Full wwPDB X-ray Structure Validation Report ⓘ

Sep 14, 2023 – 08:54 AM EDT

PDB ID	:	6REQ
Title	:	METHYLMALONYL-COA MUTASE, 3-CARBOXYPROPYL-COA INHIBITOR COMPLEX
Authors	:	Evans, P.R.; Mancia, F.
Deposited on	:	1998-09-03
Resolution	:	2.20 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

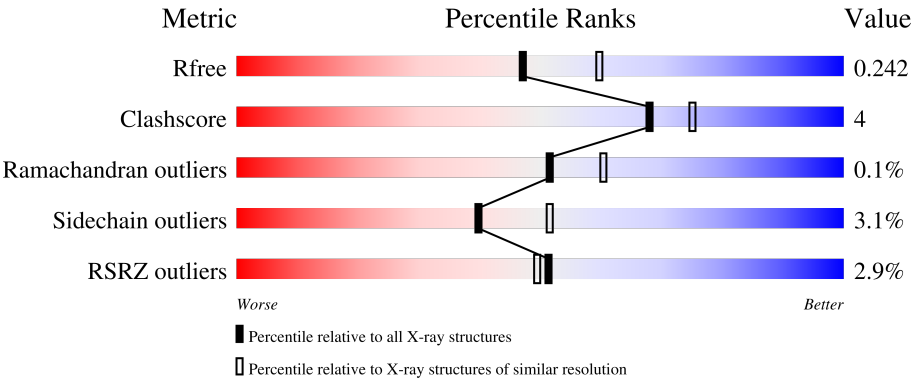
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh &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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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

Mol	Chain	Length	Quality of chain
1	A	727	71% 27%
1	C	727	2% 70% 27%
2	B	637	3% 71% 24%
2	D	637	6% 68% 25%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 22116 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 PROTEIN (METHYLMALONYL-COA MUTASE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	727	Total	C	N	O	S	0	0	0
			5601	3538	971	1068	24			
1	C	727	Total	C	N	O	S	0	0	0
			5601	3538	971	1068	24			

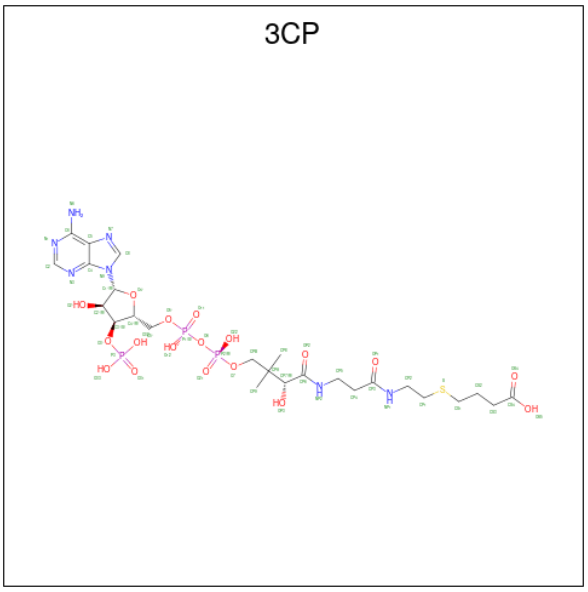
- Molecule 2 is a protein called PROTEIN (METHYLMALONYL-COA MUTASE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	619	Total	C	N	O	S	0	0	0
			4731	2982	824	912	13			
2	D	619	Total	C	N	O	S	0	0	0
			4731	2982	824	912	13			

There are 6 discrepancies between the modelled and reference sequences:

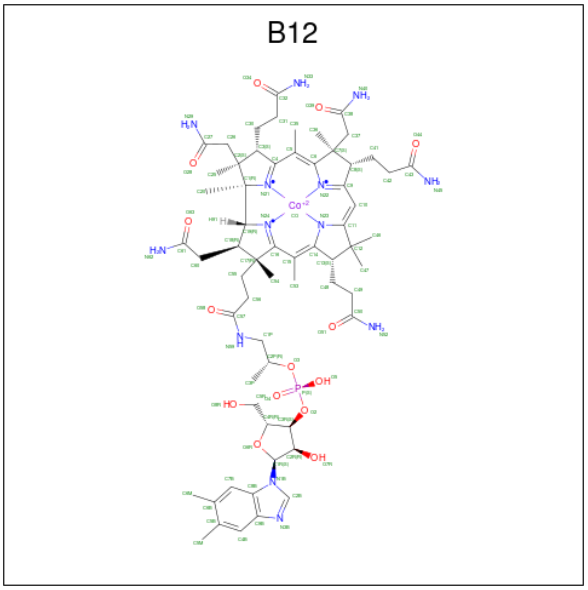
Chain	Residue	Modelled	Actual	Comment	Reference
B	203	GLY	ALA	SEE REMARK 999	UNP P11652
D	203	GLY	ALA	SEE REMARK 999	UNP P11652
B	330	GLU	ASP	SEE REMARK 999	UNP P11652
D	330	GLU	ASP	SEE REMARK 999	UNP P11652
B	331	LEU	VAL	SEE REMARK 999	UNP P11652
D	331	LEU	VAL	SEE REMARK 999	UNP P11652

- Molecule 3 is 3-CARBOXYPROPYL-COENZYME A (three-letter code: 3CP) (formula: $C_{25}H_{42}N_7O_{18}P_3S$).



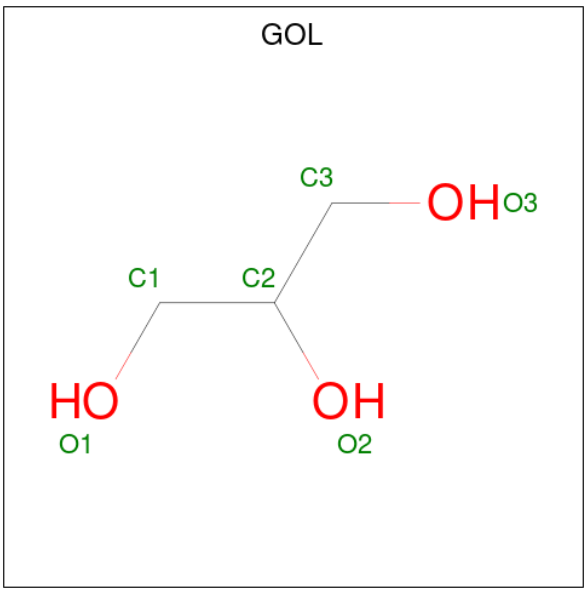
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	S	0	0
			54	25	7	18	3	1		
3	C	1	Total	C	N	O	P	S	0	0
			54	25	7	18	3	1		

- Molecule 4 is COBALAMIN (three-letter code: B12) (formula: $C_{62}H_{89}CoN_{13}O_{14}P$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total	C	Co	N	O	P	0	0
			91	62	1	13	14	1		
4	C	1	Total	C	Co	N	O	P	0	0
			91	62	1	13	14	1		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 6 3 3	0	0
5	C	1	Total C O 6 3 3	0	0

- Molecule 6 is water.

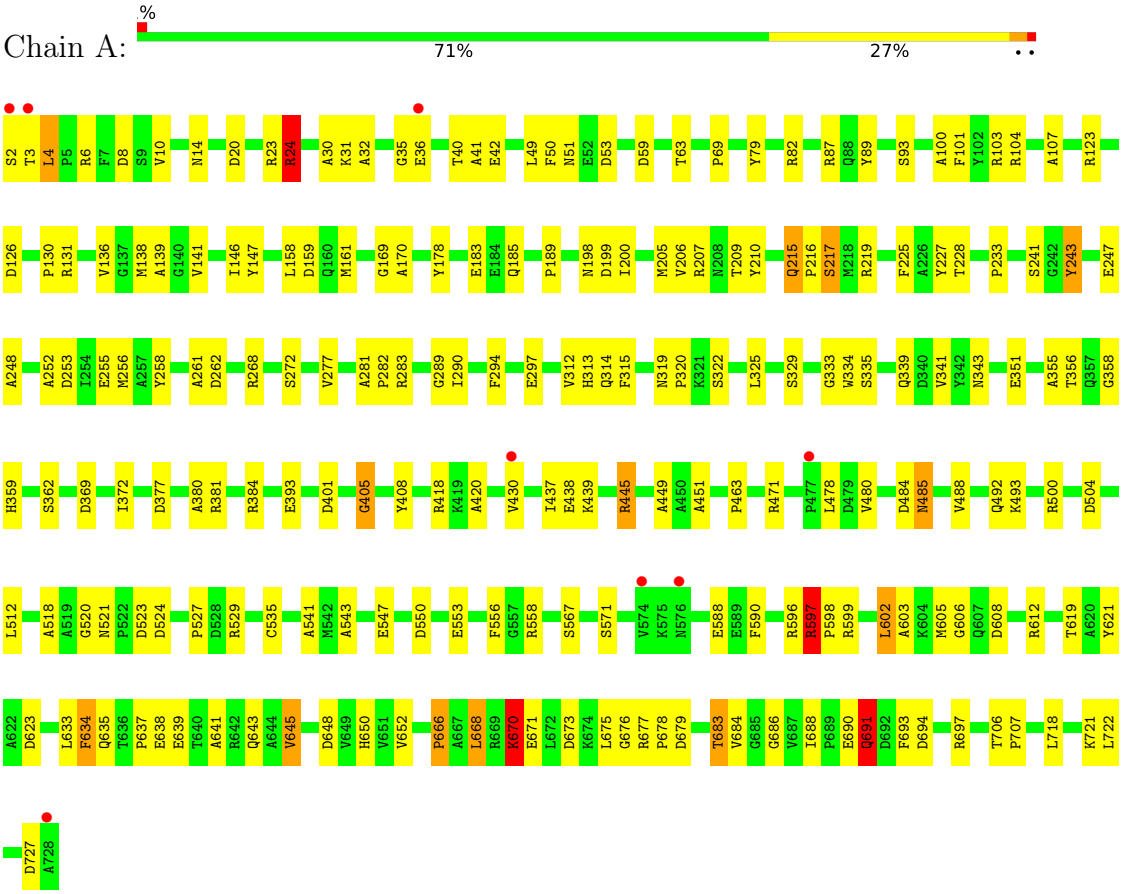
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	356	Total O 356 356	0	0
6	B	219	Total O 219 219	0	0
6	C	361	Total O 361 361	0	0
6	D	214	Total O 214 214	0	0

3 Residue-property plots (i)

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

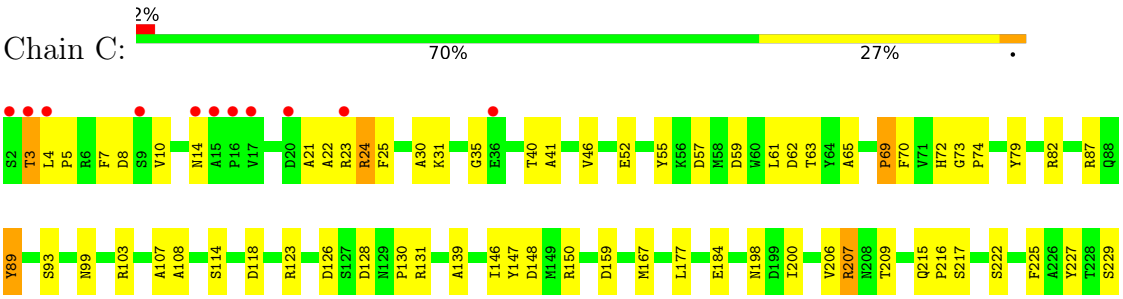
• Molecule 1: PROTEIN (METHYLMALONYL-COA MUTASE)

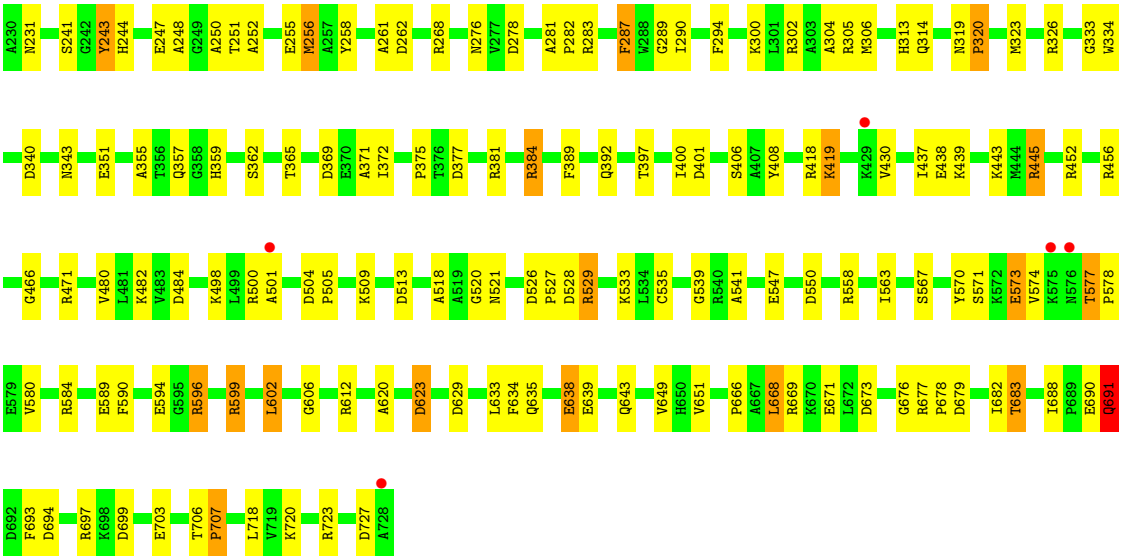
Chain A:



• Molecule 1: PROTEIN (METHYLMALONYL-COA MUTASE)

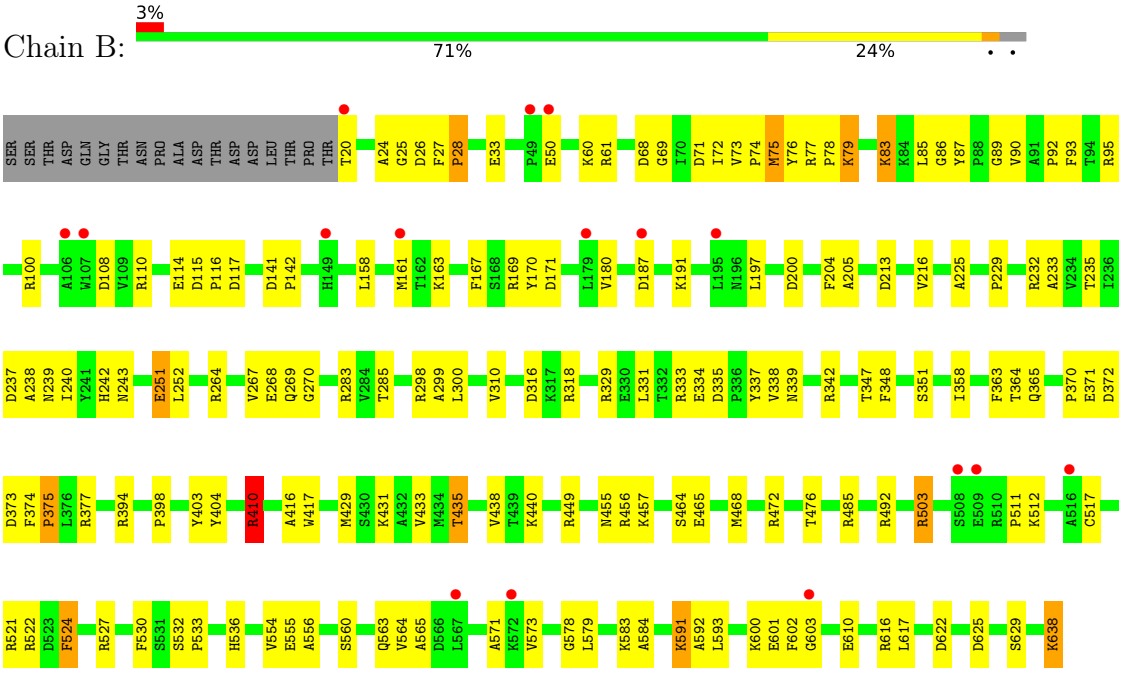
Chain C:





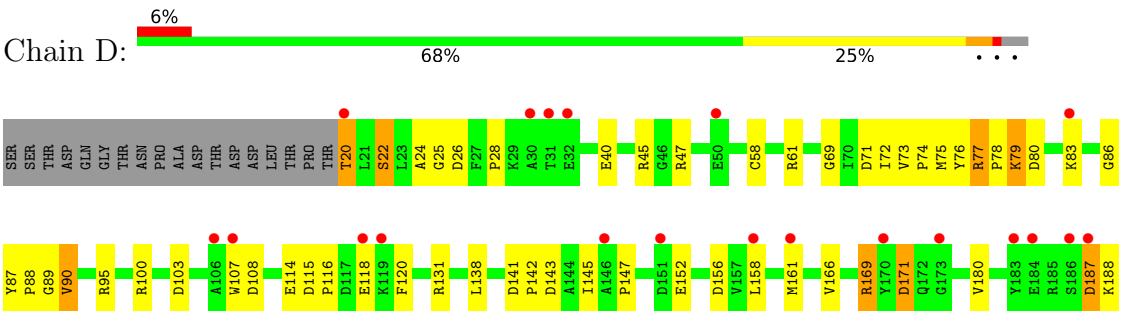
• Molecule 2: PROTEIN (METHYLMALONYL-COA MUTASE)

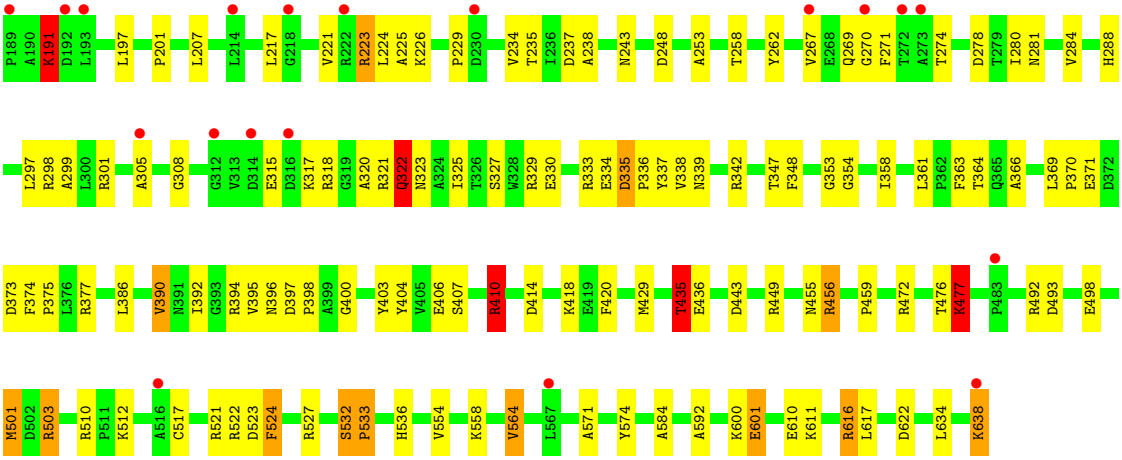
Chain B:



• Molecule 2: PROTEIN (METHYLMALONYL-COA MUTASE)

Chain D:




P189 A190 K191 D192 L193 L197 P201 L207 L214 L217 G218 V221 R222 R223 L224 A225 K226 P229 D230 V234 T235 I236 D237 A238 N243 D248 A253 T258 Y262 V267 E268 Q269 G270 F271 T272 A273 T274 D278 T279 I280 N281 V284 H288
L297 R298 A299 L300 R301 A305 G308 G312 V313 D314 E315 D316 K317 R318 G319 A320 R321 Q322 N323 A324 I325 T326 S327 W328 R329 E330 R333 E334 D335 P336 Y337 V338 N339 R342 T347 F348 G353 G354 I358 L361 P362 F363 T364 Q365 A366 L369 P370 E371 D372
D373 F374 P375 L376 R377 L386 V390 N391 I392 G393 R394 V395 N396 D397 P398 A399 G400 Y403 Y404 V405 E406 S407 R410 D414 K418 E419 F420 M429 T435 E436 D443 R449 N455 R456 P459 R472 T476 K477 P483 R492 D493 E498
M501 D502 R503 R510 P511 K512 A516 C517 R521 R522 D523 F524 R527 S532 P533 H536 V554 K558 V564 L567 A571 Y574 A584 A592 K600 E601 E610 K611 R616 L617 D622 L634 K638

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	119.95Å 160.46Å 88.48Å 90.00° 105.01° 90.00°	Depositor
Resolution (Å)	20.00 – 2.20 19.98 – 2.20	Depositor EDS
% Data completeness (in resolution range)	98.9 (20.00-2.20) 98.9 (19.98-2.20)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	0.05	Depositor
$< I/\sigma(I) >$ [1]	10.26 (at 2.19Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.206 , 0.263 0.195 , 0.242	Depositor DCC
R_{free} test set	8160 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	24.6	Xtriage
Anisotropy	0.471	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 47.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	22116	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.65% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: B12, GOL, 3CP

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	0.83	0/5717	2.17	226/7757 (2.9%)
1	C	0.85	0/5717	2.19	229/7757 (3.0%)
2	B	0.75	0/4821	2.10	167/6540 (2.6%)
2	D	0.77	2/4821 (0.0%)	2.12	169/6540 (2.6%)
All	All	0.80	2/21076 (0.0%)	2.15	791/28594 (2.8%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	C	0	1
2	D	0	1
All	All	0	3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	354	GLY	N-CA	-5.95	1.37	1.46
2	D	270	GLY	N-CA	-5.19	1.38	1.46

