



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 29, 2017 – 04:46 PM EDT

PDB ID : 3FF6
Title : Human ACC2 CT domain with CP-640186
Authors : Williams, S.P.; Madauss, K.P.; Burkhardt, W.A.
Deposited on : unknown
Resolution : 3.19 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030345
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20030345

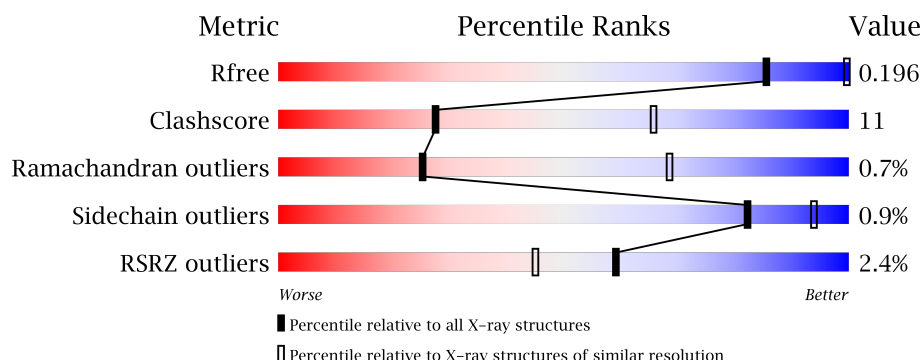
1 Overall quality at a glance ⓘ

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}	100719	1015 (3.22-3.18)
Clashscore	112137	1009 (3.20-3.20)
Ramachandran outliers	110173	1118 (3.22-3.18)
Sidechain outliers	110143	1117 (3.22-3.18)
RSRZ outliers	101464	1020 (3.22-3.18)

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. 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>3%</div> <div>78%</div> <div>20%</div> <div>..</div> </div>
1	B	760	<div> <div>%</div> <div>75%</div> <div>23%</div> <div>.</div> </div>
1	C	760	<div> <div>4%</div> <div>77%</div> <div>20%</div> <div>..</div> </div>
1	D	760	<div> <div>%</div> <div>74%</div> <div>22%</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.

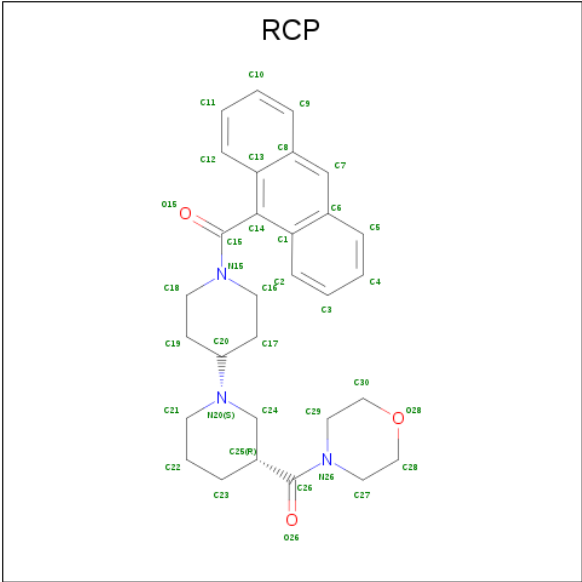
- Molecule 1 is a protein called Acetyl-CoA carboxylase 2.

