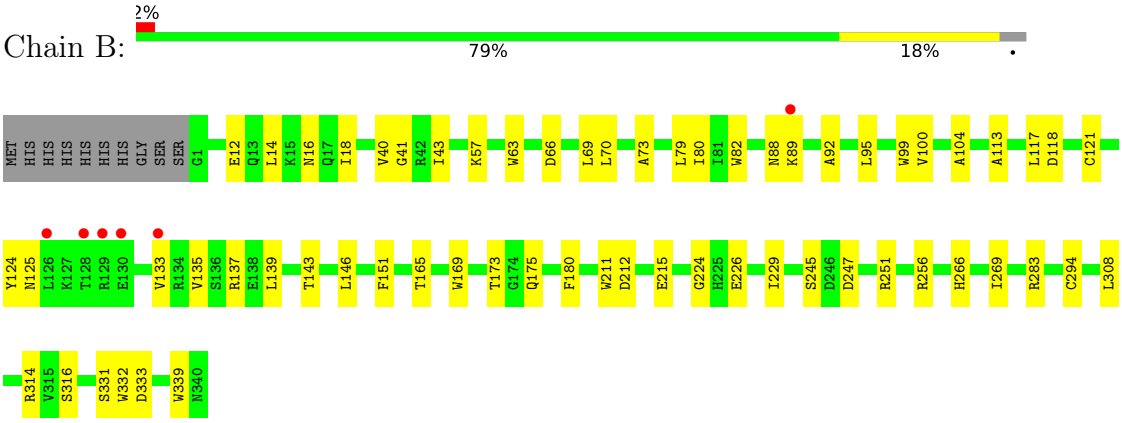
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

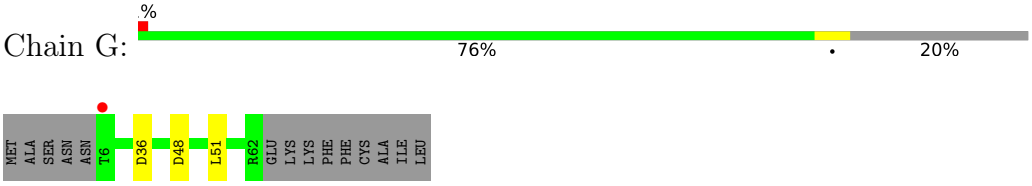
• Molecule 1: Guanine nucleotide-binding protein G(s) subunit alpha isoforms short



