Full wwPDB X-ray Structure Validation Report ⓘ

Oct 17, 2021 – 05:32 AM EDT

PDB ID	:	1JOF
Title	:	Neurospora crassa 3-carboxy-cis,cis-mucoante lactonizing enzyme
Authors	:	Kajander, T.; Merckel, M.C.; Thompson, A.; Deacon, A.M.; Mazur, P.; Kozarich, J.W.; Goldman, A.
Deposited on	:	2001-07-28
Resolution	:	2.50 Å(reported)

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

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

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

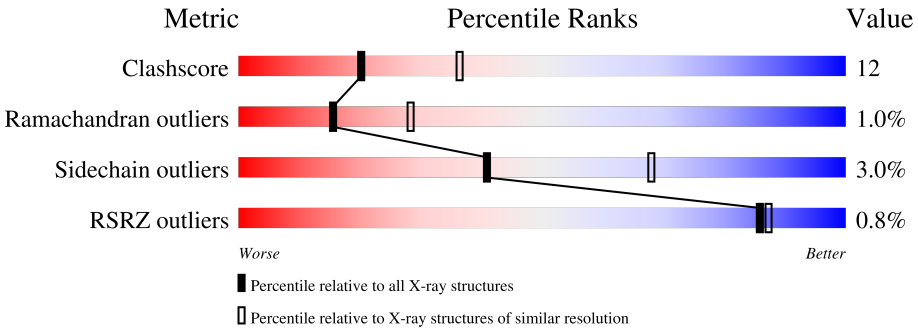
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

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 2.50 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.



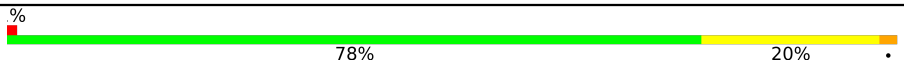
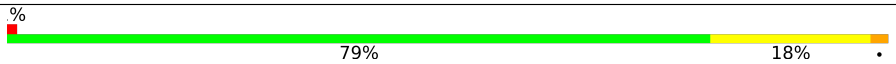
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	365	78% 21%
1	B	365	78% 20%
1	C	365	% 79% 19%
1	D	365	% 79% 19%
1	E	365	2% 80% 18%
1	F	365	% 79% 18%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	G	365	
1	H	365	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	BME	A	367	-	X	-	-
3	BME	A	368	-	X	X	-
3	BME	B	9013	-	X	-	-
3	BME	B	9014	-	X	X	-
3	BME	C	367	-	X	-	-
3	BME	C	399	-	X	X	-
3	BME	D	466	-	X	-	-
3	BME	D	499	-	X	X	-
3	BME	E	566	-	X	-	-
3	BME	E	599	-	X	X	-
3	BME	F	666	-	X	-	-
3	BME	F	699	-	X	X	-
3	BME	G	766	-	X	-	-
3	BME	G	799	-	X	-	-
3	BME	H	1866	-	X	-	-
3	BME	H	1899	-	X	X	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 23837 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 CARBOXY-CIS,CIS-MUCONATE CYCLASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	365	Total	C	N	O	S	Se	0	0	0
			2871	1845	481	530	5	10			
1	B	365	Total	C	N	O	S	Se	0	0	0
			2871	1845	481	530	5	10			
1	C	365	Total	C	N	O	S	Se	0	0	0
			2875	1847	481	532	5	10			
1	D	365	Total	C	N	O	S	Se	0	0	0
			2875	1847	481	532	5	10			
1	E	365	Total	C	N	O	S	Se	0	0	0
			2871	1845	481	530	5	10			
1	F	365	Total	C	N	O	S	Se	0	0	0
			2871	1845	481	530	5	10			
1	G	365	Total	C	N	O	S	Se	0	0	0
			2875	1847	481	532	5	10			
1	H	365	Total	C	N	O	S	Se	0	0	0
			2875	1847	481	532	5	10			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	6	MSE	MET	engineered mutation	UNP P38677
A	45	MSE	MET	engineered mutation	UNP P38677
A	59	MSE	MET	engineered mutation	UNP P38677
A	150	MSE	MET	engineered mutation	UNP P38677
A	200	MSE	MET	engineered mutation	UNP P38677
A	211	MSE	MET	engineered mutation	UNP P38677
A	228	MSE	MET	engineered mutation	UNP P38677
A	269	MSE	MET	engineered mutation	UNP P38677
A	324	MSE	MET	engineered mutation	UNP P38677
A	359	MSE	MET	engineered mutation	UNP P38677
B	6	MSE	MET	engineered mutation	UNP P38677
B	45	MSE	MET	engineered mutation	UNP P38677
B	59	MSE	MET	engineered mutation	UNP P38677

Continued on next page...

Continued from previous page...

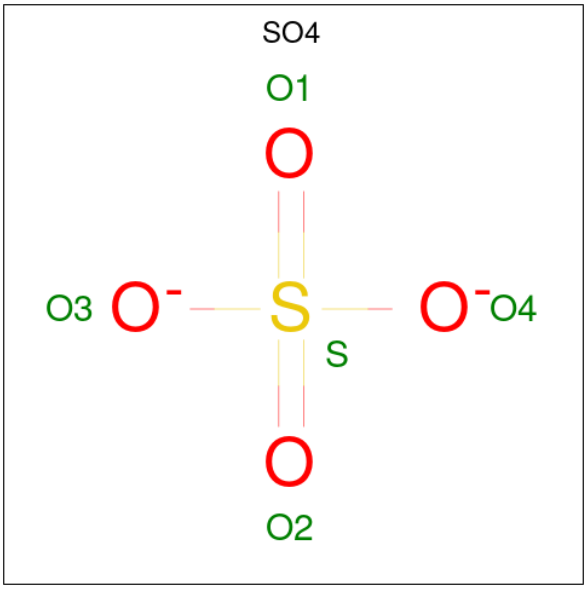
Chain	Residue	Modelled	Actual	Comment	Reference
B	150	MSE	MET	engineered mutation	UNP P38677
B	200	MSE	MET	engineered mutation	UNP P38677
B	211	MSE	MET	engineered mutation	UNP P38677
B	228	MSE	MET	engineered mutation	UNP P38677
B	269	MSE	MET	engineered mutation	UNP P38677
B	324	MSE	MET	engineered mutation	UNP P38677
B	359	MSE	MET	engineered mutation	UNP P38677
C	6	MSE	MET	engineered mutation	UNP P38677
C	45	MSE	MET	engineered mutation	UNP P38677
C	59	MSE	MET	engineered mutation	UNP P38677
C	150	MSE	MET	engineered mutation	UNP P38677
C	200	MSE	MET	engineered mutation	UNP P38677
C	211	MSE	MET	engineered mutation	UNP P38677
C	228	MSE	MET	engineered mutation	UNP P38677
C	269	MSE	MET	engineered mutation	UNP P38677
C	324	MSE	MET	engineered mutation	UNP P38677
C	359	MSE	MET	engineered mutation	UNP P38677
D	6	MSE	MET	engineered mutation	UNP P38677
D	45	MSE	MET	engineered mutation	UNP P38677
D	59	MSE	MET	engineered mutation	UNP P38677
D	150	MSE	MET	engineered mutation	UNP P38677
D	200	MSE	MET	engineered mutation	UNP P38677
D	211	MSE	MET	engineered mutation	UNP P38677
D	228	MSE	MET	engineered mutation	UNP P38677
D	269	MSE	MET	engineered mutation	UNP P38677
D	324	MSE	MET	engineered mutation	UNP P38677
D	359	MSE	MET	engineered mutation	UNP P38677
E	6	MSE	MET	engineered mutation	UNP P38677
E	45	MSE	MET	engineered mutation	UNP P38677
E	59	MSE	MET	engineered mutation	UNP P38677
E	150	MSE	MET	engineered mutation	UNP P38677
E	200	MSE	MET	engineered mutation	UNP P38677
E	211	MSE	MET	engineered mutation	UNP P38677
E	228	MSE	MET	engineered mutation	UNP P38677
E	269	MSE	MET	engineered mutation	UNP P38677
E	324	MSE	MET	engineered mutation	UNP P38677
E	359	MSE	MET	engineered mutation	UNP P38677
F	6	MSE	MET	engineered mutation	UNP P38677
F	45	MSE	MET	engineered mutation	UNP P38677
F	59	MSE	MET	engineered mutation	UNP P38677
F	150	MSE	MET	engineered mutation	UNP P38677
F	200	MSE	MET	engineered mutation	UNP P38677

Continued on next page...

Continued from previous page...

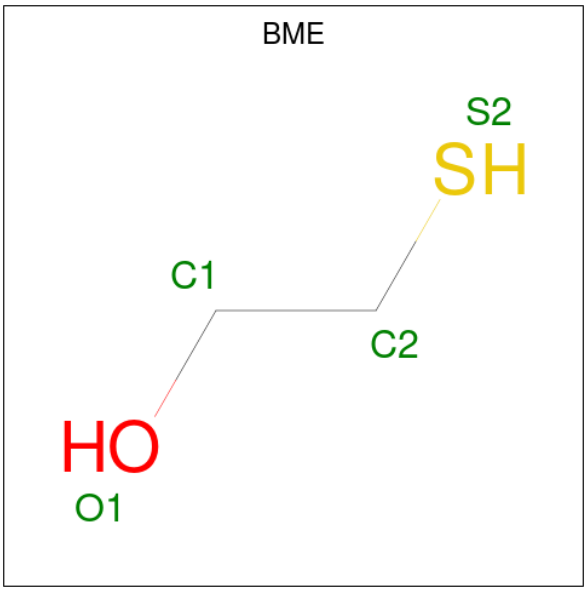
Chain	Residue	Modelled	Actual	Comment	Reference
F	211	MSE	MET	engineered mutation	UNP P38677
F	228	MSE	MET	engineered mutation	UNP P38677
F	269	MSE	MET	engineered mutation	UNP P38677
F	324	MSE	MET	engineered mutation	UNP P38677
F	359	MSE	MET	engineered mutation	UNP P38677
G	6	MSE	MET	engineered mutation	UNP P38677
G	45	MSE	MET	engineered mutation	UNP P38677
G	59	MSE	MET	engineered mutation	UNP P38677
G	150	MSE	MET	engineered mutation	UNP P38677
G	200	MSE	MET	engineered mutation	UNP P38677
G	211	MSE	MET	engineered mutation	UNP P38677
G	228	MSE	MET	engineered mutation	UNP P38677
G	269	MSE	MET	engineered mutation	UNP P38677
G	324	MSE	MET	engineered mutation	UNP P38677
G	359	MSE	MET	engineered mutation	UNP P38677
H	6	MSE	MET	engineered mutation	UNP P38677
H	45	MSE	MET	engineered mutation	UNP P38677
H	59	MSE	MET	engineered mutation	UNP P38677
H	150	MSE	MET	engineered mutation	UNP P38677
H	200	MSE	MET	engineered mutation	UNP P38677
H	211	MSE	MET	engineered mutation	UNP P38677
H	228	MSE	MET	engineered mutation	UNP P38677
H	269	MSE	MET	engineered mutation	UNP P38677
H	324	MSE	MET	engineered mutation	UNP P38677
H	359	MSE	MET	engineered mutation	UNP P38677

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0
2	E	1	Total O S 5 4 1	0	0
2	F	1	Total O S 5 4 1	0	0
2	G	1	Total O S 5 4 1	0	0
2	H	1	Total O S 5 4 1	0	0

- Molecule 3 is BETA-MERCAPTOETHANOL (three-letter code: BME) (formula: C_2H_6OS).



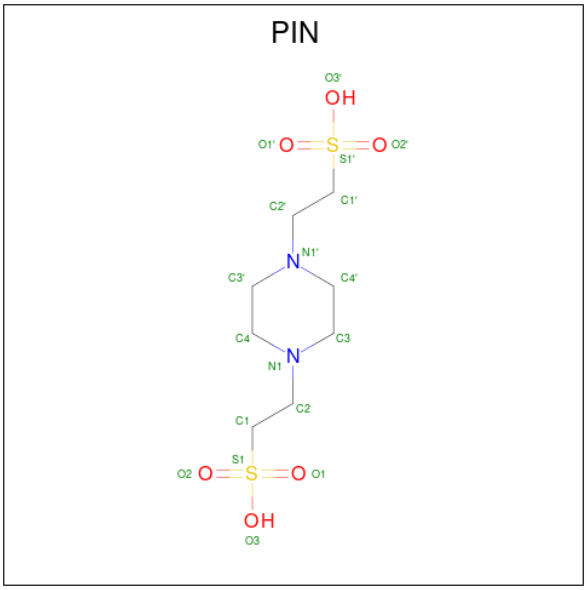
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O S 4 2 1 1	0	0
3	A	1	Total C O S 4 2 1 1	0	0
3	B	1	Total C O S 4 2 1 1	0	0
3	B	1	Total C O S 4 2 1 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	C	1	Total	C	O	S	0	0
			4	2	1	1		
3	C	1	Total	C	O	S	0	0
			4	2	1	1		
3	D	1	Total	C	O	S	0	0
			4	2	1	1		
3	D	1	Total	C	O	S	0	0
			4	2	1	1		
3	E	1	Total	C	O	S	0	0
			4	2	1	1		
3	E	1	Total	C	O	S	0	0
			4	2	1	1		
3	F	1	Total	C	O	S	0	0
			4	2	1	1		
3	F	1	Total	C	O	S	0	0
			4	2	1	1		
3	G	1	Total	C	O	S	0	0
			4	2	1	1		
3	G	1	Total	C	O	S	0	0
			4	2	1	1		
3	H	1	Total	C	O	S	0	0
			4	2	1	1		
3	H	1	Total	C	O	S	0	0
			4	2	1	1		

- Molecule 4 is PIPERAZINE-N,N'-BIS(2-ETHANESULFONIC ACID) (three-letter code: PIN) (formula: $C_8H_{18}N_2O_6S_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	N	O	S	0	0
			18	8	2	6	2		
4	H	1	Total	C	N	O	S	0	0
			18	8	2	6	2		

- Molecule 5 is water.

