



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 15, 2020 – 12:07 am BST

PDB ID : 3FF6
Title : Human ACC2 CT domain with CP-640186
Authors : Williams, S.P.; Madauss, K.P.; Burkhardt, W.A.
Deposited on : 2008-12-02
Resolution : 3.19 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 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 : 2.11
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) : 2.11

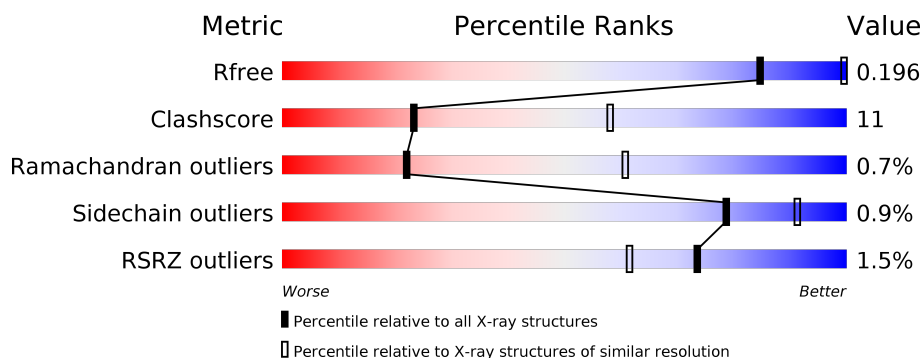
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.19 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	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on 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	760	<div> <div>2%</div> <div> <div></div> <div>78%</div> <div>20%</div> <div>..</div> </div> </div>
1	B	760	<div> <div>%</div> <div> <div></div> <div>75%</div> <div>23%</div> <div>.</div> </div> </div>
1	C	760	<div> <div>2%</div> <div> <div></div> <div>77%</div> <div>20%</div> <div>..</div> </div> </div>
1	D	760	<div> <div>%</div> <div> <div></div> <div>74%</div> <div>22%</div> <div>..</div> </div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 22989 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.

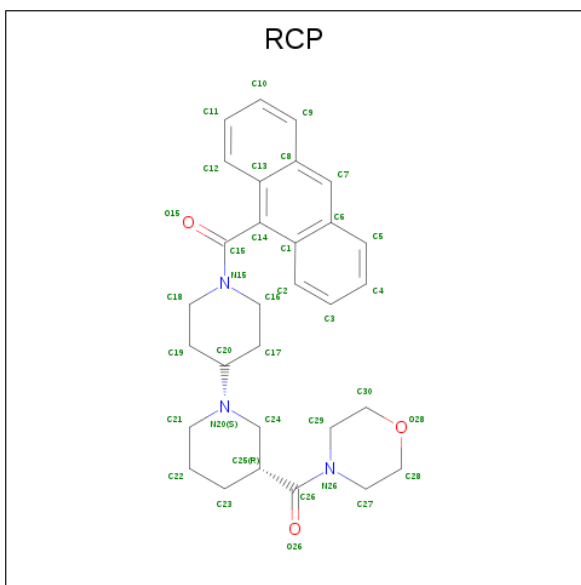
- Molecule 1 is a protein called Acetyl-CoA carboxylase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	750	Total	C	N	O	S	0	0	0
			5656	3628	961	1044	23			
1	B	748	Total	C	N	O	S	0	0	0
			5754	3684	988	1058	24			
1	C	742	Total	C	N	O	S	0	0	0
			5706	3650	980	1052	24			
1	D	733	Total	C	N	O	S	0	0	0
			5641	3615	965	1037	24			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1692	GLY	-	EXPRESSION TAG	UNP O00763
A	2451	GLU	-	EXPRESSION TAG	UNP O00763
B	1692	GLY	-	EXPRESSION TAG	UNP O00763
B	2451	GLU	-	EXPRESSION TAG	UNP O00763
C	1692	GLY	-	EXPRESSION TAG	UNP O00763
C	2451	GLU	-	EXPRESSION TAG	UNP O00763
D	1692	GLY	-	EXPRESSION TAG	UNP O00763
D	2451	GLU	-	EXPRESSION TAG	UNP O00763

- Molecule 2 is (3R)-1'-(9-ANTHRYLCARBONYL)-3-(MORPHOLIN-4-YLCARBONYL)-1, 4'-BIPIPERIDINE (three-letter code: RCP) (formula: C₃₀H₃₅N₃O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total 36	C 30	N 3	O 3	0	0
2	B	1	Total 36	C 30	N 3	O 3	0	0
2	C	1	Total 36	C 30	N 3	O 3	0	0
2	D	1	Total 36	C 30	N 3	O 3	0	0

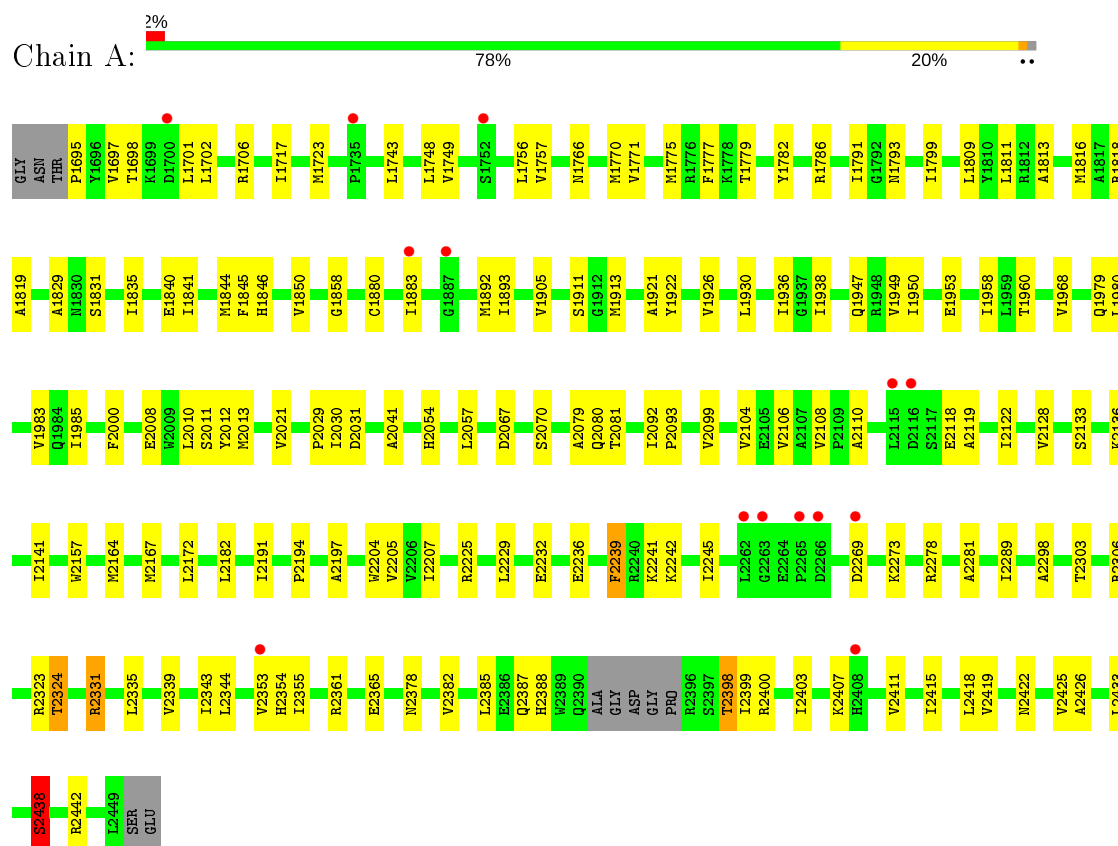
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	23	Total O 23 23	0	0
3	B	28	Total O 28 28	0	0
3	C	16	Total O 16 16	0	0
3	D	21	Total O 21 21	0	0

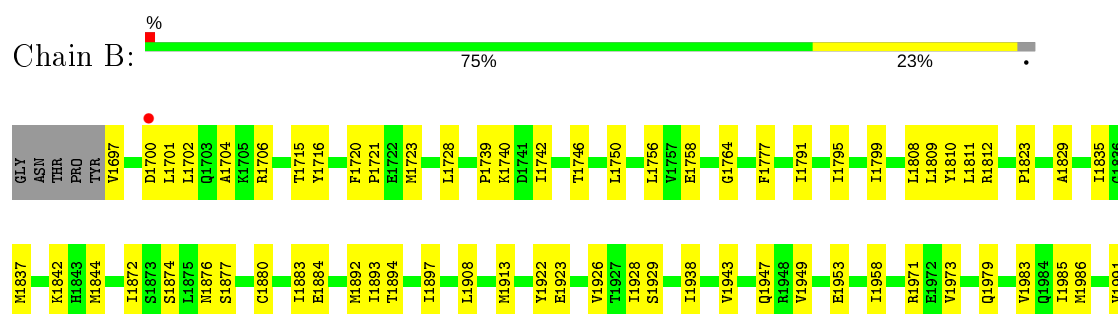
3 Residue-property plots [i](#)

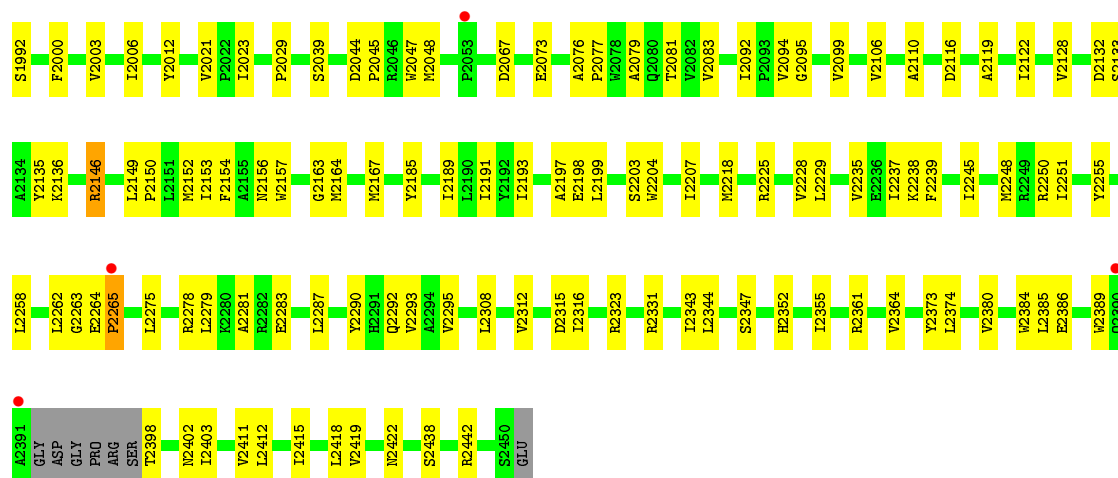
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

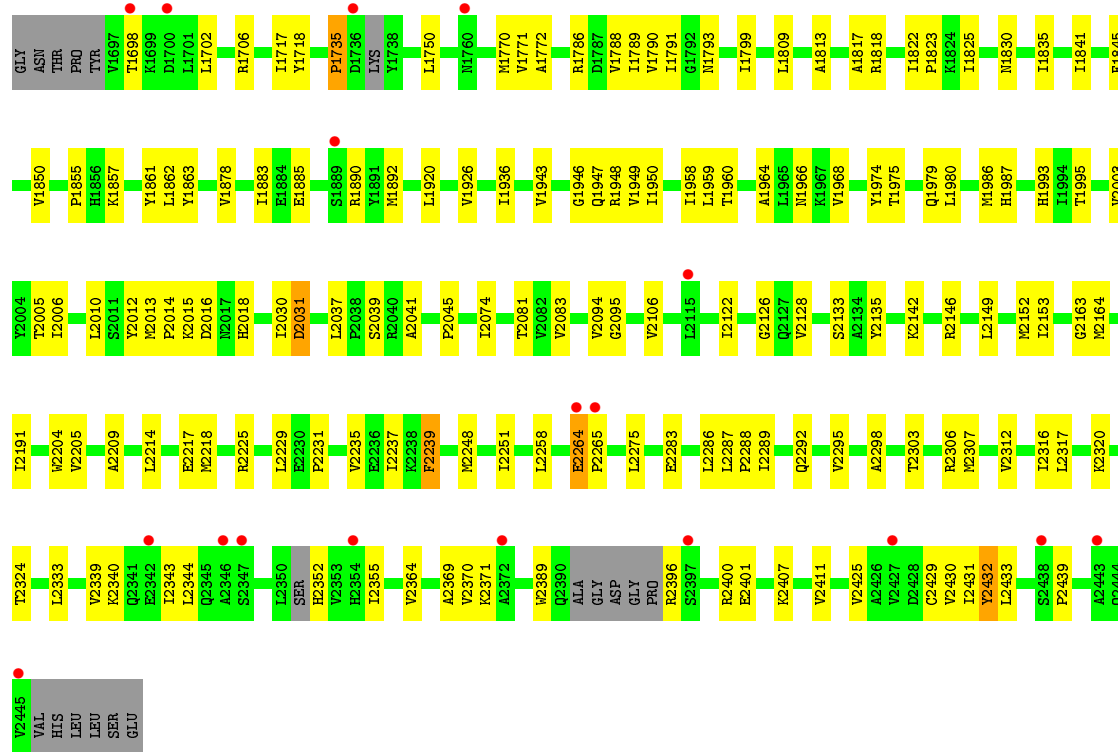
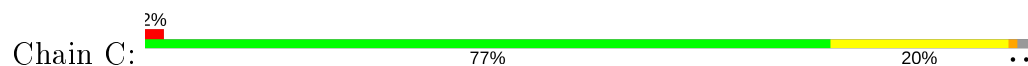