• Molecule 2: Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1

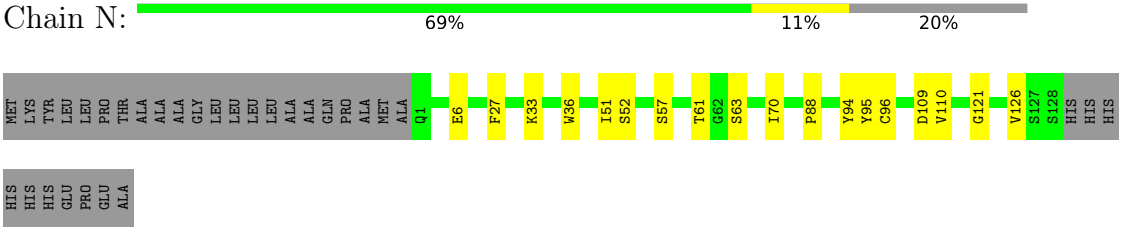


• Molecule 3: Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2



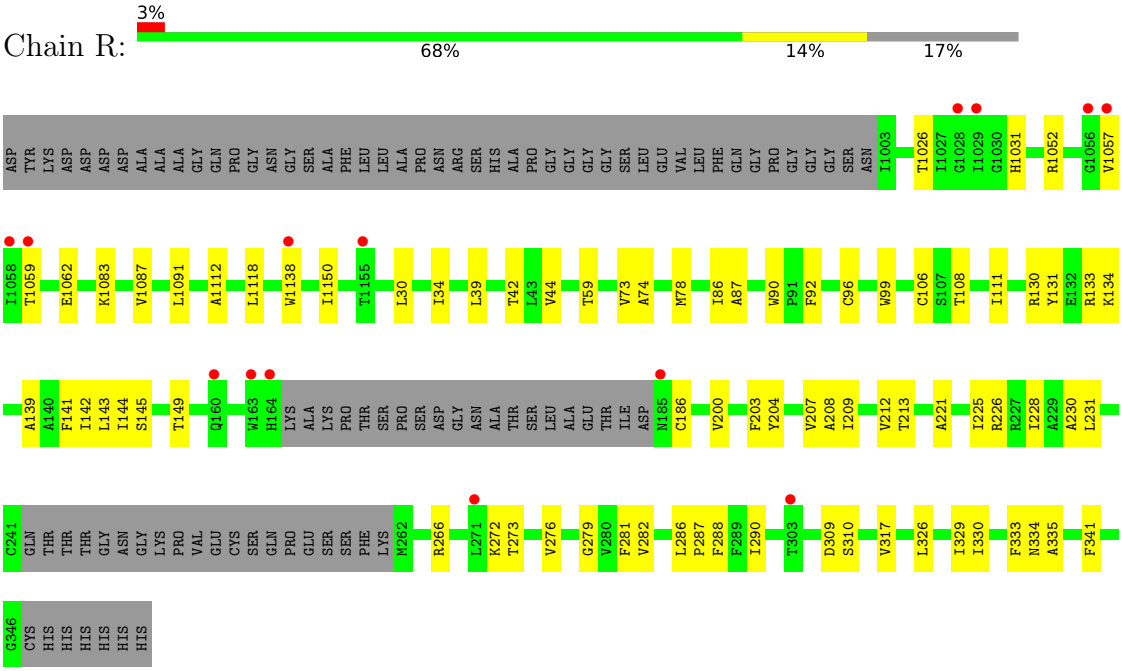
• Molecule 4: Nanobody 35

Chain N:



• Molecule 5: Endolysin,D(1A) dopamine receptor

Chain R:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 2 21	Depositor
Cell constants a, b, c, α, β, γ	99.19Å 144.31Å 147.07Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.00 – 3.80 47.00 – 3.80	Depositor EDS
% Data completeness (in resolution range)	93.2 (47.00-3.80) 93.2 (47.00-3.80)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.56 (at 3.77Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.254 , 0.297 0.253 , 0.297	Depositor DCC
R_{free} test set	1057 reflections (5.30%)	wwPDB-VP
Wilson B-factor (Å^2)	127.3	Xtriage
Anisotropy	0.372	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.24 , 101.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	0.038 for -h,l,k	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	9159	wwPDB-VP
Average B, all atoms (Å^2)	139.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.48% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 1PE, VFP

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	0.24	0/2338	0.42	0/3195
2	B	0.24	0/2493	0.46	0/3402
3	G	0.24	0/379	0.37	0/524
4	N	0.25	0/940	0.46	0/1282
5	R	0.25	0/3138	0.42	0/4304
All	All	0.25	0/9288	0.43	0/12707

There are no bond length outliers.

There are no bond angle outliers.

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	2299	0	1855	22	0
2	B	2446	0	2190	43	0
3	G	373	0	306	2	0
4	N	920	0	832	12	0
5	R	3078	0	2762	53	0
6	R	27	0	0	0	0
7	R	16	0	22	1	0
All	All	9159	0	7967	121	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 7.