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	C	N	O	0	0
			36	30	3	3		
2	B	1	Total	C	N	O	0	0
			36	30	3	3		
2	C	1	Total	C	N	O	0	0
			36	30	3	3		
2	D	1	Total	C	N	O	0	0
			36	30	3	3		

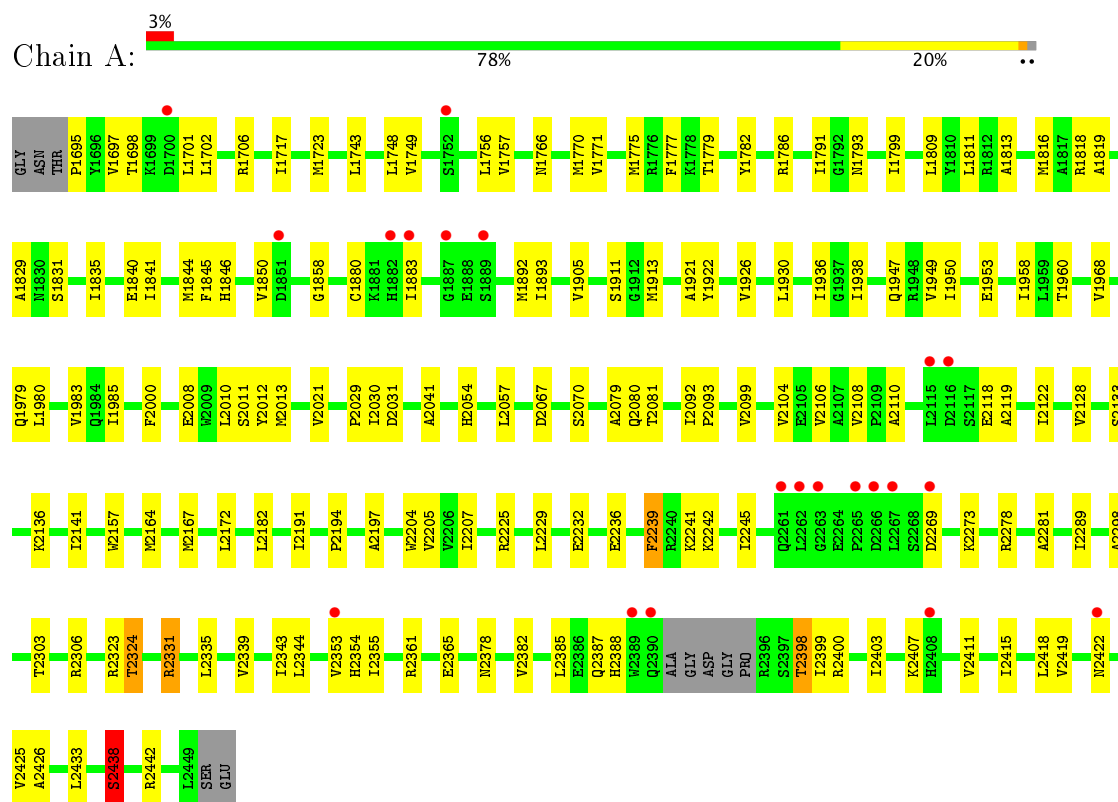
- Molecule 3 is water.

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

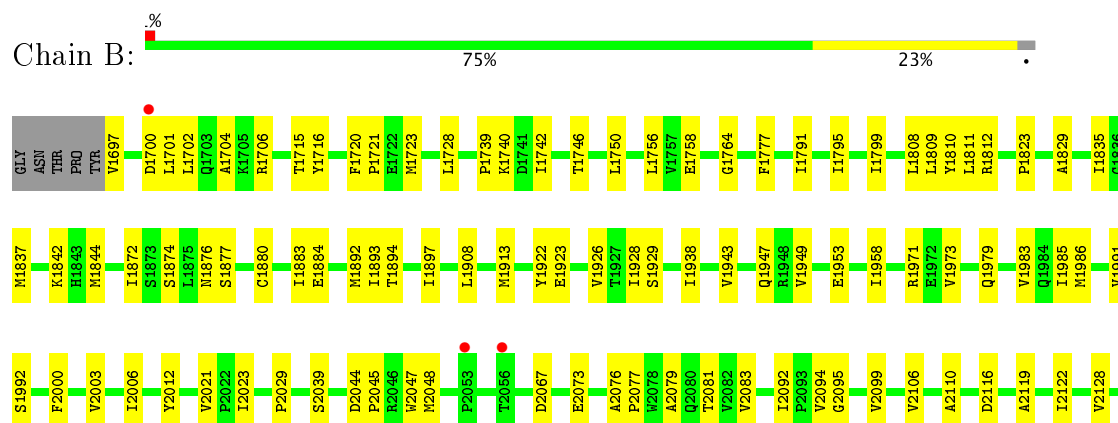
3 Residue-property plots [i](#)