• Molecule 1: Acetyl-CoA carboxylase 2

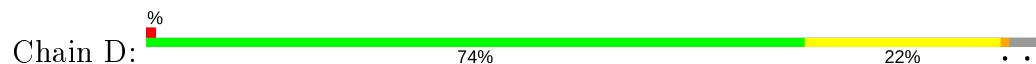




• Molecule 1: Acetyl-CoA carboxylase 2



• Molecule 1: Acetyl-CoA carboxylase 2



Q2390	L2287	L2133	T1975	I1872
A2391	P2288	S2133	L1980	L1875
ASP	I2289	R2146	H1987	I1876
GLY	Y2290	L2149	V1991	S1877
GLY	Q2291	P2150	S1992	I1883
R2396	V2292	L2151	F2000	R1890
S2397	A2293	M2152	V2003	M1891
	V2295	I2153	Y2004	M1892
K2407	T2303	A2155	T2005	I1893
V2411	R2306	F2160	I2006	I1897
R2416	V2312	G2163	Y2012	G1898
V2419	L2317	M2167	M2013	K1899
N2422	T2324	L2182	V2021	G1904
L2433	R2331	I2189	I2030	V1905
SER	R2332	L2190	P2042	E1906
GLN	L2333	I2191	M2048	I1907
HIS	Q2341	Y2192	L2049	L1908
ILE	E2342	I2193	E2073	I1914
SER	Q2345	E2198	A2076	S1918
PRO	A2346	L2199	P2077	Y1921
ALA	S2347	R2200	V2081	Y1922
ALA	G2348	M2204	V2082	V1926
GLN	E2349	I2207	V2083	V1931
VAL	L2350	E2217	R2088	I1938
VAL	S2351	M2218	I2092	L1942
HIS	H2352	Y2219	P2093	V1943
LEU	V2353	S2224	V2094	G1946
SER	I2354	V2228	G2095	Q1947
GLU	I2355	V2235	T2101	R1948
	Q2356	E2236	A2107	V1949
	S2357	I2237	A2110	I1950
	V2362	R2238	D2111	I1957
	T2366	F2239	P2112	I1958
	Y2373		D2116	L1959
	L2374		E2117	T1960
	W2375		E2118	G1961
	N2378		I2121	L1965
			V2128	L1969
			W2129	G1970
				R1971
				E1972
				V1973
				Y1974

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	81.55Å 168.84Å 293.35Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.19 20.00 – 3.19	Depositor EDS
% Data completeness (in resolution range)	95.7 (20.00-3.19) 94.5 (20.00-3.19)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.34 (at 3.22Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.197 , 0.251 0.205 , 0.196	Depositor DCC
R_{free} test set	4652 reflections (7.22%)	wwPDB-VP
Wilson B-factor (Å ²)	64.6	Xtriage
Anisotropy	0.122	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 60.8	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	0.92	EDS
Total number of atoms	22989	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.28% 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: RCP

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	0.41	1/5788 (0.0%)	0.54	1/7896 (0.0%)
1	B	0.39	0/5890	0.55	0/8012
1	C	0.38	0/5839	0.54	2/7949 (0.0%)
1	D	0.39	0/5775	0.53	0/7865
All	All	0.39	1/23292 (0.0%)	0.54	3/31722 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2438	SER	CB-OG	9.19	1.54	1.42

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	1735	PRO	N-CA-CB	6.16	110.69	103.30
1	A	1695	PRO	N-CA-CB	5.34	109.70	103.30
1	C	2031	ASP	CB-CG-OD2	5.24	123.01	118.30

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	5656	0	5369	141	0
1	B	5754	0	5528	146	0
1	C	5706	0	5470	138	0
1	D	5641	0	5414	145	0
2	A	36	0	35	3	0
2	B	36	0	35	2	0
2	C	36	0	35	1	0
2	D	36	0	35	1	0
3	A	23	0	0	0	0
3	B	28	0	0	0	0
3	C	16	0	0	0	0
3	D	21	0	0	1	0
All	All	22989	0	21921	505	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 11.