All (121) 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:202:LYS:HD3	5:R:133:ARG:HH12	1.37	0.88
2:B:104:ALA:HB3	2:B:113:ALA:HB3	1.66	0.78
5:R:228:ILE:HG21	5:R:266:ARG:HH12	1.51	0.74
4:N:94:TYR:O	4:N:121:GLY:HA3	1.94	0.68
2:B:40:VAL:HG22	2:B:283:ARG:NH1	2.10	0.65
5:R:228:ILE:HG21	5:R:266:ARG:NH1	2.11	0.65
5:R:86:ILE:HG23	5:R:87:ALA:H	1.63	0.64
1:A:202:LYS:HD3	5:R:133:ARG:NH1	2.11	0.64
2:B:99:TRP:HB3	2:B:117:LEU:HD13	1.80	0.63
1:A:363:ASN:OD1	1:A:366:ARG:NH2	2.31	0.63
5:R:73:VAL:HG22	5:R:106:CYS:HB3	1.82	0.62
2:B:70:LEU:HB2	2:B:82:TRP:HB2	1.81	0.62
5:R:108:THR:HA	5:R:111:ILE:HG22	1.83	0.61
5:R:288:PHE:HE1	5:R:317:VAL:HG22	1.67	0.60
2:B:229:ILE:HD13	2:B:245:SER:HB3	1.83	0.59
5:R:90:TRP:HD1	5:R:92:PHE:HB2	1.68	0.59
5:R:90:TRP:CZ2	5:R:186:CYS:HB2	2.40	0.56
5:R:1026:THR:OG1	5:R:1031:HIS:O	2.22	0.56
2:B:331:SER:OG	2:B:333:ASP:OD1	2.23	0.55
2:B:79:LEU:HD13	2:B:95:LEU:HD21	1.88	0.55
5:R:133:ARG:HE	5:R:134:LYS:HG3	1.71	0.54
2:B:226:GLU:OE2	4:N:27:PHE:HA	2.08	0.54
5:R:1138:TRP:HZ3	5:R:1150:ILE:HD11	1.73	0.54
2:B:40:VAL:HG22	2:B:283:ARG:HH12	1.74	0.53
4:N:6:GLU:OE2	4:N:96:CYS:HB3	2.09	0.53
5:R:200:VAL:HA	5:R:204:TYR:HB2	1.90	0.53
5:R:1052:ARG:NH1	5:R:1057:VAL:O	2.42	0.52
2:B:124:TYR:CD1	2:B:135:VAL:HA	2.45	0.52
5:R:130:ARG:HD2	5:R:133:ARG:HH21	1.73	0.52
4:N:52:SER:OG	4:N:57:SER:OG	2.20	0.52
1:A:287:VAL:HA	1:A:292:SER:HB2	1.91	0.51
5:R:1087:VAL:O	5:R:1091:LEU:HG	2.09	0.51
1:A:121:MET:O	2:B:137:ARG:NH1	2.44	0.51
1:A:269:ARG:O	1:A:343:HIS:ND1	2.44	0.50
2:B:294:CYS:SG	2:B:308:LEU:HB2	2.52	0.50
5:R:139:ALA:HA	5:R:142:ILE:HG12	1.93	0.50
5:R:279:GLY:HA2	5:R:282:VAL:HG22	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:12:GLU:O	2:B:16:ASN:ND2	2.44	0.50
1:A:26:ILE:HD11	2:B:92:ALA:HB3	1.94	0.49
1:A:193:ILE:HD12	1:A:210:VAL:HG22	1.94	0.49
2:B:73:ALA:HB1	2:B:100:VAL:HG11	1.95	0.49
1:A:217:ARG:HG2	1:A:220:TRP:HZ2	1.78	0.49
4:N:94:TYR:O	4:N:121:GLY:CA	2.60	0.49
1:A:44:LEU:HD21	1:A:46:LEU:HD23	1.95	0.49
2:B:224:GLY:O	2:B:251:ARG:NH1	2.45	0.48
4:N:61:THR:HG22	4:N:63:SER:H	1.78	0.48
2:B:245:SER:OG	2:B:247:ASP:OD1	2.31	0.48
1:A:265:ASN:HB3	1:A:268:LEU:HB2	1.95	0.48
5:R:30:LEU:O	5:R:34:ILE:HG12	2.13	0.48
5:R:90:TRP:CD1	5:R:92:PHE:HB2	2.47	0.48
2:B:316:SER:HB2	2:B:332:TRP:CD1	2.49	0.48
2:B:125:ASN:O	2:B:133:VAL:HG13	2.14	0.47
4:N:36:TRP:CZ3	4:N:96:CYS:HB2	2.50	0.47
5:R:334:ASN:OD1	5:R:335:ALA:N	2.47	0.47
4:N:88:PRO:HA	4:N:126:VAL:HG11	1.97	0.47
3:G:48:ASP:OD2	3:G:51:LEU:HG	2.15	0.47
5:R:208:ALA:O	5:R:212:VAL:HG23	2.15	0.47
1:A:379:LEU:HA	5:R:273:THR:HG21	1.97	0.47
5:R:272:LYS:O	5:R:276:VAL:HG23	2.14	0.47
1:A:23:ASN:HB2	2:B:88:ASN:OD1	2.14	0.46
2:B:139:LEU:HD13	2:B:169:TRP:CG	2.50	0.46
5:R:1059:THR:HG23	5:R:1062:GLU:H	1.81	0.46
4:N:109:ASP:OD1	4:N:110:VAL:N	2.49	0.46
1:A:234:VAL:HB	1:A:277:LEU:HD23	1.97	0.46