All (791) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	384	ARG	CD-NE-CZ	31.13	167.18	123.60
2	B	410	ARG	CD-NE-CZ	30.08	165.71	123.60
1	C	384	ARG	CD-NE-CZ	28.61	163.66	123.60
1	A	268	ARG	NE-CZ-NH2	-25.19	107.70	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	596	ARG	CD-NE-CZ	24.04	157.25	123.60
2	D	410	ARG	NE-CZ-NH1	21.16	130.88	120.30
2	B	169	ARG	CD-NE-CZ	20.05	151.66	123.60
1	A	103	ARG	CD-NE-CZ	19.01	150.21	123.60
1	A	500	ARG	NE-CZ-NH2	-18.96	110.82	120.30
2	D	410	ARG	CD-NE-CZ	18.07	148.89	123.60
2	D	410	ARG	NE-CZ-NH2	-17.61	111.50	120.30
1	C	283	ARG	NE-CZ-NH1	16.18	128.39	120.30
1	A	82	ARG	NE-CZ-NH1	15.78	128.19	120.30
1	C	283	ARG	NE-CZ-NH2	-15.44	112.58	120.30
2	B	410	ARG	NE-CZ-NH1	14.70	127.65	120.30
2	D	616	ARG	NE-CZ-NH1	-14.49	113.05	120.30
1	C	23	ARG	NE-CZ-NH1	14.40	127.50	120.30
2	D	115	ASP	CB-CG-OD1	14.21	131.09	118.30
1	A	596	ARG	NE-CZ-NH2	-14.04	113.28	120.30
1	A	500	ARG	NE-CZ-NH1	14.00	127.30	120.30
1	C	268	ARG	NE-CZ-NH2	-14.00	113.30	120.30
1	C	150	ARG	NE-CZ-NH2	-13.88	113.36	120.30
2	D	394	ARG	NE-CZ-NH2	-13.31	113.64	120.30
2	B	77	ARG	NE-CZ-NH1	13.26	126.93	120.30
2	D	169	ARG	NE-CZ-NH2	-13.23	113.69	120.30
1	C	369	ASP	CB-CG-OD2	13.02	130.02	118.30
1	C	596	ARG	NE-CZ-NH1	12.96	126.78	120.30
2	B	169	ARG	NE-CZ-NH2	-12.87	113.87	120.30
2	B	524	PHE	CB-CG-CD1	12.73	129.71	120.80
1	A	159	ASP	CB-CG-OD1	12.65	129.69	118.30
2	D	492	ARG	NE-CZ-NH2	-12.52	114.04	120.30
2	B	410	ARG	NE-CZ-NH2	-12.51	114.04	120.30
1	C	302	ARG	NE-CZ-NH1	12.47	126.53	120.30
1	C	500	ARG	NE-CZ-NH2	-12.43	114.08	120.30
1	A	381	ARG	NE-CZ-NH2	12.41	126.51	120.30
2	D	269	GLN	C-N-CA	12.09	147.69	122.30
1	A	283	ARG	NE-CZ-NH1	11.87	126.23	120.30
1	A	104	ARG	NE-CZ-NH2	11.86	126.23	120.30
1	C	381	ARG	NE-CZ-NH1	11.78	126.19	120.30
1	C	159	ASP	CB-CG-OD1	11.73	128.86	118.30
1	A	79	TYR	CB-CG-CD2	-11.63	114.02	121.00
1	A	123	ARG	NE-CZ-NH2	-11.45	114.58	120.30
2	B	503	ARG	NE-CZ-NH1	11.31	125.96	120.30
1	A	384	ARG	NE-CZ-NH1	11.25	125.93	120.30
2	D	47	ARG	NE-CZ-NH1	11.12	125.86	120.30
2	B	622	ASP	CB-CG-OD1	11.10	128.29	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	418	ARG	NE-CZ-NH1	11.05	125.83	120.30
1	C	79	TYR	CB-CG-CD2	-11.05	114.37	121.00
1	C	123	ARG	NE-CZ-NH2	-11.04	114.78	120.30
2	B	77	ARG	NE-CZ-NH2	-11.03	114.79	120.30
2	B	169	ARG	NE-CZ-NH1	10.82	125.71	120.30
2	B	394	ARG	NE-CZ-NH2	-10.82	114.89	120.30
2	B	616	ARG	NE-CZ-NH2	10.78	125.69	120.30
1	A	24	ARG	NE-CZ-NH1	10.78	125.69	120.30
2	B	616	ARG	NE-CZ-NH1	-10.64	114.98	120.30
2	B	435	THR	CA-CB-CG2	10.61	127.25	112.40
1	A	24	ARG	CG-CD-NE	10.59	134.03	111.80
1	A	82	ARG	CD-NE-CZ	10.39	138.15	123.60
1	C	82	ARG	CD-NE-CZ	10.33	138.06	123.60
2	B	100	ARG	CD-NE-CZ	10.31	138.03	123.60
2	D	322	GLN	CB-CG-CD	10.24	138.23	111.60
1	A	268	ARG	NH1-CZ-NH2	10.22	130.64	119.40
2	D	77	ARG	NE-CZ-NH2	-10.16	115.22	120.30
2	B	87	TYR	CB-CG-CD2	10.15	127.09	121.00
2	D	403	TYR	CB-CG-CD2	9.91	126.95	121.00
1	A	471	ARG	NE-CZ-NH2	-9.89	115.36	120.30
1	C	723	ARG	NE-CZ-NH1	-9.83	115.39	120.30
2	B	77	ARG	CD-NE-CZ	9.80	137.32	123.60
2	D	616	ARG	CD-NE-CZ	9.77	137.27	123.60
1	C	408	TYR	CB-CG-CD1	-9.75	115.15	121.00
2	D	348	PHE	CB-CG-CD2	9.73	127.61	120.80
1	C	484	ASP	CB-CG-OD1	9.66	127.00	118.30
1	A	484	ASP	CB-CG-OD1	9.60	126.94	118.30
1	C	723	ARG	CD-NE-CZ	9.56	136.99	123.60
1	C	456	ARG	NE-CZ-NH2	9.53	125.06	120.30
1	A	103	ARG	NE-CZ-NH1	9.52	125.06	120.30
2	D	169	ARG	NE-CZ-NH1	9.50	125.05	120.30
1	C	677	ARG	NE-CZ-NH2	-9.47	115.56	120.30
1	A	369	ASP	CB-CG-OD2	9.44	126.80	118.30
2	B	485	ARG	NE-CZ-NH1	9.39	124.99	120.30
1	C	123	ARG	CD-NE-CZ	9.32	136.65	123.60
2	D	248	ASP	CB-CG-OD2	-9.26	109.97	118.30
1	C	281	ALA	N-CA-CB	9.26	123.07	110.10
2	B	527	ARG	NE-CZ-NH2	-9.23	115.69	120.30
2	B	521	ARG	NE-CZ-NH2	-9.22	115.69	120.30
1	C	227	TYR	CB-CG-CD2	9.19	126.52	121.00
2	D	187	ASP	C-N-CA	9.17	144.63	121.70
2	D	89	GLY	C-N-CA	9.17	144.63	121.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	547	GLU	OE1-CD-OE2	-9.15	112.31	123.30
2	B	485	ARG	CD-NE-CZ	9.12	136.36	123.60
2	B	449	ARG	NE-CZ-NH1	-9.10	115.75	120.30
1	A	520	GLY	O-C-N	-9.04	108.23	122.70
1	C	408	TYR	CB-CG-CD2	8.94	126.36	121.00
2	D	435	THR	CA-CB-CG2	8.91	124.88	112.40
2	D	45	ARG	NE-CZ-NH2	-8.91	115.85	120.30
2	D	24	ALA	C-N-CA	8.90	140.99	122.30
1	A	599	ARG	CD-NE-CZ	8.89	136.05	123.60
2	D	229	PRO	C-N-CA	8.88	143.90	121.70
2	B	342	ARG	NE-CZ-NH1	8.87	124.73	120.30
1	C	314	GLN	O-C-N	-8.84	108.56	122.70
2	B	298	ARG	NE-CZ-NH1	8.83	124.71	120.30
1	C	131	ARG	NE-CZ-NH2	8.80	124.70	120.30
1	C	24	ARG	CG-CD-NE	8.79	130.26	111.80
1	C	206	VAL	CA-CB-CG1	8.78	124.08	110.90
2	B	117	ASP	CB-CG-OD1	8.72	126.14	118.30
1	C	24	ARG	NE-CZ-NH1	8.69	124.65	120.30
2	D	353	GLY	C-N-CA	8.69	140.56	122.30
1	A	24	ARG	NE-CZ-NH2	-8.67	115.97	120.30
2	D	524	PHE	CB-CG-CD1	8.67	126.87	120.80
2	D	397	ASP	CB-CG-OD2	8.66	126.10	118.30
1	A	103	ARG	NE-CZ-NH2	-8.54	116.03	120.30
2	D	449	ARG	NE-CZ-NH2	-8.47	116.06	120.30
2	D	456	ARG	O-C-N	-8.45	109.18	122.70
1	C	633	LEU	O-C-N	-8.45	109.18	122.70
2	B	373	ASP	CB-CG-OD2	8.44	125.90	118.30
2	D	321	ARG	NE-CZ-NH2	-8.44	116.08	120.30
2	D	61	ARG	CD-NE-CZ	8.43	135.41	123.60
1	C	526	ASP	CB-CG-OD2	8.43	125.89	118.30
1	A	131	ARG	NE-CZ-NH2	8.42	124.51	120.30
1	C	55	TYR	CB-CG-CD2	8.38	126.03	121.00
1	C	59	ASP	CB-CG-OD1	8.37	125.83	118.30
2	D	95	ARG	CG-CD-NE	8.36	129.35	111.80
2	B	86	GLY	CA-C-O	8.34	135.62	120.60
1	C	8	ASP	C-N-CA	8.29	142.41	121.70
1	C	89	TYR	CA-CB-CG	8.24	129.05	113.40
2	B	171	ASP	CB-CG-OD1	8.23	125.71	118.30
1	A	697	ARG	NE-CZ-NH1	8.22	124.41	120.30
2	B	616	ARG	CD-NE-CZ	8.22	135.11	123.60
2	D	492	ARG	NE-CZ-NH1	8.19	124.39	120.30
1	A	343	ASN	O-C-N	-8.14	109.68	122.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	329	ARG	NE-CZ-NH2	8.12	124.36	120.30
1	A	590	PHE	CB-CG-CD2	8.11	126.48	120.80
2	B	348	PHE	CB-CG-CD2	8.08	126.46	120.80
2	B	377	ARG	NE-CZ-NH2	-8.08	116.26	120.30
1	A	634	PHE	CB-CG-CD1	-8.03	115.18	120.80
1	C	679	ASP	CB-CG-OD2	7.99	125.49	118.30
1	C	377	ASP	CB-CG-OD1	7.99	125.49	118.30
1	C	550	ASP	CB-CG-OD2	-7.95	111.15	118.30
1	C	79	TYR	CB-CG-CD1	7.91	125.75	121.00
2	D	238	ALA	C-N-CA	7.89	141.43	121.70
2	B	89	GLY	O-C-N	-7.88	110.08	122.70
2	B	86	GLY	O-C-N	-7.83	110.17	122.70
1	C	103	ARG	NE-CZ-NH2	-7.83	116.39	120.30
1	A	294	PHE	CB-CG-CD2	7.82	126.28	120.80
1	A	6	ARG	CD-NE-CZ	7.81	134.53	123.60
1	C	596	ARG	NE-CZ-NH2	-7.78	116.41	120.30
2	B	377	ARG	NE-CZ-NH1	7.76	124.18	120.30
2	D	72	ILE	CB-CG1-CD1	7.76	135.63	113.90
1	A	599	ARG	CG-CD-NE	7.76	128.09	111.80
1	A	79	TYR	CB-CG-CD1	7.75	125.65	121.00
2	B	213	ASP	CB-CG-OD2	-7.75	111.33	118.30
1	A	207	ARG	CD-NE-CZ	7.70	134.38	123.60
1	C	146	ILE	O-C-N	-7.68	110.42	122.70
2	B	522	ARG	NE-CZ-NH1	-7.62	116.49	120.30
1	C	673	ASP	CB-CG-OD1	7.62	125.15	118.30
1	A	445	ARG	NE-CZ-NH2	-7.61	116.49	120.30
2	B	601	GLU	O-C-N	-7.61	110.52	122.70
2	D	315	GLU	C-N-CA	7.61	140.73	121.70
2	D	477	LYS	N-CA-CB	7.59	124.27	110.60
1	C	126	ASP	CB-CG-OD2	-7.57	111.49	118.30
2	B	601	GLU	C-N-CA	7.57	140.62	121.70
1	C	573	GLU	CA-C-N	7.54	133.79	117.20
1	A	89	TYR	CA-CB-CG	7.53	127.70	113.40
1	A	608	ASP	CB-CG-OD1	7.53	125.07	118.30
1	A	547	GLU	OE1-CD-OE2	-7.52	114.27	123.30
2	B	72	ILE	CB-CG1-CD1	7.52	134.95	113.90
2	B	329	ARG	NE-CZ-NH2	7.52	124.06	120.30
2	D	61	ARG	NE-CZ-NH1	7.52	124.06	120.30
1	A	377	ASP	CB-CG-OD1	7.51	125.06	118.30
2	D	278	ASP	CA-C-N	7.51	133.72	117.20
2	B	108	ASP	N-CA-CB	-7.50	97.11	110.60
2	B	232	ARG	CD-NE-CZ	7.46	134.04	123.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	178	TYR	CB-CG-CD1	-7.42	116.55	121.00
1	A	358	GLY	O-C-N	-7.42	110.82	122.70
1	C	24	ARG	CD-NE-CZ	7.42	133.98	123.60
2	B	283	ARG	NE-CZ-NH1	7.41	124.00	120.30
1	C	41	ALA	C-N-CA	7.41	140.22	121.70
2	D	634	LEU	C-N-CA	7.40	137.85	122.30
1	C	150	ARG	NH1-CZ-NH2	7.36	127.50	119.40
1	A	535	CYS	O-C-N	-7.35	110.94	122.70
1	A	553	GLU	O-C-N	-7.34	110.96	122.70
2	D	363	PHE	C-N-CA	7.32	140.01	121.70
2	B	337	TYR	O-C-N	-7.32	110.99	122.70
1	A	633	LEU	O-C-N	-7.31	111.00	122.70
2	B	71	ASP	CB-CG-OD1	7.31	124.88	118.30
2	D	398	PRO	O-C-N	-7.31	111.01	122.70
2	D	24	ALA	O-C-N	-7.30	110.78	123.20
2	D	169	ARG	CD-NE-CZ	7.29	133.81	123.60
1	A	210	TYR	CB-CG-CD1	7.29	125.37	121.00
2	D	131	ARG	CD-NE-CZ	7.29	133.80	123.60
1	A	294	PHE	CB-CG-CD1	-7.29	115.70	120.80
2	B	536	HIS	O-C-N	-7.29	111.04	122.70
1	C	676	GLY	O-C-N	-7.29	111.04	122.70
1	A	697	ARG	NE-CZ-NH2	-7.27	116.66	120.30
2	D	20	THR	O-C-N	-7.27	111.07	122.70
2	D	339	ASN	O-C-N	-7.27	111.07	122.70
2	D	301	ARG	CA-C-N	7.27	133.19	117.20
2	B	229	PRO	C-N-CA	7.25	139.82	121.70
2	D	78	PRO	O-C-N	-7.24	111.11	122.70
2	D	229	PRO	O-C-N	-7.24	111.12	122.70
1	C	22	ALA	CB-CA-C	7.22	120.94	110.10
1	A	243	TYR	CB-CG-CD2	7.22	125.33	121.00
1	C	683	THR	N-CA-CB	7.20	123.97	110.30
1	C	93	SER	N-CA-CB	-7.18	99.73	110.50
2	D	472	ARG	NE-CZ-NH2	-7.17	116.71	120.30
2	B	492	ARG	CD-NE-CZ	7.17	133.64	123.60
2	D	400	GLY	CA-C-O	7.17	133.50	120.60
2	D	600	LYS	O-C-N	-7.15	111.25	122.70
2	B	187	ASP	C-N-CA	7.14	139.56	121.70
2	D	26	ASP	CB-CA-C	-7.14	96.12	110.40
2	D	418	LYS	CA-C-N	7.14	132.91	117.20
1	A	207	ARG	NE-CZ-NH2	7.12	123.86	120.30
1	A	225	PHE	CB-CG-CD2	7.10	125.77	120.80
1	A	53	ASP	CB-CG-OD1	7.09	124.68	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	283	ARG	CD-NE-CZ	7.08	133.51	123.60
2	D	536	HIS	O-C-N	-7.08	111.38	122.70
1	C	727	ASP	C-N-CA	7.07	139.37	121.70
1	C	612	ARG	NE-CZ-NH1	-7.06	116.77	120.30
1	C	439	LYS	C-N-CA	7.06	137.12	122.30
1	A	679	ASP	CB-CG-OD1	7.05	124.65	118.30
1	C	304	ALA	O-C-N	-7.05	111.42	122.70
1	A	362	SER	N-CA-CB	7.05	121.07	110.50
2	B	229	PRO	O-C-N	-7.01	111.49	122.70
2	B	268	GLU	C-N-CA	7.00	139.21	121.70
2	D	521	ARG	NE-CZ-NH2	-7.00	116.80	120.30
1	C	439	LYS	O-C-N	-6.99	111.33	123.20
2	D	523	ASP	CB-CG-OD2	-6.98	112.02	118.30
1	A	147	TYR	CB-CG-CD2	6.96	125.18	121.00
1	A	59	ASP	CB-CG-OD1	6.95	124.56	118.30
1	C	633	LEU	CA-C-O	6.94	134.67	120.10
1	C	518	ALA	N-CA-CB	6.93	119.81	110.10
1	C	52	GLU	C-N-CA	6.92	139.01	121.70
1	A	556	PHE	CB-CG-CD2	6.92	125.64	120.80
1	A	675	LEU	C-N-CA	6.88	136.75	122.30
2	D	100	ARG	NE-CZ-NH1	6.88	123.74	120.30
2	D	404	TYR	CG-CD1-CE1	6.88	126.80	121.30
1	C	70	PHE	O-C-N	-6.87	111.71	122.70
2	B	456	ARG	NE-CZ-NH2	-6.86	116.87	120.30
2	D	143	ASP	CB-CG-OD1	6.85	124.47	118.30
2	D	348	PHE	CB-CG-CD1	-6.85	116.00	120.80
1	A	381	ARG	NH1-CZ-NH2	-6.85	111.87	119.40
2	D	617	LEU	CA-CB-CG	6.84	131.03	115.30
2	B	235	THR	N-CA-CB	6.83	123.28	110.30
2	B	225	ALA	C-N-CA	6.82	138.75	121.70
2	D	100	ARG	NE-CZ-NH2	-6.82	116.89	120.30
2	B	530	PHE	CB-CG-CD1	-6.81	116.03	120.80
2	B	283	ARG	N-CA-CB	6.80	122.85	110.60
1	A	183	GLU	O-C-N	-6.80	111.82	122.70
1	C	255	GLU	OE1-CD-OE2	-6.78	115.16	123.30
2	D	335	ASP	CB-CG-OD1	6.77	124.39	118.30
1	C	282	PRO	N-CA-CB	6.77	111.42	103.30
2	B	233	ALA	CB-CA-C	-6.76	99.96	110.10
1	C	103	ARG	CD-NE-CZ	6.76	133.06	123.60
1	A	206	VAL	CA-CB-CG1	6.75	121.03	110.90
1	A	329	SER	N-CA-CB	6.74	120.61	110.50
1	A	255	GLU	OE1-CD-OE2	-6.73	115.22	123.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	333	ARG	CD-NE-CZ	6.72	133.00	123.60
1	A	666	PRO	N-CA-CB	6.71	111.35	103.30