All (505) 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:D:2030:ILE:O	1:D:2324:THR:HG22	1.43	1.18
1:B:1723:MET:CE	1:B:2000:PHE:HA	1.89	1.02
1:A:2343:ILE:HG22	1:A:2403:ILE:HG21	1.38	1.02
1:A:1723:MET:CE	1:A:2000:PHE:HA	1.94	0.97
1:A:2191:ILE:HD13	1:A:2207:ILE:HG22	1.48	0.96
1:D:1723:MET:HE3	1:D:2000:PHE:HA	1.47	0.94
1:D:1883:ILE:HD12	1:D:1892:MET:HE3	1.48	0.94
1:A:2343:ILE:CG2	1:A:2403:ILE:HG21	1.97	0.93
1:B:1883:ILE:HD12	1:B:1892:MET:HE3	1.46	0.93
1:A:1723:MET:HE3	1:A:2000:PHE:HA	1.51	0.92
1:C:2030:ILE:O	1:C:2324:THR:HG22	1.70	0.91
1:B:2308:LEU:HD12	1:B:2316:ILE:HG23	1.52	0.90
1:C:2010:LEU:HD23	1:C:2013:MET:CE	2.01	0.90
1:C:2344:LEU:HD23	1:C:2355:ILE:HG23	1.54	0.89
1:A:1791:ILE:CD1	1:A:1813:ALA:HB1	2.03	0.89
1:C:2344:LEU:CD2	1:C:2355:ILE:HG23	2.02	0.89
1:A:1791:ILE:HD11	1:A:1813:ALA:HB1	1.53	0.89
1:C:2214:LEU:HD21	1:C:2352:HIS:NE2	1.87	0.88
1:C:1841:ILE:HD12	1:C:1878:VAL:HG21	1.54	0.88
1:A:2164:MET:HE3	1:B:1979:GLN:O	1.74	0.87
1:C:2153:ILE:HD12	1:C:2191:ILE:CD1	2.04	0.87
1:C:1772:ALA:HB1	1:C:1791:ILE:HG22	1.57	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2153:ILE:HD12	1:C:2191:ILE:HD13	1.59	0.84
1:A:2191:ILE:HD13	1:A:2207:ILE:CG2	2.08	0.84
1:C:1835:ILE:HG22	1:D:2228:VAL:HG11	1.61	0.83
1:A:2343:ILE:HG21	1:A:2403:ILE:HD13	1.59	0.82
1:A:2030:ILE:O	1:A:2324:THR:HG22	1.79	0.81
1:D:1883:ILE:HD12	1:D:1892:MET:CE	2.09	0.81
1:C:2010:LEU:HD23	1:C:2013:MET:HE3	1.59	0.81
1:A:2344:LEU:HD23	1:A:2355:ILE:HG23	1.63	0.80
1:A:2164:MET:HE3	1:B:1985:ILE:HD11	1.62	0.80
1:B:1701:LEU:HD21	1:B:1764:GLY:HA3	1.62	0.80
1:D:2081:THR:HG21	1:D:2128:VAL:O	1.80	0.80
1:A:1835:ILE:HG22	1:B:2228:VAL:HG11	1.65	0.79
1:B:2081:THR:HG21	1:B:2128:VAL:O	1.82	0.79
1:A:2343:ILE:CG2	1:A:2403:ILE:HD13	2.13	0.78
1:C:2094:VAL:HG21	1:C:2152:MET:HG3	1.64	0.78
1:C:1772:ALA:CB	1:C:1791:ILE:HG22	2.15	0.77
1:C:1788:VAL:HG21	1:C:1825:ILE:HD13	1.66	0.77
1:D:2351:SER:CB	1:D:2354:HIS:HB2	2.16	0.76
1:C:2214:LEU:HD21	1:C:2352:HIS:CE1	2.21	0.75
1:B:2067:ASP:OD1	1:B:2323:ARG:NH2	2.19	0.75
1:C:2010:LEU:HA	1:C:2013:MET:HE2	1.70	0.74
1:C:2214:LEU:HD21	1:C:2352:HIS:HE2	1.51	0.74
1:B:2263:GLY:C	1:B:2265:PRO:HD3	2.08	0.74
1:A:2081:THR:HG21	1:A:2128:VAL:O	1.87	0.73
1:B:2153:ILE:HD12	1:B:2191:ILE:CD1	2.18	0.73
1:C:1791:ILE:HG21	1:C:1813:ALA:HB1	1.71	0.73
1:C:2258:LEU:HD22	1:C:2275:LEU:HD22	1.70	0.73
1:C:2163:GLY:HA2	1:D:1980:LEU:HD22	1.70	0.73
1:C:2312:VAL:HG21	1:D:1905:VAL:HG12	1.69	0.73
1:D:1926:VAL:HG21	1:D:2013:MET:HE2	1.72	0.72
1:C:1862:LEU:HD21	1:D:2293:VAL:HG23	1.72	0.72
1:D:1723:MET:CE	1:D:2000:PHE:HA	2.20	0.72
1:D:1931:VAL:HG21	1:D:1957:ILE:HD11	1.70	0.72
1:B:1723:MET:HE3	1:B:2000:PHE:HA	1.70	0.72
1:C:1788:VAL:CG2	1:C:1825:ILE:HD13	2.20	0.71
1:C:1789:ILE:HD12	1:C:1817:ALA:HB2	1.72	0.71
1:A:2029:PRO:O	1:A:2323:ARG:NH1	2.23	0.71
1:B:2283:GLU:O	1:B:2287:LEU:HD13	1.88	0.71
1:A:2343:ILE:HG22	1:A:2403:ILE:CG2	2.19	0.71
1:A:1723:MET:HE3	1:A:2000:PHE:CA	2.21	0.71
1:A:2010:LEU:HA	1:A:2013:MET:HE2	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1926:VAL:CG2	1:D:2013:MET:HE2	2.20	0.70
1:A:2422:ASN:ND2	1:B:2411:VAL:HG21	2.06	0.70
1:A:2164:MET:CE	1:B:1985:ILE:HD11	2.22	0.70
1:B:2229:LEU:HD11	1:B:2237:ILE:HD12	1.73	0.69
1:C:2081:THR:HG21	1:C:2128:VAL:O	1.91	0.69
1:B:2248:MET:HE1	1:B:2283:GLU:HB2	1.74	0.69
1:D:2362:TRP:O	1:D:2366:THR:HG23	1.93	0.68
1:B:2116:ASP:OD2	1:C:2041:ALA:HB2	1.93	0.68
1:D:2110:ALA:HB2	1:D:2118:GLU:HA	1.75	0.68
1:A:2335:LEU:HB3	1:A:2385:LEU:HD13	1.75	0.68
1:A:1702:LEU:HD21	1:A:1706:ARG:NH2	2.09	0.67
1:B:1723:MET:HE3	1:B:2000:PHE:CA	2.23	0.67
1:A:1883:ILE:CD1	1:A:1892:MET:HE3	2.25	0.67
1:B:1823:PRO:HB3	1:B:1926:VAL:HG13	1.77	0.67
1:C:1966:ASN:HD21	1:C:1974:TYR:H	1.41	0.67
1:D:2235:VAL:HG13	1:D:2239:PHE:HB3	1.76	0.66
1:A:1880:CYS:HB3	1:A:1893:ILE:HA	1.77	0.66
1:D:1949:VAL:HG11	1:D:1991:VAL:O	1.94	0.66
1:A:2289:ILE:HD12	1:D:1975:THR:HG21	1.77	0.66
1:B:2106:VAL:HG13	1:B:2122:ILE:HB	1.78	0.66
1:A:2080:GLN:HB2	1:A:2104:VAL:HG11	1.77	0.66
1:A:2010:LEU:HD23	1:A:2013:MET:HE3	1.77	0.66
1:D:2218:MET:HE3	1:D:2312:VAL:O	1.96	0.66
1:A:1926:VAL:HG11	1:A:2013:MET:HE1	1.77	0.65
1:B:1791:ILE:HD11	1:B:1810:TYR:HA	1.78	0.65
1:B:2153:ILE:HD12	1:B:2191:ILE:HD12	1.78	0.65
1:A:2344:LEU:CD2	1:A:2355:ILE:HG23	2.26	0.65
1:B:2094:VAL:HG21	1:B:2152:MET:HG3	1.78	0.65
1:C:2344:LEU:HD21	1:C:2355:ILE:HG23	1.79	0.65
1:C:2106:VAL:HG13	1:C:2122:ILE:HB	1.78	0.64
1:A:1791:ILE:HD12	1:A:1813:ALA:CB	2.27	0.64
1:A:2010:LEU:HD23	1:A:2013:MET:CE	2.28	0.64
1:B:1883:ILE:HD12	1:B:1892:MET:CE	2.26	0.64
1:C:1835:ILE:HD11	1:D:2237:ILE:HG21	1.80	0.63
1:C:1980:LEU:HD22	1:D:2163:GLY:HA2	1.80	0.63
1:B:2203:SER:O	1:B:2207:ILE:HG22	1.98	0.63
1:C:2396:ARG:HA	1:C:2400:ARG:CB	2.29	0.62
1:D:1949:VAL:CG1	1:D:1991:VAL:O	2.47	0.62
1:C:1790:VAL:HG22	1:C:1825:ILE:HB	1.80	0.62
1:A:1791:ILE:CD1	1:A:1813:ALA:CB	2.76	0.62
1:B:2343:ILE:HG22	1:B:2403:ILE:HD13	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1841:ILE:HD12	1:C:1878:VAL:CG2	2.26	0.62
1:A:1723:MET:HE1	1:A:2000:PHE:HA	1.82	0.61
1:A:2099:VAL:HG22	1:A:2157:TRP:CE2	2.36	0.61
1:C:2433:LEU:HD22	1:D:2419:VAL:HG21	1.81	0.61
1:B:2331:ARG:NH2	1:B:2386:GLU:OE2	2.34	0.61
1:C:2081:THR:HB	1:C:2133:SER:OG	2.00	0.61
1:A:1883:ILE:HD12	1:A:1892:MET:HE3	1.81	0.61
1:D:1914:ILE:HD12	1:D:1942:LEU:HD11	1.83	0.61
1:A:1926:VAL:HG11	1:A:2013:MET:CE	2.31	0.61
1:A:1845:PHE:O	1:B:2250:ARG:NH2	2.33	0.61
1:C:2003:VAL:HA	1:C:2006:ILE:HD12	1.82	0.61
1:D:2388:HIS:O	1:D:2397:SER:HA	2.00	0.60
1:B:1953:GLU:HA	1:B:1983:VAL:HG21	1.82	0.60
1:C:1926:VAL:HG21	1:C:2013:MET:CE	2.31	0.60
1:A:2419:VAL:HG13	1:A:2426:ALA:HB2	1.83	0.60
1:A:1985:ILE:HD11	1:B:2164:MET:HG3	1.83	0.60
1:C:2225:ARG:HH12	1:C:2303:THR:HG22	1.67	0.60
1:D:2153:ILE:HD12	1:D:2191:ILE:CD1	2.31	0.60
1:B:1876:ASN:O	1:B:1876:ASN:CG	2.39	0.60
1:B:1728:LEU:HD11	1:B:1777:PHE:CB	2.31	0.60
1:C:2225:ARG:NH1	1:C:2303:THR:HG22	2.16	0.60
1:D:2081:THR:HB	1:D:2133:SER:OG	2.02	0.60
1:B:1723:MET:CE	1:B:2000:PHE:CA	2.72	0.60
1:A:1979:GLN:O	1:B:2164:MET:HE3	2.02	0.59
1:D:2182:LEU:HD22	1:D:2189:ILE:HD13	1.85	0.59
1:A:2411:VAL:HG13	1:B:2418:LEU:HD13	1.83	0.59
1:B:2290:TYR:O	1:B:2293:VAL:HG12	2.02	0.59
1:C:2286:LEU:HD21	1:D:1855:PRO:HG2	1.84	0.59
1:C:2343:ILE:HD13	1:C:2389:TRP:CE2	2.38	0.59
1:B:1949:VAL:HG13	1:B:1992:SER:HA	1.84	0.59
1:B:1811:LEU:HD22	1:B:1913:MET:SD	2.43	0.59
1:B:2343:ILE:HG22	1:B:2403:ILE:CD1	2.32	0.59
1:D:2378:ASN:O	1:D:2382:VAL:HG23	2.02	0.59
1:A:1779:THR:HG23	1:A:1782:TYR:H	1.68	0.59
1:C:1789:ILE:HG13	1:C:1822:ILE:HD11	1.84	0.59
1:B:2081:THR:HB	1:B:2133:SER:OG	2.02	0.58
1:A:1850:VAL:HG12	1:A:1858:GLY:O	2.03	0.58
1:C:1786:ARG:HB2	1:C:2015:LYS:HG3	1.85	0.58
1:A:2041:ALA:HB2	1:D:2116:ASP:OD2	2.03	0.58
1:C:2235:VAL:HG13	1:C:2239:PHE:HB3	1.85	0.58
1:D:2073:GLU:OE2	1:D:2083:VAL:HG13	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2433:LEU:CD2	1:D:2419:VAL:HG21	2.34	0.58
1:A:1717:ILE:HG12	1:A:1771:VAL:HG22	1.86	0.58
1:D:2048:MET:HE3	1:D:2049:LEU:HD12	1.85	0.57
1:A:1958:ILE:HA	1:B:2167:MET:HE2	1.85	0.57
1:C:1791:ILE:HG21	1:C:1813:ALA:CB	2.34	0.57
1:A:1953:GLU:HA	1:A:1983:VAL:HG21	1.87	0.57
1:C:1950:ILE:HD13	1:C:2005:THR:HB	1.85	0.57
1:C:2343:ILE:HD13	1:C:2389:TRP:CZ2	2.39	0.57
1:A:1841:ILE:HD13	1:A:1844:MET:SD	2.44	0.57
1:C:1698:THR:HA	1:C:1702:LEU:HB3	1.87	0.56
1:A:2388:HIS:CB	1:A:2399:ILE:CG2	2.84	0.56
1:B:1728:LEU:HD11	1:B:1777:PHE:HB2	1.87	0.56
1:C:1946:GLY:O	1:C:1948:ARG:N	2.37	0.56
1:A:2344:LEU:HD23	1:A:2355:ILE:CG2	2.36	0.56
1:A:2204:TRP:CB	1:B:1908:LEU:HD13	2.36	0.56
1:B:2116:ASP:CG	1:C:2041:ALA:HB2	2.25	0.56
1:C:2235:VAL:HG21	1:C:2295:VAL:HG12	1.86	0.55
1:D:2355:ILE:HG22	1:D:2356:GLN:N	2.21	0.55
1:C:1855:PRO:HB2	1:D:2289:ILE:HD11	1.88	0.55
1:A:2081:THR:CG2	1:A:2128:VAL:O	2.54	0.55
1:B:2343:ILE:CG2	1:B:2403:ILE:HD12	2.37	0.55
1:A:2387:GLN:HE21	1:A:2398:THR:HG21	1.72	0.55
1:A:2422:ASN:HD22	1:B:2411:VAL:HG21	1.70	0.55
1:C:1986:MET:HE1	1:D:2167:MET:CE	2.37	0.54
1:C:1835:ILE:CG2	1:D:2228:VAL:HG11	2.36	0.54
1:D:2303:THR:HG23	1:D:2306:ARG:H	1.71	0.54
1:C:2106:VAL:CG1	1:C:2122:ILE:HB	2.37	0.54
1:C:2340:LYS:HG3	1:C:2355:ILE:HG22	1.90	0.54
1:D:1750:LEU:HD23	1:D:1756:LEU:HD23	1.89	0.54
1:D:2107:ALA:HA	1:D:2121:ILE:HG22	1.90	0.54
1:A:1947:GLN:O	1:A:1949:VAL:HG23	2.08	0.54
1:B:2343:ILE:HG21	1:B:2403:ILE:HD12	1.89	0.54
1:A:2204:TRP:HB3	1:B:1908:LEU:HD13	1.90	0.54
1:B:1723:MET:HE3	1:B:2000:PHE:N	2.23	0.54
1:B:2343:ILE:HG13	1:B:2389:TRP:CZ2	2.43	0.53
1:A:2415:ILE:HG23	1:B:2415:ILE:HD12	1.91	0.53
1:D:2218:MET:CE	1:D:2312:VAL:O	2.56	0.53
1:C:2411:VAL:HG21	1:D:2422:ASN:ND2	2.23	0.53
1:A:1818:ARG:HD3	1:A:1921:ALA:HA	1.89	0.53
1:A:1846:HIS:HA	1:B:2251:ILE:HD11	1.89	0.53
1:C:1883:ILE:HG21	1:C:1892:MET:HB2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2364:VAL:HG13	1:C:2369:ALA:HA	1.89	0.53
1:B:1823:PRO:CB	1:B:1926:VAL:HG13	2.39	0.53
1:B:1715:THR:HG22	1:B:1716:TYR:O	2.08	0.53
1:A:2418:LEU:O	1:A:2422:ASN:N	2.37	0.53
1:B:1697:VAL:O	1:B:1701:LEU:N	2.42	0.53
1:C:2204:TRP:HB3	1:D:1908:LEU:HD13	1.91	0.53
1:C:2312:VAL:HG21	1:D:1905:VAL:CG1	2.36	0.53
1:A:2278:ARG:O	1:A:2281:ALA:HB3	2.09	0.52
1:C:1823:PRO:HB3	1:C:1926:VAL:HG13	1.91	0.52
1:B:1880:CYS:HB3	1:B:1893:ILE:HA	1.90	0.52
1:A:1960:THR:HG21	2:B:2:RCP:H171	1.90	0.52
1:D:2353:VAL:HG23	1:D:2354:HIS:CD2	2.44	0.52
1:A:2415:ILE:HG12	1:B:2415:ILE:HD13	1.91	0.52
1:B:1884:GLU:OE1	1:B:1884:GLU:N	2.42	0.52
1:C:2030:ILE:C	1:C:2030:ILE:HD12	2.30	0.52
1:A:1883:ILE:HD13	1:A:1892:MET:HE3	1.91	0.52
1:A:2081:THR:HB	1:A:2133:SER:OG	2.09	0.52
1:B:1746:THR:HG21	1:B:1758:GLU:OE1	2.10	0.52
1:C:1770:MET:HG2	1:C:1793:ASN:HA	1.92	0.52
1:D:1973:VAL:HG12	1:D:2112:PRO:HB2	1.92	0.52
1:A:1793:ASN:HD22	1:A:1829:ALA:H	1.57	0.52
1:C:2407:LYS:O	1:C:2411:VAL:HG23	2.10	0.52
1:B:2229:LEU:CD1	1:B:2237:ILE:HD12	2.39	0.51
1:D:1723:MET:HE3	1:D:2000:PHE:CA	2.29	0.51
1:B:2079:ALA:HB2	1:B:2132:ASP:HB2	1.92	0.51
1:B:2343:ILE:HG13	1:B:2389:TRP:HZ2	1.74	0.51
1:B:1971:ARG:NH1	1:B:1973:VAL:HG22	2.26	0.51
1:B:1723:MET:HE1	1:B:2000:PHE:HA	1.86	0.51
1:D:2347:SER:HB2	1:D:2407:LYS:HA	1.91	0.51
1:D:1947:GLN:O	1:D:1949:VAL:HG12	2.10	0.51
1:D:2262:LEU:CD1	1:D:2279:LEU:HD22	2.40	0.51
1:D:2353:VAL:O	1:D:2357:SER:CB	2.59	0.51
1:A:2232:GLU:HG2	2:A:1:RCP:C4	2.41	0.51
1:B:1723:MET:HE2	1:B:2000:PHE:HA	1.88	0.51
1:B:2248:MET:HE1	1:B:2283:GLU:CB	2.39	0.51
1:D:2110:ALA:CB	1:D:2118:GLU:HA	2.41	0.51
1:A:2194:PRO:HD2	1:A:2197:ALA:CB	2.41	0.51
1:A:1791:ILE:HD12	1:A:1813:ALA:HB1	1.81	0.51
1:A:2012:TYR:OH	1:A:2070:SER:O	2.24	0.51
1:C:2264:GLU:CB	1:C:2265:PRO:CD	2.88	0.51
1:A:1831:SER:HA	1:A:1936:ILE:HD12	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1861:TYR:OH	1:C:1885:GLU:CB	2.59	0.51
1:D:2076:ALA:HB3	1:D:2077:PRO:HD3	1.91	0.51
1:A:2099:VAL:HG22	1:A:2157:TRP:CZ2	2.46	0.50
1:B:1883:ILE:CD1	1:B:1892:MET:HE3	2.33	0.50
1:C:2411:VAL:HG21	1:D:2422:ASN:HD22	1.75	0.50
1:A:1980:LEU:HD22	1:B:2163:GLY:HA2	1.94	0.50
1:A:2099:VAL:CG2	1:A:2157:TRP:CE2	2.95	0.50
1:D:1965:LEU:O	1:D:1969:LEU:HG	2.11	0.50
1:A:2269:ASP:O	1:A:2273:LYS:CB	2.60	0.50
1:C:1788:VAL:HG23	1:C:1823:PRO:HB2	1.93	0.50
1:D:1872:ILE:HG23	1:D:1877:SER:HB2	1.93	0.50
1:B:2106:VAL:CG1	1:B:2122:ILE:HB	2.42	0.50
1:A:2021:VAL:HB	1:A:2093:PRO:HG2	1.92	0.50
1:A:1922:TYR:CE2	1:A:1947:GLN:HG3	2.47	0.50
1:A:2407:LYS:O	1:A:2411:VAL:HG23	2.12	0.50
1:B:2237:ILE:HG22	1:B:2238:LYS:HG2	1.93	0.50
1:C:1986:MET:CE	1:D:2167:MET:HE3	2.42	0.50
1:B:1928:ILE:HG22	1:B:1929:SER:N	2.27	0.49
1:B:2398:THR:CB	1:B:2402:ASN:CB	2.90	0.49
1:C:2248:MET:HE1	1:C:2283:GLU:HA	1.94	0.49
1:C:2352:HIS:C	1:C:2352:HIS:ND1	2.65	0.49
1:B:2384:TRP:CE3	1:B:2385:LEU:HD23	2.47	0.49
1:D:2292:GLN:O	1:D:2295:VAL:HG22	2.11	0.49
1:B:2029:PRO:O	1:B:2323:ARG:NH1	2.46	0.49
1:D:1946:GLY:O	1:D:1948:ARG:N	2.46	0.49
1:B:1791:ILE:CD1	1:B:1810:TYR:HA	2.43	0.49
1:B:1949:VAL:CG1	1:B:1991:VAL:O	2.60	0.49
1:B:2207:ILE:HG12	1:B:2207:ILE:O	2.13	0.49
