



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 03:34 PM UTC

PDB ID : 8W1V / pdb_00008w1v
Title : The beta2 adrenergic receptor bound to a bitopic ligand
Authors : Gaiser, B.; Danielsen, M.; Xu, X.; Jorgensen, K.; Fronik, P.; Marcher-Rorsted, E.; Wrobe, T.; Hirata, K.; Liu, X.; Mathiesen, J.; Pedersen, D.
Deposited on : 2024-02-19
Resolution : 3.00 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

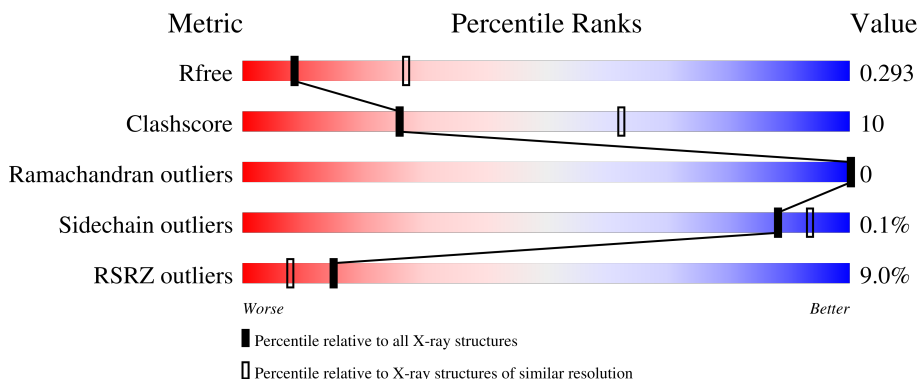
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	549	9% 62% 18% 20%
1	B	549	5% 60% 20% 20%
2	D	125	14% 77% 18% 5%
2	F	125	2% 82% 14% 5%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8913 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 Beta-2 adrenergic receptor, Endolysin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	441	Total	C	N	O	S	0	0	0
			3514	2301	582	607	24			
1	B	439	Total	C	N	O	S	0	0	0
			3515	2294	584	613	24			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-23	MET	-	initiating methionine	UNP P07550
A	-22	LYS	-	expression tag	UNP P07550
A	-21	THR	-	expression tag	UNP P07550
A	-20	ILE	-	expression tag	UNP P07550
A	-19	ILE	-	expression tag	UNP P07550
A	-18	ALA	-	expression tag	UNP P07550
A	-17	LEU	-	expression tag	UNP P07550
A	-16	SER	-	expression tag	UNP P07550
A	-15	TYR	-	expression tag	UNP P07550
A	-14	ILE	-	expression tag	UNP P07550
A	-13	PHE	-	expression tag	UNP P07550
A	-12	CYS	-	expression tag	UNP P07550
A	-11	LEU	-	expression tag	UNP P07550
A	-10	VAL	-	expression tag	UNP P07550
A	-9	PHE	-	expression tag	UNP P07550
A	-8	ALA	-	expression tag	UNP P07550
A	-7	ASP	-	expression tag	UNP P07550
A	-6	TYR	-	expression tag	UNP P07550
A	-5	LYS	-	expression tag	UNP P07550
A	-4	ASP	-	expression tag	UNP P07550
A	-3	ASP	-	expression tag	UNP P07550
A	-2	ASP	-	expression tag	UNP P07550
A	-1	ASP	-	expression tag	UNP P07550
A	0	ALA	-	expression tag	UNP P07550
A	16	ARG	GLY	conflict	UNP P07550

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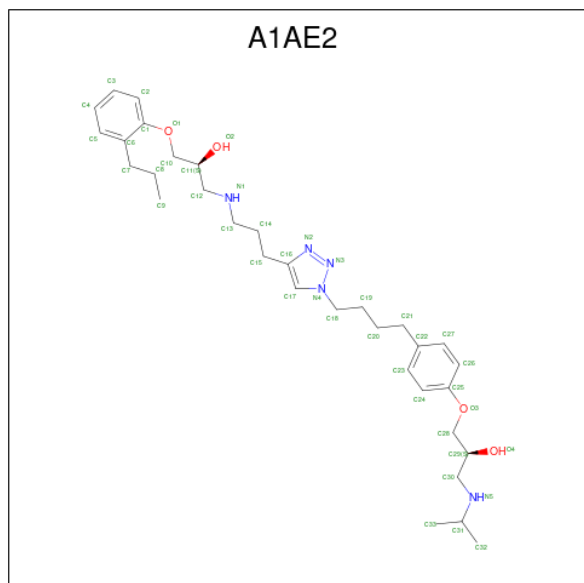
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Chain	Residue	Modelled	Actual	Comment	Reference
A	27	GLN	GLU	conflict	UNP P07550
A	187	GLU	ASN	engineered mutation	UNP P07550
A	231	TYR	GLN	conflict	UNP P07550
A	1012	GLY	ARG	conflict	UNP P00720
A	1054	THR	CYS	engineered mutation	UNP P00720
A	1097	ALA	CYS	engineered mutation	UNP P00720
A	1137	ARG	ILE	conflict	UNP P00720
B	-23	MET	-	initiating methionine	UNP P07550
B	-22	LYS	-	expression tag	UNP P07550
B	-21	THR	-	expression tag	UNP P07550
B	-20	ILE	-	expression tag	UNP P07550
B	-19	ILE	-	expression tag	UNP P07550
B	-18	ALA	-	expression tag	UNP P07550
B	-17	LEU	-	expression tag	UNP P07550
B	-16	SER	-	expression tag	UNP P07550
B	-15	TYR	-	expression tag	UNP P07550
B	-14	ILE	-	expression tag	UNP P07550
B	-13	PHE	-	expression tag	UNP P07550
B	-12	CYS	-	expression tag	UNP P07550
B	-11	LEU	-	expression tag	UNP P07550
B	-10	VAL	-	expression tag	UNP P07550
B	-9	PHE	-	expression tag	UNP P07550
B	-8	ALA	-	expression tag	UNP P07550
B	-7	ASP	-	expression tag	UNP P07550
B	-6	TYR	-	expression tag	UNP P07550
B	-5	LYS	-	expression tag	UNP P07550
B	-4	ASP	-	expression tag	UNP P07550
B	-3	ASP	-	expression tag	UNP P07550
B	-2	ASP	-	expression tag	UNP P07550
B	-1	ASP	-	expression tag	UNP P07550
B	0	ALA	-	expression tag	UNP P07550
B	16	ARG	GLY	conflict	UNP P07550
B	27	GLN	GLU	conflict	UNP P07550
B	187	GLU	ASN	engineered mutation	UNP P07550
B	231	TYR	GLN	conflict	UNP P07550
B	1012	GLY	ARG	conflict	UNP P00720
B	1054	THR	CYS	engineered mutation	UNP P00720
B	1097	ALA	CYS	engineered mutation	UNP P00720
B	1137	ARG	ILE	conflict	UNP P00720

- Molecule 2 is a protein called Nanobody60.