2:B:165:THR:HA	2:B:180:PHE:O	2.15	0.46
2:B:180:PHE:HB3	2:B:211:TRP:CZ3	2.51	0.46
2:B:57:LYS:HG2	2:B:332:TRP:O	2.15	0.45
5:R:221:ALA:O	5:R:225:ILE:HG12	2.16	0.45
5:R:286:LEU:H	5:R:287:PRO:HD2	1.81	0.45
5:R:145:SER:O	5:R:149:THR:HG23	2.16	0.45
1:A:253:GLN:O	1:A:257:ASN:ND2	2.42	0.45
1:A:371:ARG:NH1	5:R:228:ILE:HD11	2.32	0.45
5:R:203:PHE:CE2	5:R:207:VAL:HG21	2.52	0.45
5:R:329:ILE:HG13	5:R:333:PHE:CE2	2.51	0.45
5:R:209:ILE:O	5:R:213:THR:HG23	2.16	0.45
5:R:207:VAL:HG22	5:R:281:PHE:CE2	2.52	0.45
2:B:113:ALA:HB2	2:B:151:PHE:CZ	2.52	0.45
5:R:44:VAL:HG22	5:R:341:PHE:HZ	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:288:PHE:CE1	5:R:317:VAL:HG22	2.49	0.44
7:R:1202:1PE:H152	7:R:1202:1PE:H162	1.73	0.44
1:A:196:THR:HG22	1:A:198:PHE:HD2	1.82	0.44
2:B:80:ILE:HG22	2:B:92:ALA:HB2	2.00	0.44
5:R:226:ARG:NH2	5:R:230:ALA:HB2	2.32	0.44
5:R:326:LEU:O	5:R:330:ILE:HG13	2.18	0.44
2:B:121:CYS:HB2	2:B:146:LEU:HD21	1.99	0.44
5:R:59:THR:HG22	5:R:131:TYR:OH	2.17	0.44
5:R:326:LEU:O	5:R:329:ILE:HG22	2.18	0.43
5:R:1083:LYS:HD2	5:R:1112:ALA:HB1	2.00	0.43
1:A:332:LEU:HD11	1:A:347:PRO:HG3	1.99	0.43
4:N:33:LYS:HG3	4:N:51:ILE:O	2.19	0.43
2:B:143:THR:HG22	2:B:143:THR:O	2.18	0.43
1:A:217:ARG:HB3	1:A:221:ILE:HD11	1.99	0.43
2:B:124:TYR:HD1	2:B:135:VAL:HA	1.82	0.43
4:N:95:TYR:HD1	4:N:121:GLY:HA3	1.84	0.43
5:R:1083:LYS:O	5:R:1118:LEU:HD21	2.19	0.43
5:R:309:ASP:OD1	5:R:310:SER:N	2.48	0.43
5:R:73:VAL:O	5:R:78:MET:HG2	2.20	0.42
2:B:212:ASP:OD2	2:B:215:GLU:HG2	2.19	0.42
5:R:141:PHE:HA	5:R:144:ILE:HD12	2.02	0.42
2:B:40:VAL:HG22	2:B:283:ARG:CZ	2.48	0.42
2:B:41:GLY:O	2:B:43:ILE:HG12	2.20	0.42
2:B:82:TRP:CZ3	2:B:89:LYS:HB3	2.54	0.42
5:R:74:ALA:HA	5:R:78:MET:HG3	2.02	0.42
5:R:287:PRO:HA	5:R:290:ILE:HG12	2.02	0.42
5:R:143:LEU:HD23	5:R:143:LEU:HA	1.91	0.42
1:A:332:LEU:HD21	5:R:231:LEU:HD22	2.02	0.42
2:B:14:LEU:O	2:B:18:ILE:HD12	2.20	0.42
2:B:118:ASP:OD1	2:B:118:ASP:N	2.52	0.42
5:R:96:CYS:HA	5:R:99:TRP:HB3	2.01	0.42
2:B:256:ARG:NH2	3:G:36:ASP:OD2	2.52	0.41
5:R:39:LEU:HA	5:R:42:THR:HG22	2.02	0.41
2:B:80:ILE:HG22	2:B:92:ALA:CB	2.50	0.41
1:A:202:LYS:HB3	5:R:133:ARG:HH12	1.86	0.41
2:B:66:ASP:OD2	2:B:69:LEU:HD13	2.21	0.41
2:B:266:HIS:H	2:B:269:ILE:HD11	1.86	0.41
2:B:308:LEU:HD23	2:B:339:TRP:CE3	2.56	0.41
1:A:267:TRP:CH2	2:B:314:ARG:HD2	2.56	0.41
4:N:51:ILE:HD11	4:N:70:ILE:HG23	2.02	0.41
2:B:173:THR:HG23	2:B:175:GLN:HG2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:63:TRP:CD2	2:B:70:LEU:HD21	2.56	0.40
5:R:286:LEU:N	5:R:287:PRO:HD2	2.37	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	326/380 (86%)	302 (93%)	24 (7%)	0	100	100
2	B	338/350 (97%)	309 (91%)	29 (9%)	0	100	100
3	G	55/71 (78%)	52 (94%)	3 (6%)	0	100	100
4	N	126/160 (79%)	113 (90%)	13 (10%)	0	100	100
5	R	440/540 (82%)	405 (92%)	35 (8%)	0	100	100
All	All	1285/1501 (86%)	1181 (92%)	104 (8%)	0	100	100