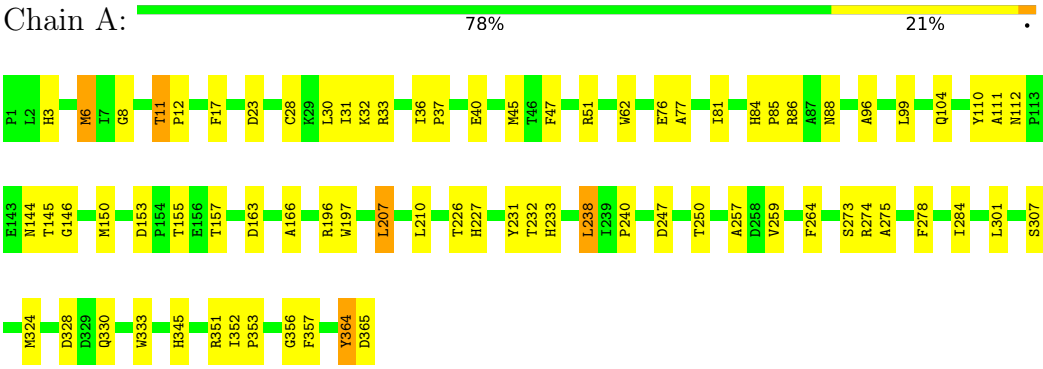
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	99	Total	O	0	0
			99	99		
5	B	79	Total	O	0	0
			79	79		
5	C	134	Total	O	0	0
			134	134		
5	D	81	Total	O	0	0
			81	81		
5	E	53	Total	O	0	0
			53	53		
5	F	88	Total	O	0	0
			88	88		
5	G	115	Total	O	0	0
			115	115		
5	H	64	Total	O	0	0
			64	64		

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.

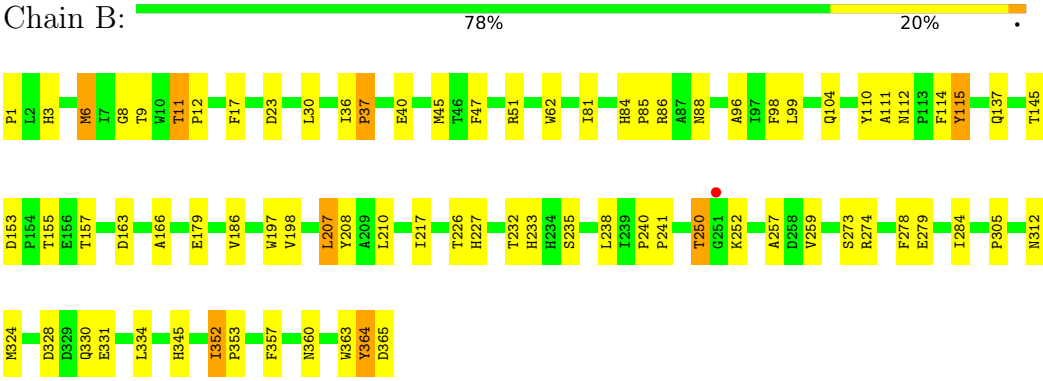
• Molecule 1: CARBOXY-CIS,CIS-MUCONATE CYCLASE

Chain A:



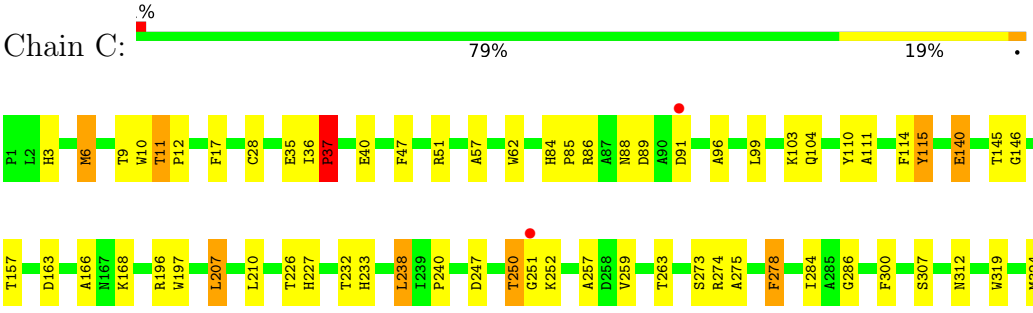
• Molecule 1: CARBOXY-CIS,CIS-MUCONATE CYCLASE

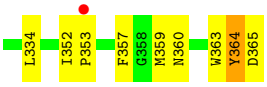
Chain B:



• Molecule 1: CARBOXY-CIS,CIS-MUCONATE CYCLASE

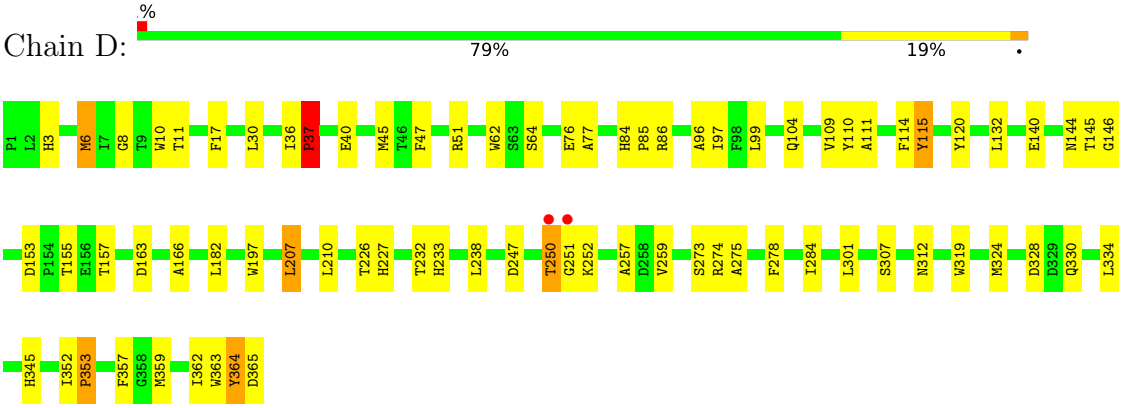
Chain C:





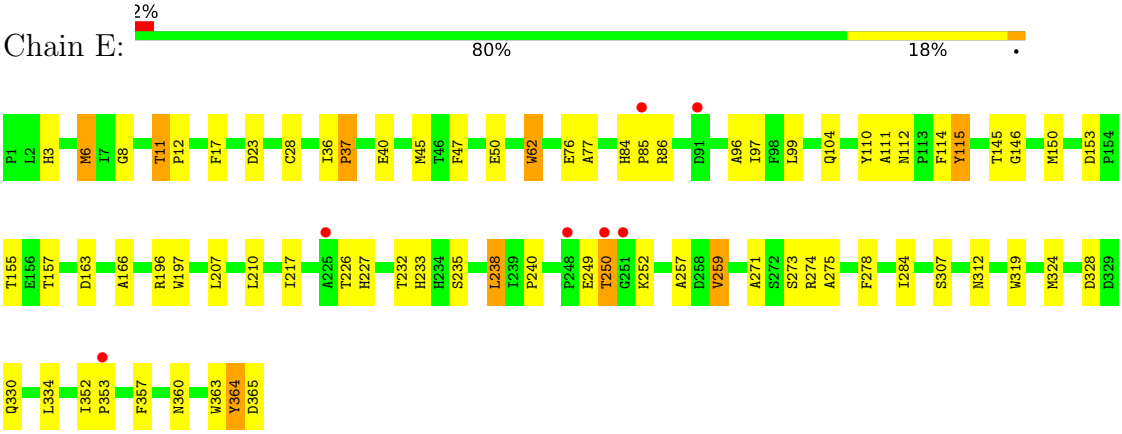
• Molecule 1: CARBOXY-CIS,CIS-MUCONATE CYCLASE

Chain D:



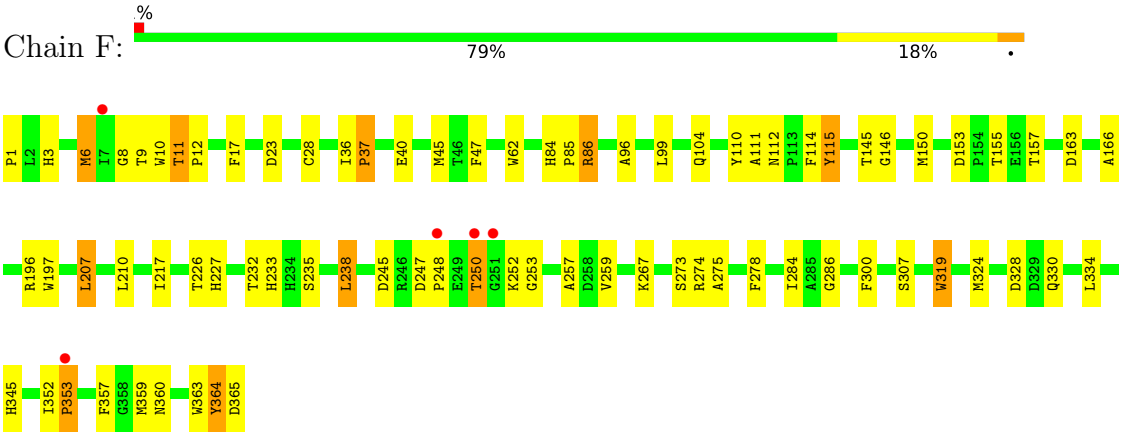
• Molecule 1: CARBOXY-CIS,CIS-MUCONATE CYCLASE

Chain E:



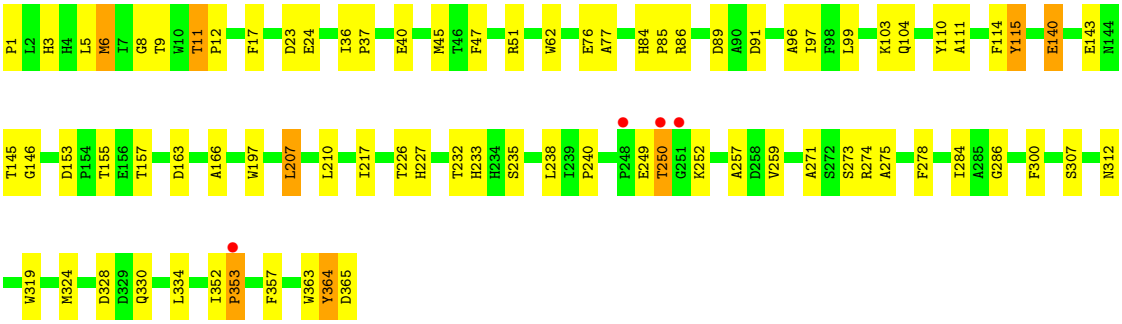
• Molecule 1: CARBOXY-CIS,CIS-MUCONATE CYCLASE

Chain F:



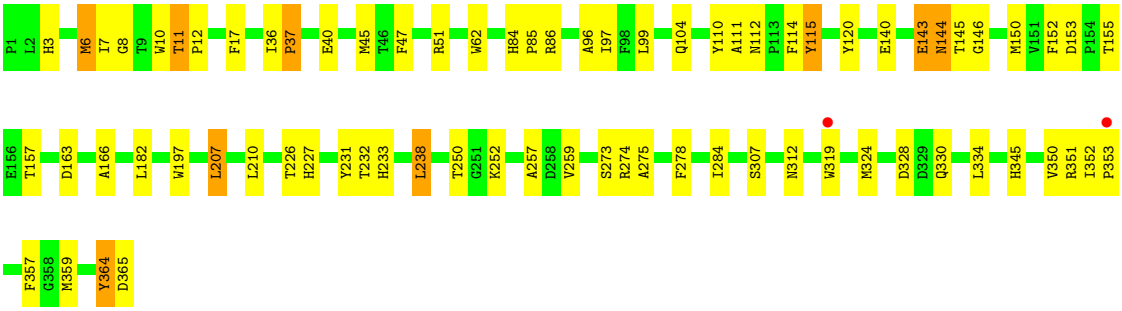
• Molecule 1: CARBOXY-CIS,CIS-MUCONATE CYCLASE

Chain G:



• Molecule 1: CARBOXY-CIS,CIS-MUCONATE CYCLASE

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	92.29Å 160.60Å 237.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.50 20.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	92.7 (20.00-2.50) 90.0 (20.00-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	5.00	Depositor
$< I/\sigma(I) >$ [1]	3.01 (at 2.50Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.212 , 0.251 0.202 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	28.6	Xtriage
Anisotropy	0.542	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 32.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	23837	wwPDB-VP
Average B, all atoms (Å^2)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.21% 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: SO4, PIN, BME

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	0.67	1/2959 (0.0%)	0.81	1/4023 (0.0%)
1	B	0.67	0/2959	0.80	2/4023 (0.0%)
1	C	0.69	2/2963 (0.1%)	0.81	3/4028 (0.1%)
1	D	0.67	0/2963	0.81	2/4028 (0.0%)
1	E	0.69	1/2959 (0.0%)	0.81	3/4023 (0.1%)
1	F	0.67	1/2959 (0.0%)	0.81	3/4023 (0.1%)
1	G	0.67	1/2963 (0.0%)	0.81	2/4028 (0.0%)
1	H	0.65	1/2963 (0.0%)	0.81	1/4028 (0.0%)
All	All	0.67	7/23688 (0.0%)	0.81	17/32204 (0.1%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	28	CYS	CB-SG	-8.55	1.67	1.82
1	F	28	CYS	CB-SG	-8.04	1.68	1.82
1	A	28	CYS	CB-SG	-7.52	1.69	1.82
1	E	28	CYS	CB-SG	-6.71	1.70	1.82
1	G	140	GLU	CD-OE2	5.35	1.31	1.25
1	H	144	ASN	CB-CG	-5.07	1.39	1.51
1	C	140	GLU	CD-OE2	5.00	1.31	1.25

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	364	TYR	N-CA-C	-6.89	92.41	111.00
1	B	364	TYR	N-CA-C	-6.85	92.50	111.00
1	C	364	TYR	N-CA-C	-6.72	92.85	111.00
1	A	364	TYR	N-CA-C	-6.71	92.87	111.00
1	D	364	TYR	N-CA-C	-6.48	93.49	111.00
1	G	364	TYR	N-CA-C	-6.39	93.75	111.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	364	TYR	N-CA-C	-6.37	93.79	111.00
1	H	364	TYR	N-CA-C	-5.97	94.88	111.00
1	F	86	ARG	NE-CZ-NH1	-5.70	117.45	120.30
1	D	334	LEU	N-CA-C	-5.67	95.69	111.00
1	E	334	LEU	N-CA-C	-5.54	96.05	111.00
1	C	334	LEU	N-CA-C	-5.48	96.20	111.00
1	F	334	LEU	N-CA-C	-5.35	96.55	111.00
1	B	334	LEU	N-CA-C	-5.31	96.65	111.00
1	E	62	TRP	N-CA-C	-5.29	96.72	111.00
1	G	334	LEU	N-CA-C	-5.06	97.34	111.00
1	C	57	ALA	N-CA-C	-5.03	97.41	111.00

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	2871	0	2704	71	0
1	B	2871	0	2704	69	0
1	C	2875	0	2708	70	0
1	D	2875	0	2708	81	0
1	E	2871	0	2704	62	0
1	F	2871	0	2704	68	0
1	G	2875	0	2708	73	0
1	H	2875	0	2708	80	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
2	D	5	0	0	1	0
2	E	5	0	0	0	0
2	F	5	0	0	0	0
2	G	5	0	0	1	0
2	H	5	0	0	0	0
3	A	8	0	8	4	0
3	B	8	0	8	4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	8	0	8	4	0
3	D	8	0	8	5	0
3	E	8	0	8	5	0
3	F	8	0	8	4	0
3	G	8	0	8	3	0
3	H	8	0	8	4	0
4	B	18	0	18	4	0
4	H	18	0	18	0	0
5	A	99	0	0	4	0
5	B	79	0	0	4	0
5	C	134	0	0	9	0
5	D	81	0	0	2	0
5	E	53	0	0	1	0
5	F	88	0	0	3	0
5	G	115	0	0	5	0
5	H	64	0	0	6	0
All	All	23837	0	21748	561	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 12.

All (561) 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:C:140:GLU:OE1	5:C:1150:HOH:O	1.60	1.19
1:D:140:GLU:OE1	5:D:1151:HOH:O	1.63	1.16
1:G:140:GLU:OE1	5:G:1157:HOH:O	1.65	1.14
1:H:140:GLU:OE1	5:H:1161:HOH:O	1.68	1.09
1:A:6:MSE:N	1:A:6:MSE:HE2	1.78	0.99
1:G:6:MSE:N	1:G:6:MSE:HE2	1.78	0.98
1:C:6:MSE:HE2	1:C:6:MSE:N	1.80	0.96
1:B:6:MSE:N	1:B:6:MSE:HE2	1.80	0.95
1:F:6:MSE:N	1:F:6:MSE:HE2	1.81	0.93
1:H:6:MSE:HE2	1:H:6:MSE:N	1.84	0.93
1:E:6:MSE:HE2	1:E:6:MSE:N	1.88	0.87
1:D:6:MSE:N	1:D:6:MSE:HE2	1.89	0.86
1:H:278:PHE:CD2	1:H:330:GLN:HG3	2.11	0.85
1:G:143:GLU:OE1	5:G:1260:HOH:O	1.95	0.84
1:F:6:MSE:HE2	1:F:6:MSE:H	1.40	0.84
1:A:6:MSE:HE2	1:A:6:MSE:H	1.39	0.83
1:D:6:MSE:HE2	1:D:6:MSE:H	1.42	0.83