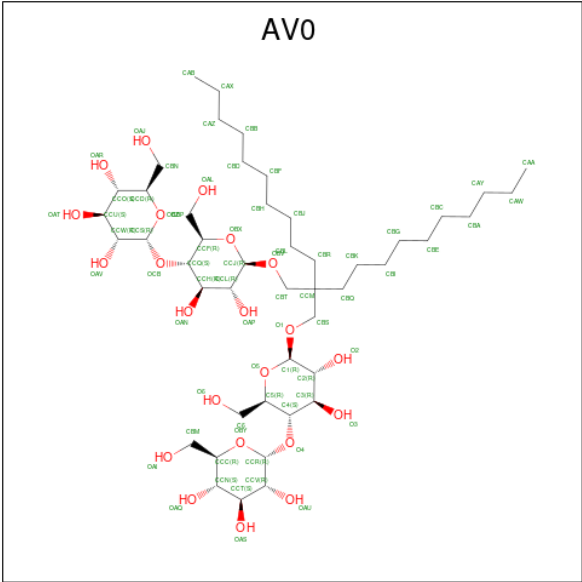
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	119	Total	C	N	O	S	0	0	0
			872	542	151	175	4			
2	F	119	Total	C	N	O	S	0	0	0
			859	536	147	172	4			

- Molecule 3 is (2S)-1-[(3-{1-[4-(4-{(2S)-2-hydroxy-3-[(propan-2-yl)amino]propoxy}phenyl)butyl]-1H-1,2,3-triazol-4-yl}propyl)amino]-3-(2-propylphenoxy)propan-2-ol (CCD ID: A1AE2) (formula: C₃₃H₅₁N₅O₄).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O		0	0
			42	33	5	4			
3	B	1	Total	C	N	O		0	0
			42	33	5	4			

- Molecule 4 is Lauryl Maltose Neopentyl Glycol (CCD ID: AV0) (formula: C₄₇H₈₈O₂₂) (labeled as "Ligand of Interest" by depositor).

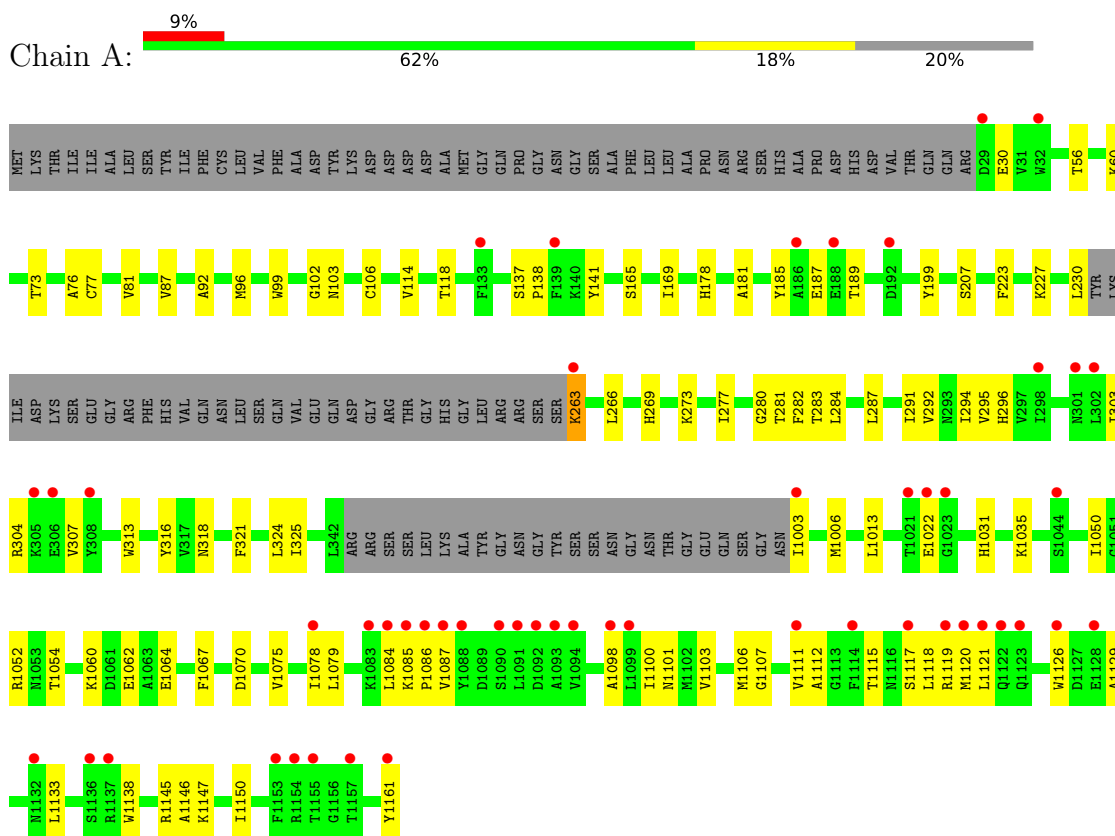


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			69	47	22		

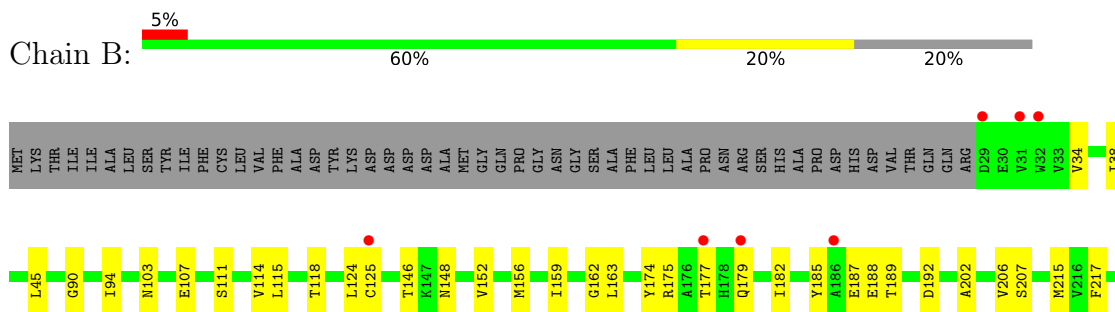
3 Residue-property plots [i](#)

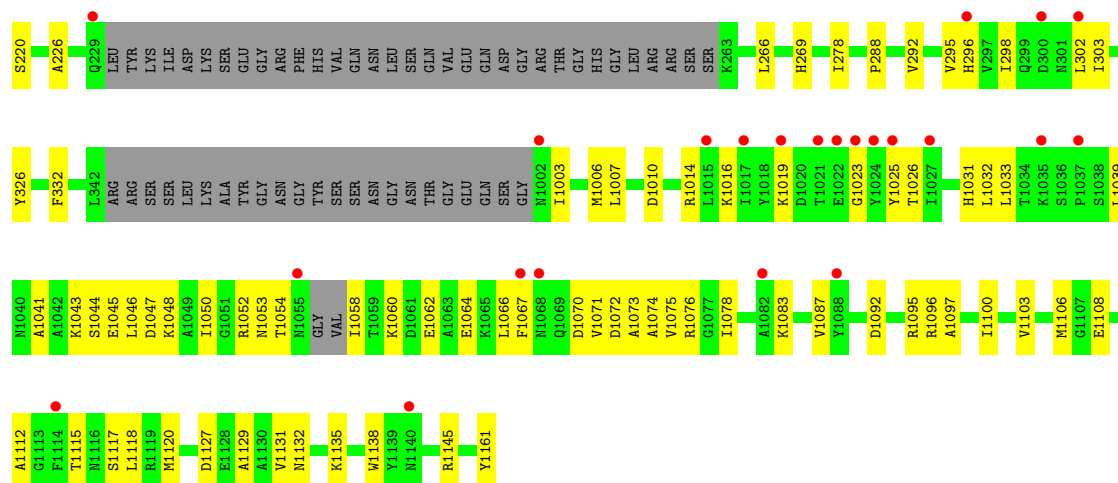
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Beta-2 adrenergic receptor,Endolysin