1	C	256	MET	CA-CB-CG	6.71	124.71	113.30
1	C	251	THR	O-C-N	-6.71	111.97	122.70
1	A	41	ALA	O-C-N	-6.71	111.97	122.70
1	C	438	GLU	O-C-N	-6.70	111.99	122.70
2	D	116	PRO	N-CA-CB	6.70	111.34	103.30
2	D	601	GLU	O-C-N	-6.69	112.00	122.70
1	A	691	GLN	CA-CB-CG	6.68	128.10	113.40
1	C	320	PRO	N-CA-CB	6.67	111.30	103.30
1	A	588	GLU	OE1-CD-OE2	6.67	131.30	123.30
2	D	342	ARG	NE-CZ-NH2	6.65	123.63	120.30
1	A	597	ARG	NE-CZ-NH2	-6.65	116.97	120.30
2	D	322	GLN	CA-C-O	6.65	134.07	120.10
2	D	403	TYR	CB-CG-CD1	-6.65	117.01	121.00
1	A	408	TYR	CB-CG-CD2	6.65	124.99	121.00
1	C	602	LEU	CB-CG-CD1	-6.65	99.70	111.00
1	C	520	GLY	O-C-N	-6.64	112.07	122.70
1	A	637	PRO	C-N-CA	6.64	138.31	121.70
1	A	6	ARG	NE-CZ-NH2	-6.63	116.98	120.30
1	C	501	ALA	CB-CA-C	6.62	120.03	110.10
1	C	52	GLU	O-C-N	-6.59	112.16	122.70
1	A	261	ALA	O-C-N	-6.58	112.17	122.70
1	A	49	LEU	CA-C-O	6.57	133.89	120.10
1	A	437	ILE	O-C-N	-6.56	112.20	122.70
1	C	69	PRO	O-C-N	-6.56	112.21	122.70
1	A	209	THR	N-CA-CB	6.55	122.74	110.30
1	C	261	ALA	O-C-N	-6.55	112.22	122.70
1	C	306	MET	CG-SD-CE	6.55	110.67	100.20
1	C	62	ASP	CA-C-O	6.54	133.83	120.10
2	D	262	TYR	CB-CG-CD2	-6.53	117.08	121.00
1	A	8	ASP	C-N-CA	6.53	138.02	121.70
2	B	171	ASP	CB-CG-OD2	-6.51	112.44	118.30
2	B	68	ASP	CB-CG-OD1	6.51	124.16	118.30
1	A	8	ASP	CB-CG-OD1	-6.50	112.45	118.30
2	B	449	ARG	NH1-CZ-NH2	6.50	126.55	119.40
2	B	492	ARG	NE-CZ-NH2	-6.50	117.05	120.30
2	B	476	THR	CA-CB-CG2	6.49	121.49	112.40
2	B	468	MET	CG-SD-CE	6.49	110.58	100.20
2	D	522	ARG	CB-CA-C	-6.49	97.43	110.40
1	A	637	PRO	O-C-N	-6.48	112.33	122.70
2	D	223	ARG	NE-CZ-NH2	-6.47	117.07	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	169	GLY	O-C-N	-6.46	112.36	122.70
1	A	170	ALA	O-C-N	-6.46	112.36	122.70
2	D	456	ARG	NE-CZ-NH2	-6.46	117.07	120.30
1	A	541	ALA	O-C-N	-6.45	112.38	122.70
2	D	58	CYS	CA-CB-SG	-6.45	102.39	114.00
1	A	621	TYR	CB-CG-CD1	6.45	124.87	121.00
1	A	169	GLY	CA-C-O	6.44	132.19	120.60
1	A	146	ILE	O-C-N	-6.43	112.41	122.70
1	A	141	VAL	CA-CB-CG1	6.43	120.54	110.90
2	D	90	VAL	CA-CB-CG2	6.42	120.53	110.90
1	A	596	ARG	NE-CZ-NH1	6.42	123.51	120.30
2	D	171	ASP	CB-CG-OD2	-6.42	112.52	118.30
2	D	269	GLN	O-C-N	-6.42	112.29	123.20
2	B	521	ARG	NE-CZ-NH1	6.42	123.51	120.30
1	C	41	ALA	O-C-N	-6.42	112.43	122.70
1	C	128	ASP	CB-CG-OD1	6.42	124.07	118.30
2	D	574	TYR	CB-CG-CD1	-6.42	117.15	121.00
1	C	302	ARG	NH1-CZ-NH2	-6.41	112.35	119.40
1	A	258	TYR	CB-CG-CD2	6.41	124.84	121.00
1	C	227	TYR	CB-CG-CD1	-6.39	117.17	121.00
1	C	430	VAL	O-C-N	-6.37	112.37	123.20
1	A	697	ARG	CD-NE-CZ	6.37	132.52	123.60
1	A	694	ASP	CB-CG-OD1	6.37	124.03	118.30
2	B	89	GLY	C-N-CA	6.37	137.62	121.70
1	A	684	VAL	CG1-CB-CG2	-6.36	100.72	110.90
1	C	623	ASP	CB-CG-OD1	6.35	124.02	118.30
2	B	372	ASP	CB-CG-OD1	6.35	124.02	118.30
1	C	123	ARG	NE-CZ-NH1	6.34	123.47	120.30
2	D	455	ASN	O-C-N	-6.34	112.55	122.70
2	D	493	ASP	CB-CG-OD1	6.34	124.01	118.30
2	B	339	ASN	O-C-N	-6.33	112.57	122.70
2	D	396	ASN	N-CA-CB	6.31	121.96	110.60
1	A	683	THR	N-CA-CB	6.31	122.29	110.30
2	D	262	TYR	CB-CG-CD1	6.31	124.79	121.00
1	C	241	SER	N-CA-C	6.31	128.03	111.00
2	B	375	PRO	N-CA-CB	6.30	110.86	103.30
1	A	493	LYS	O-C-N	-6.30	112.61	122.70
2	B	33	GLU	OE1-CD-OE2	-6.29	115.75	123.30
2	B	524	PHE	CB-CG-CD2	-6.29	116.40	120.80
1	A	677	ARG	NE-CZ-NH1	6.29	123.44	120.30
1	A	253	ASP	CB-CG-OD1	6.28	123.95	118.30
2	B	115	ASP	CB-CG-OD1	6.28	123.95	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	287	PHE	CB-CG-CD1	6.28	125.20	120.80
1	C	677	ARG	NH1-CZ-NH2	6.28	126.31	119.40
1	C	206	VAL	CG1-CB-CG2	-6.28	100.86	110.90
1	C	222	SER	O-C-N	-6.27	112.67	122.70
2	D	503	ARG	NE-CZ-NH1	6.27	123.44	120.30
2	B	25	GLY	O-C-N	-6.27	112.67	122.70
1	C	541	ALA	O-C-N	-6.27	112.67	122.70
1	C	504	ASP	CB-CG-OD1	6.27	123.94	118.30
1	C	268	ARG	O-C-N	-6.27	112.67	122.70
1	A	676	GLY	O-C-N	-6.26	112.68	122.70
1	C	590	PHE	CB-CG-CD2	6.26	125.18	120.80
1	C	570	TYR	CB-CG-CD2	6.26	124.75	121.00
2	B	76	TYR	CB-CG-CD1	-6.26	117.25	121.00
1	C	184	GLU	C-N-CA	6.25	137.32	121.70
2	D	298	ARG	CD-NE-CZ	6.24	132.34	123.60
2	B	283	ARG	NE-CZ-NH2	-6.24	117.18	120.30
1	C	381	ARG	NH1-CZ-NH2	-6.23	112.55	119.40
1	C	678	PRO	N-CA-CB	6.23	110.77	103.30
2	D	493	ASP	O-C-N	-6.22	112.74	122.70
1	C	723	ARG	O-C-N	-6.22	112.75	122.70
2	D	75	MET	CG-SD-CE	-6.21	90.26	100.20
2	D	510	ARG	NE-CZ-NH2	-6.21	117.19	120.30
1	A	605	MET	CG-SD-CE	6.19	110.11	100.20
2	B	95	ARG	CG-CD-NE	6.19	124.80	111.80
2	B	602	PHE	C-N-CA	6.19	135.30	122.30
1	A	313	HIS	C-N-CA	6.18	137.16	121.70
2	B	600	LYS	C-N-CA	6.18	137.16	121.70
2	D	527	ARG	NE-CZ-NH1	6.17	123.39	120.30
1	C	262	ASP	CB-CG-OD2	6.17	123.86	118.30
2	B	455	ASN	O-C-N	-6.17	112.83	122.70
1	A	333	GLY	O-C-N	-6.16	112.84	122.70
1	A	93	SER	N-CA-CB	-6.16	101.26	110.50
2	D	20	THR	CA-C-N	6.16	130.75	117.20
1	A	87	ARG	NE-CZ-NH1	-6.15	117.22	120.30
1	C	529	ARG	NE-CZ-NH2	-6.15	117.22	120.30
1	A	405	GLY	CA-C-N	6.15	130.73	117.20
1	A	297	GLU	OE1-CD-OE2	-6.14	115.93	123.30
1	A	281	ALA	N-CA-CB	6.14	118.70	110.10
1	A	639	GLU	OE1-CD-OE2	-6.14	115.93	123.30
2	B	299	ALA	N-CA-CB	6.14	118.70	110.10
2	B	610	GLU	O-C-N	-6.13	112.90	122.70
1	A	24	ARG	CD-NE-CZ	6.12	132.16	123.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	243	TYR	CB-CG-CD2	6.12	124.67	121.00
2	D	373	ASP	CB-CG-OD2	6.11	123.80	118.30
2	B	522	ARG	CB-CA-C	-6.11	98.19	110.40
2	B	337	TYR	CB-CG-CD2	6.11	124.66	121.00
2	D	166	VAL	N-CA-CB	6.10	124.93	111.50
2	D	414	ASP	CB-CG-OD2	6.10	123.79	118.30
2	B	555	GLU	OE1-CD-OE2	-6.09	115.99	123.30
2	D	223	ARG	O-C-N	-6.09	112.96	122.70
1	A	727	ASP	C-N-CA	6.08	136.91	121.70
1	A	41	ALA	C-N-CA	6.08	136.91	121.70
1	C	35	GLY	CA-C-O	6.07	131.53	120.60
1	C	209	THR	N-CA-CB	6.07	121.83	110.30
2	B	239	ASN	O-C-N	-6.07	112.99	122.70
1	A	688	ILE	CA-CB-CG1	6.06	122.52	111.00
1	A	206	VAL	CB-CA-C	-6.06	99.88	111.40
2	B	76	TYR	CB-CG-CD2	6.06	124.64	121.00
2	B	503	ARG	NE-CZ-NH2	-6.06	117.27	120.30
1	C	629	ASP	CB-CG-OD1	6.06	123.76	118.30
1	C	207	ARG	NE-CZ-NH1	-6.06	117.27	120.30
1	C	248	ALA	C-N-CA	6.06	135.02	122.30
2	D	22	SER	N-CA-CB	6.06	119.58	110.50
1	A	504	ASP	CB-CG-OD1	6.05	123.75	118.30
1	A	527	PRO	N-CA-CB	6.05	110.56	103.30
1	C	362	SER	N-CA-CB	6.05	119.58	110.50
1	C	498	LYS	CA-CB-CG	6.05	126.71	113.40
2	B	78	PRO	O-C-N	-6.04	113.03	122.70
1	A	553	GLU	C-N-CA	6.04	136.80	121.70
2	D	418	LYS	O-C-N	-6.04	113.04	122.70
1	C	574	VAL	N-CA-CB	6.03	124.77	111.50
1	C	676	GLY	CA-C-O	6.03	131.45	120.60
2	D	533	PRO	N-CA-CB	6.03	110.53	103.30
1	A	430	VAL	O-C-N	-6.02	112.97	123.20
1	A	228	THR	O-C-N	-6.00	113.10	122.70
2	D	377	ARG	NE-CZ-NH2	-6.00	117.30	120.30
2	D	610	GLU	O-C-N	-6.00	113.11	122.70
2	B	61	ARG	NE-CZ-NH1	5.99	123.30	120.30
2	B	457	LYS	O-C-N	-5.99	113.12	122.70
1	C	40	THR	O-C-N	-5.99	113.11	122.70
2	B	560	SER	C-N-CA	5.98	134.86	122.30
1	A	438	GLU	O-C-N	-5.98	113.13	122.70
1	A	282	PRO	O-C-N	-5.97	113.15	122.70
2	D	237	ASP	CB-CG-OD2	5.96	123.66	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	390	VAL	O-C-N	-5.95	113.18	122.70
1	A	277	VAL	C-N-CA	5.95	136.57	121.70
1	A	648	ASP	CB-CG-OD2	-5.95	112.95	118.30
1	A	334	TRP	O-C-N	-5.94	113.19	122.70
1	A	504	ASP	CB-CG-OD2	-5.93	112.96	118.30
1	A	312	VAL	CG1-CB-CG2	-5.93	101.42	110.90
2	B	591	LYS	CA-CB-CG	5.93	126.44	113.40
2	B	78	PRO	N-CA-CB	5.92	110.41	103.30
1	C	666	PRO	N-CA-CB	5.92	110.41	103.30
1	A	325	LEU	CB-CG-CD2	5.92	121.06	111.00
1	C	198	ASN	N-CA-CB	-5.91	99.97	110.60
2	D	371	GLU	CA-CB-CG	5.91	126.39	113.40
1	C	320	PRO	C-N-CA	5.90	136.45	121.70
1	C	535	CYS	O-C-N	-5.89	113.27	122.70
1	A	693	PHE	CB-CG-CD1	5.89	124.92	120.80
2	B	560	SER	O-C-N	-5.89	113.19	123.20
2	D	71	ASP	CB-CG-OD1	5.89	123.60	118.30
1	C	3	THR	N-CA-CB	5.88	121.48	110.30
1	A	210	TYR	CB-CG-CD2	-5.88	117.47	121.00
1	C	278	ASP	CB-CG-OD1	5.87	123.58	118.30
2	B	600	LYS	O-C-N	-5.87	113.31	122.70
1	C	690	GLU	O-C-N	-5.87	113.31	122.70
1	A	130	PRO	CA-C-N	5.86	130.10	117.20
1	A	283	ARG	NH1-CZ-NH2	-5.86	112.96	119.40
1	A	645	VAL	O-C-N	-5.86	113.33	122.70
1	C	466	GLY	O-C-N	-5.85	113.34	122.70
1	A	262	ASP	O-C-N	-5.85	113.26	123.20
1	C	343	ASN	O-C-N	-5.85	113.34	122.70
2	D	237	ASP	O-C-N	-5.84	113.35	122.70
2	D	238	ALA	O-C-N	-5.84	113.35	122.70
1	A	690	GLU	O-C-N	-5.83	113.37	122.70
1	C	313	HIS	O-C-N	-5.83	113.37	122.70
1	C	445	ARG	NE-CZ-NH2	-5.83	117.39	120.30
1	A	51	ASN	C-N-CA	5.82	136.25	121.70
2	D	40	GLU	OE1-CD-OE2	-5.82	116.32	123.30
1	A	633	LEU	CA-C-O	5.79	132.25	120.10
2	D	501	MET	CG-SD-CE	5.78	109.44	100.20
1	A	691	GLN	CB-CG-CD	5.77	126.60	111.60
2	B	333	ARG	NE-CZ-NH2	5.76	123.18	120.30
2	D	321	ARG	NE-CZ-NH1	5.76	123.18	120.30
2	B	578	GLY	CA-C-O	5.76	130.97	120.60
1	C	146	ILE	C-N-CA	5.76	136.10	121.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	703	GLU	CA-CB-CG	5.75	126.04	113.40
2	D	498	GLU	OE1-CD-OE2	-5.74	116.41	123.30
2	D	278	ASP	O-C-N	-5.74	113.52	122.70
2	D	622	ASP	CB-CG-OD1	5.74	123.46	118.30
1	A	23	ARG	O-C-N	-5.74	113.52	122.70
1	A	439	LYS	C-N-CA	5.73	134.34	122.30
2	D	305	ALA	CB-CA-C	-5.73	101.50	110.10
1	A	159	ASP	CB-CG-OD2	-5.72	113.15	118.30
1	A	313	HIS	O-C-N	-5.72	113.56	122.70
1	C	55	TYR	CB-CG-CD1	-5.72	117.57	121.00
2	D	299	ALA	N-CA-CB	5.71	118.10	110.10
1	C	22	ALA	N-CA-CB	-5.71	102.11	110.10
2	B	28	PRO	N-CA-CB	5.71	110.15	103.30
1	C	59	ASP	N-CA-CB	-5.70	100.34	110.60
1	C	326	ARG	CD-NE-CZ	5.69	131.57	123.60
2	D	79	LYS	O-C-N	-5.68	113.60	122.70
1	C	159	ASP	OD1-CG-OD2	-5.68	112.50	123.30
1	C	46	VAL	CG1-CB-CG2	-5.67	101.83	110.90
2	D	235	THR	N-CA-CB	5.67	121.08	110.30
2	D	503	ARG	NE-CZ-NH2	-5.67	117.47	120.30
2	B	398	PRO	N-CA-CB	5.67	110.10	103.30
1	C	357	GLN	O-C-N	-5.67	113.57	123.20
2	B	318	ARG	CD-NE-CZ	5.66	131.53	123.60
1	C	268	ARG	NE-CZ-NH1	5.66	123.13	120.30
1	C	639	GLU	OE1-CD-OE2	-5.66	116.51	123.30
1	A	393	GLU	N-CA-CB	-5.66	100.42	110.60
1	A	63	THR	O-C-N	-5.65	113.66	122.70
1	A	233	PRO	N-CA-CB	5.65	110.08	103.30
2	B	95	ARG	NE-CZ-NH2	-5.65	117.47	120.30
2	B	78	PRO	C-N-CA	5.65	135.82	121.70
2	B	363	PHE	C-N-CA	5.65	135.82	121.70
1	C	697	ARG	O-C-N	-5.64	113.67	122.70
1	A	126	ASP	CB-CG-OD2	-5.64	113.22	118.30
2	B	204	PHE	CB-CG-CD1	-5.64	116.85	120.80
1	A	612	ARG	NE-CZ-NH2	-5.64	117.48	120.30
1	C	79	TYR	O-C-N	-5.64	113.68	122.70
1	A	100	ALA	CB-CA-C	5.63	118.55	110.10
1	C	63	THR	C-N-CA	5.63	135.78	121.70
1	C	529	ARG	NE-CZ-NH1	5.63	123.11	120.30
2	D	337	TYR	O-C-N	-5.63	113.69	122.70
1	C	57	ASP	CB-CG-OD1	-5.62	113.24	118.30
1	C	300	LYS	O-C-N	-5.62	113.70	122.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	451	ALA	O-C-N	-5.62	113.71	122.70
1	A	333	GLY	C-N-CA	5.62	135.75	121.70
2	D	524	PHE	CB-CG-CD2	-5.62	116.87	120.80
1	A	523	ASP	CB-CG-OD1	5.61	123.35	118.30
1	C	484	ASP	CB-CG-OD2	-5.61	113.26	118.30
2	B	100	ARG	NE-CZ-NH1	5.60	123.10	120.30
1	A	437	ILE	CA-C-N	5.60	129.53	117.20
1	A	471	ARG	CD-NE-CZ	5.60	131.44	123.60
1	C	723	ARG	CB-CG-CD	5.60	126.16	111.60
2	B	617	LEU	CA-CB-CG	5.60	128.18	115.30
1	C	276	ASN	C-N-CA	5.60	135.69	121.70
2	D	120	PHE	CB-CG-CD2	5.59	124.72	120.80
1	C	250	ALA	CB-CA-C	-5.59	101.71	110.10
2	B	571	ALA	N-CA-CB	5.59	117.92	110.10
1	C	651	VAL	CG1-CB-CG2	-5.59	101.96	110.90
