Full wwPDB X-ray Structure Validation Report (i)

Nov 5, 2023 – 05:56 PM EST

PDB ID	:	5C9G
Title	:	Crystal Structure of a Putative enoyl-CoA hydratase/isomerase family protein from Hyphomonas neptunium
Authors	:	Szlachta, K.; Cooper, D.R.; Chapman, H.C.; Cymbrowski, M.T.; Stead, M.; Hillerich, B.S.; Ahmed, M.; Bonanno, J.; Seidel, R.; Almo, S.C.; Minor, W.; Hammonds, J.; New York Structural Genomics Research Consortium (NYSGRC)
Deposited on	:	2015-06-26
Resolution	:	2.10 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 (i) 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 (i)) were used in the production of this report:

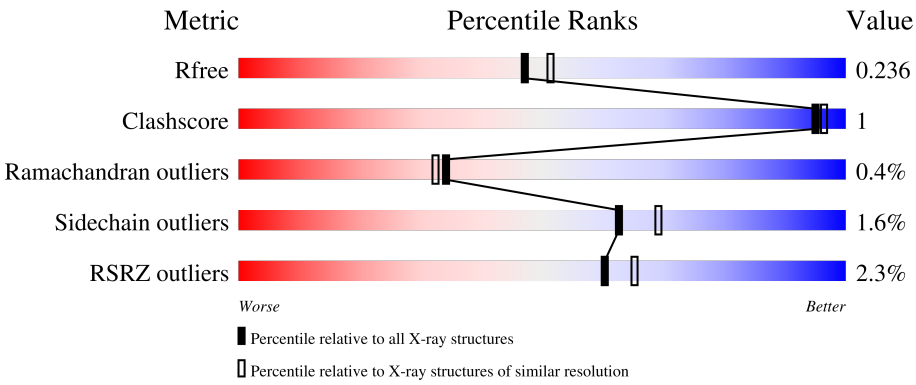
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)

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 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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	282	2% 91% 5% • •
1	B	282	2% 89% • • 7%
1	C	282	2% 88% • 8%
1	D	282	91% 5% • •

Continued on next page...

Validation Pipeline (wwPDB-VP) : 2.36

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	E	282	3% 88% • 8%
1	F	282	4% 90% • • 7%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 12870 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 Enoyl-CoA hydratase/isomerase family protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	273	1982	1254	346	377	1	4	0	0	0
1	B	261	1933	1225	340	363	1	4	0	0	0
1	C	259	1919	1216	341	358	1	3	0	1	0
1	D	273	2020	1282	353	380	1	4	0	0	0
1	E	259	1920	1216	337	363	1	3	0	0	0
1	F	262	1921	1221	335	360	1	4	0	0	0

There are 138 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-21	MSE	-	expression tag	UNP Q0C365
A	-20	HIS	-	expression tag	UNP Q0C365
A	-19	HIS	-	expression tag	UNP Q0C365
A	-18	HIS	-	expression tag	UNP Q0C365
A	-17	HIS	-	expression tag	UNP Q0C365
A	-16	HIS	-	expression tag	UNP Q0C365
A	-15	HIS	-	expression tag	UNP Q0C365
A	-14	SER	-	expression tag	UNP Q0C365
A	-13	SER	-	expression tag	UNP Q0C365
A	-12	GLY	-	expression tag	UNP Q0C365
A	-11	VAL	-	expression tag	UNP Q0C365
A	-10	ASP	-	expression tag	UNP Q0C365
A	-9	LEU	-	expression tag	UNP Q0C365
A	-8	GLY	-	expression tag	UNP Q0C365
A	-7	THR	-	expression tag	UNP Q0C365
A	-6	GLU	-	expression tag	UNP Q0C365
A	-5	ASN	-	expression tag	UNP Q0C365