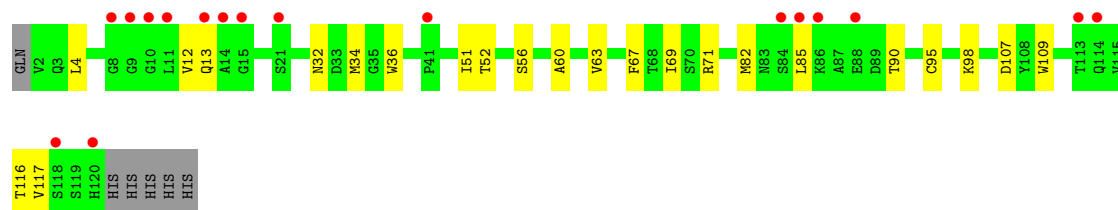
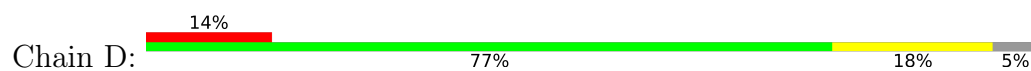


- Molecule 1: Beta-2 adrenergic receptor,Endolysin

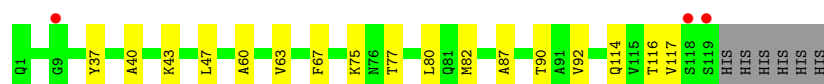
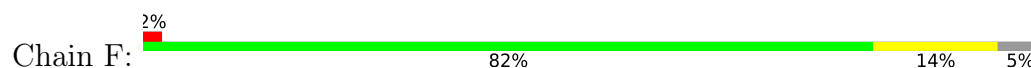




• Molecule 2: Nanobody60



• Molecule 2: Nanobody60



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	73.68Å 146.77Å 91.83Å 90.00° 107.06° 90.00°	Depositor
Resolution (Å)	48.44 – 3.00 48.44 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.44-3.00) 90.6 (48.44-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.58 (at 2.91Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.248 , 0.292 0.248 , 0.293	Depositor DCC
R_{free} test set	2246 reflections (5.54%)	wwPDB-VP
Wilson B-factor (Å ²)	40.7	Xtriage
Anisotropy	0.992	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 49.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	8913	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.67% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: A1AE2, AV0

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	0.17	0/3593	0.39	0/4877
1	B	0.15	0/3593	0.34	0/4874
2	D	0.21	0/887	0.42	0/1204
2	F	0.15	0/873	0.37	0/1185
All	All	0.16	0/8946	0.37	0/12140

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 [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	3514	0	3573	68	0
1	B	3515	0	3559	74	0
2	D	872	0	818	17	0
2	F	859	0	809	9	0
3	A	42	0	0	0	0
3	B	42	0	0	1	0
4	B	69	0	0	0	0
All	All	8913	0	8759	168	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 10.