1	C	529	ARG	N-CA-CB	-5.58	100.55	110.60
1	C	258	TYR	CB-CG-CD2	5.58	124.35	121.00
1	C	629	ASP	N-CA-CB	5.57	120.63	110.60
2	D	601	GLU	C-N-CA	5.57	135.63	121.70
1	A	30	ALA	O-C-N	-5.57	113.79	122.70
1	A	408	TYR	CB-CG-CD1	-5.57	117.66	121.00
1	C	527	PRO	N-CA-CB	5.56	109.98	103.30
2	B	90	VAL	CA-CB-CG2	5.56	119.24	110.90
1	C	107	ALA	O-C-N	-5.56	113.81	122.70
1	A	449	ALA	O-C-N	-5.55	113.82	122.70
1	C	282	PRO	O-C-N	-5.55	113.82	122.70
2	D	449	ARG	O-C-N	-5.55	113.81	122.70
1	A	185	GLN	C-N-CA	5.55	133.95	122.30
2	D	171	ASP	CB-CG-OD1	5.55	123.29	118.30
2	B	24	ALA	N-CA-CB	5.55	117.87	110.10
1	C	693	PHE	CB-CG-CD1	5.55	124.68	120.80
1	A	131	ARG	CD-NE-CZ	5.54	131.36	123.60
1	A	198	ASN	N-CA-CB	-5.54	100.62	110.60
1	C	73	GLY	N-CA-C	-5.54	99.25	113.10
1	A	147	TYR	CB-CG-CD1	-5.53	117.68	121.00
2	B	573	VAL	CA-C-N	5.53	129.36	117.20
2	B	600	LYS	CA-C-N	5.52	129.35	117.20
2	D	564	VAL	CG1-CB-CG2	-5.52	102.07	110.90
1	A	351	GLU	O-C-N	-5.52	113.87	122.70
1	A	215	GLN	CB-CG-CD	5.51	125.94	111.60
1	A	343	ASN	C-N-CA	5.51	135.47	121.70
1	C	633	LEU	C-N-CA	5.50	135.46	121.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	463	PRO	N-CA-CB	5.50	109.90	103.30
1	C	333	GLY	O-C-N	-5.50	113.91	122.70
1	A	104	ARG	CG-CD-NE	5.49	123.34	111.80
1	A	241	SER	N-CA-C	5.49	125.83	111.00
1	A	420	ALA	N-CA-CB	5.49	117.79	110.10
1	C	371	ALA	O-C-N	-5.49	113.91	122.70
1	C	578	PRO	N-CA-CB	5.49	109.89	103.30
2	D	147	PRO	N-CA-CB	5.49	109.88	103.30
1	A	199	ASP	CB-CG-OD1	5.49	123.24	118.30
1	A	524	ASP	C-N-CA	5.49	135.41	121.70
2	B	75	MET	CG-SD-CE	-5.48	91.43	100.20
1	A	207	ARG	NE-CZ-NH1	-5.48	117.56	120.30
2	D	86	GLY	C-N-CA	5.47	135.38	121.70
1	C	539	GLY	O-C-N	-5.47	113.94	122.70
2	D	26	ASP	CB-CG-OD1	-5.47	113.38	118.30
2	D	107	TRP	CA-C-O	5.47	131.58	120.10
2	D	634	LEU	O-C-N	-5.46	113.91	123.20
2	B	79	LYS	C-N-CA	5.46	135.36	121.70
2	D	95	ARG	CA-C-N	5.46	127.12	116.20
2	D	223	ARG	CD-NE-CZ	5.46	131.24	123.60
1	C	61	LEU	CA-C-N	5.46	129.20	117.20
2	D	88	PRO	N-CA-CB	5.46	109.85	103.30
1	C	177	LEU	O-C-N	-5.45	113.98	122.70
2	D	191	LYS	O-C-N	-5.45	113.98	122.70
2	B	116	PRO	N-CA-CB	5.45	109.84	103.30
2	D	89	GLY	O-C-N	-5.45	113.98	122.70
1	C	567	SER	N-CA-CB	5.45	118.67	110.50
2	B	371	GLU	CA-CB-CG	5.44	125.37	113.40
2	B	93	PHE	C-N-CA	5.44	135.30	121.70
2	B	472	ARG	NE-CZ-NH1	-5.44	117.58	120.30
2	B	251	GLU	OE1-CD-OE2	5.44	129.82	123.30
2	B	50	GLU	OE1-CD-OE2	-5.43	116.78	123.30
1	C	313	HIS	CA-C-N	5.43	129.15	117.20
1	C	82	ARG	NE-CZ-NH1	5.41	123.01	120.30
2	D	522	ARG	NE-CZ-NH2	-5.41	117.59	120.30
1	C	707	PRO	N-CA-CB	5.41	109.79	103.30
1	C	248	ALA	O-C-N	-5.41	114.01	123.20
1	A	189	PRO	N-CA-CB	5.40	109.78	103.30
1	A	101	PHE	O-C-N	-5.40	114.06	122.70
1	C	699	ASP	CB-CG-OD1	5.40	123.16	118.30
1	A	677	ARG	CD-NE-CZ	-5.38	116.06	123.60
2	B	191	LYS	O-C-N	-5.38	114.09	122.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	167	PHE	N-CA-CB	5.38	120.28	110.60
2	D	558	LYS	O-C-N	-5.38	114.09	122.70
2	B	511	PRO	N-CA-CB	5.37	109.75	103.30
2	B	170	TYR	CB-CG-CD1	-5.37	117.78	121.00
1	C	147	TYR	CB-CG-CD2	5.36	124.22	121.00
1	A	418	ARG	NE-CZ-NH2	5.36	122.98	120.30
1	C	229	SER	CA-C-N	5.36	128.99	117.20
1	C	150	ARG	CB-CA-C	-5.36	99.69	110.40
2	D	364	THR	C-N-CA	5.36	135.09	121.70
1	A	488	VAL	CB-CA-C	-5.35	101.23	111.40
2	D	69	GLY	N-CA-C	5.35	126.48	113.10
1	C	30	ALA	O-C-N	-5.35	114.14	122.70
1	C	148	ASP	CB-CG-OD2	-5.35	113.49	118.30
1	A	670	LYS	CA-CB-CG	-5.35	101.63	113.40
2	B	364	THR	O-C-N	-5.34	114.15	122.70
1	C	528	ASP	C-N-CA	5.34	135.05	121.70
2	D	600	LYS	C-N-CA	5.34	135.05	121.70
1	A	82	ARG	NE-CZ-NH2	-5.34	117.63	120.30
1	A	141	VAL	CG1-CB-CG2	-5.34	102.36	110.90
1	A	602	LEU	CB-CG-CD2	5.34	120.08	111.00
1	C	505	PRO	N-CA-CB	5.34	109.70	103.30
2	B	348	PHE	CB-CG-CD1	-5.33	117.07	120.80
2	B	110	ARG	NE-CZ-NH2	5.33	122.97	120.30
2	B	205	ALA	N-CA-CB	5.33	117.56	110.10
2	B	26	ASP	C-N-CA	5.32	135.01	121.70
2	B	417	TRP	O-C-N	-5.32	114.18	122.70
2	D	338	VAL	O-C-N	-5.32	114.18	122.70
1	A	79	TYR	O-C-N	-5.32	114.18	122.70
1	A	439	LYS	O-C-N	-5.32	114.16	123.20
1	A	315	PHE	O-C-N	-5.32	114.16	123.20
2	B	625	ASP	CB-CG-OD2	-5.32	113.52	118.30
1	C	184	GLU	O-C-N	-5.32	114.20	122.70
1	A	550	ASP	CB-CG-OD1	5.31	123.08	118.30
1	C	594	GLU	CG-CD-OE1	5.31	128.92	118.30
1	A	621	TYR	CB-CG-CD2	-5.31	117.81	121.00
2	B	269	GLN	C-N-CA	5.31	133.44	122.30
1	A	518	ALA	O-C-N	-5.30	114.22	122.70
1	C	5	PRO	N-CA-CB	5.30	109.66	103.30
2	D	253	ALA	N-CA-CB	5.30	117.52	110.10
1	A	405	GLY	O-C-N	-5.30	114.23	122.70
1	A	550	ASP	O-C-N	-5.30	114.22	122.70
1	A	49	LEU	O-C-N	-5.29	114.23	122.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	492	GLN	CG-CD-OE1	-5.29	111.02	121.60
1	C	23	ARG	O-C-N	-5.29	114.24	122.70
1	C	620	ALA	O-C-N	-5.29	114.24	122.70
1	A	524	ASP	O-C-N	-5.29	114.24	122.70
1	C	694	ASP	CB-CG-OD1	5.29	123.06	118.30
1	A	258	TYR	CB-CG-CD1	-5.29	117.83	121.00
1	C	231	ASN	O-C-N	-5.29	114.24	122.70
2	B	269	GLN	O-C-N	-5.28	114.22	123.20
1	C	513	ASP	O-C-N	-5.28	114.25	122.70
1	C	509	LYS	O-C-N	-5.28	114.25	122.70
1	C	118	ASP	CB-CG-OD2	-5.28	113.55	118.30
1	A	485	ASN	CB-CG-OD1	-5.28	111.05	121.60
1	A	603	ALA	CB-CA-C	-5.28	102.19	110.10
1	A	322	SER	O-C-N	-5.27	114.27	122.70
1	A	619	THR	O-C-N	-5.27	114.28	122.70
1	C	528	ASP	CB-CG-OD1	5.27	123.04	118.30
2	D	364	THR	O-C-N	-5.26	114.28	122.70
1	C	89	TYR	CD1-CE1-CZ	5.26	124.54	119.80
2	B	229	PRO	N-CA-CB	5.26	109.61	103.30
1	C	261	ALA	CB-CA-C	5.26	117.99	110.10
2	D	320	ALA	CB-CA-C	-5.26	102.21	110.10
2	D	330	GLU	OE1-CD-OE2	-5.26	116.99	123.30
2	D	420	PHE	CB-CG-CD1	5.26	124.48	120.80
1	A	107	ALA	CB-CA-C	-5.26	102.21	110.10
1	C	720	LYS	O-C-N	-5.25	114.29	122.70
2	B	617	LEU	N-CA-CB	5.25	120.91	110.40
1	C	528	ASP	O-C-N	-5.25	114.30	122.70
2	D	510	ARG	CD-NE-CZ	5.24	130.94	123.60
1	C	108	ALA	O-C-N	-5.24	114.29	123.20
1	C	294	PHE	CB-CG-CD1	-5.24	117.13	120.80
2	D	103	ASP	CB-CG-OD2	-5.24	113.59	118.30
1	A	217	SER	O-C-N	-5.23	114.33	122.70
2	D	107	TRP	CA-C-N	-5.23	105.69	117.20
1	A	158	LEU	O-C-N	-5.23	114.33	122.70
1	A	282	PRO	CA-C-N	5.23	128.71	117.20
1	C	550	ASP	O-C-N	-5.23	114.33	122.70
1	A	356	THR	CA-CB-CG2	-5.23	105.08	112.40
1	C	130	PRO	N-CA-CB	5.23	109.57	103.30
2	D	223	ARG	C-N-CA	5.22	134.76	121.70
2	B	521	ARG	O-C-N	-5.22	114.34	122.70
1	C	723	ARG	NH1-CZ-NH2	5.22	125.14	119.40
1	C	541	ALA	C-N-CA	5.22	134.75	121.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	227	TYR	CB-CG-CD2	5.22	124.13	121.00
1	C	305	ARG	NE-CZ-NH2	-5.21	117.69	120.30
2	B	60	LYS	O-C-N	-5.21	114.36	122.70
1	C	313	HIS	C-N-CA	5.21	134.72	121.70
1	C	397	THR	O-C-N	-5.21	114.37	122.70
2	B	556	ALA	CB-CA-C	5.21	117.91	110.10
1	A	53	ASP	CA-C-N	5.20	128.65	117.20
1	A	205	MET	O-C-N	-5.20	114.38	122.70
2	B	449	ARG	NE-CZ-NH2	-5.20	117.70	120.30
1	C	400	ILE	C-N-CA	5.20	134.71	121.70
2	B	465	GLU	O-C-N	-5.20	114.38	122.70
2	D	76	TYR	CB-CG-CD1	-5.20	117.88	121.00
1	C	375	PRO	N-CA-CB	5.20	109.54	103.30
2	D	108	ASP	N-CA-CB	-5.20	101.25	110.60
2	B	200	ASP	CB-CG-OD1	5.19	122.97	118.30
1	C	323	MET	O-C-N	-5.19	114.39	122.70
1	C	691	GLN	CB-CG-CD	5.19	125.11	111.60
1	C	357	GLN	C-N-CA	5.19	133.19	122.30
2	D	443	ASP	CB-CG-OD1	5.19	122.97	118.30
1	C	340	ASP	CB-CG-OD2	5.18	122.96	118.30
2	D	366	ALA	N-CA-CB	5.18	117.35	110.10
1	C	550	ASP	CB-CG-OD1	5.17	122.96	118.30
2	D	90	VAL	CG1-CB-CG2	-5.17	102.62	110.90
1	A	678	PRO	C-N-CA	5.17	134.63	121.70
2	D	115	ASP	CB-CG-OD2	-5.17	113.65	118.30
2	B	69	GLY	N-CA-C	5.17	126.01	113.10
2	B	404	TYR	CB-CG-CD2	-5.16	117.90	121.00
1	C	669	ARG	NE-CZ-NH1	5.16	122.88	120.30
2	D	114	GLU	CA-CB-CG	5.16	124.75	113.40
1	A	272	SER	O-C-N	-5.16	114.45	122.70
1	A	333	GLY	CA-C-O	5.16	129.88	120.60
2	B	114	GLU	CA-CB-CG	5.16	124.75	113.40
1	C	55	TYR	N-CA-C	5.16	124.92	111.00
2	B	591	LYS	N-CA-CB	-5.15	101.33	110.60
2	D	25	GLY	C-N-CA	5.15	134.58	121.70
1	C	74	PRO	CB-CA-C	-5.15	99.12	112.00
1	A	341	VAL	CA-CB-CG1	-5.14	103.19	110.90
2	B	351	SER	O-C-N	-5.14	114.47	122.70
2	B	438	VAL	CA-CB-CG2	-5.14	103.20	110.90
1	C	225	PHE	CB-CG-CD1	-5.13	117.20	120.80
2	D	327	SER	N-CA-C	5.13	124.85	111.00
2	D	86	GLY	CA-C-O	5.13	129.83	120.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	32	ALA	CA-C-N	5.13	126.45	116.20
1	C	225	PHE	CB-CG-CD2	5.13	124.39	120.80
1	C	87	ARG	NE-CZ-NH2	5.12	122.86	120.30
2	B	204	PHE	O-C-N	-5.12	114.51	122.70
1	C	558	ARG	NE-CZ-NH1	5.11	122.85	120.30
2	B	243	ASN	C-N-CA	5.11	134.46	121.70
2	B	435	THR	N-CA-CB	-5.10	100.61	110.30
1	A	558	ARG	NE-CZ-NH1	5.10	122.85	120.30
1	A	42	GLU	C-N-CA	5.10	134.44	121.70
1	C	248	ALA	CA-C-N	5.10	126.39	116.20
2	D	611	LYS	CA-C-N	5.09	128.41	117.20
1	A	50	PHE	O-C-N	-5.09	114.55	122.70
1	A	136	VAL	CA-C-O	5.09	130.79	120.10
2	B	26	ASP	O-C-N	-5.09	114.56	122.70
1	A	381	ARG	O-C-N	-5.08	114.57	122.70
1	A	673	ASP	C-N-CA	5.08	134.40	121.70
2	B	316	ASP	CB-CG-OD1	5.08	122.87	118.30
2	B	87	TYR	CG-CD1-CE1	5.08	125.36	121.30
1	A	53	ASP	O-C-N	-5.07	114.59	122.70
2	B	338	VAL	CA-C-N	5.07	128.35	117.20
1	C	99	ASN	CB-CG-OD1	-5.07	111.46	121.60
2	D	86	GLY	O-C-N	-5.07	114.59	122.70
1	C	419	LYS	O-C-N	-5.07	114.59	122.70
2	D	406	GLU	OE1-CD-OE2	-5.07	117.22	123.30
2	B	464	SER	N-CA-CB	5.07	118.10	110.50
2	B	416	ALA	N-CA-CB	5.06	117.19	110.10
2	D	28	PRO	N-CA-CB	5.06	109.38	103.30
2	B	335	ASP	CB-CG-OD1	5.06	122.86	118.30
1	C	688	ILE	CA-CB-CG1	5.06	120.61	111.00
1	A	206	VAL	CG1-CB-CG2	-5.06	102.80	110.90
1	A	596	ARG	CD-NE-CZ	5.06	130.68	123.60
2	D	476	THR	N-CA-CB	5.05	119.91	110.30
1	A	380	ALA	CB-CA-C	-5.05	102.52	110.10
1	C	589	GLU	O-C-N	-5.05	114.62	122.70
1	A	136	VAL	O-C-N	-5.05	114.62	123.20
2	D	224	LEU	CB-CG-CD2	-5.05	102.42	111.00
2	B	377	ARG	O-C-N	-5.05	114.62	122.70
2	D	298	ARG	CG-CD-NE	5.05	122.40	111.80
2	B	270	GLY	N-CA-C	5.04	125.71	113.10
1	C	437	ILE	CA-C-N	5.04	128.29	117.20
1	A	170	ALA	C-N-CA	5.04	134.30	121.70
2	B	267	VAL	O-C-N	-5.04	114.64	122.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	404	TYR	CB-CG-CD1	5.04	124.02	121.00
1	C	629	ASP	CB-CG-OD2	-5.04	113.76	118.30
1	A	40	THR	O-C-N	-5.04	114.64	122.70
1	A	248	ALA	CA-C-N	5.04	126.28	116.20
2	B	225	ALA	O-C-N	-5.04	114.64	122.70
2	B	403	TYR	CB-CG-CD2	5.04	124.02	121.00
1	A	335	SER	O-C-N	-5.03	114.65	122.70
2	B	92	PRO	O-C-N	-5.03	114.64	122.70
2	B	187	ASP	O-C-N	-5.03	114.65	122.70
1	C	351	GLU	O-C-N	-5.03	114.65	122.70
1	C	334	TRP	O-C-N	-5.03	114.65	122.70
1	A	339	GLN	O-C-N	-5.03	114.66	122.70
1	C	389	PHE	O-C-N	-5.03	114.66	122.70
2	D	225	ALA	CB-CA-C	5.03	117.64	110.10
2	B	522	ARG	CG-CD-NE	-5.02	101.25	111.80
1	C	638	GLU	OE1-CD-OE2	-5.02	117.27	123.30
2	D	243	ASN	O-C-N	-5.02	114.67	122.70
1	A	556	PHE	CB-CG-CD1	-5.02	117.28	120.80
1	A	35	GLY	C-N-CA	5.02	134.25	121.70
1	C	23	ARG	NH1-CZ-NH2	-5.02	113.88	119.40
1	C	678	PRO	C-N-CA	5.02	134.25	121.70
2	D	395	VAL	CG1-CB-CG2	-5.02	102.87	110.90
1	C	276	ASN	O-C-N	-5.02	114.67	122.70
1	A	161	MET	CA-CB-CG	5.01	121.83	113.30
1	A	314	GLN	C-N-CA	5.01	134.24	121.70
1	A	219	ARG	NE-CZ-NH1	-5.01	117.79	120.30
1	A	272	SER	CA-C-N	5.01	128.22	117.20
1	C	89	TYR	CG-CD1-CE1	-5.01	117.29	121.30
2	B	85	LEU	C-N-CA	-5.01	111.79	122.30
1	A	676	GLY	CA-C-O	5.00	129.61	120.60
1	C	443	LYS	O-C-N	-5.00	114.69	122.70