1:D:2353:VAL:O	1:D:2357:SER:HB3	2.13	0.49
1:A:2067:ASP:OD1	1:A:2323:ARG:NH2	2.46	0.49
1:A:2205:VAL:HG11	1:B:1938:ILE:HD13	1.94	0.49
1:B:2343:ILE:CG2	1:B:2403:ILE:CD1	2.89	0.49
1:C:2283:GLU:O	1:C:2287:LEU:HB2	2.13	0.49
1:B:2218:MET:HE3	1:B:2312:VAL:O	2.13	0.49
1:B:2094:VAL:HG22	1:B:2095:GLY:O	2.13	0.49
1:A:2030:ILE:HD12	1:A:2031:ASP:N	2.28	0.48
1:C:1943:VAL:HG13	1:C:1949:VAL:HG22	1.94	0.48
1:C:2370:VAL:HG23	1:C:2371:LYS:HD3	1.95	0.48
1:C:2251:ILE:HD13	1:D:1847:VAL:HG23	1.95	0.48
1:A:1770:MET:CE	1:A:1791:ILE:HG22	2.43	0.48
1:B:1700:ASP:O	1:B:1704:ALA:HB3	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1850:VAL:CG1	1:C:1857:LYS:CB	2.91	0.48
1:C:2340:LYS:CG	1:C:2355:ILE:HG22	2.42	0.48
1:A:1779:THR:HG21	1:A:1786:ARG:HD2	1.94	0.48
1:A:2388:HIS:CB	1:A:2399:ILE:HG22	2.44	0.48
1:B:2374:LEU:HD23	1:B:2380:VAL:HG21	1.96	0.48
1:B:2199:LEU:HD23	1:B:2204:TRP:CE3	2.48	0.48
1:C:1750:LEU:HG	1:C:1809:LEU:HD12	1.96	0.48
1:B:1756:LEU:HG	1:B:1812:ARG:HB3	1.96	0.48
1:C:2307:MET:HG2	1:D:1905:VAL:HG11	1.94	0.48
1:C:2298:ALA:HA	1:D:1837:MET:CE	2.44	0.48
1:A:1697:VAL:O	1:A:1701:LEU:N	2.46	0.48
1:A:1930:LEU:HD12	1:A:1950:ILE:O	2.14	0.48
1:A:2079:ALA:HB3	1:A:2136:LYS:HD3	1.96	0.48
1:B:1750:LEU:HD13	1:B:1808:LEU:HD23	1.95	0.48
1:C:2292:GLN:O	1:C:2295:VAL:HG22	2.13	0.48
1:D:2217:GLU:OE2	1:D:2333:LEU:HD11	2.14	0.48
1:B:2258:LEU:HB2	1:B:2279:LEU:HD13	1.95	0.47
1:C:1823:PRO:CB	1:C:1926:VAL:HG13	2.44	0.47
1:C:2339:VAL:HA	1:C:2343:ILE:HD12	1.96	0.47
1:B:2099:VAL:HG22	1:B:2157:TRP:CE2	2.49	0.47
1:D:1757:VAL:HG23	1:D:1759:MET:CE	2.44	0.47
1:A:2194:PRO:HD2	1:A:2197:ALA:HB3	1.97	0.47
1:B:1702:LEU:HD21	1:B:1706:ARG:NH2	2.29	0.47
1:B:1795:ILE:HD13	1:B:1829:ALA:HB1	1.95	0.47
1:D:2155:ALA:HB1	1:D:2199:LEU:HD13	1.96	0.47
1:D:1707:PHE:O	1:D:1711:THR:HG23	2.15	0.47
1:D:2199:LEU:HD23	1:D:2204:TRP:CE3	2.49	0.47
1:D:2290:TYR:HA	1:D:2293:VAL:HG12	1.95	0.47
1:B:2021:VAL:HG11	1:B:2150:PRO:HD3	1.96	0.47
1:C:1964:ALA:O	1:C:1968:VAL:HG13	2.14	0.47
1:C:2229:LEU:HD11	1:C:2237:ILE:HD12	1.95	0.47
1:A:1717:ILE:CG1	1:A:1771:VAL:HG22	2.45	0.47
1:C:1862:LEU:HD21	1:D:2293:VAL:CG2	2.43	0.47
1:D:1950:ILE:HD13	1:D:2005:THR:HB	1.97	0.47
1:C:1926:VAL:HG21	1:C:2013:MET:HE1	1.96	0.47
1:C:1835:ILE:HG22	1:D:2228:VAL:CG1	2.40	0.47
1:D:2193:ILE:CG2	1:D:2224:SER:HB2	2.45	0.47
1:A:2411:VAL:HG21	1:B:2422:ASN:HD22	1.80	0.47
1:A:1905:VAL:HG11	1:B:2312:VAL:HG21	1.97	0.47
1:C:2264:GLU:CB	1:C:2265:PRO:HD3	2.45	0.47
1:B:2373:TYR:CZ	1:B:2374:LEU:HD11	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2030:ILE:HD12	1:A:2030:ILE:C	2.35	0.46
1:B:2344:LEU:HD23	1:B:2355:ILE:HG12	1.96	0.46
1:C:1717:ILE:HG12	1:C:1771:VAL:HG22	1.97	0.46
1:D:2384:TRP:CD1	1:D:2388:HIS:CE1	3.03	0.46
1:C:1770:MET:O	1:C:1809:LEU:HD22	2.15	0.46
1:D:2332:ARG:HH21	1:D:2381:VAL:HG21	1.80	0.46
1:A:2378:ASN:O	1:A:2382:VAL:HG23	2.16	0.46
1:B:1922:TYR:CE2	1:B:1947:GLN:HG3	2.50	0.46
1:D:1743:LEU:HD13	1:D:1777:PHE:HB3	1.97	0.46
1:C:1986:MET:HE1	1:D:2167:MET:HE3	1.97	0.46
1:C:2248:MET:HE1	1:C:2283:GLU:HG3	1.97	0.46
1:B:1756:LEU:HD21	1:B:1809:LEU:HD12	1.98	0.46
1:C:2037:LEU:HD21	1:C:2320:LYS:HD3	1.98	0.46
1:A:2339:VAL:CG1	1:A:2399:ILE:HD11	2.45	0.46
1:D:2012:TYR:O	1:D:2149:LEU:HD21	2.16	0.46
1:D:2021:VAL:HG11	1:D:2150:PRO:HD3	1.97	0.46
1:B:2193:ILE:HG22	1:B:2197:ALA:HB3	1.98	0.46
1:C:2163:GLY:O	1:C:2164:MET:C	2.54	0.46
1:C:2209:ALA:H	1:C:2218:MET:HE2	1.81	0.46
1:C:2396:ARG:O	1:C:2401:GLU:N	2.48	0.46
1:D:1875:LEU:HD13	1:D:1899:LYS:HD3	1.97	0.46
1:A:2415:ILE:HG23	1:B:2415:ILE:CD1	2.45	0.45
1:B:2045:PRO:O	1:B:2048:MET:HG2	2.16	0.45
1:D:2345:GLN:HE22	1:D:2349:GLU:CA	2.29	0.45
1:A:2399:ILE:HG23	1:A:2400:ARG:N	2.31	0.45
1:C:2030:ILE:HD11	1:C:2031:ASP:OD1	2.16	0.45
1:C:2231:PRO:O	1:C:2235:VAL:HG23	2.16	0.45
1:A:2106:VAL:HG13	1:A:2122:ILE:HB	1.98	0.45
1:D:2290:TYR:O	1:D:2293:VAL:HG12	2.16	0.45
1:A:2232:GLU:HG2	2:A:1:RCP:C5	2.46	0.45
1:A:2236:GLU:HG2	2:A:1:RCP:H9	1.97	0.45
1:A:2353:VAL:HG13	1:A:2354:HIS:N	2.31	0.45
1:B:2076:ALA:HB3	1:B:2077:PRO:HD3	1.98	0.45
1:C:1835:ILE:HD11	1:D:2237:ILE:CG2	2.45	0.45
1:D:2048:MET:CE	1:D:2049:LEU:HD12	2.47	0.45
1:A:2241:LYS:O	1:A:2245:ILE:HG23	2.16	0.45
1:A:2092:ILE:HD11	1:A:2331:ARG:HG3	1.97	0.45
1:B:2099:VAL:HG11	1:B:2156:ASN:O	2.17	0.45
1:C:1993:HIS:HD2	1:C:2074:ILE:HD12	1.82	0.45
1:D:1883:ILE:HG23	1:D:1890:ARG:HB2	1.99	0.45
1:D:2198:GLU:OE1	1:D:2200:ARG:NH1	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2167:MET:HE2	1:B:1958:ILE:HA	1.99	0.45
1:C:1936:ILE:HG23	1:C:1958:ILE:HG13	1.99	0.45
1:A:2225:ARG:NH1	1:A:2303:THR:HG22	2.32	0.45
1:D:2191:ILE:HG21	1:D:2207:ILE:HD11	1.97	0.45
1:D:2345:GLN:HE22	1:D:2349:GLU:C	2.21	0.45
1:A:2008:GLU:O	1:A:2011:SER:HB3	2.17	0.45
1:D:2191:ILE:HG21	1:D:2207:ILE:CD1	2.46	0.45
1:B:1872:ILE:HG23	1:B:1877:SER:HB3	1.99	0.44
1:B:2262:LEU:HD21	1:B:2275:LEU:HB2	2.00	0.44
1:B:2292:GLN:O	1:B:2295:VAL:HG22	2.17	0.44
1:C:1786:ARG:CB	1:C:2015:LYS:HG3	2.47	0.44
1:D:2332:ARG:NH2	1:D:2375:TRP:O	2.50	0.44
1:C:2432:TYR:HE2	1:D:2416:ARG:CB	2.31	0.44
1:A:2239:PHE:CD1	1:B:1842:LYS:HE3	2.53	0.44
1:B:1844:MET:HB2	1:B:1844:MET:HE3	1.85	0.44
1:A:1766:ASN:N	1:A:1766:ASN:OD1	2.50	0.44
1:C:1818:ARG:CZ	1:C:1920:LEU:HD23	2.48	0.44
1:D:2095:GLY:O	1:D:2151:LEU:HD12	2.18	0.44
1:C:1718:TYR:CE1	1:C:1771:VAL:HG11	2.52	0.44
1:C:1863:TYR:CD2	1:C:1890:ARG:HG2	2.52	0.44
1:A:2110:ALA:HB2	1:A:2118:GLU:HA	1.99	0.44
1:C:1986:MET:HE1	1:D:2167:MET:HE1	2.00	0.44
1:C:1987:HIS:NE2	1:C:1995:THR:HG22	2.33	0.44
1:D:1931:VAL:HG21	1:D:1957:ILE:CD1	2.45	0.44
1:A:1835:ILE:HG22	1:B:2228:VAL:CG1	2.42	0.43
1:A:2306:ARG:HA	1:B:1897:ILE:HD12	2.00	0.43
1:D:1918:SER:OG	1:D:1942:LEU:HD22	2.18	0.43
1:D:1971:ARG:O	1:D:1973:VAL:HG23	2.17	0.43
1:A:1770:MET:HE1	1:A:1791:ILE:HG22	1.99	0.43
1:D:1825:ILE:HG21	1:D:2006:ILE:HD13	2.00	0.43
1:D:2153:ILE:HB	1:D:2191:ILE:HG23	2.01	0.43
1:D:2204:TRP:O	1:D:2207:ILE:HG22	2.19	0.43
1:C:2016:ASP:OD2	1:C:2018:HIS:ND1	2.52	0.43
1:B:1923:GLU:OE1	1:B:2146:ARG:NH1	2.50	0.43
1:A:1985:ILE:HD11	1:B:2164:MET:HE3	1.99	0.43
1:D:1723:MET:HE1	1:D:2003:VAL:CG2	2.49	0.43
1:D:2271:ASP:O	1:D:2275:LEU:HD12	2.17	0.43
1:D:2331:ARG:HD3	1:D:2382:VAL:HG11	1.98	0.43
1:C:1975:THR:N	1:C:1979:GLN:OE1	2.43	0.43
1:C:2014:PRO:HB2	1:C:2016:ASP:O	2.18	0.43
1:D:1872:ILE:CG2	1:D:1877:SER:HB2	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1959:LEU:HD13	1:D:2160:PHE:HB2	2.01	0.43
1:A:1698:THR:HG23	1:A:1702:LEU:HD23	2.00	0.43
1:A:1840:GLU:HG3	1:A:1841:ILE:N	2.34	0.43
1:C:2217:GLU:OE2	1:C:2333:LEU:HD21	2.18	0.43
1:C:2430:VAL:HG23	1:C:2431:ILE:N	2.33	0.43
1:A:1968:VAL:HG12	2:B:2:RCP:C6	2.49	0.43
1:C:2289:ILE:HD13	1:D:1856:HIS:ND1	2.34	0.43
1:D:1922:TYR:CZ	1:D:2146:ARG:HD3	2.53	0.43
1:A:1749:VAL:O	1:A:1757:VAL:HG22	2.19	0.43
1:D:1958:ILE:HD12	1:D:1961:GLY:HA2	2.01	0.43
1:D:2081:THR:CG2	1:D:2128:VAL:O	2.60	0.43
1:D:2153:ILE:HD12	1:D:2191:ILE:HD12	1.98	0.43
1:B:2248:MET:HE3	1:B:2255:TYR:CE2	2.53	0.43
1:B:2235:VAL:HG21	1:B:2295:VAL:HA	2.01	0.43
1:A:2433:LEU:CD2	1:B:2419:VAL:HG21	2.49	0.43
1:C:2425:VAL:HG12	1:C:2429:CYS:HB2	2.01	0.43
1:D:1864:LEU:CD2	1:D:1893:ILE:HD11	2.48	0.43
1:A:2298:ALA:HA	1:B:1837:MET:CE	2.49	0.42
1:B:2003:VAL:HA	1:B:2006:ILE:HD12	2.01	0.42
2:C:3:RCP:H25	2:C:3:RCP:H292	1.74	0.42
1:A:1723:MET:HE2	1:A:1723:MET:HB3	1.81	0.42
1:A:1743:LEU:HD13	1:A:1777:PHE:HB3	2.02	0.42
1:B:2308:LEU:CD1	1:B:2316:ILE:HG23	2.34	0.42
1:C:2030:ILE:CD1	1:C:2031:ASP:OD1	2.67	0.42
1:D:2331:ARG:CZ	1:D:2386:GLU:OE2	2.68	0.42
1:C:1845:PHE:CE1	1:C:1862:LEU:HD22	2.54	0.42
1:C:2306:ARG:HA	1:D:1897:ILE:HD12	2.01	0.42
1:C:2316:ILE:O	1:C:2317:LEU:HD23	2.19	0.42
1:D:1926:VAL:CG2	1:D:2013:MET:CE	2.93	0.42
1:D:2094:VAL:HG21	1:D:2152:MET:HG3	2.01	0.42
1:D:2407:LYS:O	1:D:2411:VAL:HG23	2.20	0.42
1:A:1756:LEU:HD21	1:A:1809:LEU:CD1	2.49	0.42
1:C:1789:ILE:HD12	1:C:1817:ALA:CB	2.46	0.42
1:D:1756:LEU:HG	1:D:1812:ARG:HB3	2.01	0.42
1:B:1739:PRO:HD2	1:B:1742:ILE:HD12	2.02	0.42
1:B:2361:ARG:O	1:B:2364:VAL:HG22	2.19	0.42
1:D:1700:ASP:O	1:D:1704:ALA:HB3	2.19	0.42
1:D:2252:ASP:OD2	1:D:2286:LEU:HD11	2.19	0.42
1:A:2419:VAL:CG1	1:A:2426:ALA:HB2	2.48	0.42
1:B:2245:ILE:HD12	1:B:2283:GLU:OE1	2.19	0.42
1:C:2142:LYS:O	1:C:2146:ARG:HD3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2339:VAL:O	1:C:2343:ILE:HB	2.19	0.42
1:D:1772:ALA:HA	1:D:1790:VAL:O	2.19	0.42
1:D:1926:VAL:HG13	1:D:2013:MET:HE1	2.01	0.42
1:A:1811:LEU:HD22	1:A:1913:MET:SD	2.60	0.42
1:D:1757:VAL:HG23	1:D:1759:MET:HE3	2.02	0.42
1:A:2110:ALA:HB2	1:A:2119:ALA:N	2.34	0.42
1:B:2110:ALA:HB2	1:B:2119:ALA:N	2.35	0.42
1:A:2361:ARG:O	1:A:2365:GLU:HB2	2.20	0.42
1:D:2345:GLN:O	1:D:2345:GLN:NE2	2.52	0.42
1:A:2425:VAL:HG13	1:B:2412:LEU:HD21	2.02	0.42
1:B:2044:ASP:HB3	1:B:2047:TRP:CD2	2.54	0.42
1:B:2438:SER:O	1:B:2442:ARG:N	2.53	0.42
1:C:2094:VAL:HG22	1:C:2095:GLY:O	2.20	0.42
1:B:2278:ARG:O	1:B:2281:ALA:HB3	2.20	0.41
1:D:2042:PRO:HB3	1:D:2101:THR:O	2.19	0.41
1:A:2343:ILE:HG21	1:A:2403:ILE:HG21	1.93	0.41
1:B:2048:MET:HE1	1:B:2154:PHE:CD2	2.55	0.41
1:C:2205:VAL:HG11	1:D:1938:ILE:HD13	2.02	0.41
1:D:1717:ILE:HG12	1:D:1771:VAL:HG22	2.02	0.41
1:D:2191:ILE:CG2	1:D:2207:ILE:HD11	2.50	0.41
1:C:1960:THR:HG21	2:D:4:RCP:H20	2.01	0.41
1:A:2141:ILE:HD13	1:A:2182:LEU:HD21	2.02	0.41
1:B:2352:HIS:HA	1:B:2355:ILE:HD12	2.02	0.41
1:D:1844:MET:CE	1:D:1864:LEU:HD13	2.50	0.41
1:D:1864:LEU:HD21	1:D:1893:ILE:HD11	2.02	0.41
1:B:1883:ILE:CD1	1:B:1892:MET:CE	2.96	0.41
1:C:1702:LEU:HD21	1:C:1706:ARG:HH11	1.84	0.41
1:C:2012:TYR:O	1:C:2149:LEU:HD21	2.20	0.41
1:B:2094:VAL:HG21	1:B:2152:MET:CG	2.49	0.41
1:B:2012:TYR:O	1:B:2149:LEU:HD21	2.21	0.41
1:A:1905:VAL:CG1	1:B:2312:VAL:HG21	2.50	0.41
1:D:1926:VAL:CG1	1:D:2013:MET:HE2	2.51	0.41
1:D:1987:HIS:O	1:D:2077:PRO:HG2	2.21	0.41
1:A:1911:SER:HB3	1:A:1938:ILE:HD13	2.01	0.41
1:B:1700:ASP:O	1:B:1704:ALA:CB	2.68	0.41
1:B:1985:ILE:HG22	1:B:1986:MET:HE2	2.03	0.41
1:B:2198:GLU:HA	1:B:2225:ARG:O	2.20	0.41
1:C:1698:THR:HA	1:C:1702:LEU:CB	2.49	0.41
1:A:2387:GLN:NE2	1:A:2398:THR:HG21	2.34	0.41
1:B:1943:VAL:CG1	1:B:1949:VAL:HG21	2.51	0.41
1:D:1804:PRO:HD3	1:D:1907:ASN:OD1	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2219:TYR:HB3	1:D:2317:LEU:HD12	2.02	0.41
1:C:2045:PRO:HG2	1:C:2083:VAL:HG21	2.03	0.41
1:A:2054:HIS:CD2	1:A:2057:LEU:HB2	2.56	0.41
1:A:2339:VAL:HG11	1:A:2399:ILE:HD11	2.03	0.41
1:A:2229:LEU:HD12	1:B:1835:ILE:HD12	2.03	0.41
1:B:2264:GLU:N	1:B:2265:PRO:HD3	2.36	0.41
1:D:1743:LEU:HD12	1:D:1744:THR:N	2.36	0.41
1:D:1949:VAL:HG13	1:D:1992:SER:HA	2.03	0.41
1:A:2172:LEU:HA	1:A:2172:LEU:HD12	1.94	0.41
1:B:2023:ILE:HD13	1:B:2092:ILE:HG12	2.03	0.41
1:B:2073:GLU:OE2	1:B:2083:VAL:HG13	2.21	0.41
1:A:1748:LEU:HB3	1:A:1756:LEU:HD22	2.03	0.41
1:A:1775:MET:HB3	1:A:1775:MET:HE2	1.90	0.41
1:A:2438:SER:O	1:A:2442:ARG:N	2.49	0.41
1:C:1793:ASN:ND2	1:C:1830:ASN:HD22	2.19	0.41
1:C:2205:VAL:CG1	1:D:1938:ILE:HD13	2.51	0.41
1:D:1723:MET:HE2	1:D:1723:MET:HB3	1.94	0.41
1:D:1926:VAL:HG22	1:D:2013:MET:CE	2.50	0.41
1:B:1720:PHE:N	1:B:1721:PRO:CD	2.85	0.40
1:B:2079:ALA:HB3	1:B:2136:LYS:HD3	2.02	0.40
1:B:2185:TYR:CB	1:B:2189:ILE:HD11	2.52	0.40
1:D:1931:VAL:HG22	1:D:1943:VAL:HG21	2.02	0.40
1:B:1880:CYS:HA	1:B:1894:THR:HG23	2.02	0.40
1:D:1818:ARG:HD3	1:D:1921:ALA:HA	2.03	0.40
1:D:2088:ARG:HA	1:D:2092:ILE:O	2.20	0.40
1:A:1816:MET:O	1:A:1819:ALA:HB3	2.21	0.40
1:C:2126:GLY:O	1:C:2128:VAL:HG23	2.21	0.40
1:C:2287:LEU:N	1:C:2288:PRO:CD	2.85	0.40
1:D:1702:LEU:HD21	1:D:1706:ARG:NH2	2.37	0.40
1:D:1707:PHE:HB3	3:D:12:HOH:O	2.21	0.40
1:B:2099:VAL:HG22	1:B:2157:TRP:CZ2	2.56	0.40
1:D:1723:MET:HE1	1:D:2003:VAL:HG23	2.03	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	746/760 (98%)	693 (93%)	50 (7%)	3 (0%)	34	69
1	B	744/760 (98%)	691 (93%)	49 (7%)	4 (0%)	29	67
1	C	734/760 (97%)	684 (93%)	45 (6%)	5 (1%)	22	61
1	D	729/760 (96%)	682 (94%)	38 (5%)	9 (1%)	13	49
All	All	2953/3040 (97%)	2750 (93%)	182 (6%)	21 (1%)	22	61