All (168) 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:B:1106:MET:HE1	1:B:1138:TRP:HB2	1.63	0.79
1:B:295:VAL:HA	1:B:298:ILE:HG22	1.69	0.75
1:A:1035:LYS:HD3	1:A:1035:LYS:H	1.52	0.74
1:A:187:GLU:HG3	1:A:189:THR:H	1.57	0.70
1:A:1103:VAL:O	1:A:1107:GLY:N	2.24	0.68
1:A:263:LYS:HA	1:A:1161:TYR:C	2.19	0.67
1:B:146:THR:HG22	1:B:148:ASN:H	1.63	0.62
1:A:292:VAL:HA	1:A:295:VAL:HG22	1.82	0.61
1:B:1045:GLU:HA	1:B:1048:LYS:HB2	1.82	0.61
1:A:118:THR:HG22	1:A:207:SER:HB3	1.81	0.61
1:A:304:ARG:HB2	1:A:307:VAL:HG12	1.85	0.59
1:B:1072:ASP:OD1	1:B:1073:ALA:N	2.36	0.58
1:A:1035:LYS:H	1:A:1035:LYS:CD	2.16	0.57
1:A:137:SER:OG	1:A:138:PRO:HD2	2.04	0.57
1:A:1064:GLU:HA	1:A:1067:PHE:HB3	1.87	0.57
1:B:1019:LYS:HG3	1:B:1023:GLY:HA2	1.86	0.57
1:B:1050:ILE:HG13	1:B:1054:THR:HG21	1.86	0.57
2:D:63:VAL:HB	2:D:67:PHE:CD1	2.39	0.57
1:A:92:ALA:HB1	1:A:96:MET:HE2	1.86	0.57
1:B:1132:ASN:HA	1:B:1135:LYS:HE2	1.87	0.56
2:D:60:ALA:HB3	2:D:63:VAL:HG22	1.87	0.56
1:A:1115:THR:HA	1:A:1118:LEU:HD12	1.86	0.56
1:B:125:CYS:HB3	1:B:215:MET:HB2	1.88	0.56
1:A:1084:LEU:HD12	1:A:1087:VAL:HG21	1.87	0.55
2:F:87:ALA:HA	2:F:117:VAL:HB	1.88	0.55
1:B:1026:THR:HG22	1:B:1032:LEU:HA	1.89	0.55
1:B:1010:ASP:HB2	1:B:1145:ARG:HG3	1.88	0.55
1:A:1121:LEU:HD23	1:A:1126:TRP:HD1	1.71	0.55
1:B:1039:LEU:HD22	1:B:1043:LYS:HE3	1.89	0.55
1:A:1006:MET:HE1	1:A:1098:ALA:HA	1.90	0.54
1:B:292:VAL:HA	1:B:295:VAL:HG22	1.89	0.54
1:A:1075:VAL:HG12	1:A:1100:ILE:HD13	1.89	0.54
1:B:1054:THR:HG21	1:B:1058:ILE:HG22	1.90	0.53
1:A:114:VAL:HG23	1:A:165:SER:HB2	1.89	0.53
1:A:1006:MET:HE2	1:A:1101:ASN:HD22	1.73	0.53
1:A:1121:LEU:HD23	1:A:1126:TRP:CD1	2.44	0.53
1:B:1117:SER:OG	1:B:1132:ASN:ND2	2.38	0.52
1:B:179:GLN:HA	1:B:182:ILE:HD12	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:67:PHE:CE2	2:D:82:MET:HB3	2.44	0.52
2:F:67:PHE:CZ	2:F:82:MET:HE3	2.46	0.51
1:A:296:HIS:HB2	1:A:303:ILE:HG12	1.92	0.51
1:B:202:ALA:O	1:B:206:VAL:HG12	2.11	0.51
1:B:1117:SER:HA	1:B:1120:MET:HE3	1.93	0.51
1:A:1117:SER:HA	1:A:1120:MET:HB2	1.92	0.51
1:B:115:LEU:HD13	1:B:162:GLY:HA2	1.92	0.51
1:B:1083:LYS:HE2	1:B:1112:ALA:HB1	1.93	0.51
1:B:288:PRO:O	1:B:292:VAL:HG22	2.10	0.51
1:B:1071:VAL:O	1:B:1075:VAL:HG23	2.11	0.51
2:D:63:VAL:HB	2:D:67:PHE:CE1	2.46	0.51
1:A:103:ASN:HA	1:A:106:CYS:HB3	1.93	0.50
1:B:107:GLU:O	1:B:111:SER:OG	2.26	0.50
1:B:175:ARG:HG2	1:B:185:TYR:CE2	2.45	0.50
2:D:52:THR:HG22	2:D:56:SER:H	1.77	0.50
2:F:37:TYR:CZ	2:F:47:LEU:HD12	2.46	0.50
1:A:313:TRP:HA	1:A:316:TYR:HB2	1.93	0.50
1:A:1084:LEU:HD22	1:A:1112:ALA:HB2	1.93	0.50
1:B:1033:LEU:HD13	1:B:1046:LEU:HB2	1.94	0.50
1:B:124:LEU:HD21	1:B:278:ILE:HG22	1.93	0.49
1:A:1084:LEU:HD13	1:A:1118:LEU:HD13	1.94	0.49
1:A:277:ILE:O	1:A:281:THR:HG23	2.12	0.49
1:A:227:LYS:HB2	1:A:263:LYS:HD2	1.94	0.49
1:B:177:THR:O	1:B:182:ILE:HD11	2.12	0.49
1:B:226:ALA:HB1	1:B:269:HIS:CD2	2.47	0.49
2:D:32:ASN:HB2	2:D:34:MET:HE2	1.95	0.49
1:A:1084:LEU:HD21	1:A:1111:VAL:HG23	1.95	0.49
2:D:4:LEU:HD23	2:D:95:CYS:SG	2.53	0.49
1:B:1003:ILE:HD13	1:B:1097:ALA:HA	1.95	0.49
1:B:1092:ASP:OD1	1:B:1095:ARG:N	2.40	0.49
1:A:181:ALA:HB1	1:A:185:TYR:CZ	2.48	0.48
1:B:302:LEU:O	1:B:302:LEU:HD13	2.12	0.48
2:F:90:THR:HG23	2:F:116:THR:HA	1.95	0.48
1:B:152:VAL:O	1:B:156:MET:HG3	2.13	0.48
1:A:99:TRP:NE1	1:A:102:GLY:O	2.37	0.48
1:A:1101:ASN:OD1	1:A:1145:ARG:NH1	2.47	0.48
1:A:1106:MET:HE3	1:A:1111:VAL:HG12	1.95	0.48
1:B:1047:ASP:HB2	1:B:1052:ARG:O	2.14	0.48
1:B:1087:VAL:HG21	1:B:1118:LEU:HD12	1.95	0.48
1:B:1096:ARG:O	1:B:1100:ILE:HG13	2.13	0.48
2:F:92:VAL:HG22	2:F:114:GLN:HG3	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:326:TYR:HB3	1:B:332:PHE:HD2	1.79	0.48
1:B:1041:ALA:O	1:B:1044:SER:OG	2.30	0.48
2:F:67:PHE:HB3	2:F:80:LEU:HD11	1.94	0.48
1:A:169:ILE:HD11	1:A:199:TYR:OH	2.14	0.48
2:D:67:PHE:HE2	2:D:82:MET:HE2	1.79	0.48
1:B:114:VAL:O	1:B:118:THR:HG23	2.14	0.47
1:A:291:ILE:O	1:A:294:ILE:HG22	2.14	0.47
1:A:1129:ALA:O	1:A:1133:LEU:HG	2.15	0.47
1:B:107:GLU:OE2	1:B:174:TYR:OH	2.27	0.47
2:F:40:ALA:HB3	2:F:43:LYS:HD2	1.97	0.47
1:A:1050:ILE:HD12	1:A:1062:GLU:HB3	1.97	0.47
1:B:1060:LYS:HB3	1:B:1060:LYS:HE3	1.79	0.47
2:D:12:VAL:HG12	2:D:13:GLN:O	2.15	0.47
2:D:52:THR:HG22	2:D:56:SER:N	2.30	0.47
1:A:1003:ILE:HA	1:A:1006:MET:HB3	1.96	0.46
1:B:159:ILE:O	1:B:163:LEU:HG	2.16	0.46
1:B:1115:THR:HA	1:B:1118:LEU:HB2	1.96	0.46
1:A:87:VAL:HG22	1:A:316:TYR:CD2	2.51	0.46
1:A:277:ILE:HG22	1:A:325:ILE:HD13	1.98	0.46
1:A:1060:LYS:O	1:A:1064:GLU:HG2	2.14	0.46
1:B:34:VAL:O	1:B:38:ILE:HG23	2.16	0.46
1:B:1127:ASP:O	1:B:1131:VAL:HG23	2.15	0.46
1:B:1074:ALA:O	1:B:1078:ILE:HG13	2.15	0.46
1:B:1031:HIS:ND1	1:B:1070:ASP:OD2	2.49	0.46
2:F:75:LYS:O	2:F:77:THR:HG23	2.17	0.45
2:D:51:ILE:HG12	2:D:71:ARG:HD2	1.98	0.45
1:A:1078:ILE:HD12	1:A:1078:ILE:HA	1.77	0.45
1:B:146:THR:HG22	1:B:148:ASN:N	2.29	0.45
1:B:1076:ARG:HE	1:B:1076:ARG:HB2	1.53	0.45
1:B:103:ASN:ND2	1:B:188:GLU:HG2	2.31	0.45
1:B:1078:ILE:HG12	1:B:1103:VAL:HG21	1.98	0.45
1:A:1013:LEU:HD21	1:A:1060:LYS:HG3	1.98	0.45
1:B:118:THR:HG22	1:B:207:SER:HB3	1.99	0.45
1:A:282:PHE:HA	1:A:318:ASN:OD1	2.17	0.45
1:B:1006:MET:HE3	1:B:1161:TYR:CE2	2.52	0.45
2:D:98:LYS:NZ	2:D:107:ASP:OD1	2.51	0.44
1:B:326:TYR:HB3	1:B:332:PHE:CD2	2.52	0.44
1:A:30:GLU:O	1:A:30:GLU:HG2	2.17	0.44
2:D:82:MET:HB2	2:D:85:LEU:HD21	1.98	0.44
1:A:230:LEU:HD23	1:A:230:LEU:HA	1.86	0.44
1:B:217:PHE:O	1:B:220:SER:OG	2.30	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:36:TRP:HD1	2:D:69:ILE:HD13	1.82	0.44
2:D:90:THR:HG23	2:D:116:THR:HA	2.00	0.44
1:B:1007:LEU:HA	1:B:1010:ASP:OD1	2.18	0.43
1:B:1052:ARG:HH21	1:B:1062:GLU:HG3	1.83	0.43
1:A:1006:MET:HE3	1:A:1161:TYR:CE2	2.53	0.43
1:A:1060:LYS:HB3	1:A:1060:LYS:HE3	1.75	0.43
1:A:141:TYR:HH	1:A:269:HIS:CD2	2.34	0.43
1:A:230:LEU:HD21	1:A:266:LEU:HD11	2.00	0.43
1:B:266:LEU:HD12	1:B:269:HIS:CE1	2.54	0.43
1:B:90:GLY:O	1:B:94:ILE:HG12	2.18	0.43
1:A:1052:ARG:NH1	1:A:1054:THR:HA	2.34	0.43
2:D:85:LEU:HB3	2:D:117:VAL:HG21	2.01	0.43
1:A:1147:LYS:HA	1:A:1150:ILE:HB	2.01	0.43
2:F:60:ALA:HB3	2:F:63:VAL:HG22	2.01	0.43
1:B:1043:LYS:HA	1:B:1046:LEU:HB3	2.01	0.43
1:A:283:THR:O	1:A:287:LEU:HB2	2.19	0.42
1:A:1078:ILE:HD11	1:A:1084:LEU:HB3	2.01	0.42
1:A:1085:LYS:HB3	1:A:1086:PRO:HD3	2.01	0.42
1:A:1087:VAL:HG13	1:A:1119:ARG:HH22	1.84	0.42
1:B:192:ASP:HB3	3:B:1201:A1AE2:C27	2.49	0.42
1:A:1022:GLU:N	1:A:1022:GLU:OE1	2.53	0.42
1:A:77:CYS:O	1:A:81:VAL:HG23	2.20	0.42
1:A:1075:VAL:O	1:A:1079:LEU:HG	2.20	0.42
1:A:1138:TRP:CZ2	1:A:1146:ALA:HA	2.54	0.42
1:B:266:LEU:HB2	1:B:269:HIS:ND1	2.35	0.42
1:A:181:ALA:HB1	1:A:185:TYR:CE2	2.54	0.41
1:B:1075:VAL:HG22	1:B:1100:ILE:HD13	2.02	0.41
1:A:223:PHE:HZ	1:A:273:LYS:HA	1.85	0.41
1:B:1010:ASP:OD1	1:B:1010:ASP:N	2.51	0.41
1:B:1060:LYS:O	1:B:1064:GLU:HG3	2.21	0.41
1:B:1047:ASP:CB	1:B:1053:ASN:HA	2.51	0.41
1:A:178:HIS:CE1	1:A:181:ALA:HB2	2.55	0.41
1:A:1031:HIS:ND1	1:A:1070:ASP:OD2	2.54	0.41
1:B:296:HIS:CD2	1:B:303:ILE:HB	2.55	0.41
1:B:1025:TYR:CE2	1:B:1039:LEU:HG	2.56	0.41
1:B:1120:MET:HB3	1:B:1129:ALA:HB2	2.03	0.41
1:B:45:LEU:HD12	1:B:45:LEU:HA	1.97	0.41
1:B:1050:ILE:HD13	1:B:1066:LEU:HD11	2.03	0.41
1:A:56:THR:O	1:A:60:LYS:HG2	2.21	0.40
1:A:321:PHE:O	1:A:324:LEU:HG	2.21	0.40
1:B:1014:ARG:HG3	1:B:1016:LYS:H	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:280:GLY:O	1:A:284:LEU:HG	2.20	0.40
2:D:95:CYS:O	2:D:109:TRP:HA	2.21	0.40
1:A:1075:VAL:O	1:A:1078:ILE:HG22	2.21	0.40
1:B:1067:PHE:O	1:B:1071:VAL:HG23	2.22	0.40
1:B:1108:GLU:H	1:B:1108:GLU:HG3	1.73	0.40
1:A:73:THR:O	1:A:76:ALA:N	2.54	0.40
1:B:187:GLU:HG2	1:B:189:THR:HB	2.02	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	435/549 (79%)	416 (96%)	19 (4%)	0	100	100
1	B	431/549 (78%)	416 (96%)	15 (4%)	0	100	100
2	D	117/125 (94%)	112 (96%)	5 (4%)	0	100	100
2	F	117/125 (94%)	114 (97%)	3 (3%)	0	100	100
All	All	1100/1348 (82%)	1058 (96%)	42 (4%)	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	376/471 (80%)	375 (100%)	1 (0%)	86	91
1	B	378/471 (80%)	378 (100%)	0	100	100
2	D	88/99 (89%)	88 (100%)	0	100	100
2	F	85/99 (86%)	85 (100%)	0	100	100
All	All	927/1140 (81%)	926 (100%)	1 (0%)	88	93