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	405	GLY	Mainchain
1	C	167	MET	Mainchain
2	D	456	ARG	Mainchain

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	5601	0	5540	41	0
1	C	5601	0	5539	39	0
2	B	4731	0	4667	28	0
2	D	4731	0	4665	43	0
3	A	54	0	37	1	0
3	C	54	0	37	1	0
4	A	91	0	88	13	0
4	C	91	0	88	9	0
5	A	6	0	8	0	0
5	C	6	0	8	0	0
6	A	356	0	0	0	0
6	B	219	0	0	0	0
6	C	361	0	0	1	0
6	D	214	0	0	0	0
All	All	22116	0	20677	160	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 4.

All (160) 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)
4:A:1800:B12:H531	4:A:1800:B12:H552	1.23	1.14
1:A:638:GLU:HA	1:A:671:GLU:HG2	1.58	0.86
1:A:635:GLN:HE22	1:A:643:GLN:HE21	1.28	0.79
2:D:374:PHE:HB3	2:D:375:PRO:HD3	1.67	0.77
1:C:635:GLN:HE22	1:C:643:GLN:HE21	1.35	0.74
4:A:1800:B12:H362	4:A:1800:B12:H351	1.70	0.74
4:C:2800:B12:H552	4:C:2800:B12:H531	1.71	0.72
2:B:374:PHE:HB3	2:B:375:PRO:HD3	1.71	0.72
1:A:650:HIS:HB3	1:A:722:LEU:HD11	1.74	0.70
2:D:180:VAL:HG13	2:D:197:LEU:HD21	1.74	0.68
1:C:290:ILE:HG13	1:C:355:ALA:HB2	1.76	0.68
1:A:706:THR:HB	1:A:707:PRO:HD2	1.75	0.68
1:A:247:GLU:HB3	4:A:1800:B12:H532	1.76	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:2800:B12:H351	4:C:2800:B12:H362	1.76	0.67
2:B:532:SER:HB3	2:B:533:PRO:HD3	1.77	0.66
2:D:308:GLY:HA3	2:D:318:ARG:HG2	1.77	0.66
1:A:290:ILE:HG13	1:A:355:ALA:HB2	1.76	0.66
1:A:14:ASN:HA	2:B:410:ARG:HH22	1.60	0.65
1:C:638:GLU:HA	1:C:671:GLU:HG2	1.78	0.65
2:D:532:SER:HB3	2:D:533:PRO:HD3	1.80	0.64
2:D:370:PRO:HB3	2:D:375:PRO:HG2	1.80	0.64
1:C:706:THR:HB	1:C:707:PRO:CD	2.30	0.62
2:D:80:ASP:HB3	2:D:407:SER:HB2	1.81	0.62
4:A:1800:B12:H531	4:A:1800:B12:C55	2.10	0.62
2:D:347:THR:HG23	2:D:358:ILE:HG21	1.81	0.61
2:B:180:VAL:HG13	2:B:197:LEU:HD21	1.83	0.61
2:D:138:LEU:HD23	2:D:145:ILE:HD13	1.83	0.61
1:A:359:HIS:CE1	1:A:401:ASP:H	2.18	0.60
1:C:706:THR:HB	1:C:707:PRO:HD2	1.82	0.60
4:C:2800:B12:C61	4:C:2800:B12:H551	2.33	0.59
1:A:706:THR:HB	1:A:707:PRO:CD	2.32	0.59
1:C:359:HIS:CE1	1:C:401:ASP:H	2.20	0.59
2:B:565:ALA:HB3	2:B:593:LEU:HD23	1.88	0.56
1:A:4:LEU:HD13	2:B:264:ARG:HG2	1.86	0.56
2:D:141:ASP:HB3	2:D:142:PRO:HD2	1.86	0.56
2:B:503:ARG:HD2	2:B:638:LYS:HD3	1.88	0.56
1:C:247:GLU:HB3	4:C:2800:B12:H532	1.86	0.56
1:A:14:ASN:HA	2:B:410:ARG:NH2	2.21	0.55
4:A:1800:B12:H353	4:A:1800:B12:H302	1.89	0.55
2:B:141:ASP:HB3	2:B:142:PRO:HD2	1.88	0.55
4:C:2800:B12:H531	4:C:2800:B12:C55	2.36	0.55
1:C:139:ALA:HB1	4:C:2800:B12:H362	1.89	0.55
2:B:27:PHE:HB3	2:B:28:PRO:HD2	1.89	0.55
2:D:386:LEU:HD23	2:D:390:VAL:HG21	1.88	0.54
1:A:635:GLN:HE22	1:A:643:GLN:NE2	2.01	0.54
2:D:435:THR:HG22	2:D:436:GLU:H	1.72	0.54
1:A:635:GLN:NE2	1:A:643:GLN:HE21	2.03	0.54
2:B:370:PRO:HB3	2:B:375:PRO:HG2	1.91	0.53
4:C:2800:B12:H351	4:C:2800:B12:H372	1.90	0.53
2:D:201:PRO:HG3	2:D:217:LEU:HD21	1.90	0.53
4:A:1800:B12:H362	4:A:1800:B12:C35	2.39	0.53
2:B:563:GLN:HE21	2:B:591:LYS:HD3	1.73	0.53
4:A:1800:B12:H552	4:A:1800:B12:C53	2.14	0.53
1:C:14:ASN:HA	2:D:410:ARG:NH2	2.24	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:564:VAL:HG22	2:B:592:ALA:HB3	1.92	0.52
2:D:141:ASP:CB	2:D:142:PRO:HD2	2.40	0.52
2:D:281:ASN:ND2	2:D:323:ASN:HD21	2.07	0.52
2:D:369:LEU:HB2	2:D:477:LYS:HG3	1.92	0.52
1:C:571:SER:HB3	1:C:623:ASP:HB3	1.91	0.52
4:A:1800:B12:H351	4:A:1800:B12:H372	1.91	0.52
2:D:223:ARG:HD2	2:D:226:LYS:HZ1	1.75	0.52
2:D:281:ASN:HD22	2:D:323:ASN:HD21	1.58	0.51
1:A:200:ILE:HG12	1:A:217:SER:HB3	1.93	0.51
1:C:252:ALA:O	1:C:256:MET:HG3	2.11	0.51
1:A:652:VAL:HG11	1:A:668:LEU:HD11	1.91	0.51
2:D:564:VAL:HG22	2:D:592:ALA:HB3	1.91	0.51
1:A:359:HIS:HE1	1:A:401:ASP:H	1.59	0.51
2:D:554:VAL:HG21	2:D:584:ALA:HB1	1.93	0.51
2:D:158:LEU:HD12	2:D:161:MET:SD	2.51	0.50
1:C:668:LEU:HD13	1:C:682:ILE:HG12	1.92	0.50
1:A:372:ILE:HG22	1:A:480:VAL:HG11	1.93	0.50
2:D:517:CYS:HB3	2:D:524:PHE:CG	2.46	0.50
1:A:512:LEU:HD21	1:A:543:ALA:HB1	1.94	0.50
1:C:577:THR:HG22	1:C:580:VAL:H	1.77	0.50
1:C:7:PHE:HA	1:C:10:VAL:HG23	1.95	0.49
1:C:635:GLN:HE22	1:C:643:GLN:NE2	2.05	0.49
1:A:139:ALA:HB1	4:A:1800:B12:H362	1.95	0.49
1:C:21:ALA:HA	2:D:90:VAL:HG11	1.95	0.48
1:A:243:TYR:HD1	1:A:289:GLY:HA2	1.78	0.48
2:D:284:VAL:HG21	2:D:297:LEU:HD22	1.95	0.48
1:A:666:PRO:O	1:A:670:LYS:HD2	2.12	0.48
2:B:237:ASP:HB3	2:B:240:ILE:HD12	1.96	0.48
2:D:374:PHE:CB	2:D:375:PRO:HD3	2.41	0.47
1:C:25:PHE:HB2	2:D:87:TYR:HB3	1.97	0.47
1:C:359:HIS:HE1	1:C:401:ASP:H	1.61	0.47
1:C:683:THR:HG21	1:C:718:LEU:HD13	1.96	0.47
1:A:606:GLY:O	1:A:634:PHE:HA	2.15	0.47
1:C:243:TYR:HD1	1:C:289:GLY:HA2	1.78	0.47
2:B:579:LEU:HG	2:B:583:LYS:HD2	1.97	0.47
2:B:141:ASP:CB	2:B:142:PRO:HD2	2.45	0.47
1:C:563:ILE:HD11	6:C:3184:HOH:O	2.15	0.47
2:D:325:ILE:HD11	2:D:361:LEU:HD21	1.96	0.47
1:A:597:ARG:HB3	1:A:598:PRO:HD2	1.96	0.46
1:A:691:GLN:NE2	1:A:691:GLN:H	2.14	0.46
1:A:215:GLN:HB3	1:A:216:PRO:HD3	1.96	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:215:GLN:HB3	1:C:216:PRO:HD3	1.97	0.46
1:C:691:GLN:HE21	1:C:691:GLN:H	1.63	0.46
2:B:73:VAL:HB	2:B:74:PRO:HD2	1.98	0.46
1:C:691:GLN:H	1:C:691:GLN:NE2	2.13	0.46
2:D:73:VAL:HB	2:D:74:PRO:HD2	1.98	0.46
2:D:191:LYS:HD2	2:D:226:LYS:O	2.15	0.46
1:A:635:GLN:NE2	1:A:643:GLN:NE2	2.63	0.46
1:C:392:GLN:HB3	2:D:459:PRO:HG2	1.97	0.46
2:D:258:THR:OG1	2:D:429:MET:HG2	2.16	0.46
1:C:452:ARG:HA	1:C:573:GLU:HG2	1.98	0.46
4:A:1800:B12:H351	4:A:1800:B12:C36	2.38	0.45
2:B:517:CYS:HB3	2:B:524:PHE:CG	2.51	0.45
2:D:390:VAL:HG12	2:D:392:ILE:HG23	1.98	0.45
1:C:571:SER:HB2	1:C:584:ARG:HH22	1.81	0.45
2:B:158:LEU:HD12	2:B:161:MET:SD	2.56	0.45
1:C:287:PHE:CE2	3:C:2801:3CP:HP11	2.52	0.45
1:A:571:SER:HB3	1:A:623:ASP:HB3	1.97	0.45
1:A:10:VAL:HG11	2:B:310:VAL:HG21	1.97	0.45
1:A:521:ASN:O	1:A:529:ARG:HD3	2.16	0.45
2:B:554:VAL:HG21	2:B:584:ALA:HB1	1.99	0.45
1:A:20:ASP:OD2	1:A:24:ARG:HD2	2.16	0.44
1:C:200:ILE:HG21	1:C:217:SER:HB3	1.98	0.44
1:C:599:ARG:HG2	1:C:649:VAL:HA	1.99	0.44
2:D:571:ALA:HA	2:D:601:GLU:HB3	2.00	0.44
2:D:503:ARG:HD2	2:D:638:LYS:HD3	1.99	0.44
1:A:691:GLN:H	1:A:691:GLN:HE21	1.65	0.44
1:A:319:ASN:HA	1:A:320:PRO:HD2	1.86	0.44
1:A:602:LEU:HD22	4:A:1800:B12:HM52	2.00	0.44
1:C:602:LEU:HD22	4:C:2800:B12:HM52	1.99	0.44
2:D:118:GLU:HG3	2:D:152:GLU:OE1	2.18	0.44
3:A:1801:3CP:OP2	3:A:1801:3CP:HB1	2.17	0.44
1:A:372:ILE:HD13	1:A:478:LEU:HD23	1.99	0.43
2:D:274:THR:HG23	2:D:317:LYS:HD3	1.99	0.43
2:D:284:VAL:HG11	2:D:322:GLN:HE21	1.83	0.43
1:A:686:GLY:O	1:A:707:PRO:HD3	2.18	0.43
1:A:252:ALA:O	1:A:256:MET:HG3	2.18	0.43
2:B:238:ALA:HB1	2:B:251:GLU:HG3	2.01	0.43
2:B:429:MET:HE3	2:B:433:VAL:HG23	1.99	0.43
1:A:138:MET:SD	1:A:485:ASN:HB2	2.59	0.43
4:C:2800:B12:H362	4:C:2800:B12:C35	2.45	0.43
1:C:606:GLY:O	1:C:634:PHE:HA	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:169:ARG:HG2	2:D:207:LEU:HD13	2.01	0.43
1:C:521:ASN:O	1:C:529:ARG:HD3	2.19	0.42
1:A:641:ALA:O	1:A:645:VAL:HG23	2.19	0.42
1:C:319:ASN:HA	1:C:320:PRO:HD2	1.83	0.42
1:C:635:GLN:NE2	1:C:643:GLN:HE21	2.10	0.42
1:A:683:THR:HG21	1:A:718:LEU:HD13	2.02	0.42
2:D:532:SER:CB	2:D:533:PRO:HD3	2.49	0.42
2:B:347:THR:HG23	2:B:358:ILE:HG21	2.01	0.42
1:A:721:LYS:HA	1:A:721:LYS:HD3	1.95	0.41
1:A:36:GLU:CD	1:A:36:GLU:H	2.24	0.41
4:A:1800:B12:H351	4:A:1800:B12:C37	2.49	0.41
2:B:242:HIS:CD2	2:B:285:THR:HG21	2.55	0.41
4:A:1800:B12:C35	4:A:1800:B12:H372	2.51	0.41
2:B:252:LEU:HD11	2:B:300:LEU:HA	2.02	0.41
2:D:217:LEU:O	2:D:221:VAL:HG23	2.21	0.41
2:D:141:ASP:HB3	2:D:142:PRO:CD	2.51	0.41
2:D:234:VAL:HB	2:D:280:ILE:HA	2.03	0.41
2:D:267:VAL:HA	2:D:271:PHE:O	2.21	0.41
1:C:65:ALA:HA	1:C:72:HIS:HB2	2.03	0.41
1:C:207:ARG:HD2	1:C:244:HIS:CD2	2.56	0.41
2:B:83:LYS:HE3	2:B:83:LYS:HA	2.03	0.40
2:B:331:LEU:HD13	2:B:365:GLN:HB3	2.04	0.40
1:C:372:ILE:HG22	1:C:480:VAL:HG11	2.03	0.40
1:C:89:TYR:HA	1:C:114:SER:HB3	2.04	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	725/727 (100%)	695 (96%)	30 (4%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	725/727 (100%)	694 (96%)	31 (4%)	0	100	100
2	B	617/637 (97%)	601 (97%)	15 (2%)	1 (0%)	47	55
2	D	617/637 (97%)	594 (96%)	21 (3%)	2 (0%)	41	46
All	All	2684/2728 (98%)	2584 (96%)	97 (4%)	3 (0%)	51	60

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	435	THR
2	D	171	ASP
2	B	603	GLY

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	582/590 (99%)	570 (98%)	12 (2%)	53	67
1	C	582/590 (99%)	564 (97%)	18 (3%)	40	51
2	B	483/509 (95%)	469 (97%)	14 (3%)	42	54
2	D	483/509 (95%)	462 (96%)	21 (4%)	29	36
All	All	2130/2198 (97%)	2065 (97%)	65 (3%)	40	51

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	SER
1	A	3	THR
1	A	4	LEU
1	A	24	ARG
1	A	31	LYS
1	A	69	PRO
1	A	445	ARG
1	A	567	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	597	ARG
1	A	668	LEU
1	A	670	LYS
1	A	691	GLN
2	B	20	THR
2	B	75	MET
2	B	79	LYS
2	B	83	LYS
2	B	163	LYS
2	B	216	VAL
2	B	334	GLU
2	B	410	ARG
2	B	431	LYS
2	B	435	THR
2	B	440	LYS
2	B	512	LYS
2	B	629	SER
2	B	638	LYS
1	C	3	THR
1	C	4	LEU
1	C	24	ARG
1	C	31	LYS
1	C	69	PRO
1	C	365	THR
1	C	384	ARG
1	C	406	SER
1	C	419	LYS
1	C	445	ARG
1	C	471	ARG
1	C	482	LYS
1	C	533	LYS
1	C	577	THR
1	C	596	ARG
1	C	599	ARG
1	C	668	LEU
1	C	691	GLN
2	D	20	THR
2	D	22	SER
2	D	77	ARG
2	D	79	LYS
2	D	83	LYS
2	D	156	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	187	ASP
2	D	188	LYS
2	D	191	LYS
2	D	288	HIS
2	D	322	GLN
2	D	334	GLU
2	D	335	ASP
2	D	336	PRO
2	D	410	ARG
2	D	477	LYS
2	D	501	MET
2	D	512	LYS
2	D	532	SER
2	D	616	ARG
2	D	638	LYS

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

Mol	Chain	Res	Type
1	A	51	ASN
1	A	359	HIS
1	A	385	ASN
1	A	462	GLN
1	A	643	GLN
1	A	691	GLN
2	B	323	ASN
2	B	563	GLN
1	C	359	HIS
1	C	385	ASN
1	C	462	GLN
1	C	643	GLN
1	C	691	GLN
2	D	149	HIS
2	D	322	GLN
2	D	323	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

6 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	$\#\|Z\| > 2$
5	GOL	C	3002	-	5,5,5	0.48	0	5,5,5	0.65	0
3	3CP	A	1801	-	48,56,56	1.15	5 (10%)	60,82,82	1.95	12 (20%)
4	B12	A	1800	1	90,101,101	1.24	10 (11%)	137,166,166	1.99	43 (31%)
3	3CP	C	2801	-	48,56,56	1.22	6 (12%)	60,82,82	1.85	13 (21%)
4	B12	C	2800	1	90,101,101	1.10	6 (6%)	137,166,166	1.78	30 (21%)
5	GOL	A	3001	-	5,5,5	0.62	0	5,5,5	1.05	0

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
5	GOL	C	3002	-	-	0/4/4/4	-
3	3CP	A	1801	-	-	7/50/70/70	0/3/3/3
4	B12	A	1800	1	-	5/52/223/223	0/3/11/11
3	3CP	C	2801	-	-	8/50/70/70	0/3/3/3
4	B12	C	2800	1	-	6/52/223/223	0/3/11/11
5	GOL	A	3001	-	-	0/4/4/4	-

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1800	B12	C14-N23	3.85	1.40	1.35
4	A	1800	B12	C54-C17	3.84	1.61	1.54
3	C	2801	3CP	CP2-NP1	3.75	1.54	1.46
3	A	1801	3CP	CP5-NP2	3.52	1.54	1.46
4	A	1800	B12	C35-C5	3.37	1.57	1.50
4	C	2800	B12	C48-C13	3.13	1.61	1.54
4	C	2800	B12	C14-N23	3.06	1.39	1.35
4	C	2800	B12	C54-C17	2.79	1.59	1.54
3	A	1801	3CP	CP2-NP1	2.78	1.52	1.46
3	A	1801	3CP	C2-N1	2.72	1.39	1.33
4	A	1800	B12	O8R-C5R	2.67	1.53	1.42
4	A	1800	B12	C41-C8	2.62	1.60	1.54
4	C	2800	B12	C55-C17	-2.41	1.49	1.54
3	A	1801	3CP	P2-O7	-2.41	1.49	1.59
3	C	2801	3CP	P1-O11	-2.39	1.42	1.50
3	C	2801	3CP	P2-O7	-2.39	1.49	1.59
3	C	2801	3CP	CP5-NP2	2.36	1.51	1.46
3	C	2801	3CP	CP9-CPA	-2.35	1.48	1.53
4	C	2800	B12	C41-C8	2.29	1.59	1.54
4	A	1800	B12	C55-C17	-2.23	1.49	1.54
4	A	1800	B12	C55-C56	2.23	1.58	1.53
4	C	2800	B12	C30-C3	2.19	1.59	1.54
3	A	1801	3CP	P2-O22	-2.16	1.45	1.55
3	C	2801	3CP	C2-N1	2.11	1.37	1.33
4	A	1800	B12	P-O2	2.08	1.66	1.60
4	A	1800	B12	C13-C14	-2.01	1.48	1.52
4	A	1800	B12	C19-N24	-2.00	1.45	1.48