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:6:MSE:HE2	1:C:6:MSE:H	1.43	0.83
1:A:356:GLY:HA2	5:A:1191:HOH:O	1.78	0.82
1:B:6:MSE:HE2	1:B:6:MSE:H	1.43	0.82
1:E:6:MSE:HE2	1:E:6:MSE:H	1.45	0.81
1:G:278:PHE:CD2	1:G:330:GLN:HG3	2.16	0.81
1:D:250:THR:HG22	1:D:252:LYS:CB	2.12	0.80
1:C:84:HIS:HD2	1:C:86:ARG:H	1.29	0.80
1:G:6:MSE:HE2	1:G:6:MSE:H	1.45	0.80
1:D:278:PHE:CD2	1:D:330:GLN:HG3	2.18	0.79
1:F:278:PHE:CD2	1:F:330:GLN:HG3	2.17	0.78
1:B:278:PHE:CD2	1:B:330:GLN:HG3	2.18	0.78
1:C:278:PHE:CD2	1:C:330:GLN:HG3	2.18	0.78
1:H:6:MSE:HE2	1:H:6:MSE:H	1.47	0.77
1:D:155:THR:HG22	1:D:157:THR:OG1	1.84	0.77
1:E:278:PHE:CD2	1:E:330:GLN:HG3	2.20	0.77
1:H:155:THR:HG22	1:H:157:THR:OG1	1.84	0.76
1:D:144:ASN:HB2	1:H:182:LEU:HD23	1.67	0.76
1:A:278:PHE:CD2	1:A:330:GLN:HG3	2.20	0.75
1:B:155:THR:HG22	1:B:157:THR:OG1	1.87	0.75
1:C:35:GLU:HG3	5:C:1167:HOH:O	1.88	0.74
1:A:155:THR:HG22	1:A:157:THR:OG1	1.88	0.74
1:D:6:MSE:HE3	1:D:47:PHE:CZ	2.23	0.73
1:H:84:HIS:HD2	1:H:86:ARG:H	1.37	0.72
1:E:155:THR:HG22	1:E:157:THR:OG1	1.88	0.72
1:A:84:HIS:HD2	1:A:86:ARG:H	1.35	0.72
1:G:84:HIS:HD2	1:G:86:ARG:H	1.37	0.71
1:B:84:HIS:HD2	1:B:86:ARG:H	1.38	0.71
1:F:267:LYS:HE3	5:F:1457:HOH:O	1.90	0.71
1:G:155:THR:HG22	1:G:157:THR:OG1	1.90	0.71
1:D:250:THR:CG2	1:D:252:LYS:CB	2.69	0.70
1:H:143:GLU:CD	5:H:1381:HOH:O	2.30	0.69
1:D:250:THR:C	1:D:252:LYS:H	1.95	0.69
1:G:143:GLU:CD	5:G:1260:HOH:O	2.30	0.69
1:A:364:TYR:O	1:A:365:ASP:HB2	1.93	0.68
1:E:84:HIS:HD2	1:E:86:ARG:H	1.43	0.67
1:H:364:TYR:O	1:H:365:ASP:HB2	1.92	0.67
1:F:84:HIS:HD2	1:F:86:ARG:H	1.43	0.67
1:D:120:TYR:CE1	1:H:140:GLU:OE2	2.48	0.67
1:C:155:THR:HG22	1:C:157:THR:OG1	1.95	0.67
1:D:364:TYR:O	1:D:365:ASP:HB2	1.93	0.66
1:G:249:GLU:O	1:G:250:THR:OG1	2.13	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:103:LYS:HE2	5:G:1544:HOH:O	1.95	0.66
1:D:226:THR:O	1:D:227:HIS:HB2	1.95	0.66
1:G:226:THR:O	1:G:227:HIS:HB2	1.96	0.66
1:A:197:TRP:CE2	1:A:259:VAL:HG22	2.31	0.66
1:F:364:TYR:O	1:F:365:ASP:HB2	1.96	0.66
1:E:6:MSE:HE3	1:E:47:PHE:CZ	2.31	0.65
1:D:6:MSE:HE3	1:D:47:PHE:HZ	1.62	0.65
1:H:226:THR:O	1:H:227:HIS:HB2	1.96	0.65
1:D:99:LEU:HD13	1:D:111:ALA:HB2	1.79	0.64
1:E:226:THR:O	1:E:227:HIS:HB2	1.98	0.64
1:C:364:TYR:O	1:C:365:ASP:HB2	1.97	0.63
1:H:250:THR:CG2	1:H:252:LYS:CB	2.76	0.63
1:A:226:THR:O	1:A:227:HIS:HB2	1.99	0.63
1:D:155:THR:CG2	1:D:157:THR:OG1	2.46	0.63
1:C:226:THR:O	1:C:227:HIS:HB2	1.99	0.62
1:G:284:ILE:CD1	1:G:324:MSE:HE1	2.28	0.62
1:G:284:ILE:HD11	1:G:324:MSE:HE1	1.80	0.62
2:D:461:SO4:O1	5:D:1082:HOH:O	2.14	0.62
1:C:35:GLU:CG	5:C:1167:HOH:O	2.45	0.62
1:H:250:THR:HG22	1:H:252:LYS:H	1.65	0.62
1:F:155:THR:HG22	1:F:157:THR:OG1	1.99	0.62
1:A:196:ARG:NH1	5:A:1244:HOH:O	2.32	0.62
1:E:197:TRP:CE2	1:E:259:VAL:HG22	2.35	0.62
1:H:6:MSE:HE3	1:H:47:PHE:CZ	2.35	0.62
1:G:153:ASP:OD1	1:G:155:THR:HB	2.01	0.61
1:H:197:TRP:CE2	1:H:259:VAL:HG22	2.36	0.61
1:C:6:MSE:HE3	1:C:47:PHE:CZ	2.36	0.61
1:F:84:HIS:CD2	1:F:85:PRO:HD2	2.35	0.61
1:H:250:THR:HG22	1:H:252:LYS:CB	2.31	0.61
1:B:197:TRP:CE2	1:B:259:VAL:HG22	2.35	0.61
1:F:6:MSE:HE3	1:F:47:PHE:CZ	2.35	0.61
1:E:155:THR:CG2	1:E:157:THR:OG1	2.49	0.60
1:A:284:ILE:CD1	1:A:324:MSE:HE1	2.31	0.60
1:D:250:THR:HG22	1:D:252:LYS:H	1.67	0.59
1:C:250:THR:C	1:C:252:LYS:H	2.04	0.59
1:H:278:PHE:CE2	1:H:330:GLN:HG3	2.37	0.59
1:B:226:THR:O	1:B:227:HIS:HB2	2.02	0.59
1:F:197:TRP:CE2	1:F:259:VAL:HG22	2.37	0.59
1:B:331:GLU:OE1	4:B:9012:PIN:H12	2.01	0.59
1:B:155:THR:CG2	1:B:157:THR:OG1	2.51	0.59
1:D:153:ASP:OD1	1:D:155:THR:HB	2.02	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:364:TYR:O	1:G:365:ASP:HB2	2.02	0.59
1:H:284:ILE:HD11	1:H:324:MSE:HE1	1.84	0.59
1:A:284:ILE:HD11	1:A:324:MSE:HE1	1.84	0.59
1:D:37:PRO:HB2	1:D:40:GLU:HB2	1.85	0.58
1:A:155:THR:CG2	1:A:157:THR:OG1	2.52	0.58
1:B:364:TYR:O	1:B:365:ASP:HB2	2.03	0.58
1:F:226:THR:O	1:F:227:HIS:HB2	2.03	0.58
1:H:155:THR:CG2	1:H:157:THR:OG1	2.51	0.58
1:E:284:ILE:CD1	1:E:324:MSE:HE1	2.33	0.58
1:H:62:TRP:CH2	1:H:111:ALA:HB1	2.39	0.58
1:A:6:MSE:HE3	1:A:47:PHE:CZ	2.37	0.58
1:B:284:ILE:CD1	1:B:324:MSE:HE1	2.34	0.58
1:D:84:HIS:HD2	1:D:86:ARG:H	1.50	0.58
1:C:250:THR:HG22	1:C:250:THR:O	2.03	0.57
1:H:284:ILE:CD1	1:H:324:MSE:HE1	2.33	0.57
1:C:197:TRP:CE2	1:C:259:VAL:HG22	2.39	0.57
1:D:144:ASN:HB2	1:H:182:LEU:CD2	2.33	0.57
1:G:232:THR:O	1:G:233:HIS:HB2	2.05	0.57
1:E:207:LEU:C	1:E:207:LEU:HD23	2.24	0.57
1:A:84:HIS:CD2	1:A:85:PRO:HD2	2.39	0.57
1:A:278:PHE:HD2	1:A:330:GLN:HG3	1.66	0.57
1:C:284:ILE:CD1	1:C:324:MSE:HE1	2.35	0.57
1:F:207:LEU:C	1:F:207:LEU:HD23	2.25	0.57
1:H:99:LEU:HD13	1:H:111:ALA:HB2	1.87	0.57
1:C:84:HIS:CD2	1:C:85:PRO:HD2	2.40	0.56
1:A:62:TRP:CZ3	1:A:96:ALA:HB1	2.41	0.56
1:B:284:ILE:HD11	1:B:324:MSE:HE1	1.85	0.56
1:E:62:TRP:CZ3	1:E:96:ALA:HB1	2.39	0.56
1:E:99:LEU:CD1	1:E:111:ALA:HB2	2.35	0.56
1:E:364:TYR:O	1:E:365:ASP:HB2	2.04	0.56
1:G:197:TRP:CE2	1:G:259:VAL:HG22	2.40	0.56
1:H:99:LEU:CD1	1:H:111:ALA:HB2	2.35	0.56
1:D:99:LEU:CD1	1:D:111:ALA:HB2	2.34	0.56
1:G:155:THR:CG2	1:G:157:THR:OG1	2.52	0.56
1:C:37:PRO:HB2	1:C:40:GLU:HB2	1.87	0.56
1:E:3:HIS:ND1	3:E:599:BME:H21	2.20	0.56
1:C:35:GLU:CD	5:C:1167:HOH:O	2.43	0.56
1:F:232:THR:O	1:F:233:HIS:HB2	2.06	0.56
1:E:232:THR:O	1:E:233:HIS:HB2	2.06	0.56
1:B:232:THR:O	1:B:233:HIS:HB2	2.06	0.56
1:E:284:ILE:HD11	1:E:324:MSE:HE1	1.87	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:153:ASP:OD1	1:C:155:THR:HB	2.07	0.55
1:A:352:ILE:HB	1:A:357:PHE:CD2	2.41	0.55
1:A:319:TRP:HE3	3:A:368:BME:H12	1.72	0.55
1:B:112:ASN:HD21	1:B:150:MSE:HE2	1.71	0.55
1:G:250:THR:C	1:G:252:LYS:H	2.09	0.55
1:D:207:LEU:HD23	1:D:207:LEU:C	2.27	0.55
1:A:3:HIS:ND1	3:A:368:BME:H21	2.22	0.55
1:B:331:GLU:OE2	4:B:9012:PIN:N1	2.39	0.55
1:F:250:THR:C	1:F:252:LYS:H	2.09	0.55
1:D:250:THR:C	1:D:252:LYS:N	2.60	0.55
1:G:352:ILE:HB	1:G:357:PHE:CD2	2.42	0.55
1:B:99:LEU:CD1	1:B:111:ALA:HB2	2.37	0.54
1:C:84:HIS:CD2	1:C:86:ARG:H	2.18	0.54
1:C:207:LEU:C	1:C:207:LEU:HD23	2.28	0.54
1:G:9:THR:HG22	1:G:357:PHE:HA	1.89	0.54
1:H:232:THR:O	1:H:233:HIS:HB2	2.07	0.54
1:C:232:THR:O	1:C:233:HIS:HB2	2.07	0.54
1:E:37:PRO:HB2	1:E:40:GLU:HB2	1.88	0.54
1:H:112:ASN:HD21	1:H:150:MSE:HE2	1.72	0.54
1:E:319:TRP:HE3	3:E:599:BME:H12	1.71	0.54
1:F:112:ASN:ND2	1:F:150:MSE:HE2	2.23	0.54
1:A:351:ARG:NH2	5:A:1578:HOH:O	2.39	0.54
1:D:250:THR:HG22	1:D:250:THR:O	2.06	0.54
1:E:110:TYR:N	1:E:110:TYR:CD1	2.76	0.54
1:G:84:HIS:CD2	1:G:85:PRO:HD2	2.42	0.54
1:G:84:HIS:CD2	1:G:86:ARG:H	2.24	0.54
1:H:112:ASN:ND2	1:H:150:MSE:HE2	2.22	0.54
1:B:352:ILE:HB	1:B:357:PHE:CD2	2.43	0.53
1:H:250:THR:HG21	1:H:252:LYS:CB	2.37	0.53
1:B:6:MSE:HE3	1:B:47:PHE:CZ	2.44	0.53
1:F:319:TRP:HE3	3:F:699:BME:H12	1.74	0.53
1:H:37:PRO:HB2	1:H:40:GLU:HB2	1.90	0.53
1:D:3:HIS:ND1	3:D:499:BME:H21	2.23	0.53
1:F:99:LEU:CD1	1:F:111:ALA:HB2	2.39	0.53
1:F:112:ASN:HD21	1:F:150:MSE:HE2	1.74	0.53
1:F:352:ILE:HB	1:F:357:PHE:CD2	2.43	0.53
1:D:62:TRP:CH2	1:D:111:ALA:HB1	2.44	0.53
1:F:62:TRP:CH2	1:F:111:ALA:HB1	2.43	0.53
1:F:250:THR:HG22	1:F:252:LYS:CB	2.39	0.53
1:G:37:PRO:HB2	1:G:40:GLU:HB2	1.90	0.53
1:E:6:MSE:HE3	1:E:47:PHE:HZ	1.73	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:278:PHE:CE2	1:F:330:GLN:HG3	2.44	0.53
1:E:196:ARG:NH2	5:E:1001:HOH:O	2.42	0.53
1:H:3:HIS:ND1	3:H:1899:BME:H21	2.24	0.53
1:B:30:LEU:HD13	1:B:352:ILE:CD1	2.38	0.53
1:A:240:PRO:CB	1:B:345:HIS:HB3	2.38	0.52
1:E:99:LEU:HD13	1:E:111:ALA:HB2	1.90	0.52
1:H:6:MSE:HE3	1:H:47:PHE:HZ	1.75	0.52
1:E:250:THR:C	1:E:252:LYS:H	2.13	0.52
1:F:10:TRP:HB2	1:F:359:MSE:SE	2.60	0.52
1:B:112:ASN:ND2	1:B:150:MSE:HE2	2.23	0.52
1:C:6:MSE:HE3	1:C:47:PHE:HZ	1.73	0.52
1:E:153:ASP:OD1	1:E:155:THR:HB	2.09	0.52
1:E:112:ASN:HD21	1:E:150:MSE:HE2	1.75	0.52
1:G:207:LEU:C	1:G:207:LEU:HD23	2.29	0.52
1:B:153:ASP:OD1	1:B:155:THR:HB	2.10	0.52
1:E:249:GLU:O	1:E:250:THR:OG1	2.26	0.52
1:H:51:ARG:HD2	5:H:1604:HOH:O	2.09	0.52
1:G:62:TRP:CZ3	1:G:96:ALA:HB1	2.45	0.52
1:A:232:THR:O	1:A:233:HIS:HB2	2.10	0.51
1:G:278:PHE:HD1	1:G:278:PHE:H	1.58	0.51
1:C:99:LEU:CD1	1:C:111:ALA:HB2	2.40	0.51
1:C:155:THR:CG2	1:C:157:THR:OG1	2.59	0.51
1:F:62:TRP:CZ3	1:F:96:ALA:HB1	2.45	0.51
1:G:36:ILE:O	1:G:37:PRO:C	2.48	0.51
1:A:6:MSE:HE3	1:A:47:PHE:HZ	1.75	0.51
1:B:114:PHE:O	1:B:115:TYR:HB2	2.10	0.51
1:F:284:ILE:CD1	1:F:324:MSE:HE1	2.40	0.51
1:B:197:TRP:CD2	1:B:259:VAL:HG22	2.46	0.51
1:F:250:THR:C	1:F:252:LYS:N	2.62	0.51
1:B:36:ILE:O	1:B:37:PRO:C	2.48	0.51
1:B:84:HIS:CD2	1:B:85:PRO:HD2	2.46	0.51
1:H:36:ILE:O	1:H:37:PRO:C	2.48	0.51
1:D:197:TRP:CE2	1:D:259:VAL:HG22	2.45	0.51
1:H:319:TRP:HE3	3:H:1899:BME:H12	1.76	0.51
1:C:247:ASP:O	1:C:251:GLY:N	2.38	0.51
1:C:284:ILE:HD11	1:C:324:MSE:HE1	1.93	0.51
1:H:84:HIS:CD2	1:H:85:PRO:HD2	2.46	0.51
1:E:250:THR:HG22	1:E:250:THR:O	2.10	0.51
1:G:319:TRP:HE3	3:G:799:BME:H12	1.75	0.51
1:G:278:PHE:CD1	1:G:278:PHE:N	2.79	0.51
1:D:84:HIS:CD2	1:D:85:PRO:HD2	2.46	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:182:LEU:HD23	1:H:144:ASN:HB2	1.92	0.50
1:D:352:ILE:HB	1:D:357:PHE:CD2	2.47	0.50
1:F:36:ILE:O	1:F:37:PRO:C	2.50	0.50
1:C:3:HIS:ND1	3:C:399:BME:H21	2.27	0.50
1:C:99:LEU:HD13	1:C:111:ALA:HB2	1.93	0.50
1:C:250:THR:C	1:C:252:LYS:N	2.64	0.50
1:E:145:THR:CG2	1:E:146:GLY:N	2.74	0.50
1:F:155:THR:CG2	1:F:157:THR:OG1	2.59	0.50
1:F:278:PHE:CD1	1:F:278:PHE:N	2.80	0.50
1:D:110:TYR:CD1	1:D:110:TYR:N	2.80	0.50
1:B:207:LEU:C	1:B:207:LEU:HD23	2.32	0.50
1:C:103:LYS:NZ	5:C:1595:HOH:O	2.45	0.50
1:E:84:HIS:CD2	1:E:85:PRO:HD2	2.47	0.50
1:H:152:PHE:HB2	5:H:1088:HOH:O	2.11	0.50
1:H:352:ILE:HB	1:H:357:PHE:CD2	2.47	0.50
1:A:197:TRP:CD2	1:A:259:VAL:HG22	2.46	0.50
1:A:345:HIS:HB3	1:B:240:PRO:CB	2.42	0.50
1:B:3:HIS:ND1	3:B:9014:BME:H21	2.27	0.50
1:H:62:TRP:CZ3	1:H:96:ALA:HB1	2.47	0.50
1:C:62:TRP:CH2	1:C:111:ALA:HB1	2.47	0.50
1:D:140:GLU:OE2	1:H:120:TYR:CE1	2.64	0.50
1:G:8:GLY:CA	1:G:45:MSE:HE3	2.42	0.50
1:H:197:TRP:CD2	1:H:259:VAL:HG22	2.47	0.50
1:C:250:THR:HG22	1:C:252:LYS:H	1.76	0.49
1:E:36:ILE:HB	1:E:37:PRO:HD2	1.93	0.49
1:A:76:GLU:O	1:A:77:ALA:HB2	2.12	0.49
1:C:250:THR:HG22	1:C:252:LYS:CB	2.42	0.49
1:C:319:TRP:HE3	3:C:399:BME:H12	1.77	0.49
1:D:8:GLY:CA	1:D:45:MSE:HE3	2.42	0.49
1:F:196:ARG:NH2	5:F:1002:HOH:O	2.46	0.49
1:F:278:PHE:HD1	1:F:278:PHE:H	1.58	0.49
1:G:8:GLY:HA3	1:G:45:MSE:HE3	1.94	0.49
1:G:197:TRP:CD2	1:G:259:VAL:HG22	2.47	0.49
1:D:6:MSE:HA	1:D:17:PHE:O	2.13	0.49
1:E:197:TRP:CD2	1:E:259:VAL:HG22	2.48	0.49
1:H:110:TYR:N	1:H:110:TYR:CD1	2.80	0.49
1:C:278:PHE:CE2	1:C:330:GLN:HG3	2.48	0.49
1:D:319:TRP:HE3	3:D:499:BME:H12	1.77	0.49
1:F:163:ASP:CG	1:F:166:ALA:HB3	2.33	0.49
1:A:275:ALA:HB3	1:A:307:SER:HB2	1.95	0.49
1:D:145:THR:CG2	1:D:146:GLY:N	2.75	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:163:ASP:CG	1:E:166:ALA:HB3	2.32	0.49
1:G:99:LEU:HD13	1:G:111:ALA:HB2	1.95	0.49
1:H:364:TYR:O	1:H:365:ASP:CB	2.59	0.49
1:H:365:ASP:N	5:H:1604:HOH:O	2.22	0.49
1:G:99:LEU:CD1	1:G:111:ALA:HB2	2.42	0.49
1:G:275:ALA:HB3	1:G:307:SER:HB2	1.93	0.49
1:H:8:GLY:HA3	1:H:45:MSE:HE3	1.93	0.49
1:H:153:ASP:OD1	1:H:155:THR:HB	2.13	0.49
1:A:207:LEU:C	1:A:207:LEU:HD23	2.33	0.49
1:E:112:ASN:ND2	1:E:150:MSE:HE2	2.28	0.49
1:B:37:PRO:HB2	1:B:40:GLU:HB2	1.95	0.48
1:C:62:TRP:CZ3	1:C:96:ALA:HB1	2.48	0.48
1:D:232:THR:O	1:D:233:HIS:HB2	2.13	0.48
1:D:284:ILE:CD1	1:D:324:MSE:HE1	2.43	0.48
1:E:240:PRO:CB	1:F:345:HIS:HB3	2.42	0.48
2:G:761:SO4:O3	5:G:1283:HOH:O	2.20	0.48
1:A:153:ASP:OD1	1:A:155:THR:HB	2.12	0.48
1:D:182:LEU:HB3	1:H:143:GLU:OE2	2.13	0.48
1:E:84:HIS:CD2	1:E:86:ARG:H	2.27	0.48
1:A:114:PHE:O	1:A:115:TYR:HB2	2.13	0.48
1:C:36:ILE:O	1:C:37:PRO:C	2.51	0.48
1:F:197:TRP:CD2	1:F:259:VAL:HG22	2.48	0.48
1:E:278:PHE:CE2	1:E:330:GLN:HG3	2.49	0.48
1:C:352:ILE:HB	1:C:357:PHE:CD2	2.48	0.48
1:D:275:ALA:HB3	1:D:307:SER:HB2	1.94	0.48
1:E:352:ILE:HB	1:E:357:PHE:CD2	2.48	0.48
1:G:3:HIS:ND1	3:G:799:BME:H21	2.28	0.48
1:H:207:LEU:C	1:H:207:LEU:HD23	2.33	0.48
1:A:163:ASP:CG	1:A:166:ALA:HB3	2.34	0.48
1:F:267:LYS:CE	5:F:1457:HOH:O	2.57	0.48