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	263	LYS

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	296	HIS
1	B	148	ASN
1	B	299	GLN
1	B	312	ASN
1	B	1053	ASN
2	F	81	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

3 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
3	A1AE2	B	1201	-	44,44,44	2.50	8 (18%)	54,55,55	1.13	6 (11%)
3	A1AE2	A	1201	-	44,44,44	2.47	8 (18%)	54,55,55	1.43	7 (12%)
4	AV0	B	1202	-	72,72,72	1.15	6 (8%)	92,98,98	1.36	13 (14%)

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	A1AE2	B	1201	-	-	19/33/33/33	0/3/3/3
3	A1AE2	A	1201	-	-	21/33/33/33	0/3/3/3
4	AV0	B	1202	-	-	20/50/130/130	0/4/4/4

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1201	A1AE2	C5-C6	8.52	1.53	1.39
3	B	1201	A1AE2	C5-C6	8.31	1.53	1.39
3	B	1201	A1AE2	C3-C4	6.74	1.53	1.38
3	A	1201	A1AE2	C3-C4	6.72	1.53	1.38
3	A	1201	A1AE2	C2-C1	6.51	1.53	1.39
3	B	1201	A1AE2	C2-C1	6.45	1.52	1.39
3	B	1201	A1AE2	N2-N3	5.11	1.40	1.32
3	B	1201	A1AE2	C1-C6	-4.92	1.32	1.39
3	A	1201	A1AE2	N2-N3	4.84	1.39	1.32
3	A	1201	A1AE2	C1-C6	-4.39	1.32	1.39
3	B	1201	A1AE2	C4-C5	-4.17	1.31	1.38
3	A	1201	A1AE2	C4-C5	-4.12	1.31	1.38
3	B	1201	A1AE2	C3-C2	-4.02	1.32	1.38
3	A	1201	A1AE2	C3-C2	-3.94	1.32	1.38
4	B	1202	AV0	CBQ-CCM	3.61	1.60	1.54
4	B	1202	AV0	CBR-CCM	3.54	1.60	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1201	A1AE2	C17-N4	3.17	1.40	1.34
3	A	1201	A1AE2	C17-N4	3.14	1.39	1.34
4	B	1202	AV0	CBT-CCM	2.31	1.58	1.53
4	B	1202	AV0	CBS-CCM	2.13	1.58	1.53
4	B	1202	AV0	CBQ-CBK	2.12	1.59	1.52
4	B	1202	AV0	O1-C1	2.00	1.43	1.40

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1202	AV0	CCU-CCO-CCD	4.52	118.43	110.23
4	B	1202	AV0	OBZ-CCD-CCO	4.27	117.40	109.70
3	A	1201	A1AE2	C14-C15-C16	-4.18	105.12	113.56
3	A	1201	A1AE2	O1-C1-C6	3.97	121.02	115.89
4	B	1202	AV0	OBV-CCJ-CCL	3.26	113.22	108.27
3	A	1201	A1AE2	C17-N4-N3	-3.22	107.62	110.75
4	B	1202	AV0	CCR-O4-C4	-3.19	110.42	117.98
4	B	1202	AV0	OBX-CCF-CCQ	2.93	115.77	109.72
4	B	1202	AV0	CCJ-CCL-CCH	-2.67	104.39	110.01
3	B	1201	A1AE2	O1-C1-C6	2.50	119.12	115.89
3	A	1201	A1AE2	C15-C16-C17	-2.40	125.60	130.26
4	B	1202	AV0	CCS-CCW-CCU	-2.23	105.31	110.01
3	B	1201	A1AE2	C12-C11-C10	-2.23	107.13	110.54
3	B	1201	A1AE2	C18-N4-N3	2.22	125.24	120.78
3	B	1201	A1AE2	C17-N4-N3	-2.22	108.59	110.75
4	B	1202	AV0	OBX-CCJ-CCL	-2.21	105.84	110.37
4	B	1202	AV0	CBR-CBL-CBJ	-2.18	106.69	113.19
3	B	1201	A1AE2	C12-N1-C13	-2.16	108.67	113.38
3	B	1201	A1AE2	C28-O3-C25	-2.16	113.10	117.85
3	A	1201	A1AE2	N4-N3-N2	2.15	108.96	107.02
4	B	1202	AV0	OCB-CCQ-CCF	-2.15	103.83	109.48
3	A	1201	A1AE2	C12-N1-C13	-2.08	108.84	113.38
3	A	1201	A1AE2	C28-O3-C25	-2.06	113.32	117.85
4	B	1202	AV0	CBR-CCM-CBQ	2.05	113.78	109.96
4	B	1202	AV0	CCS-OBZ-CCD	-2.05	109.72	113.72
4	B	1202	AV0	OBZ-CCD-CBN	2.01	111.42	106.44

There are no chirality outliers.