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	1735	PRO
1	C	1947	GLN
1	D	2349	GLU
1	D	2355	ILE
1	B	2265	PRO
1	D	1947	GLN
1	D	2351	SER
1	A	2398	THR
1	A	2438	SER
1	B	1740	LYS
1	B	2347	SER
1	C	2264	GLU
1	D	1904	GLY
1	D	2341	GLN
1	B	1799	ILE
1	C	1799	ILE
1	D	1799	ILE
1	D	2288	PRO
1	D	2348	GLY
1	A	1799	ILE
1	C	2439	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	558/650 (86%)	553 (99%)	5 (1%)	78	91
1	B	578/650 (89%)	572 (99%)	6 (1%)	76	90
1	C	576/650 (89%)	572 (99%)	4 (1%)	84	94
1	D	568/650 (87%)	563 (99%)	5 (1%)	78	91
All	All	2280/2600 (88%)	2260 (99%)	20 (1%)	78	91

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2108	VAL
1	A	2239	PHE
1	A	2242	LYS
1	A	2324	THR
1	A	2331	ARG
1	B	1874	SER
1	B	2039	SER
1	B	2135	TYR
1	B	2146	ARG
1	B	2239	PHE
1	B	2315	ASP
1	C	2039	SER
1	C	2135	TYR
1	C	2239	PHE
1	C	2432	TYR
1	D	1864	LEU
1	D	1960	THR
1	D	2129	TRP
1	D	2146	ARG
1	D	2239	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1793	ASN
1	A	1993	HIS
1	A	2054	HIS
1	A	2387	GLN
1	A	2408	HIS
1	A	2422	ASN