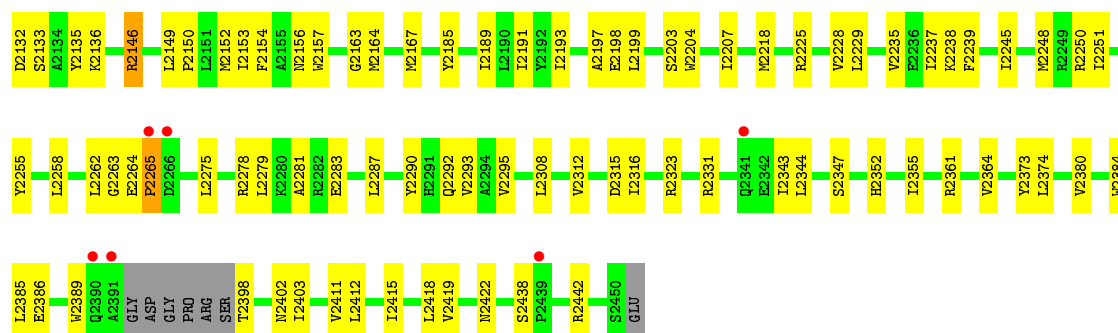
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

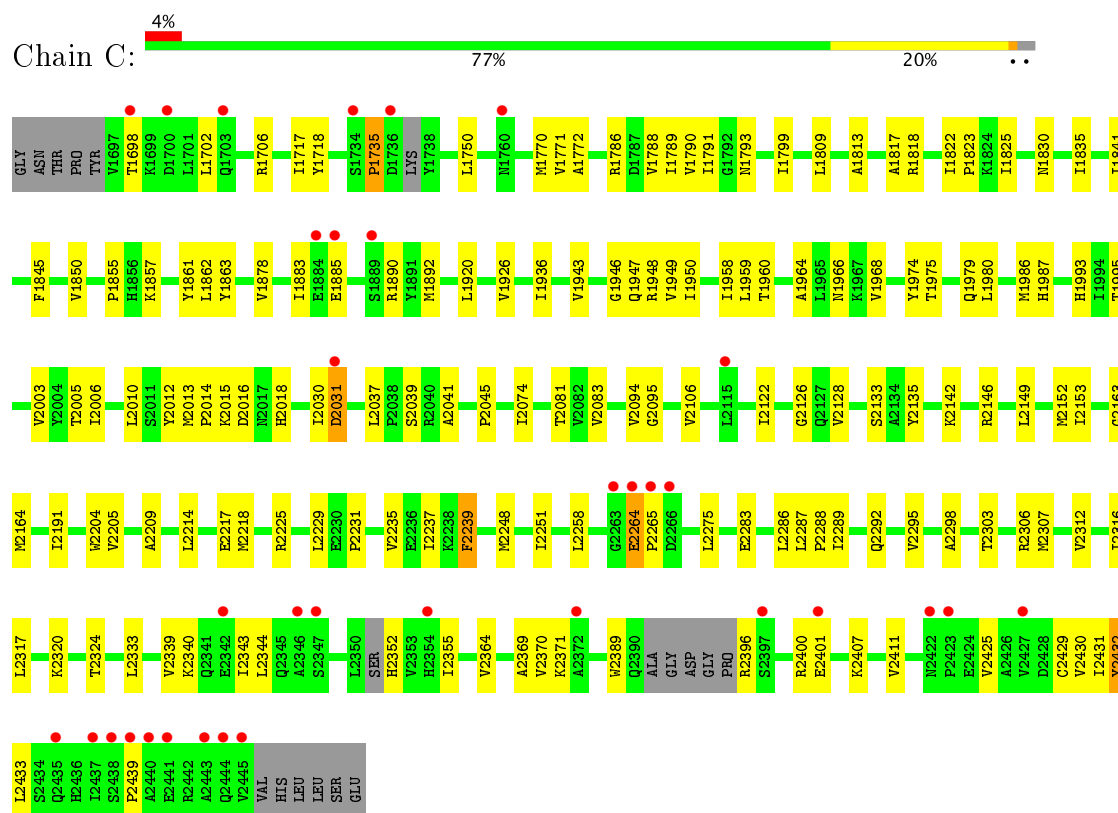


• Molecule 1: Acetyl-CoA carboxylase 2

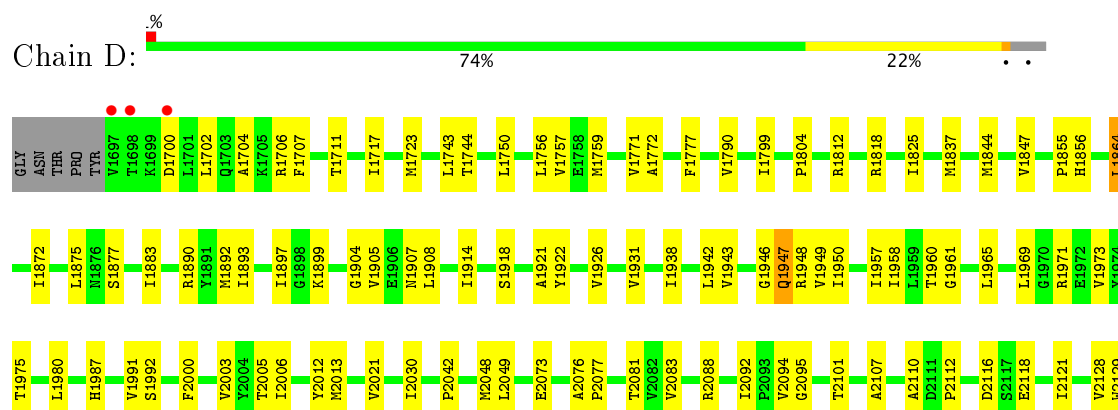




• Molecule 1: Acetyl-CoA carboxylase 2



• Molecule 1: Acetyl-CoA carboxylase 2



Q2390	L2287	S2133
A2391	F2288	
GLY	I2289	
ASP	Y2290	R2146
GLY	H2291	
PRO	Q2292	L2149
R2396	V2293	P2150
S2397	A2294	L2151
	V2295	M2152
R2407		I2153
	T2303	F2154
V2411		A2155
	R2306	
R2416	V2312	F2160
V2419	L2317	G2163
N2422		M2167
	T2324	
L2433		L2182
SER	R2331	
GLN	R2332	I2189
HIS	L2333	L2190
ILE		I2191
SER	Q2341	Y2192
PRO	E2342	I2193
ALA		
GLU	Q2345	E2198
ARG	A2346	L2199
ALA	S2347	R2200
GLN	G2348	
VAL	E2349	W2204
VAL	L2350	
HIS	S2351	I2207
LEU	V2353	E2217
LEU	H2354	M2218
SER	I2355	Y2219
GLU	Q2356	
	S2357	S2224
	W2362	V2228
	T2366	V2235
		E2236
	Y2373	I2237
	L2374	K2238
	W2375	F2239
	N2378	D2252
	V2381	L2262
	V2382	
	Q2383	D2271
	W2384	
	I2385	L2275
	E2386	
	Q2387	L2279
	H2388	
	W2389	L2286

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 (7.79%)	DCC
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 , 36.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	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.