All (98) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1801	3CP	CP8-CPA-CPB	6.88	119.46	108.23
3	C	2801	3CP	CP9-CPA-CPB	6.33	118.55	108.23
4	A	1800	B12	C20-C1-C19	6.01	115.14	109.36
3	A	1801	3CP	CP1-CP2-NP1	-5.68	100.48	112.42
4	C	2800	B12	C55-C17-C16	5.20	126.91	116.65
4	A	1800	B12	C55-C17-C18	5.10	121.00	111.15
4	A	1800	B12	C54-C17-C16	-4.79	87.53	112.40
4	A	1800	B12	C15-C16-N24	4.71	129.21	122.42
4	A	1800	B12	C10-C9-N22	-4.55	120.51	125.73
3	A	1801	3CP	CP5-NP2-CP6	-4.45	114.65	122.59
4	A	1800	B12	C16-C15-C14	-4.41	114.56	121.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	2800	B12	C41-C8-C9	-4.38	103.47	111.19
4	C	2800	B12	C1P-N59-C57	-4.38	113.16	122.69
3	C	2801	3CP	CP8-CPA-CPB	4.29	115.23	108.23
4	C	2800	B12	C16-C15-C14	-4.26	114.78	121.25
4	C	2800	B12	C36-C7-C8	4.21	119.86	112.08
3	C	2801	3CP	CS2-CS3-CS4	-4.04	104.30	114.47
4	C	2800	B12	C54-C17-C16	-4.02	91.54	112.40
3	A	1801	3CP	CP9-CPA-CPB	3.89	114.57	108.23
4	A	1800	B12	C7B-C8B-C9B	3.88	124.38	120.54
4	A	1800	B12	C55-C56-C57	-3.87	102.79	111.23
4	C	2800	B12	C20-C1-C19	3.85	113.07	109.36
4	C	2800	B12	C7B-C8B-C9B	3.72	124.22	120.54
3	C	2801	3CP	CP5-NP2-CP6	-3.65	116.07	122.59
4	C	2800	B12	O44-C43-N45	-3.53	112.88	122.50
3	A	1801	3CP	O7-CPB-CPA	-3.50	104.93	110.55
4	A	1800	B12	C13-C14-N23	3.48	113.83	109.10
4	A	1800	B12	C1-C19-N24	-3.40	102.41	106.24
4	C	2800	B12	C4B-C9B-C8B	-3.40	117.62	121.10
4	A	1800	B12	O28-C27-N29	-3.36	113.33	122.50
3	C	2801	3CP	CP1-CP2-NP1	-3.34	105.39	112.42
3	A	1801	3CP	CP2-NP1-CP3	-3.34	116.63	122.84
3	C	2801	3CP	C4-C5-N7	3.28	112.82	109.40
3	C	2801	3CP	O7-CPB-CPA	-3.28	105.28	110.55
4	C	2800	B12	C56-C55-C17	-3.27	109.21	115.52
4	A	1800	B12	O58-C57-N59	3.27	129.18	123.01
3	C	2801	3CP	C5-C6-N6	3.26	125.31	120.35
4	C	2800	B12	C18-C17-C16	3.26	104.63	100.67
4	A	1800	B12	C36-C7-C8	3.25	118.08	112.08
4	A	1800	B12	C41-C8-C9	-3.23	105.50	111.19
4	A	1800	B12	C13-C14-C15	-3.23	119.39	124.32
4	C	2800	B12	C42-C43-N45	3.20	126.48	116.51
4	C	2800	B12	O34-C32-C31	-3.20	111.67	121.07
3	A	1801	3CP	CS2-CS3-CS4	-3.19	106.42	114.47
4	C	2800	B12	C15-C16-N24	3.19	127.01	122.42
4	A	1800	B12	C10-C11-N23	3.12	129.76	124.43
4	A	1800	B12	C18-C17-C16	3.11	104.45	100.67
4	A	1800	B12	C48-C13-C12	-3.06	108.05	116.63
4	C	2800	B12	C54-C17-C55	-2.98	104.33	109.25
4	A	1800	B12	C41-C8-C7	-2.95	106.02	114.14
4	A	1800	B12	C12-C11-C10	-2.95	119.53	123.37
4	A	1800	B12	C30-C3-C4	2.94	116.48	109.63
4	A	1800	B12	C7-C6-C5	-2.94	123.44	128.07

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	1800	B12	O3-C2P-C1P	-2.88	101.16	106.92
4	C	2800	B12	C18-C19-N24	2.88	106.70	102.31
4	A	1800	B12	C35-C5-C6	-2.86	117.88	122.43
4	C	2800	B12	O58-C57-N59	2.85	128.39	123.01
4	C	2800	B12	C49-C50-N52	2.79	125.21	116.51
4	C	2800	B12	C36-C7-C37	-2.76	106.25	110.80
4	A	1800	B12	C5B-C4B-C9B	-2.75	117.33	121.22
3	A	1801	3CP	CP9-CPA-CP7	-2.74	104.06	108.82
4	C	2800	B12	C55-C17-C18	2.73	116.42	111.15
4	A	1800	B12	C7-C6-N22	2.72	112.92	107.94
4	A	1800	B12	C12-C13-C14	-2.71	97.72	102.26
4	C	2800	B12	C55-C56-C57	-2.70	105.34	111.23
4	A	1800	B12	C9-C10-C11	-2.70	122.07	125.97
3	A	1801	3CP	OS5-CS4-OS4	-2.64	116.71	123.30
3	A	1801	3CP	C5-C6-N6	2.64	124.36	120.35
4	A	1800	B12	C3-C4-N21	2.59	115.21	111.97
4	C	2800	B12	C54-C17-C18	-2.58	109.17	112.98
3	C	2801	3CP	O32-P3-O31	2.57	120.75	110.68
4	C	2800	B12	O6R-C1R-C2R	-2.55	103.20	106.93
4	A	1800	B12	C7-C8-C9	2.51	104.11	100.90
4	A	1800	B12	C2-C1-C19	-2.49	114.67	118.60
4	C	2800	B12	C2-C1-C19	-2.47	114.71	118.60
3	C	2801	3CP	CP8-CPA-CP9	-2.45	104.17	109.17
4	A	1800	B12	O6R-C1R-C2R	-2.44	103.36	106.93
4	C	2800	B12	C53-C15-C16	2.43	124.56	120.38
4	A	1800	B12	C37-C7-C8	-2.42	101.91	108.39
4	C	2800	B12	C49-C48-C13	-2.40	107.81	114.73
3	C	2801	3CP	OP2-CP6-NP2	2.37	128.09	122.99
4	A	1800	B12	C18-C19-N24	2.35	105.90	102.31
3	A	1801	3CP	C4-C5-N7	2.34	111.84	109.40
4	A	1800	B12	O58-C57-C56	-2.29	117.83	122.02
3	A	1801	3CP	CP8-CPA-CP9	-2.27	104.54	109.17
4	A	1800	B12	O44-C43-N45	-2.19	116.53	122.50
4	C	2800	B12	C1-C19-C18	-2.17	118.33	121.88
4	A	1800	B12	C17-C16-N24	-2.16	107.83	111.15
3	C	2801	3CP	OP1-CP3-CP4	-2.15	118.08	122.02
4	A	1800	B12	C17-C16-C15	-2.13	122.91	126.26
4	C	2800	B12	C31-C30-C3	-2.11	108.64	114.73
4	A	1800	B12	C53-C15-C16	2.10	124.00	120.38
4	C	2800	B12	C31-C32-N33	2.07	122.95	116.51
3	C	2801	3CP	CP9-CPA-CP7	-2.06	105.26	108.82
4	A	1800	B12	C60-C18-C19	-2.04	109.29	114.62

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	1800	B12	C56-C57-N59	-2.04	112.98	116.42
4	A	1800	B12	C25-C2-C1	2.03	116.84	113.78
4	A	1800	B12	C26-C27-N29	2.02	122.92	116.52

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1801	3CP	P1-O6-P2-O7
3	C	2801	3CP	P1-O6-P2-O7
4	A	1800	B12	C42-C41-C8-C9
4	C	2800	B12	C42-C41-C8-C9
3	A	1801	3CP	S-CS1-CS2-CS3
3	C	2801	3CP	S-CS1-CS2-CS3
4	A	1800	B12	C16-C17-C55-C56
4	A	1800	B12	C30-C31-C32-O34
4	A	1800	B12	C30-C31-C32-N33
4	C	2800	B12	C2P-O3-P-O2
4	A	1800	B12	C2P-O3-P-O2
3	A	1801	3CP	CS1-CS2-CS3-CS4
3	C	2801	3CP	C3'-O3'-P3-O32
3	A	1801	3CP	P2-O6-P1-O12
3	C	2801	3CP	CP2-CP1-S-CS1
4	C	2800	B12	C30-C31-C32-N33
3	C	2801	3CP	P2-O6-P1-O12
4	C	2800	B12	C30-C31-C32-O34
3	A	1801	3CP	CS2-CS3-CS4-OS4
3	A	1801	3CP	CS2-CS3-CS4-OS5
3	C	2801	3CP	CS2-CS3-CS4-OS4
3	C	2801	3CP	CS2-CS3-CS4-OS5
4	C	2800	B12	C55-C56-C57-O58
3	A	1801	3CP	CP2-CP1-S-CS1
4	C	2800	B12	C55-C56-C57-N59
3	C	2801	3CP	P2-O6-P1-O11

There are no ring outliers.

4 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1801	3CP	1	0
4	A	1800	B12	13	0

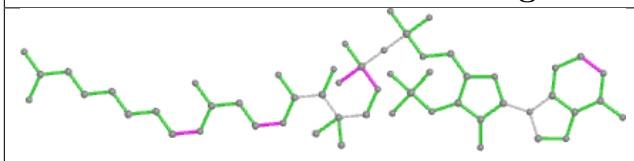
Continued on next page...

Continued from previous page...

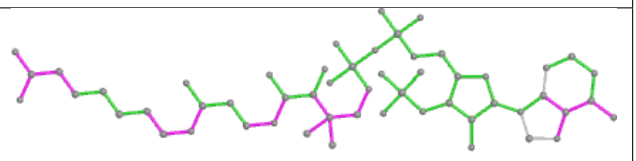
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	2801	3CP	1	0
4	C	2800	B12	9	0