All (60) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1201	A1AE2	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
3	A	1201	A1AE2	O3-C28-C29-C30
3	A	1201	A1AE2	C28-C29-C30-N5
3	A	1201	A1AE2	O4-C29-C30-N5
3	A	1201	A1AE2	C29-C30-N5-C31
3	B	1201	A1AE2	O3-C28-C29-C30
3	B	1201	A1AE2	O3-C28-C29-O4
3	B	1201	A1AE2	C28-C29-C30-N5
3	B	1201	A1AE2	O4-C29-C30-N5
4	B	1202	AV0	CBL-CBR-CCM-CBQ
4	B	1202	AV0	CBL-CBR-CCM-CBS
4	B	1202	AV0	CBL-CBR-CCM-CBT
4	B	1202	AV0	OBZ-CCS-OCB-CCQ
4	B	1202	AV0	OAJ-CBN-CCD-OBZ
4	B	1202	AV0	OAL-CBP-CCF-OBX
4	B	1202	AV0	OAJ-CBN-CCD-CCO
3	A	1201	A1AE2	C24-C25-O3-C28
3	A	1201	A1AE2	C26-C25-O3-C28
3	B	1201	A1AE2	C19-C20-C21-C22
3	A	1201	A1AE2	C19-C20-C21-C22
4	B	1202	AV0	OAL-CBP-CCF-CCQ
3	A	1201	A1AE2	O3-C28-C29-O4
3	B	1201	A1AE2	C26-C25-O3-C28
4	B	1202	AV0	OAI-CBM-CCC-OBY
3	B	1201	A1AE2	C24-C25-O3-C28
4	B	1202	AV0	CBC-CBE-CBG-CBI
4	B	1202	AV0	CBG-CBI-CBK-CBQ
4	B	1202	AV0	CBB-CBD-CBF-CBH
3	B	1201	A1AE2	N4-C18-C19-C20
4	B	1202	AV0	CBA-CBC-CBE-CBG
4	B	1202	AV0	O5-C5-C6-O6
4	B	1202	AV0	CBD-CBF-CBH-CBJ
3	A	1201	A1AE2	N4-C18-C19-C20
3	B	1201	A1AE2	C33-C31-N5-C30
4	B	1202	AV0	CBE-CBG-CBI-CBK
4	B	1202	AV0	CAZ-CBB-CBD-CBF
3	A	1201	A1AE2	C29-C28-O3-C25
3	B	1201	A1AE2	C29-C30-N5-C31
3	B	1201	A1AE2	C11-C12-N1-C13
3	A	1201	A1AE2	C18-C19-C20-C21
3	B	1201	A1AE2	C32-C31-N5-C30
3	B	1201	A1AE2	C19-C18-N4-C17
3	B	1201	A1AE2	C13-C14-C15-C16