1:B:319:TRP:HE3	3:B:9014:BME:H12	1.78	0.48
1:B:99:LEU:HD13	1:B:111:ALA:HB2	1.94	0.48
1:A:99:LEU:CD1	1:A:111:ALA:HB2	2.44	0.48
1:D:47:PHE:CG	1:D:51:ARG:HG2	2.49	0.48
1:C:163:ASP:CG	1:C:166:ALA:HB3	2.34	0.48
1:G:62:TRP:CH2	1:G:111:ALA:HB1	2.48	0.48
1:C:278:PHE:N	1:C:278:PHE:CD1	2.82	0.47
1:C:257:ALA:HA	1:C:273:SER:CB	2.44	0.47
1:E:36:ILE:O	1:E:37:PRO:C	2.50	0.47
1:E:76:GLU:O	1:E:77:ALA:HB2	2.14	0.47
1:G:278:PHE:CE2	1:G:330:GLN:HG3	2.47	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:163:ASP:CG	1:B:166:ALA:HB3	2.35	0.47
1:C:9:THR:HG22	1:C:357:PHE:HA	1.95	0.47
1:E:257:ALA:HA	1:E:273:SER:CB	2.45	0.47
1:D:250:THR:O	1:D:252:LYS:N	2.48	0.47
1:D:278:PHE:N	1:D:278:PHE:CD1	2.82	0.47
1:A:84:HIS:CD2	1:A:86:ARG:H	2.23	0.47
1:D:10:TRP:HB2	1:D:359:MSE:SE	2.65	0.47
1:D:30:LEU:HD13	1:D:352:ILE:CD1	2.45	0.47
1:D:99:LEU:HD11	1:D:109:VAL:CG1	2.44	0.47
1:D:278:PHE:CE2	1:D:330:GLN:HG3	2.48	0.47
1:F:62:TRP:CZ2	1:F:111:ALA:HB1	2.50	0.47
1:F:210:LEU:C	1:F:210:LEU:HD23	2.35	0.47
1:F:257:ALA:HA	1:F:273:SER:CB	2.44	0.47
1:G:163:ASP:CG	1:G:166:ALA:HB3	2.34	0.47
1:H:36:ILE:HB	1:H:37:PRO:HD2	1.96	0.47
1:A:3:HIS:CE1	3:A:368:BME:H21	2.49	0.47
1:B:11:THR:HG22	1:B:12:PRO:O	2.14	0.47
1:C:278:PHE:HD1	5:C:1539:HOH:O	1.98	0.47
1:E:97:ILE:HB	1:E:114:PHE:HB2	1.96	0.47
1:F:284:ILE:HD11	1:F:324:MSE:HE1	1.97	0.47
1:H:278:PHE:HD2	1:H:330:GLN:HG3	1.71	0.47
1:A:110:TYR:CD1	1:A:110:TYR:N	2.83	0.46
1:B:186:VAL:HG22	5:B:1605:HOH:O	2.16	0.46
1:B:145:THR:CG2	1:B:146:GLY:N	2.78	0.46
1:D:76:GLU:O	1:D:77:ALA:HB2	2.15	0.46
1:G:257:ALA:HA	1:G:273:SER:CB	2.46	0.46
1:B:313:ALA:HB1	5:B:1592:HOH:O	2.15	0.46
1:D:197:TRP:CD2	1:D:259:VAL:HG22	2.50	0.46
1:A:99:LEU:HD13	1:A:111:ALA:HB2	1.96	0.46
1:B:279:GLU:HA	4:B:9012:PIN:O1'	2.15	0.46
1:C:275:ALA:HB3	1:C:307:SER:HB2	1.96	0.46
1:F:6:MSE:HA	1:F:17:PHE:O	2.16	0.46
1:H:257:ALA:HA	1:H:273:SER:CB	2.46	0.46
1:A:37:PRO:HB2	1:A:40:GLU:HB2	1.96	0.46
1:A:112:ASN:ND2	1:A:150:MSE:HE2	2.31	0.46
1:B:257:ALA:HA	1:B:273:SER:CB	2.45	0.46
1:F:11:THR:HG22	1:F:12:PRO:O	2.16	0.46
1:H:163:ASP:CG	1:H:166:ALA:HB3	2.36	0.46
1:A:36:ILE:O	1:A:37:PRO:C	2.53	0.46
1:A:278:PHE:CE2	1:A:330:GLN:HG3	2.51	0.46
1:B:8:GLY:HA3	1:B:45:MSE:HE3	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:278:PHE:HD2	1:E:330:GLN:HG3	1.76	0.46
1:F:3:HIS:ND1	3:F:699:BME:H21	2.30	0.46
1:F:110:TYR:N	1:F:110:TYR:CD1	2.84	0.46
1:B:62:TRP:CH2	1:B:111:ALA:HB1	2.51	0.46
1:C:210:LEU:C	1:C:210:LEU:HD23	2.35	0.46
1:D:257:ALA:HA	1:D:273:SER:CB	2.46	0.46
1:A:264:PHE:CE2	1:E:50:GLU:HG2	2.50	0.46
1:B:47:PHE:CG	1:B:51:ARG:HG2	2.51	0.46
1:F:245:ASP:O	1:F:253:GLY:HA2	2.16	0.46
1:H:8:GLY:CA	1:H:45:MSE:HE3	2.45	0.46
1:G:97:ILE:HB	1:G:114:PHE:HB2	1.98	0.45
1:D:36:ILE:HB	1:D:37:PRO:HD2	1.98	0.45
1:D:364:TYR:O	1:D:365:ASP:CB	2.58	0.45
1:A:36:ILE:HB	1:A:37:PRO:HD2	1.98	0.45
1:A:247:ASP:HB3	1:A:250:THR:HB	1.99	0.45
1:C:88:ASN:O	1:C:89:ASP:C	2.52	0.45
1:A:142:GLN:HG3	1:A:144:ASN:HB3	1.98	0.45
1:H:84:HIS:CD2	1:H:86:ARG:H	2.24	0.45
1:A:196:ARG:NH2	5:A:998:HOH:O	2.49	0.45
1:C:10:TRP:HB2	1:C:359:MSE:SE	2.67	0.45
1:F:9:THR:HG22	1:F:357:PHE:HA	1.98	0.45
1:A:6:MSE:HA	1:A:17:PHE:O	2.16	0.45
1:G:5:LEU:C	1:G:6:MSE:HE2	2.36	0.45
1:B:3:HIS:CE1	3:B:9014:BME:H21	2.52	0.45
1:C:250:THR:O	1:C:252:LYS:N	2.50	0.45
1:E:62:TRP:CH2	1:E:111:ALA:HB1	2.51	0.45
1:B:84:HIS:CD2	1:B:86:ARG:H	2.25	0.45
1:F:114:PHE:O	1:F:115:TYR:HB2	2.16	0.45
1:F:153:ASP:OD1	1:F:155:THR:HB	2.17	0.45
1:A:62:TRP:CH2	1:A:111:ALA:HB1	2.52	0.45
1:C:6:MSE:HA	1:C:17:PHE:O	2.17	0.45
1:C:155:THR:HG22	1:C:155:THR:O	2.15	0.45
1:D:163:ASP:CG	1:D:166:ALA:HB3	2.37	0.45
1:H:364:TYR:HA	5:H:1604:HOH:O	2.16	0.45
1:E:8:GLY:HA3	1:E:45:MSE:HE3	1.98	0.45
1:G:6:MSE:HE3	1:G:47:PHE:CZ	2.52	0.45
1:A:8:GLY:CA	1:A:45:MSE:HE3	2.47	0.44
1:D:250:THR:HG21	1:D:252:LYS:CB	2.45	0.44
1:G:47:PHE:CG	1:G:51:ARG:HG2	2.52	0.44
1:G:240:PRO:CB	1:H:345:HIS:HB3	2.47	0.44
1:A:62:TRP:CZ2	1:A:111:ALA:HB1	2.52	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:305:PRO:HD2	5:B:1074:HOH:O	2.16	0.44
1:D:250:THR:HG22	1:D:252:LYS:N	2.32	0.44
1:C:278:PHE:HD1	1:C:278:PHE:H	1.65	0.44
1:E:319:TRP:CZ3	3:E:599:BME:S2	3.10	0.44
1:H:62:TRP:CZ2	1:H:111:ALA:HB1	2.52	0.44
1:F:238:LEU:HD12	1:F:238:LEU:HA	1.78	0.44
1:H:250:THR:HG22	1:H:252:LYS:N	2.29	0.44
1:H:275:ALA:HB3	1:H:307:SER:HB2	1.99	0.44
1:A:112:ASN:HD21	1:A:150:MSE:HE2	1.83	0.44
1:C:36:ILE:HB	1:C:37:PRO:HD2	1.99	0.44
1:B:186:VAL:CG2	5:B:1605:HOH:O	2.66	0.44
1:E:23:ASP:OD1	1:E:23:ASP:C	2.56	0.44
1:G:286:GLY:HA3	1:G:300:PHE:CE2	2.52	0.44
1:B:250:THR:C	1:B:252:LYS:H	2.21	0.44
1:B:278:PHE:N	1:B:278:PHE:CD1	2.85	0.44
1:C:263:THR:HB	5:C:884:HOH:O	2.18	0.44
1:D:8:GLY:HA3	1:D:45:MSE:HE3	2.00	0.44
1:D:62:TRP:CZ3	1:D:96:ALA:HB1	2.52	0.44
1:F:6:MSE:HE3	1:F:47:PHE:HZ	1.77	0.44
1:F:47:PHE:CZ	1:F:364:TYR:HB2	2.53	0.44
1:G:110:TYR:N	1:G:110:TYR:CD1	2.85	0.44
1:H:97:ILE:HB	1:H:114:PHE:HB2	2.00	0.44
1:B:47:PHE:CZ	1:B:364:TYR:HB2	2.53	0.44
1:C:47:PHE:CG	1:C:51:ARG:HG2	2.52	0.44
1:D:120:TYR:HE1	1:H:140:GLU:OE2	1.98	0.44
1:E:3:HIS:CE1	3:E:599:BME:H21	2.53	0.44
1:F:36:ILE:HB	1:F:37:PRO:HD2	2.00	0.44
1:C:145:THR:CG2	1:C:146:GLY:N	2.81	0.44
1:E:363:TRP:CE3	3:E:599:BME:S2	3.11	0.44
1:G:363:TRP:CE3	3:G:799:BME:S2	3.11	0.44
1:A:11:THR:CG2	1:A:12:PRO:O	2.65	0.43
1:A:257:ALA:HA	1:A:273:SER:CB	2.48	0.43
1:B:62:TRP:CZ3	1:B:96:ALA:HB1	2.53	0.43
1:E:114:PHE:O	1:E:115:TYR:HB2	2.18	0.43
1:A:238:LEU:HD12	1:A:238:LEU:HA	1.87	0.43
1:B:217:ILE:O	1:B:235:SER:HA	2.18	0.43
1:D:250:THR:CG2	1:D:250:THR:O	2.65	0.43
1:C:89:ASP:HB3	1:C:91:ASP:OD2	2.19	0.43
1:E:259:VAL:O	1:E:271:ALA:HA	2.18	0.43
1:D:247:ASP:HB3	1:D:250:THR:HB	2.00	0.43
1:F:145:THR:CG2	1:F:146:GLY:N	2.81	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:6:MSE:HA	1:G:17:PHE:O	2.18	0.43
1:G:76:GLU:O	1:G:77:ALA:HB2	2.18	0.43
1:C:286:GLY:HA3	1:C:300:PHE:CE2	2.53	0.43
1:F:8:GLY:HA3	1:F:45:MSE:HE3	1.99	0.43
1:G:364:TYR:O	1:G:365:ASP:CB	2.63	0.43
1:E:275:ALA:HB3	1:E:307:SER:HB2	2.00	0.43
1:F:37:PRO:HB2	1:F:40:GLU:HB2	2.00	0.43
1:G:11:THR:CG2	1:G:12:PRO:O	2.67	0.43
1:G:47:PHE:CZ	1:G:364:TYR:HB2	2.53	0.43
1:H:10:TRP:HB2	1:H:359:MSE:SE	2.69	0.43
1:C:238:LEU:HD12	1:C:238:LEU:HA	1.88	0.43
1:A:364:TYR:O	1:A:365:ASP:CB	2.57	0.43
1:C:110:TYR:CD1	1:C:110:TYR:N	2.86	0.43
1:F:352:ILE:HA	1:F:353:PRO:HD3	1.70	0.43
1:B:278:PHE:CE2	1:B:330:GLN:HG3	2.52	0.43
1:D:62:TRP:CZ2	1:D:111:ALA:HB1	2.54	0.43
1:H:84:HIS:HD2	1:H:86:ARG:N	2.09	0.43
1:H:231:TYR:CE2	1:H:233:HIS:HA	2.54	0.43
1:E:364:TYR:O	1:E:365:ASP:CB	2.64	0.43
1:H:11:THR:CG2	1:H:12:PRO:O	2.67	0.43
1:A:81:ILE:O	1:A:88:ASN:ND2	2.51	0.42
1:C:114:PHE:O	1:C:115:TYR:HB2	2.18	0.42
1:E:62:TRP:CH2	1:E:96:ALA:HB1	2.54	0.42
1:E:210:LEU:HD23	1:E:210:LEU:C	2.40	0.42
1:H:3:HIS:CE1	3:H:1899:BME:H21	2.53	0.42
1:H:114:PHE:O	1:H:115:TYR:HB2	2.19	0.42
1:A:8:GLY:HA3	1:A:45:MSE:HE3	2.00	0.42
1:B:36:ILE:HB	1:B:37:PRO:HD2	2.01	0.42
1:C:250:THR:CG2	1:C:252:LYS:CB	2.97	0.42
1:E:8:GLY:CA	1:E:45:MSE:HE3	2.48	0.42
1:F:11:THR:CG2	1:F:12:PRO:O	2.67	0.42
1:H:6:MSE:HA	1:H:17:PHE:O	2.18	0.42
1:D:278:PHE:HD1	1:D:278:PHE:H	1.67	0.42
1:E:11:THR:HG22	1:E:12:PRO:O	2.19	0.42
1:E:278:PHE:N	1:E:278:PHE:CD1	2.88	0.42
1:G:145:THR:CG2	1:G:146:GLY:N	2.82	0.42
1:D:319:TRP:CZ3	3:D:499:BME:S2	3.12	0.42
1:C:363:TRP:CE3	3:C:399:BME:S2	3.13	0.42
1:D:114:PHE:O	1:D:115:TYR:HB2	2.20	0.42
1:D:120:TYR:CZ	1:H:140:GLU:OE2	2.73	0.42
1:E:217:ILE:O	1:E:235:SER:HA	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:363:TRP:CE3	3:F:699:BME:S2	3.12	0.42
1:H:47:PHE:CG	1:H:51:ARG:HG2	2.55	0.42
1:B:363:TRP:CE3	3:B:9014:BME:S2	3.12	0.42
1:C:247:ASP:HB3	1:C:250:THR:HB	2.01	0.42
1:D:210:LEU:C	1:D:210:LEU:HD23	2.39	0.42
1:G:36:ILE:HB	1:G:37:PRO:HD2	2.02	0.42
1:G:240:PRO:HB2	1:H:345:HIS:HB3	2.02	0.42
1:B:30:LEU:HD13	1:B:352:ILE:HD11	2.01	0.42
1:B:232:THR:O	1:B:233:HIS:CB	2.68	0.42
1:F:8:GLY:CA	1:F:45:MSE:HE3	2.50	0.42
1:G:250:THR:O	1:G:252:LYS:N	2.48	0.42
1:G:259:VAL:O	1:G:271:ALA:HA	2.20	0.42
1:G:352:ILE:HA	1:G:353:PRO:HD2	1.80	0.42
1:A:47:PHE:CG	1:A:51:ARG:HG2	2.54	0.42
1:D:99:LEU:HD13	1:D:111:ALA:CB	2.47	0.42
1:B:110:TYR:CD1	1:B:110:TYR:N	2.87	0.42
1:B:198:VAL:HA	1:B:208:TYR:O	2.19	0.42
1:D:3:HIS:CE1	3:D:499:BME:H21	2.55	0.42
1:F:217:ILE:O	1:F:235:SER:HA	2.20	0.42
1:G:210:LEU:HD23	1:G:210:LEU:C	2.40	0.42
1:D:6:MSE:HE2	1:D:362:ILE:O	2.19	0.42
1:A:145:THR:CG2	1:A:146:GLY:N	2.83	0.41
1:G:11:THR:HG22	1:G:12:PRO:O	2.20	0.41
1:H:210:LEU:C	1:H:210:LEU:HD23	2.41	0.41
1:F:3:HIS:CE1	3:F:699:BME:H21	2.54	0.41
1:G:217:ILE:O	1:G:235:SER:HA	2.20	0.41
1:A:84:HIS:HA	1:A:85:PRO:HD3	1.93	0.41
1:B:6:MSE:HA	1:B:17:PHE:O	2.19	0.41
1:B:11:THR:CG2	1:B:12:PRO:O	2.68	0.41
1:B:81:ILE:O	1:B:88:ASN:ND2	2.53	0.41
1:C:240:PRO:CB	1:D:345:HIS:HB3	2.50	0.41
1:C:319:TRP:CZ3	3:C:399:BME:S2	3.13	0.41
1:D:8:GLY:N	1:D:45:MSE:HE3	2.35	0.41
1:D:64:SER:HB2	1:D:132:LEU:HB2	2.01	0.41
1:E:6:MSE:HA	1:E:17:PHE:O	2.19	0.41
1:H:7:ILE:HD12	1:H:7:ILE:N	2.35	0.41
1:B:1:PRO:HD2	1:B:23:ASP:OD1	2.20	0.41
1:D:84:HIS:CD2	1:D:86:ARG:H	2.35	0.41
1:D:284:ILE:HD11	1:D:324:MSE:HE1	2.03	0.41
1:D:301:LEU:HD12	1:D:301:LEU:HA	1.91	0.41
1:A:30:LEU:HD13	1:A:352:ILE:CD1	2.49	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:210:LEU:C	1:A:210:LEU:HD23	2.41	0.41
1:A:333:TRP:CZ3	1:A:351:ARG:HB2	2.55	0.41
1:B:210:LEU:C	1:B:210:LEU:HD23	2.41	0.41
1:C:196:ARG:NH2	5:C:1000:HOH:O	2.54	0.41
1:F:364:TYR:O	1:F:365:ASP:CB	2.62	0.41
1:G:114:PHE:O	1:G:115:TYR:HB2	2.21	0.41
1:H:145:THR:CG2	1:H:146:GLY:N	2.82	0.41
1:A:23:ASP:OD1	1:A:23:ASP:C	2.59	0.41
1:A:112:ASN:HD21	1:A:150:MSE:HG3	1.85	0.41
1:B:98:PHE:CG	1:B:99:LEU:N	2.88	0.41
1:C:250:THR:O	1:C:250:THR:CG2	2.67	0.41
1:A:231:TYR:CE2	1:A:233:HIS:HA	2.56	0.41
1:F:247:ASP:HA	1:F:248:PRO:HD3	1.90	0.41
1:G:62:TRP:CZ2	1:G:111:ALA:HB1	2.56	0.41
1:H:319:TRP:CZ3	3:H:1899:BME:S2	3.14	0.41
1:H:334:LEU:HD13	1:H:334:LEU:C	2.41	0.41
1:B:9:THR:HG22	1:B:357:PHE:HA	2.03	0.41
1:D:84:HIS:HA	1:D:85:PRO:HD3	1.97	0.41
1:D:210:LEU:HD21	1:D:257:ALA:CB	2.51	0.41
1:F:275:ALA:HB3	1:F:307:SER:HB2	2.02	0.41
1:A:31:ILE:O	1:A:32:LYS:HB2	2.21	0.41
1:A:99:LEU:HD12	1:A:99:LEU:HA	1.81	0.41
1:A:319:TRP:CZ3	3:A:368:BME:S2	3.14	0.41
1:C:168:LYS:NZ	5:C:1326:HOH:O	2.53	0.41
1:G:155:THR:HG22	1:G:155:THR:O	2.19	0.41
1:H:238:LEU:HD12	1:H:238:LEU:HA	1.88	0.41
1:A:301:LEU:HD12	1:A:301:LEU:HA	1.92	0.41
1:F:232:THR:O	1:F:233:HIS:CB	2.68	0.41
1:H:350:VAL:HG22	1:H:351:ARG:N	2.35	0.41
1:C:11:THR:HA	1:C:12:PRO:HD3	1.98	0.40
1:D:363:TRP:CE3	3:D:499:BME:S2	3.14	0.40
1:G:1:PRO:HD2	1:G:23:ASP:OD1	2.21	0.40
1:G:1:PRO:HD3	1:G:24:GLU:OE2	2.21	0.40
1:G:84:HIS:HA	1:G:85:PRO:HD3	1.89	0.40
1:G:284:ILE:HD11	1:G:324:MSE:CE	2.48	0.40
1:A:33:ARG:HG2	1:A:33:ARG:HH11	1.85	0.40
1:B:8:GLY:CA	1:B:45:MSE:HE3	2.51	0.40
1:B:137:GLN:OE1	1:B:179:GLU:HB3	2.21	0.40
1:D:97:ILE:HB	1:D:114:PHE:HB2	2.01	0.40
1:G:84:HIS:HD2	1:G:86:ARG:N	2.11	0.40
1:F:99:LEU:HD13	1:F:111:ALA:HB2	2.02	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:278:PHE:N	1:H:278:PHE:CD1	2.88	0.40
1:B:240:PRO:HA	1:B:241:PRO:HD3	1.99	0.40
1:D:352:ILE:HA	1:D:353:PRO:HD3	1.68	0.40
1:E:238:LEU:HD12	1:E:238:LEU:HA	1.86	0.40
1:F:286:GLY:HA3	1:F:300:PHE:CE2	2.57	0.40
1:G:232:THR:O	1:G:233:HIS:CB	2.69	0.40
1:B:331:GLU:CD	4:B:9012:PIN:H12	2.41	0.40
1:F:1:PRO:HD2	1:F:23:ASP:OD1	2.22	0.40
1:F:84:HIS:HA	1:F:85:PRO:HD3	1.90	0.40
1:G:89:ASP:HB3	1:G:91:ASP:OD2	2.21	0.40
1:H:6:MSE:N	1:H:6:MSE:CE	2.71	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	363/365 (100%)	341 (94%)	20 (6%)	2 (1%)	25	43
1	B	363/365 (100%)	344 (95%)	15 (4%)	4 (1%)	14	26
1	C	363/365 (100%)	340 (94%)	19 (5%)	4 (1%)	14	26
1	D	363/365 (100%)	340 (94%)	18 (5%)	5 (1%)	11	20
1	E	363/365 (100%)	339 (93%)	20 (6%)	4 (1%)	14	26
1	F	363/365 (100%)	342 (94%)	17 (5%)	4 (1%)	14	26
1	G	363/365 (100%)	340 (94%)	20 (6%)	3 (1%)	19	35
1	H	363/365 (100%)	341 (94%)	19 (5%)	3 (1%)	19	35
All	All	2904/2920 (100%)	2727 (94%)	148 (5%)	29 (1%)	15	28