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Mol	Chain	Res	Type
1	B	2139	GLN
1	B	2170	GLN
1	B	2184	GLN
1	B	2352	HIS
1	B	2422	ASN
1	C	1780	GLN
1	C	1793	ASN
1	C	1879	HIS
1	C	1966	ASN
1	C	1993	HIS
1	C	2127	GLN
1	C	2187	GLN
1	D	2123	GLN
1	D	2127	GLN
1	D	2345	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

4 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
2	RCP	A	1	-	41,41,41	1.31	5 (12%)	58,58,58	1.57	10 (17%)
2	RCP	D	4	-	41,41,41	1.28	4 (9%)	58,58,58	1.54	11 (18%)
2	RCP	C	3	-	41,41,41	1.23	4 (9%)	58,58,58	1.46	11 (18%)
2	RCP	B	2	-	41,41,41	1.35	5 (12%)	58,58,58	1.74	12 (20%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	RCP	A	1	-	-	6/20/48/48	0/6/6/6
2	RCP	D	4	-	-	3/20/48/48	0/6/6/6
2	RCP	C	3	-	-	3/20/48/48	0/6/6/6
2	RCP	B	2	-	-	9/20/48/48	0/6/6/6

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1	RCP	C14-C15	-4.02	1.46	1.50
2	B	2	RCP	C14-C15	-3.89	1.46	1.50
2	D	4	RCP	C14-C15	-3.60	1.46	1.50
2	B	2	RCP	C26-N26	2.90	1.39	1.34
2	A	1	RCP	C1-C6	-2.84	1.37	1.43
2	C	3	RCP	C14-C15	-2.82	1.47	1.50
2	A	1	RCP	C13-C8	-2.76	1.38	1.43
2	B	2	RCP	C13-C8	-2.63	1.38	1.43
2	D	4	RCP	C26-N26	2.62	1.38	1.34
2	C	3	RCP	C1-C6	-2.54	1.38	1.43
2	C	3	RCP	C26-N26	2.48	1.38	1.34
2	D	4	RCP	C13-C8	-2.48	1.38	1.43
2	C	3	RCP	C13-C8	-2.47	1.38	1.43
2	D	4	RCP	C1-C6	-2.43	1.38	1.43
2	B	2	RCP	C1-C6	-2.40	1.38	1.43
2	A	1	RCP	C26-N26	2.36	1.38	1.34
2	B	2	RCP	C14-C13	-2.16	1.38	1.41
2	A	1	RCP	C18-N15	-2.02	1.43	1.47

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1	RCP	C25-C26-N26	-5.55	112.44	118.80
2	C	3	RCP	O15-C15-C14	-5.32	116.44	121.59
2	B	2	RCP	C25-C26-N26	-5.08	112.98	118.80
2	B	2	RCP	O15-C15-C14	-4.88	116.86	121.59
2	D	4	RCP	O15-C15-C14	-4.34	117.39	121.59
2	D	4	RCP	C27-N26-C29	3.91	120.15	112.62
2	B	2	RCP	C23-C25-C24	3.86	116.85	109.92
2	B	2	RCP	C21-N20-C24	3.67	111.81	108.19
2	A	1	RCP	O15-C15-C14	-3.63	118.08	121.59
2	D	4	RCP	C25-C24-N20	3.52	116.03	111.14
2	B	2	RCP	C25-C24-N20	3.42	115.90	111.14
2	C	3	RCP	C22-C21-N20	-3.27	105.77	111.28
2	C	3	RCP	C23-C25-C24	3.25	115.74	109.92
2	D	4	RCP	C22-C21-N20	-3.05	106.14	111.28
2	B	2	RCP	O26-C26-N26	3.05	125.24	121.67
2	B	2	RCP	C23-C22-C21	-3.01	106.63	110.85
2	D	4	RCP	C28-C27-N26	2.99	116.20	109.84
2	D	4	RCP	C23-C22-C21	-2.86	106.84	110.85
2	A	1	RCP	O26-C26-N26	2.83	124.98	121.67
2	A	1	RCP	C23-C25-C24	2.82	114.98	109.92
2	D	4	RCP	C25-C26-N26	-2.75	115.65	118.80
2	A	1	RCP	O28-C28-C27	-2.72	105.80	111.80
2	C	3	RCP	C14-C15-N15	2.72	120.92	117.86
2	A	1	RCP	C27-N26-C29	2.67	117.75	112.62
2	A	1	RCP	O15-C15-N15	2.65	126.72	122.34
2	B	2	RCP	O28-C28-C27	-2.62	106.01	111.80
2	A	1	RCP	C16-N15-C18	2.59	117.61	112.62
2	C	3	RCP	C18-C19-C20	-2.58	105.90	110.81
2	D	4	RCP	C23-C25-C24	2.36	114.16	109.92
2	A	1	RCP	C14-C15-N15	-2.36	115.21	117.86
2	C	3	RCP	C25-C24-N20	2.31	114.36	111.14
2	B	2	RCP	C29-N26-C26	-2.31	114.72	123.28
2	D	4	RCP	C29-N26-C26	-2.29	114.77	123.28
2	D	4	RCP	C30-C29-N26	2.27	114.68	109.84
2	B	2	RCP	O15-C15-N15	2.27	126.08	122.34
2	B	2	RCP	C23-C25-C26	-2.27	105.73	109.83
2	C	3	RCP	C9-C8-C7	-2.22	118.36	122.00
2	C	3	RCP	C25-C26-N26	-2.17	116.32	118.80
2	C	3	RCP	C16-N15-C18	2.14	116.74	112.62
2	C	3	RCP	O28-C30-C29	-2.08	107.22	111.80
2	D	4	RCP	C18-C19-C20	-2.06	106.89	110.81
2	A	1	RCP	C18-C19-C20	-2.03	106.96	110.81
2	C	3	RCP	C5-C6-C7	-2.02	118.69	122.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2	RCP	C27-N26-C29	2.01	116.50	112.62

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1	RCP	O26-C26-N26-C29
2	A	1	RCP	C25-C26-N26-C29
2	B	2	RCP	O26-C26-N26-C27
2	B	2	RCP	C25-C26-N26-C27
2	D	4	RCP	O15-C15-N15-C16
2	A	1	RCP	C17-C20-N20-C24
2	A	1	RCP	C19-C20-N20-C21
2	B	2	RCP	C17-C20-N20-C24
2	B	2	RCP	C19-C20-N20-C21
2	B	2	RCP	O15-C15-N15-C16
2	D	4	RCP	C14-C15-N15-C16
2	C	3	RCP	C17-C20-N20-C24
2	A	1	RCP	C19-C20-N20-C24
2	C	3	RCP	C19-C20-N20-C21
2	B	2	RCP	C19-C20-N20-C24
2	B	2	RCP	C14-C15-N15-C16
2	B	2	RCP	C1-C14-C15-N15
2	B	2	RCP	C13-C14-C15-N15
2	A	1	RCP	C17-C20-N20-C21
2	C	3	RCP	O26-C26-N26-C27
2	D	4	RCP	C17-C20-N20-C24

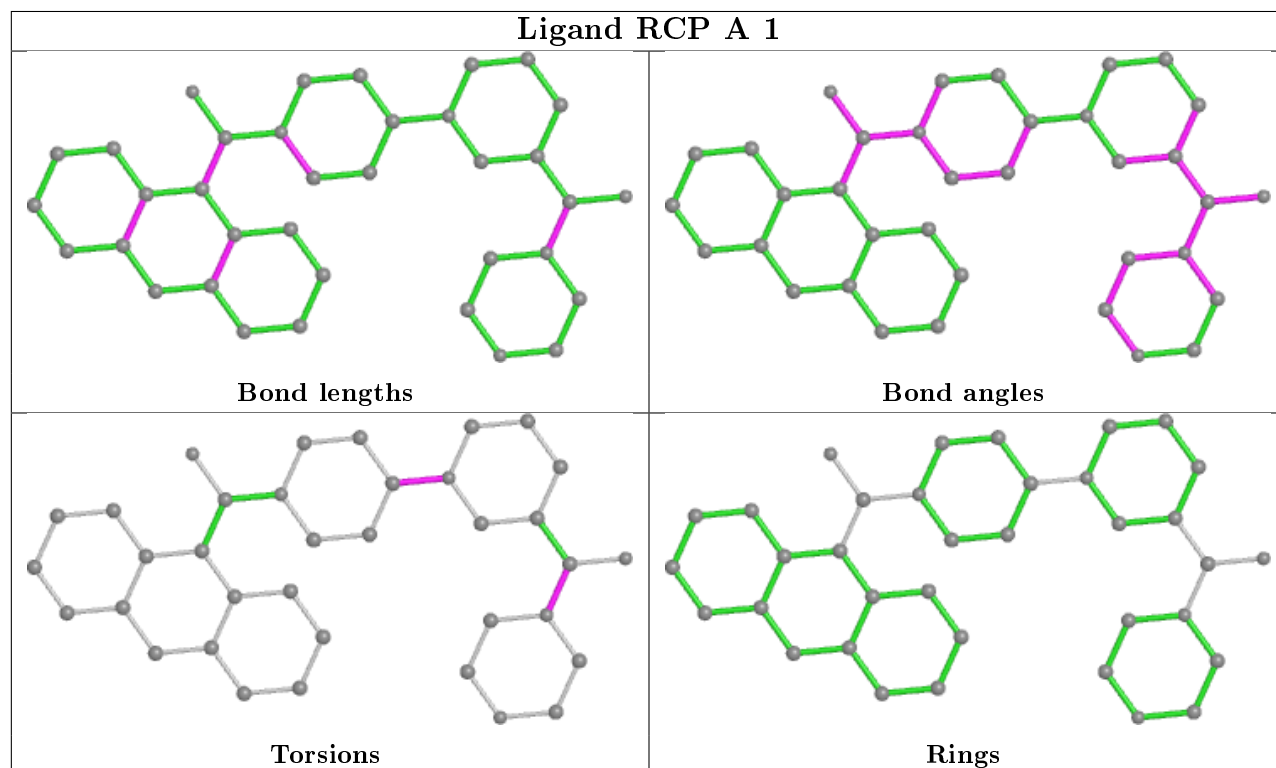
There are no ring outliers.