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	LEU	-	expression tag	UNP Q0C365
A	-3	TYR	-	expression tag	UNP Q0C365
A	-2	PHE	-	expression tag	UNP Q0C365
A	-1	GLN	-	expression tag	UNP Q0C365
A	0	SER	-	expression tag	UNP Q0C365
A	1	MSE	-	expression tag	UNP Q0C365
B	-21	MSE	-	expression tag	UNP Q0C365
B	-20	HIS	-	expression tag	UNP Q0C365
B	-19	HIS	-	expression tag	UNP Q0C365
B	-18	HIS	-	expression tag	UNP Q0C365
B	-17	HIS	-	expression tag	UNP Q0C365
B	-16	HIS	-	expression tag	UNP Q0C365
B	-15	HIS	-	expression tag	UNP Q0C365
B	-14	SER	-	expression tag	UNP Q0C365
B	-13	SER	-	expression tag	UNP Q0C365
B	-12	GLY	-	expression tag	UNP Q0C365
B	-11	VAL	-	expression tag	UNP Q0C365
B	-10	ASP	-	expression tag	UNP Q0C365
B	-9	LEU	-	expression tag	UNP Q0C365
B	-8	GLY	-	expression tag	UNP Q0C365
B	-7	THR	-	expression tag	UNP Q0C365
B	-6	GLU	-	expression tag	UNP Q0C365
B	-5	ASN	-	expression tag	UNP Q0C365
B	-4	LEU	-	expression tag	UNP Q0C365
B	-3	TYR	-	expression tag	UNP Q0C365
B	-2	PHE	-	expression tag	UNP Q0C365
B	-1	GLN	-	expression tag	UNP Q0C365
B	0	SER	-	expression tag	UNP Q0C365
B	1	MSE	-	expression tag	UNP Q0C365
C	-21	MSE	-	expression tag	UNP Q0C365
C	-20	HIS	-	expression tag	UNP Q0C365
C	-19	HIS	-	expression tag	UNP Q0C365
C	-18	HIS	-	expression tag	UNP Q0C365
C	-17	HIS	-	expression tag	UNP Q0C365
C	-16	HIS	-	expression tag	UNP Q0C365
C	-15	HIS	-	expression tag	UNP Q0C365
C	-14	SER	-	expression tag	UNP Q0C365
C	-13	SER	-	expression tag	UNP Q0C365
C	-12	GLY	-	expression tag	UNP Q0C365
C	-11	VAL	-	expression tag	UNP Q0C365
C	-10	ASP	-	expression tag	UNP Q0C365
C	-9	LEU	-	expression tag	UNP Q0C365

Continued on next page...

Continued from previous page...

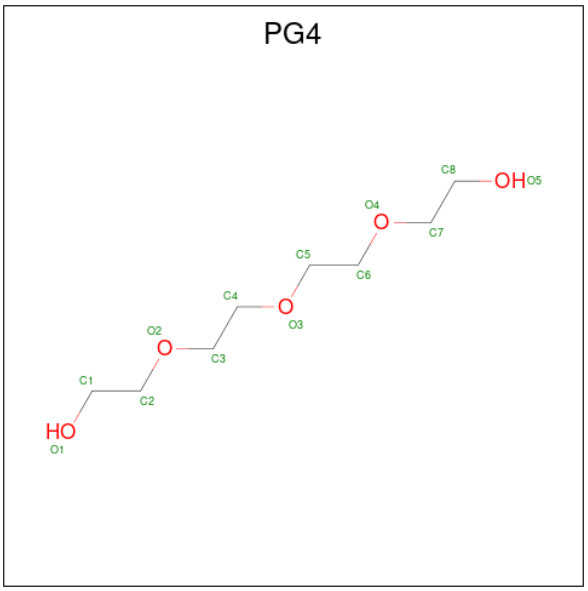
Chain	Residue	Modelled	Actual	Comment	Reference
C	-8	GLY	-	expression tag	UNP Q0C365
C	-7	THR	-	expression tag	UNP Q0C365
C	-6	GLU	-	expression tag	UNP Q0C365
C	-5	ASN	-	expression tag	UNP Q0C365
C	-4	LEU	-	expression tag	UNP Q0C365
C	-3	TYR	-	expression tag	UNP Q0C365
C	-2	PHE	-	expression tag	UNP Q0C365
C	-1	GLN	-	expression tag	UNP Q0C365
C	0	SER	-	expression tag	UNP Q0C365
C	1	MSE	-	expression tag	UNP Q0C365
D	-21	MSE	-	expression tag	UNP Q0C365
D	-20	HIS	-	expression tag	UNP Q0C365
D	-19	HIS	-	expression tag	UNP Q0C365
D	-18	HIS	-	expression tag	UNP Q0C365
D	-17	HIS	-	expression tag	UNP Q0C365
D	-16	HIS	-	expression tag	UNP Q0C365
D	-15	HIS	-	expression tag	UNP Q0C365
D	-14	SER	-	expression tag	UNP Q0C365
D	-13	SER	-	expression tag	UNP Q0C365
D	-12	GLY	-	expression tag	UNP Q0C365
D	-11	VAL	-	expression tag	UNP Q0C365
D	-10	ASP	-	expression tag	UNP Q0C365
D	-9	LEU	-	expression tag	UNP Q0C365
D	-8	GLY	-	expression tag	UNP Q0C365
D	-7	THR	-	expression tag	UNP Q0C365
D	-6	GLU	-	expression tag	UNP Q0C365
D	-5	ASN	-	expression tag	UNP Q0C365
D	-4	LEU	-	expression tag	UNP Q0C365
D	-3	TYR	-	expression tag	UNP Q0C365
D	-2	PHE	-	expression tag	UNP Q0C365
D	-1	GLN	-	expression tag	UNP Q0C365
D	0	SER	-	expression tag	UNP Q0C365
D	1	MSE	-	expression tag	UNP Q0C365
E	-21	MSE	-	expression tag	UNP Q0C365
E	-20	HIS	-	expression tag	UNP Q0C365
E	-19	HIS	-	expression tag	UNP Q0C365
E	-18	HIS	-	expression tag	UNP Q0C365
E	-17	HIS	-	expression tag	UNP Q0C365
E	-16	HIS	-	expression tag	UNP Q0C365
E	-15	HIS	-	expression tag	UNP Q0C365
E	-14	SER	-	expression tag	UNP Q0C365
E	-13	SER	-	expression tag	UNP Q0C365