There are no Ramachandran outliers to report.

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	169/341 (50%)	169 (100%)	0	100	100
2	B	234/291 (80%)	234 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	G	28/58 (48%)	28 (100%)	0	100	100
4	N	91/129 (70%)	91 (100%)	0	100	100
5	R	263/455 (58%)	263 (100%)	0	100	100
All	All	785/1274 (62%)	785 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
5	R	224	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

2 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	$\#\|Z\| > 2$
7	1PE	R	1202	-	15,15,15	0.54	0	14,14,14	0.36	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	VFP	R	1201	-	24,30,30	1.11	1 (4%)	32,44,44	1.61	5 (15%)

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
7	1PE	R	1202	-	-	9/13/13/13	-
6	VFP	R	1201	-	-	0/8/27/27	0/4/4/4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	R	1201	VFP	C4-C3	2.73	1.40	1.36

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	R	1201	VFP	C1-C2-N1	-4.14	120.88	124.37
6	R	1201	VFP	C20-N2-C18	3.77	125.65	121.17
6	R	1201	VFP	C3-C4-C5	-3.09	116.67	119.31
6	R	1201	VFP	C8-O2-C2	2.99	124.05	118.16
6	R	1201	VFP	C7-C1-C5	-2.54	106.03	109.97

There are no chirality outliers.

All (9) torsion outliers are listed below:

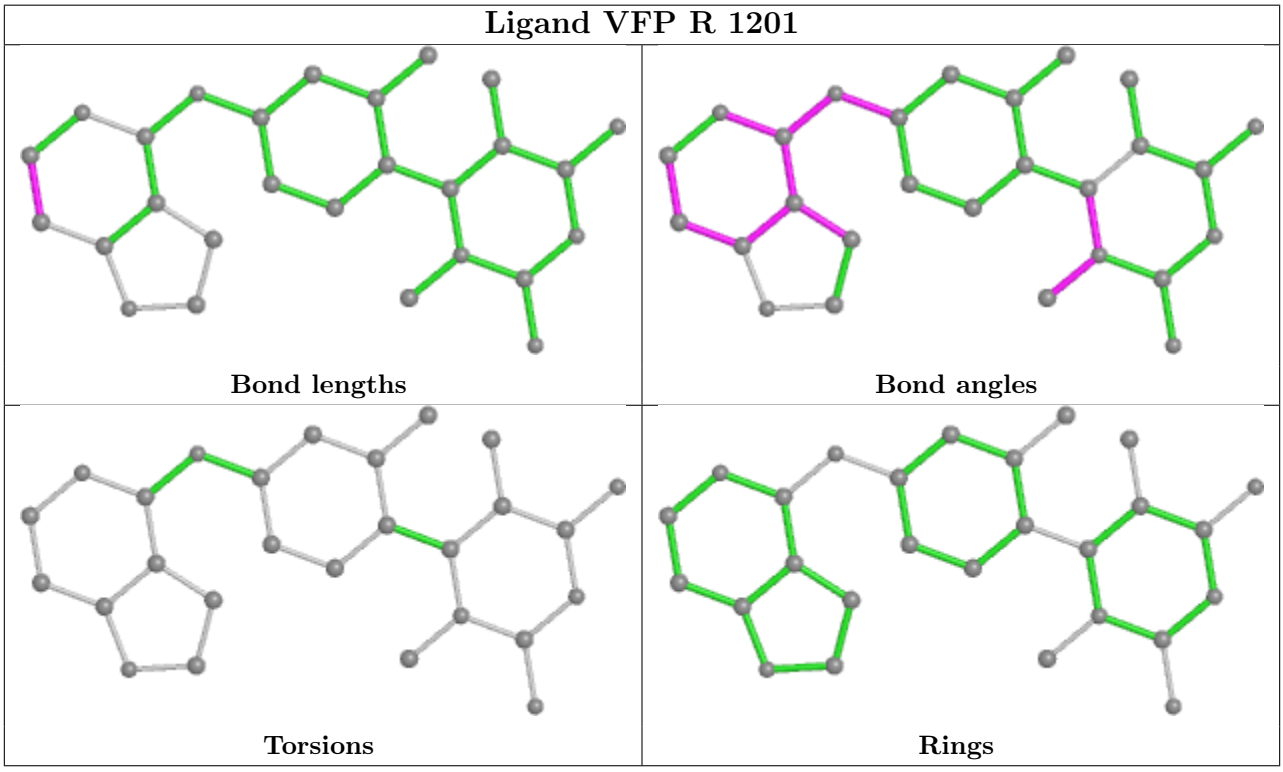
Mol	Chain	Res	Type	Atoms
7	R	1202	1PE	OH6-C15-C25-OH5
7	R	1202	1PE	OH2-C12-C22-OH3
7	R	1202	1PE	C16-C26-OH6-C15
7	R	1202	1PE	C14-C24-OH4-C13
7	R	1202	1PE	OH4-C13-C23-OH3
7	R	1202	1PE	C15-C25-OH5-C14
7	R	1202	1PE	C23-C13-OH4-C24
7	R	1202	1PE	C12-C22-OH3-C23
7	R	1202	1PE	OH7-C16-C26-OH6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	R	1202	1PE	1	0

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



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

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, 95^{th} 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	338/380 (88%)	-0.25	7 (2%)	63	55	69, 143, 250, 326	0
2	B	340/350 (97%)	-0.23	6 (1%)	68	61	63, 113, 169, 210	0
3	G	57/71 (80%)	-0.36	1 (1%)	68	61	105, 135, 213, 237	0
4	N	128/160 (80%)	-0.31	0	100	100	80, 109, 150, 191	0
5	R	446/540 (82%)	-0.19	14 (3%)	49	40	86, 164, 219, 248	0
All	All	1309/1501 (87%)	-0.23	28 (2%)	63	55	63, 137, 219, 326	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	G	6	THR	4.2
5	R	1056	GLY	3.9
5	R	160	GLN	3.8
1	A	91	THR	3.7
1	A	380	LEU	3.3
2	B	129	ARG	3.2
5	R	1059	THR	3.2
5	R	163	TRP	2.9
5	R	1057	VAL	2.8
2	B	130	GLU	2.7
5	R	164	HIS	2.6
1	A	138	ALA	2.6
1	A	129	PRO	2.6
5	R	1058	ILE	2.5
5	R	271	LEU	2.5
2	B	89	LYS	2.4
2	B	133	VAL	2.4
5	R	185	ASN	2.3
1	A	178	PRO	2.3
2	B	128	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	90	GLU	2.2
5	R	1029	ILE	2.1
5	R	1155	THR	2.1
1	A	379	LEU	2.1
5	R	1138	TRP	2.1
5	R	1028	GLY	2.1
2	B	126	LEU	2.1
5	R	303	THR	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