4 monomers are involved in 7 short contacts:

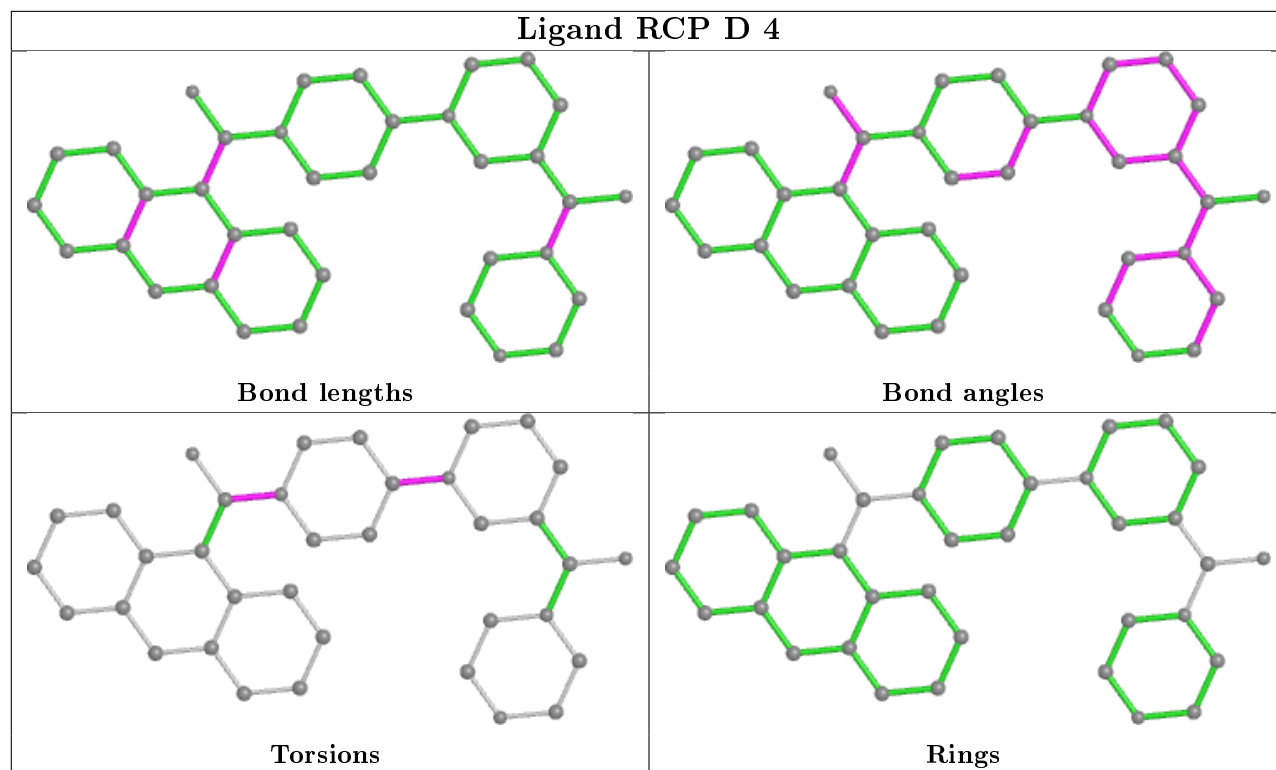
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1	RCP	3	0
2	D	4	RCP	1	0
2	C	3	RCP	1	0
2	B	2	RCP	2	0

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.

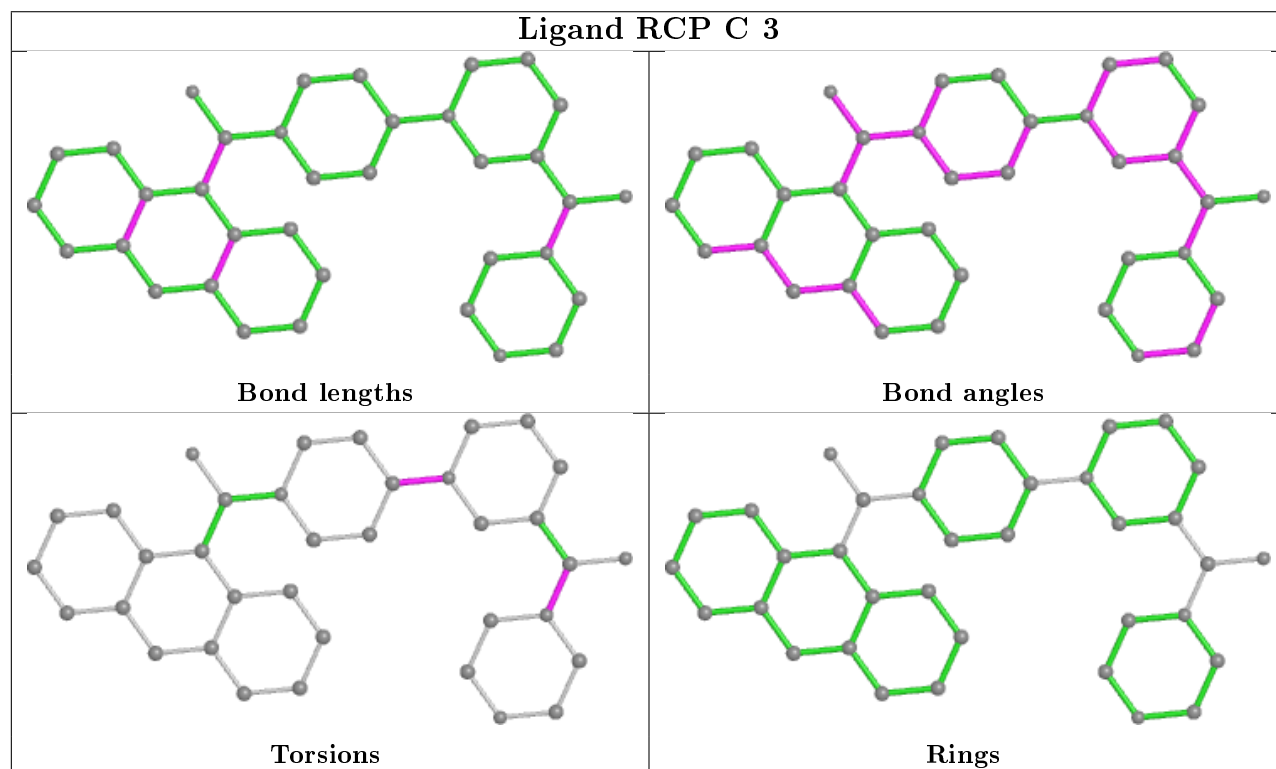
Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD 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.

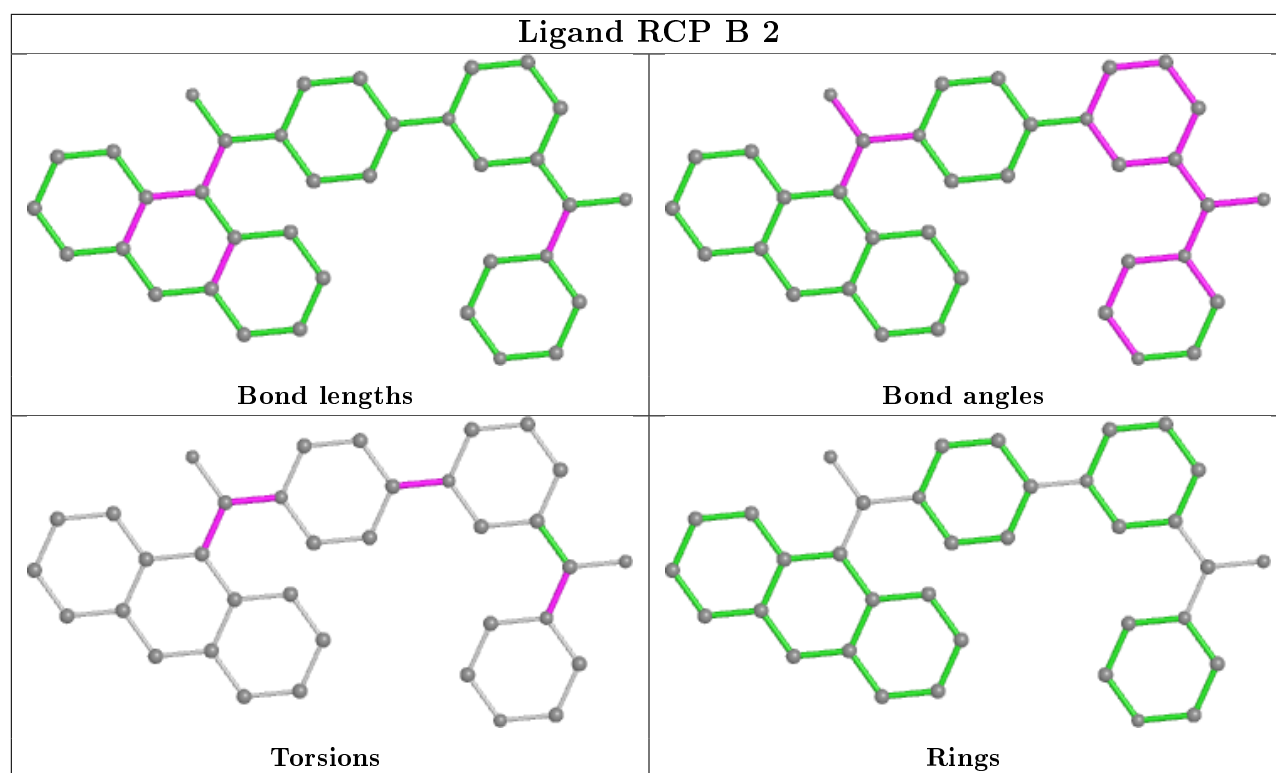


Ligand RCP D 4



Ligand RCP C 3





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	750/760 (98%)	-0.38	14 (1%) 66 53	27, 37, 48, 62	0
1	B	748/760 (98%)	-0.45	5 (0%) 87 81	30, 37, 51, 65	0
1	C	742/760 (97%)	-0.28	18 (2%) 59 44	27, 37, 53, 62	0
1	D	733/760 (96%)	-0.42	9 (1%) 79 67	29, 36, 50, 61	0
All	All	2973/3040 (97%)	-0.38	46 (1%) 73 61	27, 37, 51, 65	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	2342	GLU	4.2
1	C	1700	ASP	3.9
1	A	1883	ILE	3.4
1	B	2391	ALA	3.3
1	D	2390	GLN	3.2
1	D	1697	VAL	3.1
1	A	1700	ASP	3.1
1	B	2265	PRO	3.1
1	A	2263	GLY	3.0
1	C	1736	ASP	3.0
1	C	2443	ALA	3.0
1	D	1698	THR	3.0
1	C	1698	THR	2.9
1	C	1889	SER	2.9
1	C	2397	SER	2.9
1	C	2342	GLU	2.9
1	D	2391	ALA	2.8
1	A	2269	ASP	2.8
1	B	1700	ASP	2.7
1	A	2262	LEU	2.6
1	C	2346	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	2266	ASP	2.5
1	B	2390	GLN	2.5
1	D	2373	TYR	2.4
1	D	1700	ASP	2.4
1	A	1752	SER	2.4
1	C	2264	GLU	2.3
1	A	2115	LEU	2.3
1	C	2265	PRO	2.3
1	C	2372	ALA	2.3
1	D	2374	LEU	2.3
1	C	1760	ASN	2.3
1	C	2347	SER	2.2
1	D	2353	VAL	2.2
1	A	1887	GLY	2.2
1	A	2408	HIS	2.2
1	A	2265	PRO	2.2
1	A	2353	VAL	2.2
1	C	2438	SER	2.1
1	C	2354	HIS	2.1
1	C	2427	VAL	2.1
1	A	2116	ASP	2.1
1	C	2445	VAL	2.1
1	C	2115	LEU	2.1
1	B	2053	PRO	2.0
1	A	1735	PRO	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](#)