Continued on next page...

Continued from previous page...

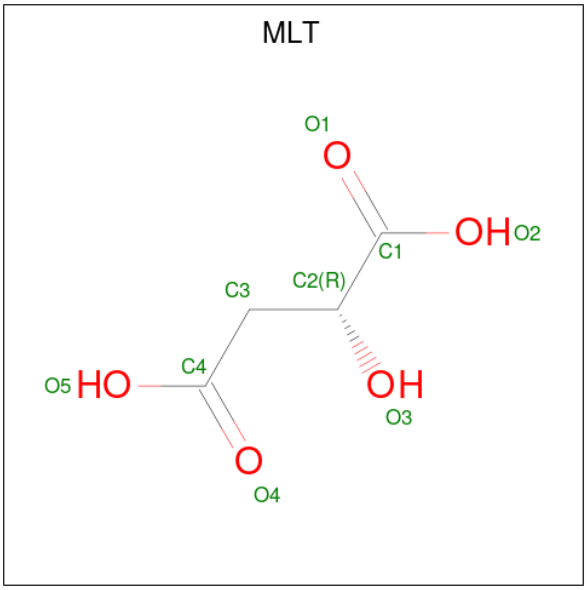
Chain	Residue	Modelled	Actual	Comment	Reference
E	-12	GLY	-	expression tag	UNP Q0C365
E	-11	VAL	-	expression tag	UNP Q0C365
E	-10	ASP	-	expression tag	UNP Q0C365
E	-9	LEU	-	expression tag	UNP Q0C365
E	-8	GLY	-	expression tag	UNP Q0C365
E	-7	THR	-	expression tag	UNP Q0C365
E	-6	GLU	-	expression tag	UNP Q0C365
E	-5	ASN	-	expression tag	UNP Q0C365
E	-4	LEU	-	expression tag	UNP Q0C365
E	-3	TYR	-	expression tag	UNP Q0C365
E	-2	PHE	-	expression tag	UNP Q0C365
E	-1	GLN	-	expression tag	UNP Q0C365
E	0	SER	-	expression tag	UNP Q0C365
E	1	MSE	-	expression tag	UNP Q0C365
F	-21	MSE	-	expression tag	UNP Q0C365
F	-20	HIS	-	expression tag	UNP Q0C365
F	-19	HIS	-	expression tag	UNP Q0C365
F	-18	HIS	-	expression tag	UNP Q0C365
F	-17	HIS	-	expression tag	UNP Q0C365
F	-16	HIS	-	expression tag	UNP Q0C365
F	-15	HIS	-	expression tag	UNP Q0C365
F	-14	SER	-	expression tag	UNP Q0C365
F	-13	SER	-	expression tag	UNP Q0C365
F	-12	GLY	-	expression tag	UNP Q0C365
F	-11	VAL	-	expression tag	UNP Q0C365
F	-10	ASP	-	expression tag	UNP Q0C365
F	-9	LEU	-	expression tag	UNP Q0C365
F	-8	GLY	-	expression tag	UNP Q0C365
F	-7	THR	-	expression tag	UNP Q0C365
F	-6	GLU	-	expression tag	UNP Q0C365
F	-5	ASN	-	expression tag	UNP Q0C365
F	-4	LEU	-	expression tag	UNP Q0C365
F	-3	TYR	-	expression tag	UNP Q0C365
F	-2	PHE	-	expression tag	UNP Q0C365
F	-1	GLN	-	expression tag	UNP Q0C365
F	0	SER	-	expression tag	UNP Q0C365
F	1	MSE	-	expression tag	UNP Q0C365