All (29) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	250	THR
1	G	250	THR
1	A	115	TYR
1	B	353	PRO
1	C	353	PRO
1	B	115	TYR
1	B	250	THR
1	C	115	TYR
1	D	115	TYR
1	E	115	TYR
1	E	353	PRO
1	F	115	TYR
1	F	353	PRO
1	G	115	TYR
1	G	353	PRO
1	H	353	PRO
1	A	353	PRO
1	C	250	THR
1	D	250	THR
1	D	353	PRO
1	H	115	TYR
1	F	250	THR
1	E	37	PRO
1	H	37	PRO
1	B	37	PRO
1	C	37	PRO
1	D	37	PRO
1	F	37	PRO
1	D	251	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	299/298 (100%)	291 (97%)	8 (3%)	44 71
1	B	299/298 (100%)	289 (97%)	10 (3%)	38 64
1	C	300/298 (101%)	289 (96%)	11 (4%)	34 60

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	D	300/298 (101%)	291 (97%)	9 (3%)	41 68
1	E	299/298 (100%)	290 (97%)	9 (3%)	41 68
1	F	299/298 (100%)	290 (97%)	9 (3%)	41 68
1	G	300/298 (101%)	292 (97%)	8 (3%)	44 71
1	H	300/298 (101%)	291 (97%)	9 (3%)	41 68
All	All	2396/2384 (100%)	2323 (97%)	73 (3%)	41 68