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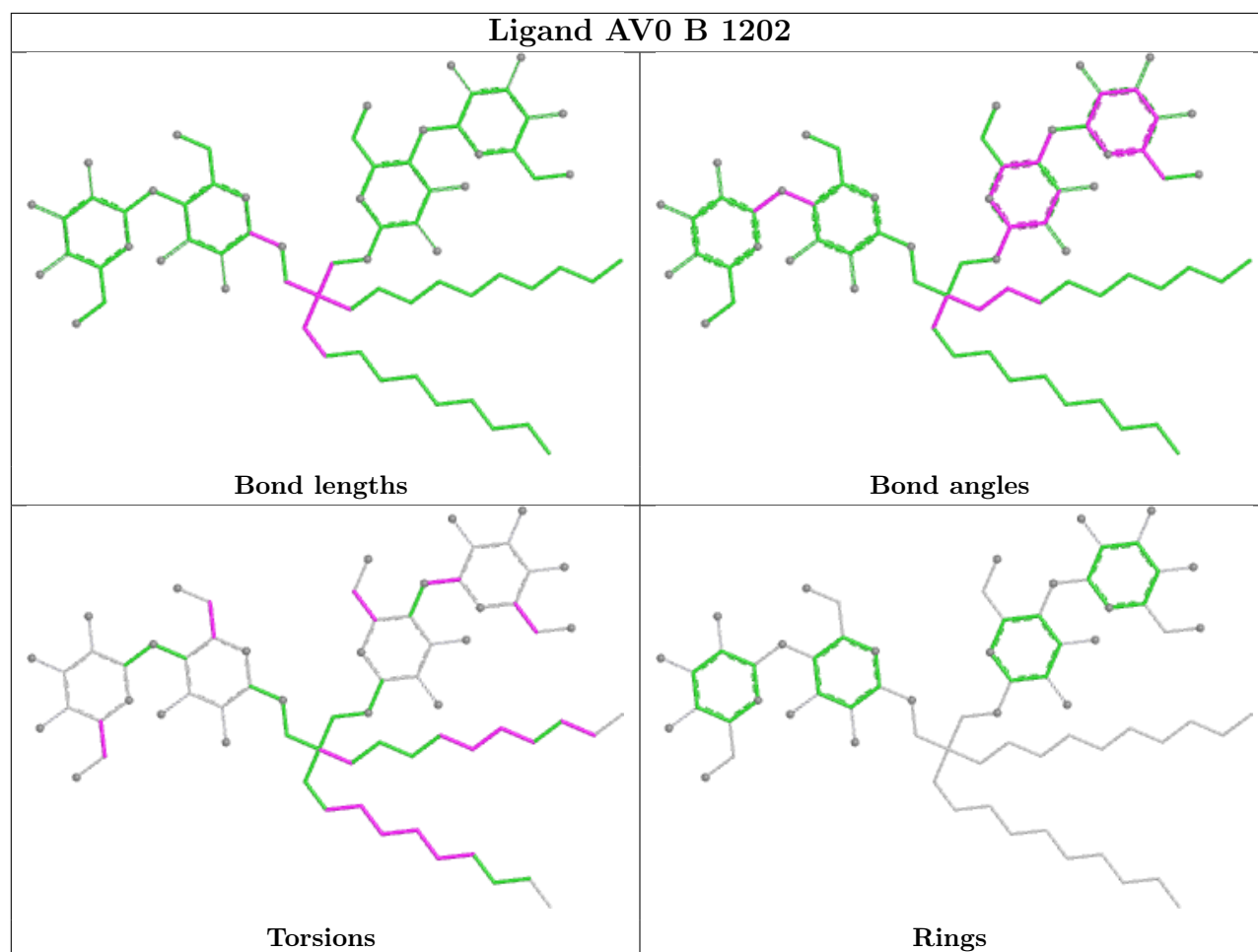
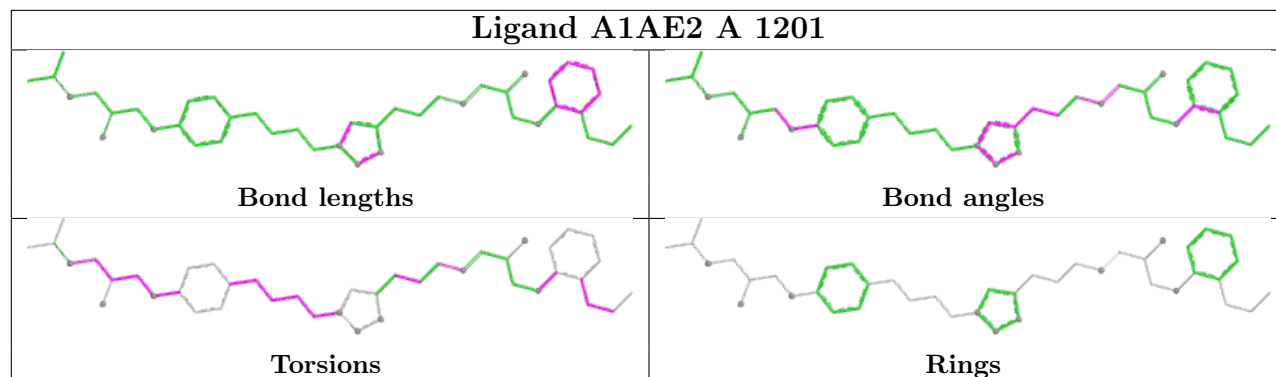
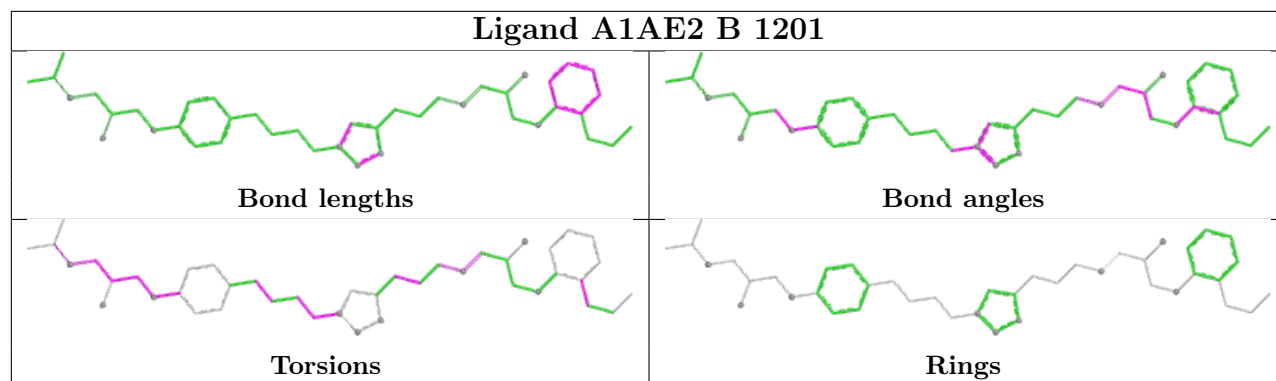
Mol	Chain	Res	Type	Atoms
3	B	1201	A1AE2	C1-C6-C7-C8
3	B	1201	A1AE2	C5-C6-C7-C8
4	B	1202	AV0	OAI-CBM-CCC-CCN
3	A	1201	A1AE2	C1-C6-C7-C8
3	A	1201	A1AE2	C2-C1-O1-C10
3	B	1201	A1AE2	C29-C28-O3-C25
3	A	1201	A1AE2	C6-C7-C8-C9
3	A	1201	A1AE2	C6-C1-O1-C10
3	B	1201	A1AE2	C19-C18-N4-N3
3	A	1201	A1AE2	C5-C6-C7-C8
4	B	1202	AV0	CAB-CAX-CAZ-CBB
3	A	1201	A1AE2	C20-C21-C22-C27
3	A	1201	A1AE2	C20-C21-C22-C23
3	A	1201	A1AE2	C14-C13-N1-C12
3	B	1201	A1AE2	C14-C13-N1-C12
4	B	1202	AV0	CAY-CBA-CBC-CBE
3	A	1201	A1AE2	C19-C18-N4-N3

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1201	A1AE2	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 [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, 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	441/549 (80%)	0.71	51 (11%) 9 5	27, 49, 94, 105	0
1	B	439/549 (79%)	0.68	30 (6%) 23 12	28, 60, 100, 113	0
2	D	119/125 (95%)	1.16	17 (14%) 6 3	34, 72, 96, 116	0
2	F	119/125 (95%)	0.40	3 (2%) 58 35	36, 49, 64, 79	0
All	All	1118/1348 (82%)	0.72	101 (9%) 15 8	27, 54, 96, 116	0

All (101) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	10	GLY	11.5
1	A	1086	PRO	5.4
1	A	1094	VAL	4.5
1	A	1084	LEU	4.3
1	A	1119	ARG	4.3
2	F	9	GLY	4.2
1	A	1090	SER	3.9
1	A	263	LYS	3.8
1	A	1155	THR	3.8
2	D	88	GLU	3.8
1	A	1092	ASP	3.7
1	A	1087	VAL	3.7
1	A	1128	GLU	3.7
2	D	84	SER	3.6
2	F	118	SER	3.6
1	A	1121	LEU	3.5
1	B	1023	GLY	3.4
1	A	1083	LYS	3.4
1	B	1114	PHE	3.4
2	D	9	GLY	3.4
1	B	1025	TYR	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	1088	TYR	3.3
1	A	29	ASP	3.2
1	B	1022	GLU	3.2
1	B	1027	ILE	3.2
2	D	85	LEU	3.2
1	B	1024	TYR	3.2
1	A	1123	GLN	3.2
1	B	1082	ALA	3.1
2	D	113	THR	3.1
1	B	296	HIS	3.1
2	D	15	GLY	2.9
2	D	120	HIS	2.9
2	D	118	SER	2.9
1	A	302	LEU	2.9
1	B	1019	LYS	2.9
1	B	179	GLN	2.8
2	F	119	SER	2.8
1	A	1120	MET	2.8
1	A	1122	GLN	2.8
1	A	1023	GLY	2.7
1	A	1136	SER	2.7
1	A	1091	LEU	2.7
2	D	11	LEU	2.6
1	B	229	GLN	2.6
1	A	1161	TYR	2.6
1	A	1153	PHE	2.6
1	B	31	VAL	2.6
1	B	186	ALA	2.6
1	B	302	LEU	2.5
2	D	114	GLN	2.5
1	A	301	ASN	2.5
1	B	1021	THR	2.5
1	A	1098	ALA	2.4
1	A	192	ASP	2.4
1	A	306	GLU	2.4
1	A	1132	ASN	2.4
2	D	14	ALA	2.4
1	A	305	LYS	2.4
1	A	1154	ARG	2.4
1	A	1114	PHE	2.4
1	B	1002	ASN	2.3
1	A	308	TYR	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	1088	TYR	2.3
2	D	86	LYS	2.3
1	A	1022	GLU	2.3
1	A	1093	ALA	2.3
1	A	1117	SER	2.3
1	B	1037	PRO	2.2
1	A	1099	LEU	2.2
1	A	1126	TRP	2.2
1	B	1055	ASN	2.2
1	B	1068	ASN	2.2
1	A	188	GLU	2.2
1	B	29	ASP	2.2
1	A	1157	THR	2.2
1	A	186	ALA	2.2
1	A	139	PHE	2.2
1	B	300	ASP	2.2
1	A	1085	LYS	2.1
1	A	133	PHE	2.1
1	B	125	CYS	2.1
1	A	1021	THR	2.1
1	B	1140	ASN	2.1
1	B	32	TRP	2.1
1	B	1017	ILE	2.1
2	D	8	GLY	2.1
2	D	41	PRO	2.1
1	A	1044	SER	2.1
1	B	1067	PHE	2.1
1	A	1111	VAL	2.1
1	A	1078	ILE	2.1
1	B	1015	LEU	2.1
2	D	21	SER	2.1
1	B	1035	LYS	2.1
1	A	32	TRP	2.1
1	A	298	ILE	2.1
1	A	1003	ILE	2.1
1	A	1137	ARG	2.1
1	B	177	THR	2.0
2	D	13	GLN	2.0