- Molecule 2 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	E	1	13	8	5	0	0

- Molecule 3 is D-MALATE (three-letter code: MLT) (formula: $C_4H_6O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
3	E	1	9	4	5	0	0

- Molecule 4 is water.

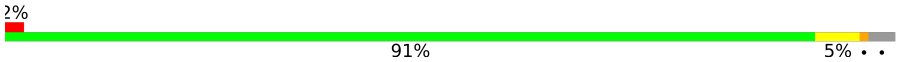
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	182	182	182	0	0
			Total	O		
4	B	181	181	181	0	0
			Total	O		
4	C	162	162	162	0	0
			Total	O		
4	D	243	243	243	0	0
			Total	O		
4	E	179	179	179	0	0
			Total	O		
4	F	206	206	206	0	0

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: Enoyl-CoA hydratase/isomerase family protein

Chain A:

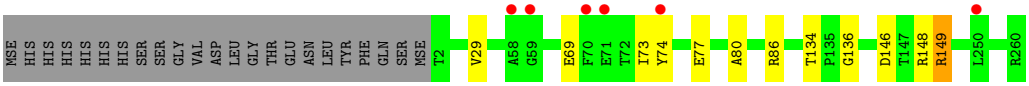


• Molecule 1: Enoyl-CoA hydratase/isomerase family protein

Chain B:

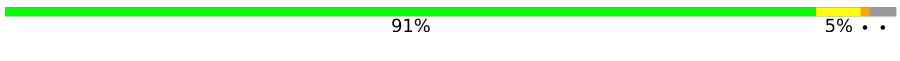
• Molecule 1: Enoyl-CoA hydratase/isomerase family protein

Chain C:



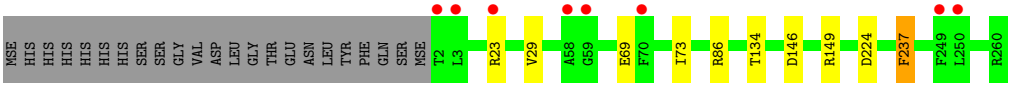
• Molecule 1: Enoyl-CoA hydratase/isomerase family protein

Chain D:



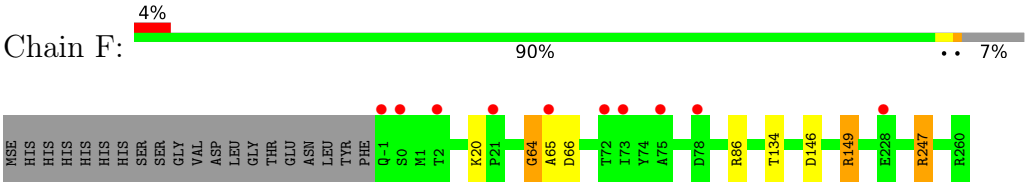
• Molecule 1: Enoyl-CoA hydratase/isomerase family protein

Chain E:



• Molecule 1: Enoyl-CoA hydratase/isomerase family protein

Chain F:


4%
90%
7%
MSE
HIS
HIS
HIS
HIS
HIS
HIS
SER
SER
GLY
VAL
ASP
LEU
GLY
THR
GLU
ASN
LEU
TYR
PHE
Q-1
SO
M1
T2
K20
P21
G64
A65
D66
T72
I73
Y74
A75
D78
R86
T134
D146
R149
E228
R247
R260