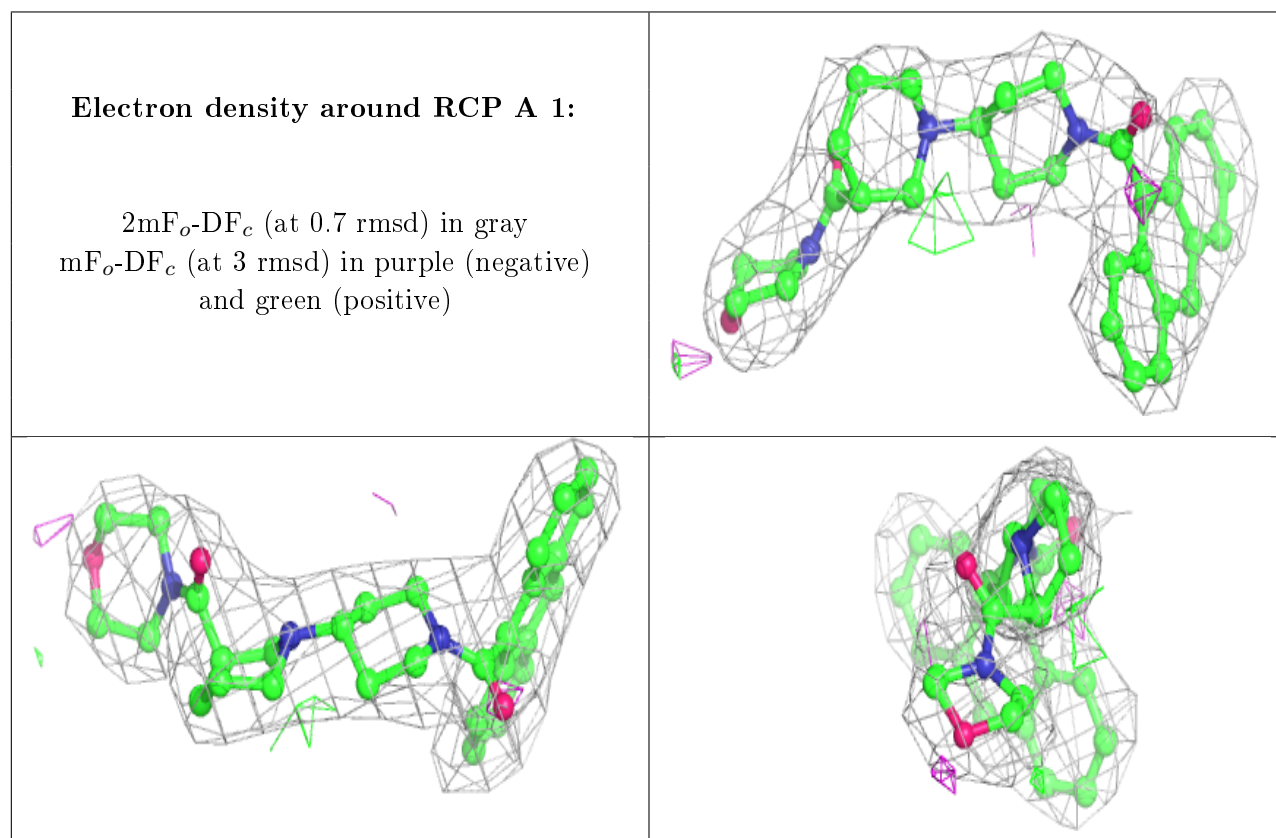
There are no carbohydrates in this entry.

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.

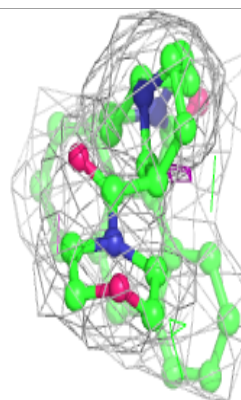
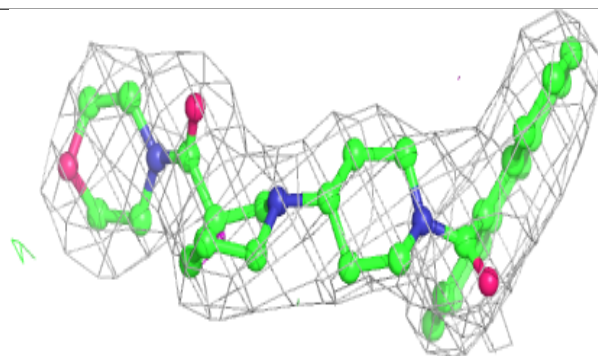
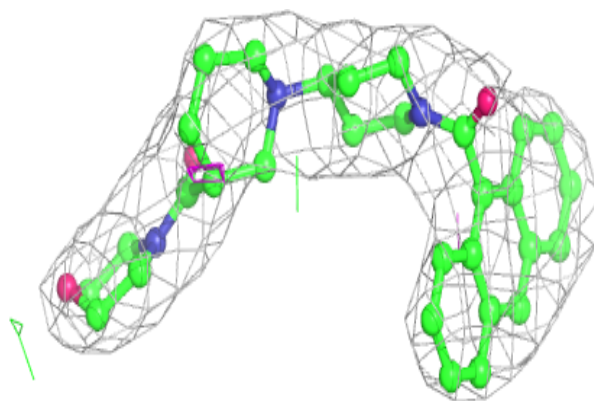
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	RCP	A	1	36/36	0.93	0.21	35,36,46,47	0
2	RCP	D	4	36/36	0.93	0.21	32,35,36,37	0
2	RCP	C	3	36/36	0.95	0.18	34,37,38,39	0
2	RCP	B	2	36/36	0.95	0.22	41,46,50,51	0

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.

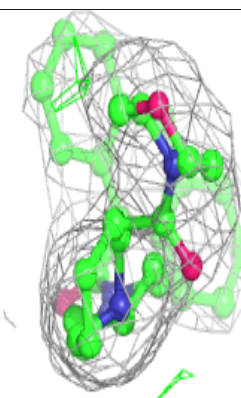
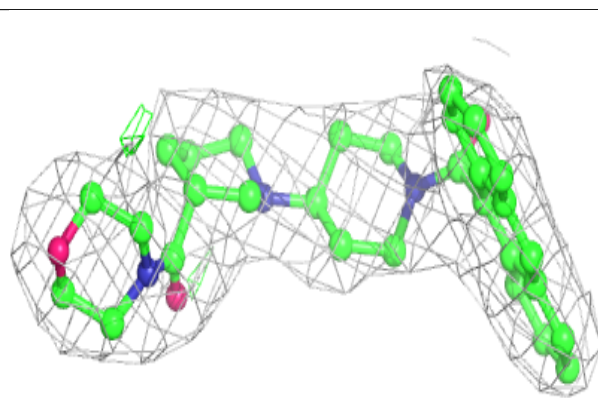
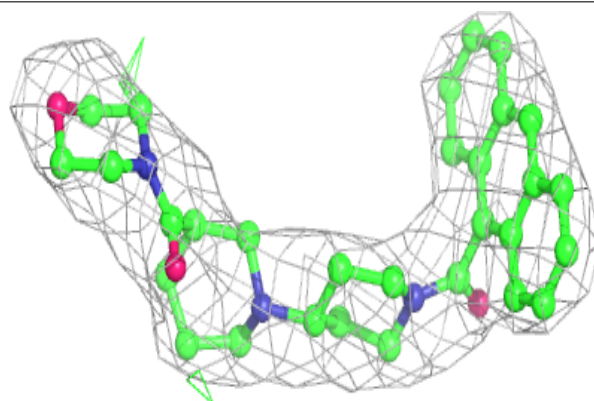


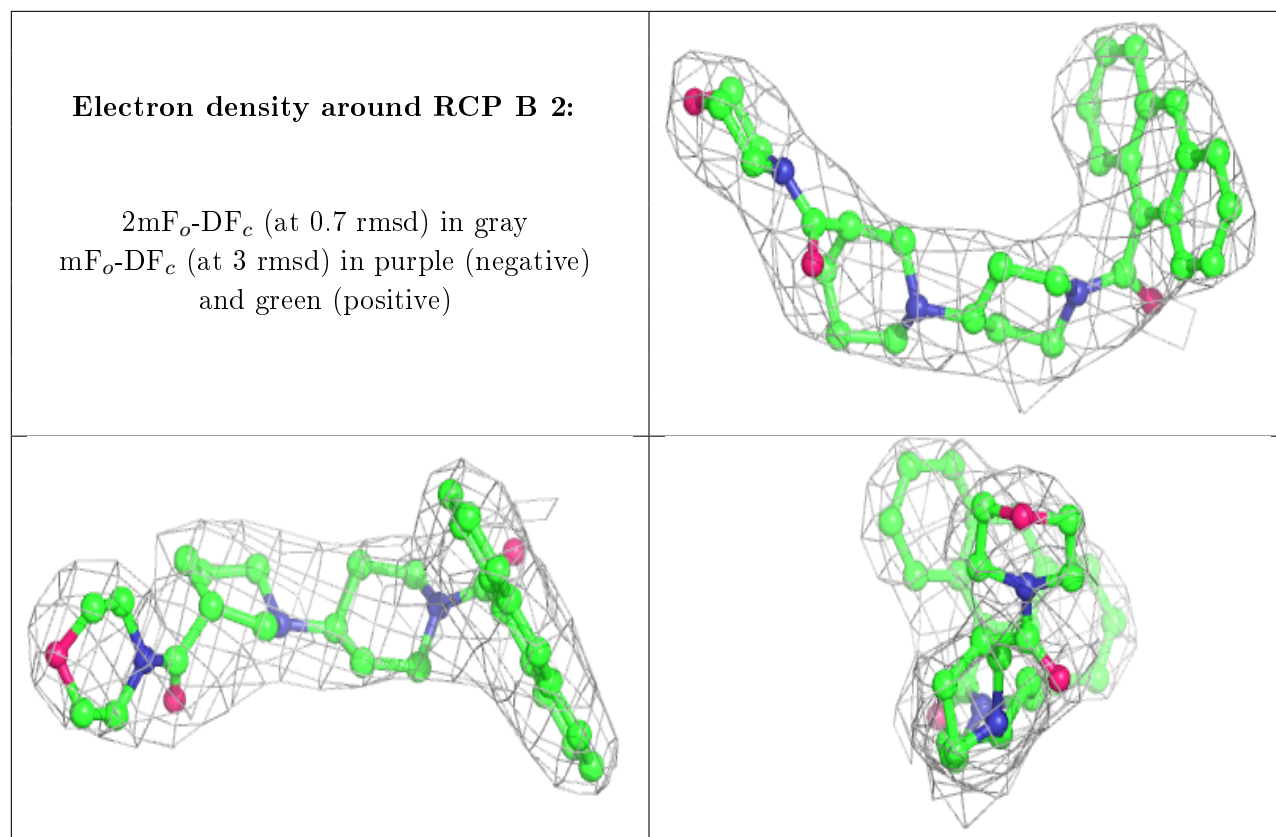
Electron density around RCP D 4:

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

**Electron density around RCP C 3:**

$2mF_o-DF_c$ (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.