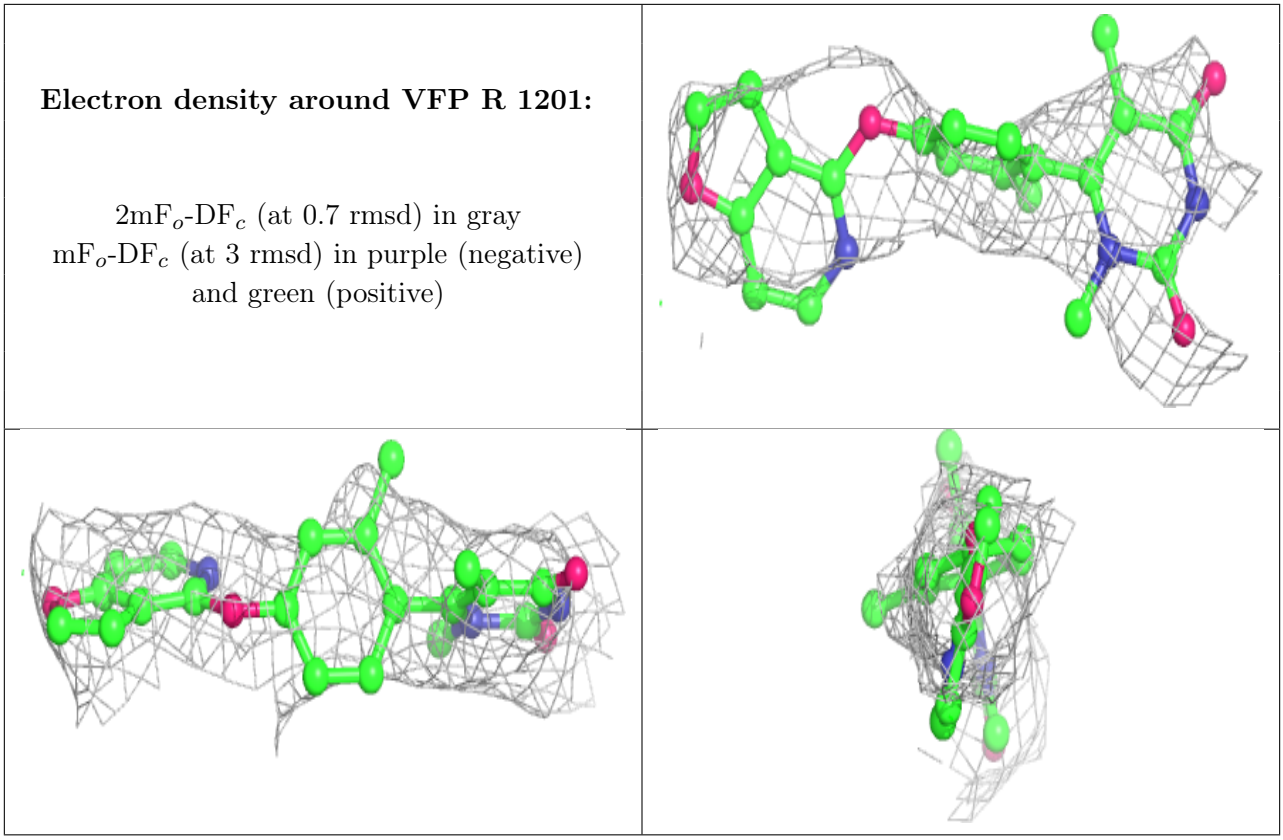
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	1PE	R	1202	16/16	0.80	0.36	101,117,135,135	0
6	VFP	R	1201	27/27	0.84	0.52	104,152,169,182	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 VFP R 1201:

$2mF_o$-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.