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	63.48Å 128.12Å 209.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.10 39.85 – 2.09	Depositor EDS
% Data completeness (in resolution range)	97.7 (40.00-2.10) 97.4 (39.85-2.09)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.95 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.8.0107	Depositor
R, R_{free}	0.198 , 0.232 0.207 , 0.236	Depositor DCC
R_{free} test set	4957 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	30.2	Xtriage
Anisotropy	0.287	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 41.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	12870	wwPDB-VP
Average B, all atoms (Å^2)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 45.11 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.3852e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MLT, PG4

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	0.58	0/2011	0.81	8/2720 (0.3%)
1	B	0.59	0/1962	0.82	7/2651 (0.3%)
1	C	0.59	0/1952	0.81	5/2637 (0.2%)
1	D	0.60	0/2051	0.83	9/2773 (0.3%)
1	E	0.59	0/1950	0.91	9/2638 (0.3%)
1	F	0.60	0/1950	0.83	5/2636 (0.2%)
All	All	0.59	0/11876	0.84	43/16055 (0.3%)

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	F	0	1

There are no bond length outliers.

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	86	ARG	NE-CZ-NH2	17.62	129.11	120.30
1	E	86	ARG	NE-CZ-NH1	-11.27	114.67	120.30
1	C	149	ARG	NE-CZ-NH2	-8.97	115.82	120.30
1	B	86	ARG	NE-CZ-NH2	-7.86	116.37	120.30
1	F	66	ASP	N-CA-CB	7.39	123.89	110.60
1	E	86	ARG	CD-NE-CZ	7.35	133.90	123.60
1	D	23	ARG	NE-CZ-NH1	7.23	123.91	120.30
1	C	149	ARG	NE-CZ-NH1	7.10	123.85	120.30
1	B	149	ARG	NE-CZ-NH2	-6.88	116.86	120.30
1	A	86	ARG	NE-CZ-NH1	6.79	123.70	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	86	ARG	NE-CZ-NH2	-6.72	116.94	120.30
1	F	86	ARG	NE-CZ-NH2	-6.67	116.96	120.30
1	D	86	ARG	NE-CZ-NH1	6.63	123.61	120.30
1	B	23	ARG	NE-CZ-NH1	6.48	123.54	120.30
1	D	86	ARG	NE-CZ-NH2	-6.47	117.07	120.30
1	E	149	ARG	NE-CZ-NH2	-6.41	117.10	120.30
1	F	86	ARG	NE-CZ-NH1	6.25	123.42	120.30
1	A	149	ARG	NE-CZ-NH1	6.18	123.39	120.30
1	E	23	ARG	NE-CZ-NH1	6.12	123.36	120.30
1	E	237	PHE	CB-CG-CD1	-6.06	116.56	120.80
1	D	148	ARG	NE-CZ-NH1	6.03	123.31	120.30
1	B	86	ARG	NE-CZ-NH1	5.83	123.22	120.30
1	A	149	ARG	NE-CZ-NH2	-5.69	117.45	120.30
1	B	149	ARG	NE-CZ-NH1	5.60	123.10	120.30
1	D	149	ARG	NE-CZ-NH2	-5.59	117.50	120.30
1	C	86[A]	ARG	NE-CZ-NH1	5.55	123.08	120.30
1	C	86[B]	ARG	NE-CZ-NH1	5.55	123.08	120.30
1	F	247	ARG	NE-CZ-NH1	5.53	123.06	120.30
1	C	148	ARG	NE-CZ-NH1	5.51	123.05	120.30
1	B	247	ARG	NE-CZ-NH1	5.35	122.98	120.30
1	E	149	ARG	NE-CZ-NH1	5.33	122.96	120.30
1	D	23	ARG	NE-CZ-NH2	-5.28	117.66	120.30
1	E	224	ASP	CB-CG-OD1	5.25	123.02	118.30
1	A	138	LEU	CA-CB-CG	5.24	127.34	115.30
1	A	228	GLU	CB-CA-C	-5.22	99.97	110.40
1	E	237	PHE	N-CA-CB	5.21	119.98	110.60
1	F	149	ARG	NE-CZ-NH2	-5.21	117.69	120.30
1	D	149	ARG	NE-CZ-NH1	5.21	122.90	120.30
1	D	224	ASP	CB-CG-OD1	5.18	122.97	118.30
1	A	148	ARG	NE-CZ-NH1	5.13	122.86	120.30
1	A	224	ASP	CB-CG-OD1	5.08	122.88	118.30
1	B	224	ASP	CB-CG-OD1	5.04	122.84	118.30
1	D	138	LEU	CA-CB-CG	5.04	126.89	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	F	64	GLY	Peptide