All (73) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	MSE
1	A	11	THR
1	A	104	GLN
1	A	207	LEU
1	A	238	LEU
1	A	274	ARG
1	A	312	ASN
1	A	328	ASP
1	B	6	MSE
1	B	11	THR
1	B	104	GLN
1	B	207	LEU
1	B	238	LEU
1	B	274	ARG
1	B	312	ASN
1	B	328	ASP
1	B	352	ILE
1	B	360	ASN
1	C	6	MSE
1	C	11	THR
1	C	37	PRO
1	C	104	GLN
1	C	207	LEU
1	C	238	LEU
1	C	274	ARG
1	C	278	PHE
1	C	312	ASN
1	C	328	ASP
1	C	360	ASN
1	D	6	MSE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	11	THR
1	D	37	PRO
1	D	104	GLN
1	D	207	LEU
1	D	238	LEU
1	D	274	ARG
1	D	312	ASN
1	D	328	ASP
1	E	6	MSE
1	E	11	THR
1	E	104	GLN
1	E	238	LEU
1	E	259	VAL
1	E	274	ARG
1	E	312	ASN
1	E	328	ASP
1	E	360	ASN
1	F	6	MSE
1	F	11	THR
1	F	104	GLN
1	F	207	LEU
1	F	238	LEU
1	F	274	ARG
1	F	319	TRP
1	F	328	ASP
1	F	360	ASN
1	G	6	MSE
1	G	11	THR
1	G	104	GLN
1	G	207	LEU
1	G	238	LEU
1	G	274	ARG
1	G	312	ASN
1	G	328	ASP
1	H	6	MSE
1	H	11	THR
1	H	104	GLN
1	H	143	GLU
1	H	207	LEU
1	H	238	LEU
1	H	274	ARG
1	H	312	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	H	328	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	GLN
1	A	49	HIS
1	A	84	HIS
1	A	104	GLN
1	A	112	ASN
1	B	20	GLN
1	B	84	HIS
1	B	112	ASN
1	C	20	GLN
1	C	84	HIS
1	D	20	GLN
1	D	84	HIS
1	D	112	ASN
1	E	20	GLN
1	E	84	HIS
1	E	112	ASN
1	E	227	HIS
1	F	20	GLN
1	F	84	HIS
1	F	112	ASN
1	G	20	GLN
1	G	84	HIS
1	G	112	ASN
1	H	84	HIS
1	H	112	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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)

26 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	BME	A	367	1	3,3,3	2.04	1 (33%)	1,2,2	2.60	1 (100%)
3	BME	D	466	1	3,3,3	2.04	1 (33%)	1,2,2	2.59	1 (100%)
3	BME	G	766	1	3,3,3	2.04	1 (33%)	1,2,2	2.60	1 (100%)
3	BME	H	1899	1	3,3,3	2.03	1 (33%)	1,2,2	2.59	1 (100%)
3	BME	B	9014	1	3,3,3	2.04	1 (33%)	1,2,2	2.58	1 (100%)
3	BME	H	1866	1	3,3,3	2.05	1 (33%)	1,2,2	2.60	1 (100%)
2	SO4	H	861	-	4,4,4	0.78	0	6,6,6	0.70	0
3	BME	D	499	1	3,3,3	2.03	1 (33%)	1,2,2	2.59	1 (100%)
2	SO4	G	761	-	4,4,4	1.28	0	6,6,6	0.33	0
2	SO4	D	461	-	4,4,4	1.06	0	6,6,6	0.53	0
2	SO4	C	366	-	4,4,4	0.95	0	6,6,6	0.41	0
3	BME	G	799	1	3,3,3	2.03	1 (33%)	1,2,2	2.58	1 (100%)
2	SO4	B	366	-	4,4,4	0.60	0	6,6,6	0.26	0
2	SO4	A	366	-	4,4,4	0.55	0	6,6,6	0.26	0
3	BME	E	599	1	3,3,3	2.03	1 (33%)	1,2,2	2.60	1 (100%)
4	PIN	B	9012	-	18,18,18	3.20	5 (27%)	22,26,26	1.77	4 (18%)
2	SO4	F	661	-	4,4,4	0.60	0	6,6,6	0.20	0
3	BME	C	399	1	3,3,3	2.03	1 (33%)	1,2,2	2.59	1 (100%)
3	BME	F	699	1	3,3,3	2.04	1 (33%)	1,2,2	2.60	1 (100%)
3	BME	B	9013	1	3,3,3	2.03	1 (33%)	1,2,2	2.61	1 (100%)
4	PIN	H	9078	-	18,18,18	3.34	5 (27%)	22,26,26	2.45	5 (22%)
3	BME	A	368	1	3,3,3	2.03	1 (33%)	1,2,2	2.59	1 (100%)
3	BME	F	666	1	3,3,3	2.04	1 (33%)	1,2,2	2.58	1 (100%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	SO4	E	561	-	4,4,4	0.70	0	6,6,6	0.26	0
3	BME	C	367	1	3,3,3	2.05	1 (33%)	1,2,2	2.59	1 (100%)
3	BME	E	566	1	3,3,3	2.04	1 (33%)	1,2,2	2.60	1 (100%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	BME	G	799	1	-	1/1/1/1	-
3	BME	A	367	1	-	1/1/1/1	-
3	BME	D	466	1	-	1/1/1/1	-
3	BME	G	766	1	-	1/1/1/1	-
3	BME	H	1866	1	-	1/1/1/1	-
3	BME	H	1899	1	-	1/1/1/1	-
3	BME	D	499	1	-	1/1/1/1	-
3	BME	B	9014	1	-	1/1/1/1	-
4	PIN	H	9078	-	-	3/12/22/22	0/1/1/1
3	BME	A	368	1	-	1/1/1/1	-
3	BME	F	666	1	-	1/1/1/1	-
3	BME	E	599	1	-	1/1/1/1	-
4	PIN	B	9012	-	-	1/12/22/22	0/1/1/1
3	BME	C	367	1	-	1/1/1/1	-
3	BME	E	566	1	-	1/1/1/1	-
3	BME	F	699	1	-	1/1/1/1	-
3	BME	B	9013	1	-	1/1/1/1	-
3	BME	C	399	1	-	1/1/1/1	-

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	9078	PIN	C1-S1	-8.29	1.65	1.77
4	H	9078	PIN	C1'-S1'	-7.75	1.66	1.77
4	B	9012	PIN	C1-S1	-7.47	1.66	1.77
4	B	9012	PIN	C1'-S1'	-7.42	1.67	1.77
4	H	9078	PIN	O3-S1	6.10	1.69	1.47
4	B	9012	PIN	O3-S1	5.93	1.68	1.47
4	B	9012	PIN	O3'-S1'	4.61	1.63	1.47
4	H	9078	PIN	O3'-S1'	3.97	1.61	1.47
3	H	1866	BME	O1-C1	-3.52	1.23	1.42
3	C	367	BME	O1-C1	-3.52	1.23	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	766	BME	O1-C1	-3.51	1.23	1.42
3	E	566	BME	O1-C1	-3.51	1.24	1.42
3	F	666	BME	O1-C1	-3.50	1.24	1.42
3	A	367	BME	O1-C1	-3.50	1.24	1.42
3	D	466	BME	O1-C1	-3.50	1.24	1.42
3	B	9014	BME	O1-C1	-3.50	1.24	1.42
3	F	699	BME	O1-C1	-3.50	1.24	1.42
3	B	9013	BME	O1-C1	-3.50	1.24	1.42
3	H	1899	BME	O1-C1	-3.50	1.24	1.42
3	C	399	BME	O1-C1	-3.50	1.24	1.42
3	A	368	BME	O1-C1	-3.49	1.24	1.42
3	E	599	BME	O1-C1	-3.49	1.24	1.42
3	G	799	BME	O1-C1	-3.49	1.24	1.42
3	D	499	BME	O1-C1	-3.49	1.24	1.42
4	B	9012	PIN	C2'-N1'	-2.52	1.41	1.47
4	H	9078	PIN	O2'-S1'	2.27	1.51	1.45

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	H	9078	PIN	O1'-S1'-C1'	7.22	115.61	106.92
4	H	9078	PIN	O3'-S1'-C1'	-4.95	97.76	105.77
4	B	9012	PIN	O1'-S1'-C1'	4.86	112.77	106.92
4	H	9078	PIN	O2-S1-C1	3.98	111.71	106.92
4	H	9078	PIN	O2'-S1'-C1'	-3.59	102.59	106.92
4	B	9012	PIN	O2-S1-C1	3.31	110.91	106.92
4	B	9012	PIN	O3-S1-C1	-3.19	100.61	105.77
4	H	9078	PIN	O3-S1-C1	-2.99	100.94	105.77
3	B	9013	BME	O1-C1-C2	2.61	121.12	110.83
3	H	1866	BME	O1-C1-C2	2.60	121.11	110.83
3	E	566	BME	O1-C1-C2	2.60	121.11	110.83
3	E	599	BME	O1-C1-C2	2.60	121.09	110.83
3	F	699	BME	O1-C1-C2	2.60	121.08	110.83
3	G	766	BME	O1-C1-C2	2.60	121.08	110.83
3	A	367	BME	O1-C1-C2	2.60	121.08	110.83
3	H	1899	BME	O1-C1-C2	2.59	121.07	110.83
3	D	466	BME	O1-C1-C2	2.59	121.06	110.83
3	D	499	BME	O1-C1-C2	2.59	121.05	110.83
3	A	368	BME	O1-C1-C2	2.59	121.05	110.83
3	C	367	BME	O1-C1-C2	2.59	121.05	110.83
3	C	399	BME	O1-C1-C2	2.59	121.04	110.83
3	G	799	BME	O1-C1-C2	2.58	121.02	110.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	666	BME	O1-C1-C2	2.58	121.01	110.83
3	B	9014	BME	O1-C1-C2	2.58	121.00	110.83
4	B	9012	PIN	O3'-S1'-C1'	-2.31	102.04	105.77

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	367	BME	O1-C1-C2-S2
3	A	368	BME	O1-C1-C2-S2
3	B	9013	BME	O1-C1-C2-S2
3	B	9014	BME	O1-C1-C2-S2
3	C	367	BME	O1-C1-C2-S2
3	C	399	BME	O1-C1-C2-S2
3	D	466	BME	O1-C1-C2-S2
3	D	499	BME	O1-C1-C2-S2
3	E	566	BME	O1-C1-C2-S2
3	E	599	BME	O1-C1-C2-S2
3	F	666	BME	O1-C1-C2-S2
3	F	699	BME	O1-C1-C2-S2
3	G	766	BME	O1-C1-C2-S2
3	G	799	BME	O1-C1-C2-S2
3	H	1866	BME	O1-C1-C2-S2
3	H	1899	BME	O1-C1-C2-S2
4	H	9078	PIN	C1'-C2'-N1'-C4'
4	H	9078	PIN	C1'-C2'-N1'-C3'
4	H	9078	PIN	C2-C1-S1-O2
4	B	9012	PIN	C1-C2-N1-C4

There are no ring outliers.