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

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](#)

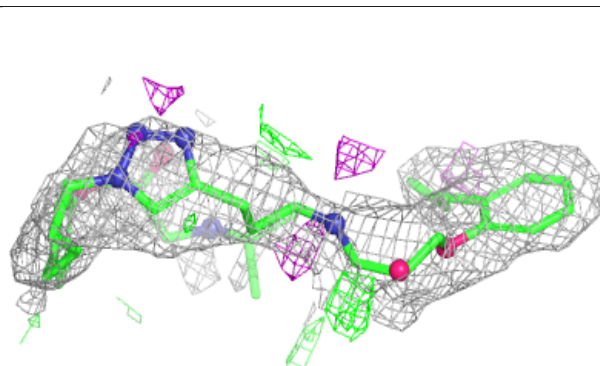
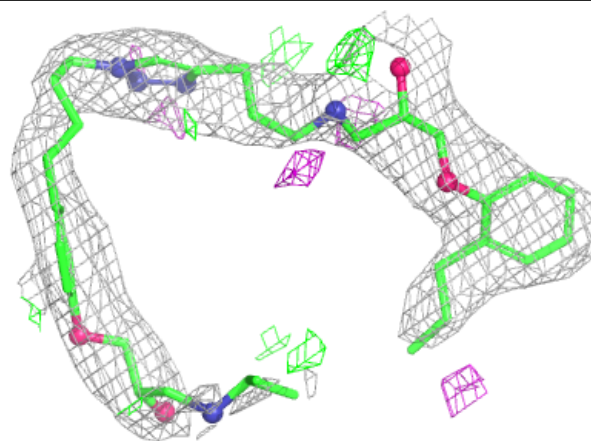
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	A1AE2	A	1201	42/42	0.83	0.22	39,62,86,89	0
3	A1AE2	B	1201	42/42	0.85	0.20	42,67,85,89	0
4	AV0	B	1202	69/69	0.86	0.15	37,54,77,88	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.

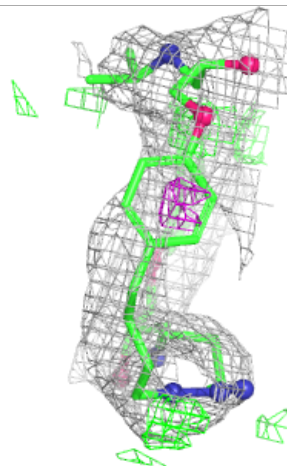
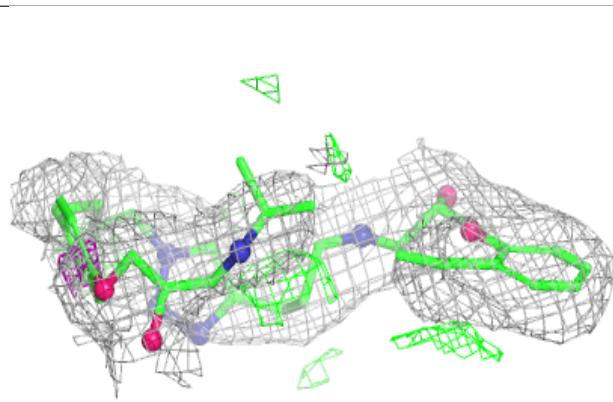
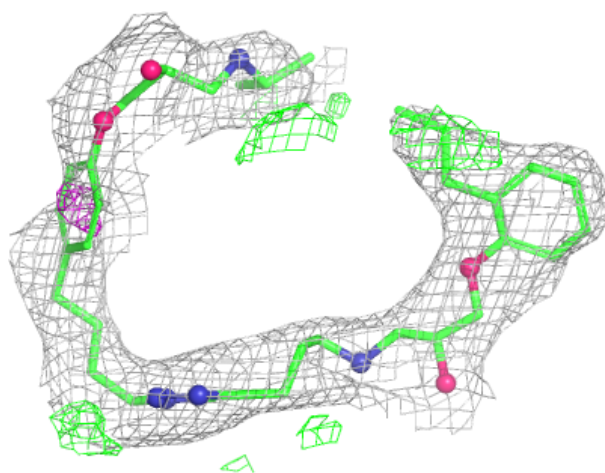
Electron density around A1AE2 A 1201:

2mF_o-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



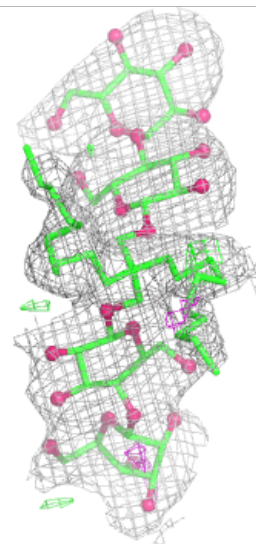
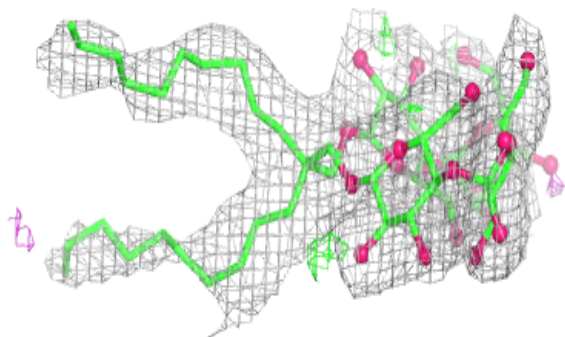
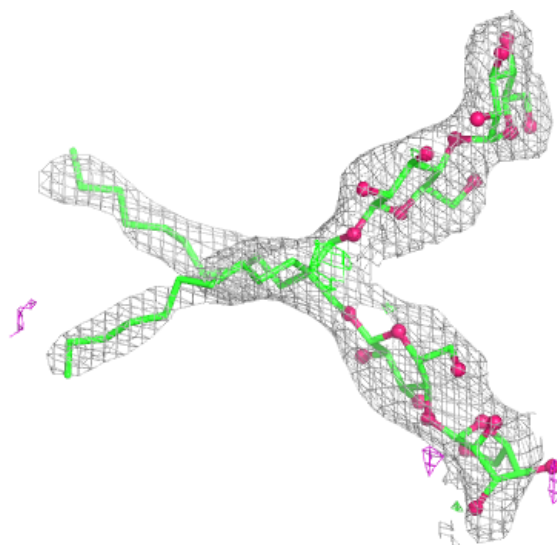
Electron density around A1AE2 B 1201:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around AV0 B 1202:

$2mF_o-DF_c$ (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.