The worst 5 of 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

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%)	38 77

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	744/760 (98%)	691 (93%)	49 (7%)	4 (0%)	32	74
1	C	734/760 (97%)	684 (93%)	45 (6%)	5 (1%)	25	68
1	D	729/760 (96%)	682 (94%)	38 (5%)	9 (1%)	15	56
All	All	2953/3040 (97%)	2750 (93%)	182 (6%)	21 (1%)	25	68

5 of 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

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%)	82	94
1	B	578/650 (89%)	572 (99%)	6 (1%)	80	93
1	C	576/650 (89%)	572 (99%)	4 (1%)	87	96
1	D	568/650 (87%)	563 (99%)	5 (1%)	82	94
All	All	2280/2600 (88%)	2260 (99%)	20 (1%)	82	94

5 of 20 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	2239	PHE
1	B	2315	ASP
1	D	1960	THR
1	B	2135	TYR
1	B	2146	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 21 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	2352	HIS
1	C	1780	GLN
1	C	2187	GLN
1	B	2184	GLN
1	D	2123	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	1.30	5 (12%)	57,58,58	1.51	10 (17%)
2	RCP	B	2	-	41,41,41	1.34	5 (12%)	57,58,58	1.65	11 (19%)
2	RCP	C	3	-	41,41,41	1.22	4 (9%)	57,58,58	1.40	10 (17%)
2	RCP	D	4	-	41,41,41	1.27	4 (9%)	57,58,58	1.50	9 (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
2	RCP	A	1	-	-	0/20/48/48	0/6/6/6
2	RCP	B	2	-	-	0/20/48/48	0/6/6/6
2	RCP	C	3	-	-	0/20/48/48	0/6/6/6
2	RCP	D	4	-	-	0/20/48/48	0/6/6/6

The worst 5 of 18 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1	RCP	C14-C15	-3.96	1.46	1.50
2	B	2	RCP	C14-C15	-3.83	1.46	1.50
2	D	4	RCP	C14-C15	-3.54	1.46	1.50
2	A	1	RCP	C1-C6	-2.82	1.37	1.43
2	C	3	RCP	C14-C15	-2.78	1.47	1.50

The worst 5 of 40 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1	RCP	C25-C26-N26	-5.35	112.44	118.72
2	C	3	RCP	O15-C15-C14	-5.23	116.44	121.59
2	B	2	RCP	C25-C26-N26	-4.89	112.98	118.72
2	B	2	RCP	O15-C15-C14	-4.80	116.86	121.59
2	D	4	RCP	O15-C15-C14	-4.27	117.39	121.59

There are no chirality outliers.

There are no torsion outliers.

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	B	2	RCP	2	0
2	C	3	RCP	1	0
2	D	4	RCP	1	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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%)	-0.12	21 (2%) 53 39	27, 37, 48, 62	0
1	B	748/760 (98%)	-0.22	9 (1%) 79 67	30, 37, 51, 65	0
1	C	742/760 (97%)	-0.03	34 (4%) 33 20	27, 37, 53, 62	0
1	D	733/760 (96%)	-0.21	8 (1%) 80 68	29, 36, 50, 61	0
All	All	2973/3040 (97%)	-0.14	72 (2%) 59 45	27, 37, 51, 65	0

The worst 5 of 72 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	2342	GLU	4.4
1	C	2443	ALA	4.2
1	C	2438	SER	3.8
1	C	1700	ASP	3.8
1	C	1889	SER	3.6

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
2	RCP	A	1	36/36	0.91	0.24	1.46	35,36,46,47	0
2	RCP	B	2	36/36	0.94	0.21	0.50	41,46,50,51	0
2	RCP	D	4	36/36	0.93	0.22	0.25	32,35,36,37	0
2	RCP	C	3	36/36	0.94	0.20	0.14	34,37,38,39	0

6.5 Other polymers [i](#)

There are no such residues in this entry.