11 monomers are involved in 39 short contacts:

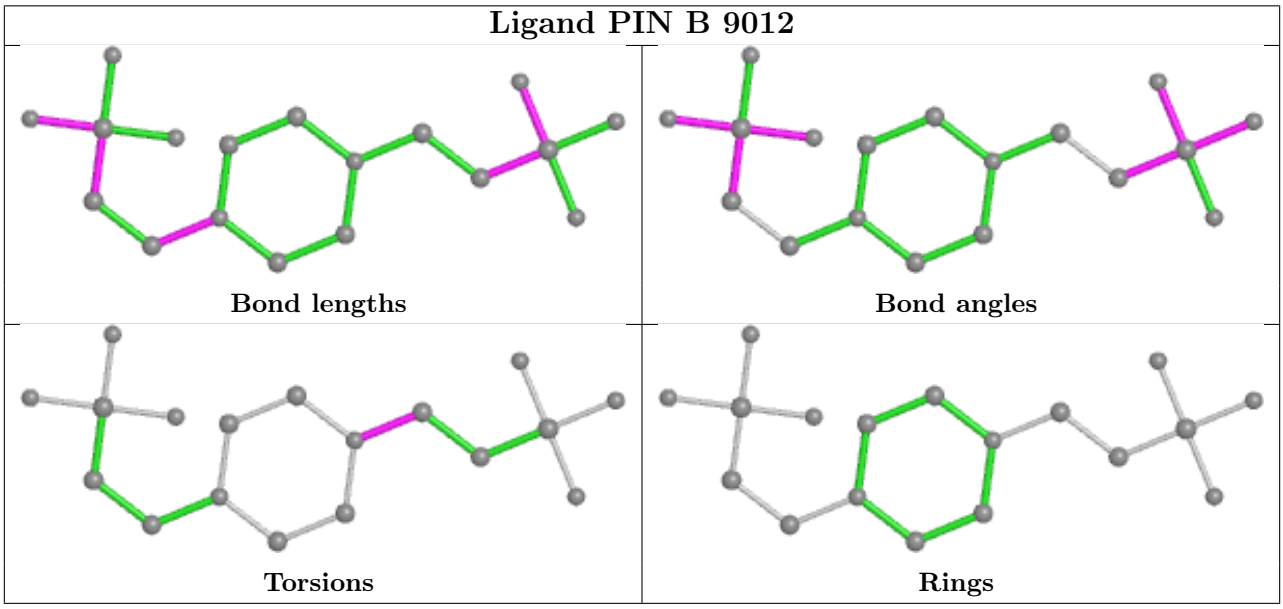
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	H	1899	BME	4	0
3	B	9014	BME	4	0
3	D	499	BME	5	0
2	G	761	SO4	1	0
2	D	461	SO4	1	0
3	G	799	BME	3	0
3	E	599	BME	5	0
4	B	9012	PIN	4	0

Continued on next page...

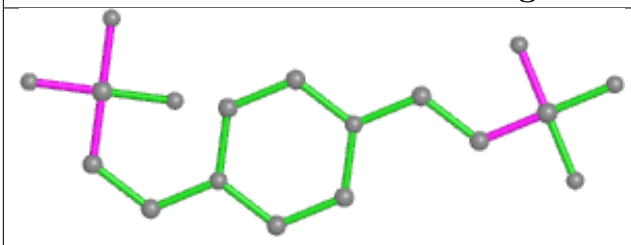
Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	399	BME	4	0
3	F	699	BME	4	0
3	A	368	BME	4	0

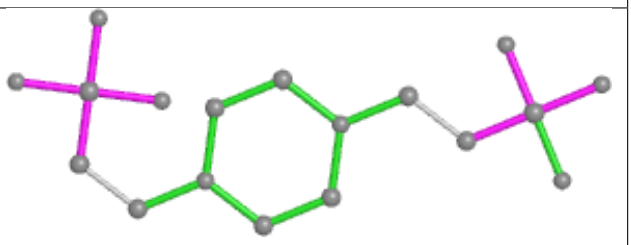
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.



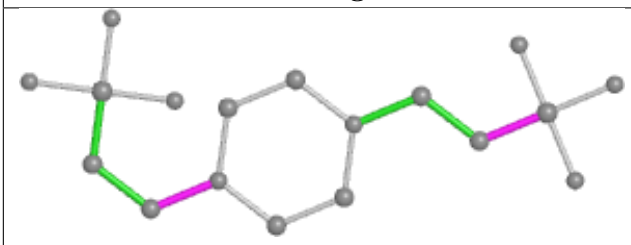
Ligand PIN H 9078



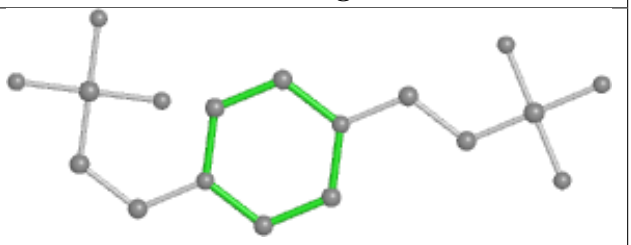
Bond lengths



Bond angles



Torsions



Rings

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	355/365 (97%)	-0.41	0 100 100	11, 22, 39, 58	0
1	B	355/365 (97%)	-0.39	1 (0%) 94 94	11, 23, 42, 76	0
1	C	355/365 (97%)	-0.43	3 (0%) 86 87	10, 21, 39, 70	0
1	D	355/365 (97%)	-0.31	2 (0%) 89 90	11, 25, 47, 66	0
1	E	355/365 (97%)	-0.09	7 (1%) 65 68	16, 32, 53, 79	0
1	F	355/365 (97%)	-0.26	5 (1%) 75 77	14, 25, 45, 85	0
1	G	355/365 (97%)	-0.34	4 (1%) 80 82	11, 23, 40, 81	0
1	H	355/365 (97%)	-0.22	2 (0%) 89 90	10, 27, 50, 85	0
All	All	2840/2920 (97%)	-0.30	24 (0%) 86 87	10, 25, 46, 85	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	353	PRO	4.4
1	G	248	PRO	4.2
1	E	251	GLY	4.1
1	G	251	GLY	4.0
1	F	251	GLY	3.9
1	E	353	PRO	3.8
1	C	251	GLY	3.4
1	H	353	PRO	3.4
1	G	353	PRO	3.2
1	C	91	ASP	3.2
1	F	248	PRO	2.9
1	D	251	GLY	2.9
1	F	250	THR	2.8
1	D	250	THR	2.6
1	C	353	PRO	2.5
1	E	248	PRO	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	251	GLY	2.3
1	E	225	ALA	2.3
1	G	250	THR	2.3
1	H	319	TRP	2.2
1	E	85	PRO	2.2
1	E	250	THR	2.2
1	F	7	ILE	2.2
1	E	91	ASP	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
3	BME	D	466	4/4	0.82	0.47	30,46,47,48	0
3	BME	H	1866	4/4	0.82	0.57	30,46,47,48	0
3	BME	G	766	4/4	0.84	0.47	30,46,47,48	0
2	SO4	G	761	5/5	0.85	0.20	73,73,73,73	0
3	BME	B	9013	4/4	0.85	0.41	30,46,47,48	0
3	BME	C	367	4/4	0.85	0.55	30,46,47,48	0
3	BME	A	367	4/4	0.86	0.44	30,46,47,48	0
3	BME	G	799	4/4	0.87	0.37	30,46,47,48	0
3	BME	B	9014	4/4	0.87	0.28	30,46,47,48	0
3	BME	F	666	4/4	0.88	0.43	30,46,47,48	0
3	BME	C	399	4/4	0.88	0.27	30,46,47,48	0
3	BME	H	1899	4/4	0.88	0.37	30,46,47,48	0
3	BME	D	499	4/4	0.89	0.30	30,46,47,48	0
3	BME	F	699	4/4	0.89	0.34	30,46,47,48	0
3	BME	E	566	4/4	0.89	0.44	30,46,47,48	0

Continued on next page...

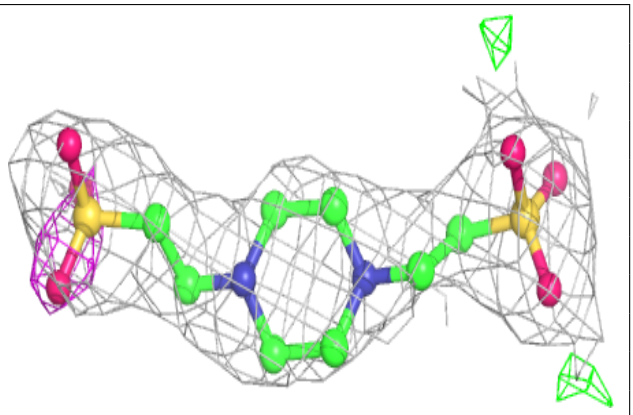
Continued from previous page...

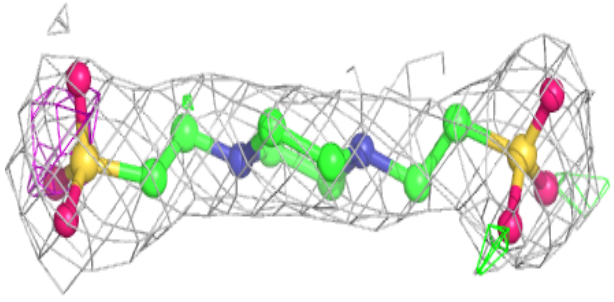
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	PIN	B	9012	18/18	0.89	0.21	44,44,44,44	0
4	PIN	H	9078	18/18	0.89	0.26	61,61,61,61	0
3	BME	A	368	4/4	0.90	0.33	30,46,47,48	0
2	SO4	D	461	5/5	0.90	0.20	52,52,52,52	0
3	BME	E	599	4/4	0.94	0.36	30,46,47,48	0
2	SO4	C	366	5/5	0.95	0.15	70,70,70,70	0
2	SO4	H	861	5/5	0.95	0.19	54,54,54,54	0
2	SO4	A	366	5/5	0.98	0.12	37,37,37,37	0
2	SO4	B	366	5/5	0.98	0.19	34,34,34,34	0
2	SO4	E	561	5/5	0.98	0.15	47,47,47,47	0
2	SO4	F	661	5/5	0.98	0.20	45,45,45,45	0

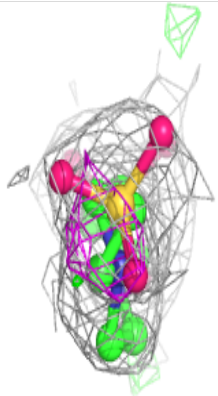
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around PIN B 9012:

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

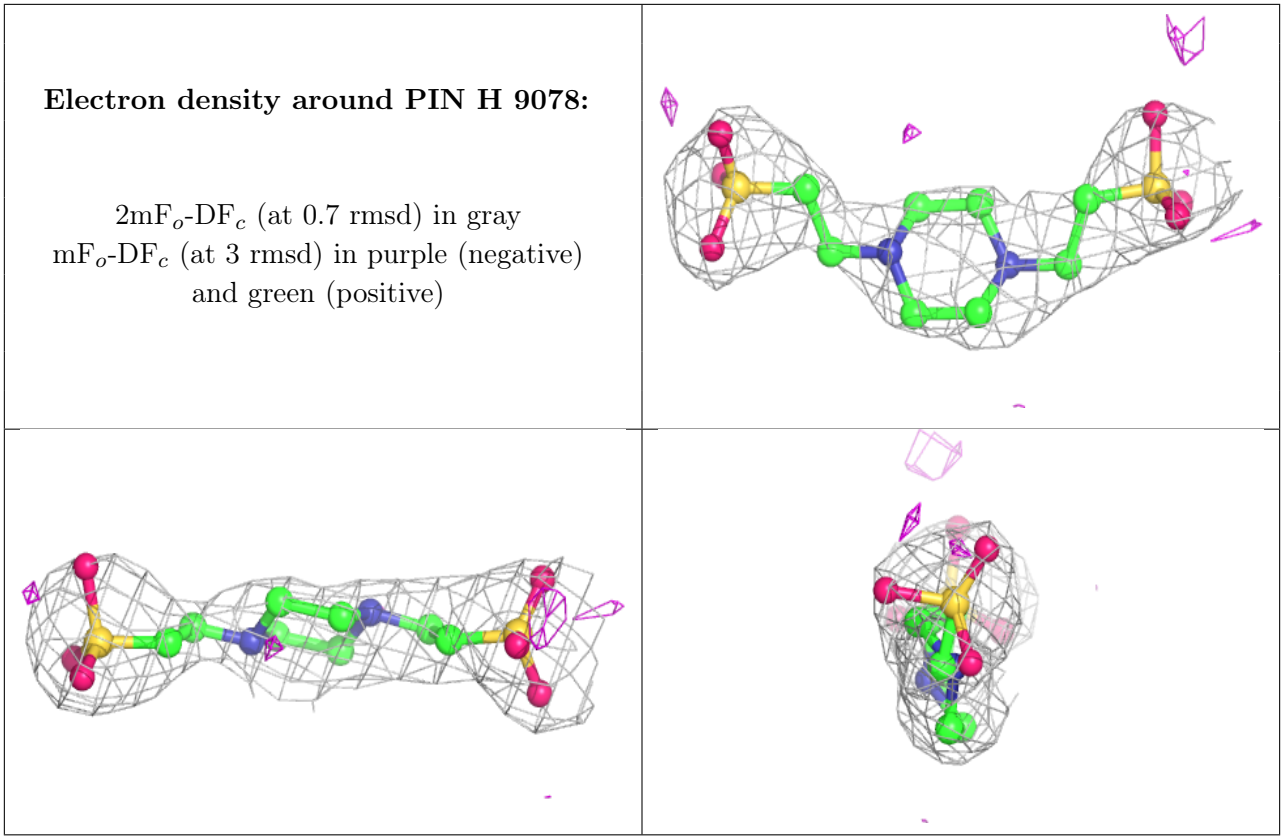






Electron density around PIN H 9078:

$2mF_o$-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.