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

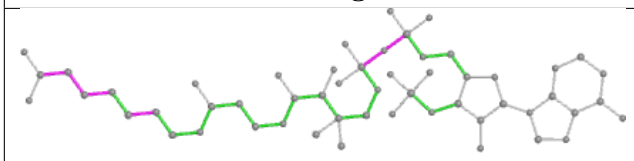
Ligand 3CP A 1801



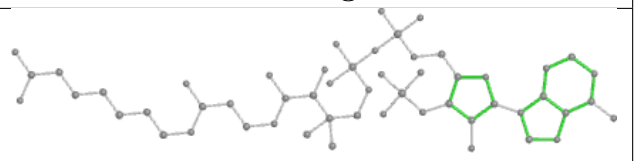
Bond lengths



Bond angles

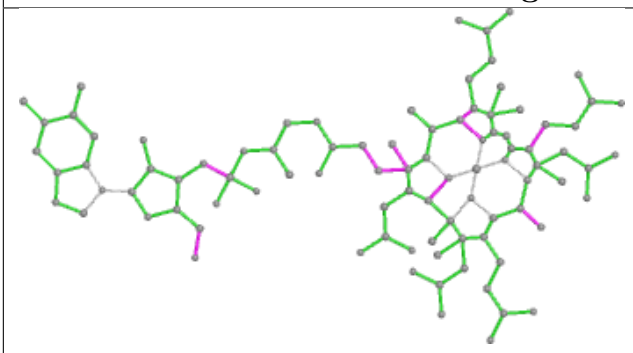


Torsions

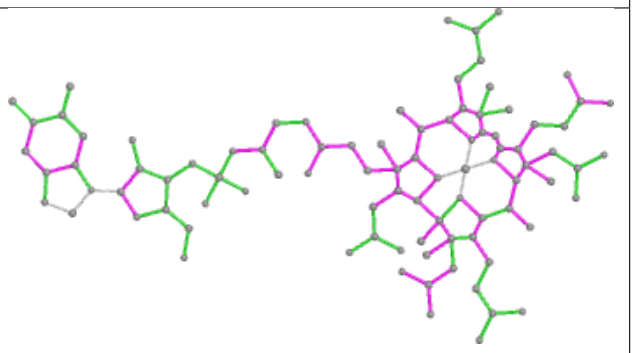


Rings

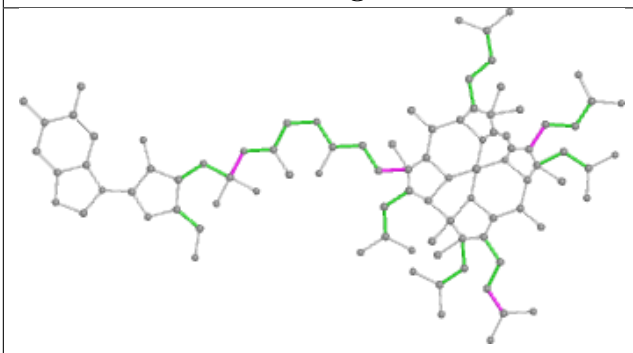
Ligand B12 A 1800



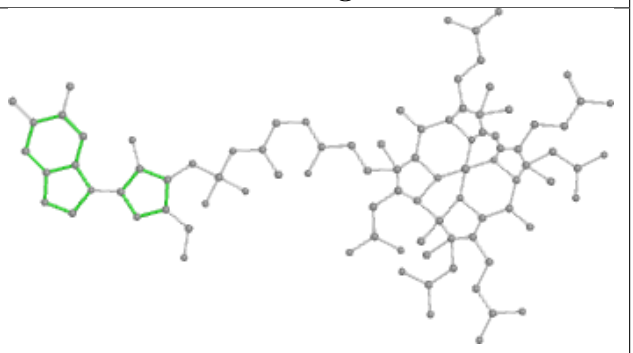
Bond lengths



Bond angles

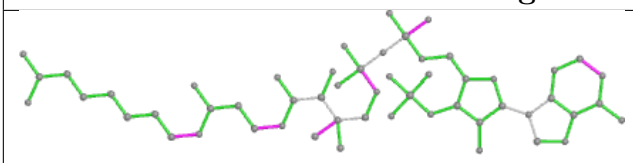


Torsions

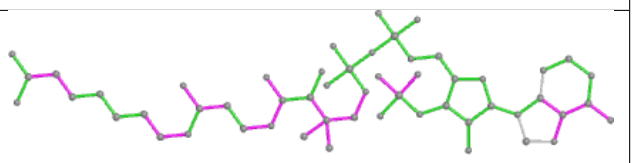


Rings

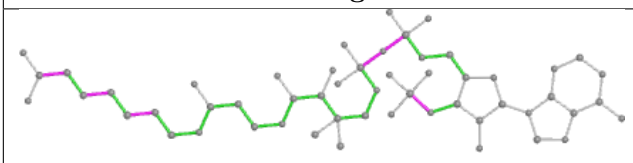
Ligand 3CP C 2801



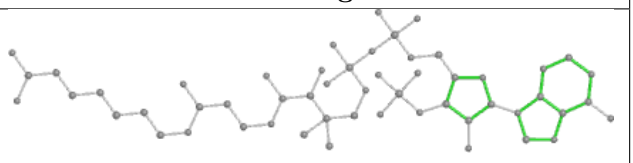
Bond lengths



Bond angles

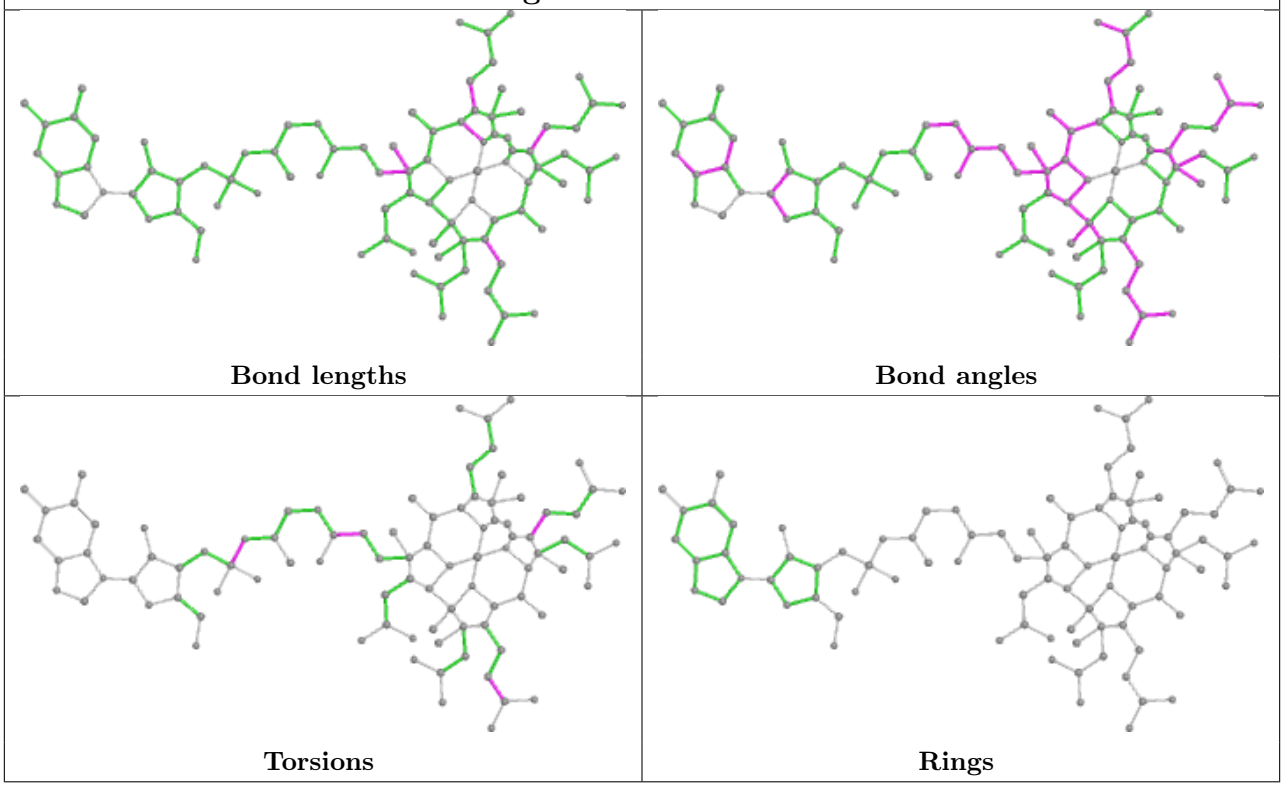


Torsions



Rings

Ligand B12 C 2800



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	727/727 (100%)	-0.34	8 (1%)	80	79	16, 30, 53, 108	0
1	C	727/727 (100%)	-0.28	16 (2%)	62	59	14, 29, 53, 109	0
2	B	619/637 (97%)	-0.13	16 (2%)	56	53	19, 37, 61, 93	0
2	D	619/637 (97%)	0.26	39 (6%)	20	19	19, 41, 64, 93	0
All	All	2692/2728 (98%)	-0.14	79 (2%)	51	49	14, 33, 59, 109	0

All (79) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	2	SER	10.3
1	C	2	SER	7.1
1	A	3	THR	6.0
1	C	3	THR	5.9
1	C	728	ALA	5.6
2	D	270	GLY	5.3
2	D	107	TRP	5.2
1	A	728	ALA	4.8
2	D	106	ALA	4.5
1	C	23	ARG	4.5
2	D	187	ASP	4.0
2	D	230	ASP	4.0
2	D	158	LEU	3.7
2	D	161	MET	3.7
1	C	36	GLU	3.5
2	D	189	PRO	3.5
2	D	30	ALA	3.5
2	B	508	SER	3.4
2	D	192	ASP	3.4
2	D	193	LEU	3.4
2	D	567	LEU	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	20	THR	3.2
2	D	305	ALA	3.1
2	D	272	THR	3.1
2	D	312	GLY	3.0
1	C	15	ALA	3.0
2	B	187	ASP	3.0
2	B	603	GLY	3.0
2	B	567	LEU	2.9
1	C	575	LYS	2.9
2	D	638	LYS	2.9
2	D	20	THR	2.8
2	D	170	TYR	2.8
1	A	576	ASN	2.8
2	D	50	GLU	2.8
1	C	429	LYS	2.7
1	A	430	VAL	2.7
2	D	316	ASP	2.7
2	B	50	GLU	2.6
2	B	107	TRP	2.6
2	B	106	ALA	2.6
2	B	509	GLU	2.6
1	C	20	ASP	2.6
2	D	184	GLU	2.5
1	C	9	SER	2.5
2	D	267	VAL	2.4
2	B	49	PRO	2.4
2	D	483	PRO	2.4
1	C	576	ASN	2.4
1	C	4	LEU	2.4
2	D	183	TYR	2.4
2	B	516	ALA	2.4
2	B	195	LEU	2.3
2	D	186	SER	2.3
2	D	173	GLY	2.3
2	D	218	GLY	2.3
1	A	36	GLU	2.3
2	D	273	ALA	2.2
2	D	222	ARG	2.2
1	C	14	ASN	2.2
2	D	314	ASP	2.2
2	D	516	ALA	2.2
1	C	501	ALA	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	D	31	THR	2.1
1	C	16	PRO	2.1
2	D	83	LYS	2.1
2	B	149	HIS	2.1
1	A	574	VAL	2.1
2	B	179	LEU	2.1
2	D	32	GLU	2.1
2	D	146	ALA	2.1
2	D	151	ASP	2.1
2	B	161	MET	2.1
2	B	572	LYS	2.1
2	D	119	LYS	2.1
1	C	17	VAL	2.1
2	D	214	LEU	2.0
2	D	118	GLU	2.0
1	A	477	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 monosaccharides in this entry.

6.4 Ligands (i)

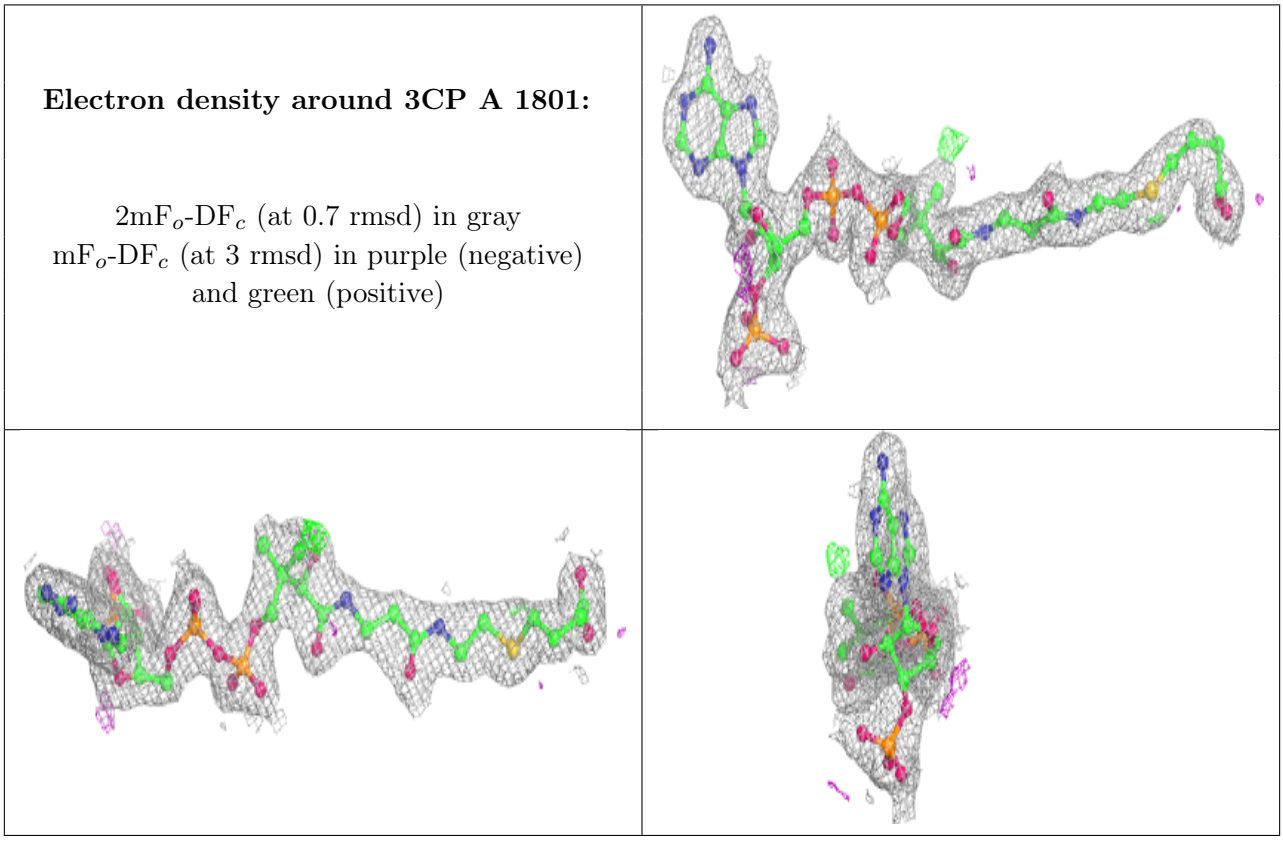
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	GOL	A	3001	6/6	0.95	0.14	29,34,37,40	0
5	GOL	C	3002	6/6	0.95	0.11	31,31,34,34	0
3	3CP	A	1801	54/54	0.97	0.09	17,24,31,35	0
3	3CP	C	2801	54/54	0.97	0.10	15,23,30,36	0
4	B12	A	1800	91/91	0.98	0.08	13,21,27,31	0
4	B12	C	2800	91/91	0.98	0.08	11,19,25,28	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.

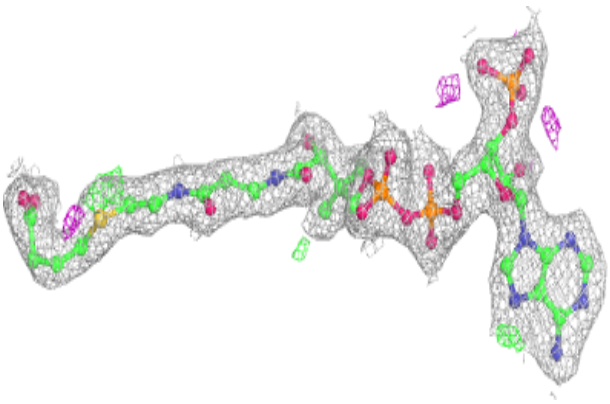
Electron density around 3CP A 1801:

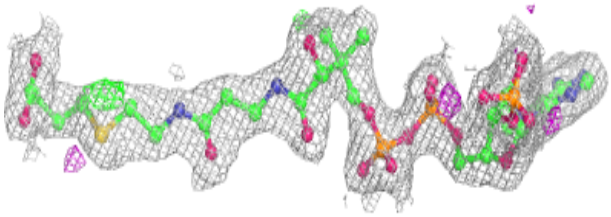
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

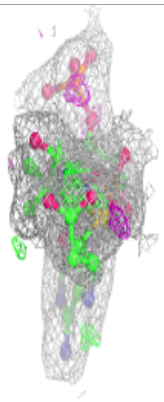


Electron density around 3CP C 2801:

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

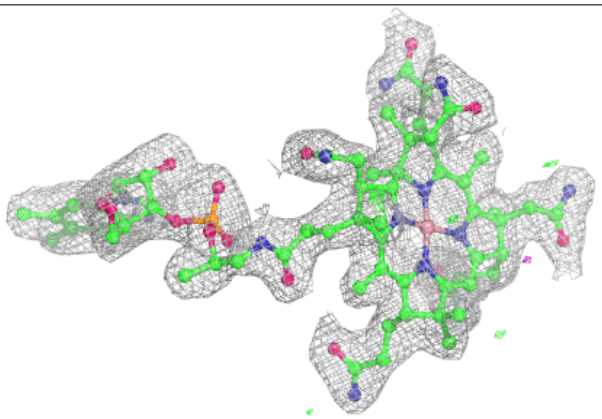


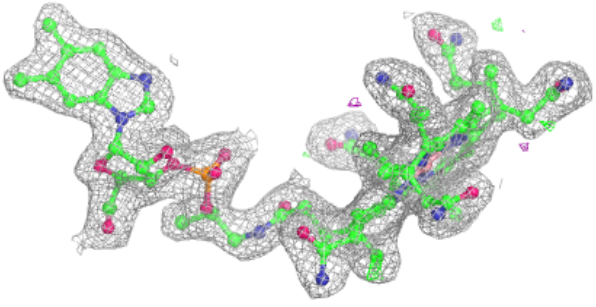


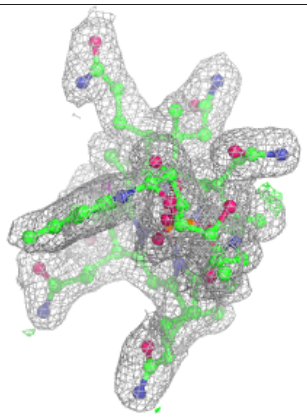


Electron density around B12 A 1800:

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

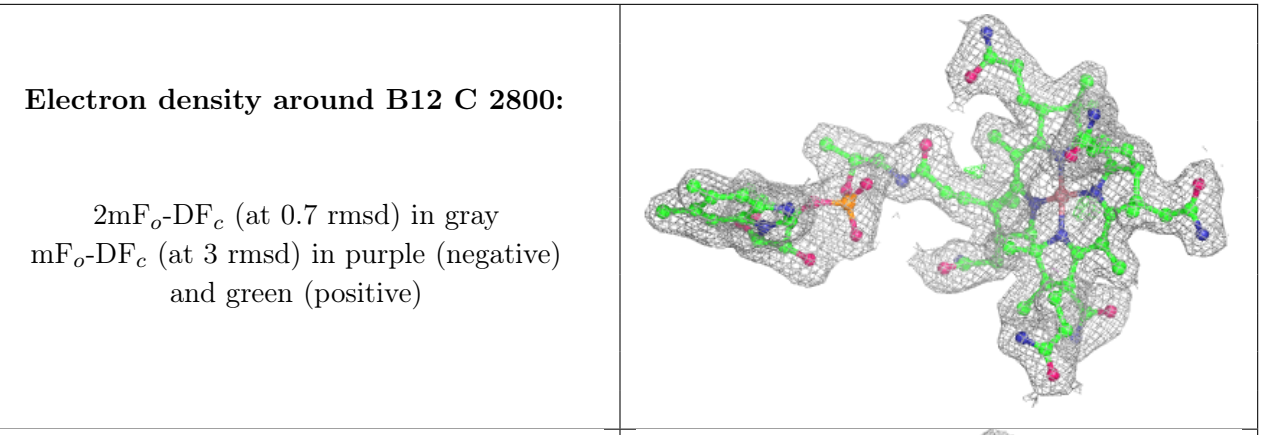


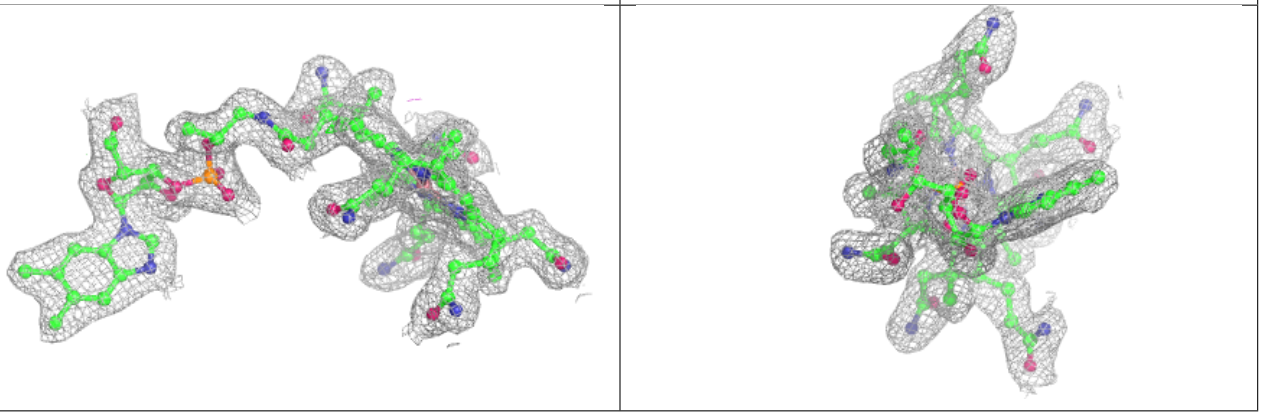




Electron density around B12 C 2800:

$2mF_o$-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.