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	1982	0	1969	10	0
1	B	1933	0	1956	2	0
1	C	1919	0	1933	8	0
1	D	2020	0	2032	6	1
1	E	1920	0	1932	3	0
1	F	1921	0	1934	2	0
2	E	13	0	18	0	0
3	E	9	0	4	0	0
4	A	182	0	0	0	0
4	B	181	0	0	1	0
4	C	162	0	0	1	0
4	D	243	0	0	2	0
4	E	179	0	0	0	0
4	F	206	0	0	1	0
All	All	12870	0	11778	27	1

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 1.

All (27) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:16:ILE:HB	1:B:53:ILE:HD13	1.68	0.75
1:A:222:TRP:CH2	1:A:228:GLU:HG2	2.23	0.73
1:A:222:TRP:CZ2	1:A:228:GLU:HG2	2.32	0.64
1:C:29:VAL:CG2	1:C:73:ILE:HD11	2.31	0.61
1:A:237:PHE:CE1	1:C:74:TYR:CE1	2.89	0.61
1:A:237:PHE:CE1	1:C:74:TYR:HE1	2.21	0.59
1:B:19:ASN:ND2	4:B:301:HOH:O	2.26	0.56
1:E:29:VAL:CG2	1:E:73:ILE:HD11	2.36	0.56
1:A:237:PHE:CD2	1:C:80:ALA:HB1	2.43	0.54
1:D:138:LEU:HD23	1:D:140:LEU:HD12	1.92	0.52
1:A:138:LEU:HD23	1:A:140:LEU:HD12	1.91	0.51
1:D:44:ALA:HB3	4:D:453:HOH:O	2.09	0.51
1:E:69:GLU:HG3	1:E:73:ILE:HG12	1.95	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:69:GLU:HG3	1:C:73:ILE:HG12	1.96	0.47
1:F:149:ARG:NH1	4:F:302:HOH:O	2.47	0.46
1:C:29:VAL:HG21	1:C:73:ILE:HD11	1.98	0.44
1:C:149:ARG:NH1	4:C:303:HOH:O	2.50	0.44
1:D:2:THR:HG22	1:D:2:THR:O	2.17	0.44
1:E:29:VAL:HG21	1:E:73:ILE:HD11	2.00	0.44
1:A:2:THR:HG22	1:A:2:THR:O	2.19	0.43
1:A:207:SER:CB	1:C:136:GLY:HA2	2.49	0.42
1:F:64:GLY:O	1:F:65:ALA:O	2.38	0.41
1:A:138:LEU:HD23	1:A:140:LEU:CD1	2.51	0.41
1:A:142:TYR:CZ	1:A:146:ASP:HB3	2.55	0.41
1:D:130:LYS:HG2	4:D:348:HOH:O	2.21	0.41
1:D:138:LEU:HD23	1:D:140:LEU:CD1	2.51	0.40
1:D:142:TYR:CZ	1:D:146:ASP:HB3	2.57	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:-10:ASP:OD2	1:D:23:ARG:NH2[4_556]	2.07	0.13

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	271/282 (96%)	266 (98%)	4 (2%)	1 (0%)	34	32
1	B	259/282 (92%)	255 (98%)	3 (1%)	1 (0%)	34	32
1	C	258/282 (92%)	253 (98%)	4 (2%)	1 (0%)	34	32
1	D	271/282 (96%)	266 (98%)	4 (2%)	1 (0%)	34	32
1	E	257/282 (91%)	252 (98%)	4 (2%)	1 (0%)	34	32

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	260/282 (92%)	254 (98%)	5 (2%)	1 (0%)	34	32
All	All	1576/1692 (93%)	1546 (98%)	24 (2%)	6 (0%)	34	32

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	134	THR
1	B	134	THR
1	C	134	THR
1	D	134	THR
1	E	134	THR
1	F	134	THR

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	187/202 (93%)	183 (98%)	4 (2%)	53	59
1	B	186/202 (92%)	183 (98%)	3 (2%)	62	69
1	C	182/202 (90%)	180 (99%)	2 (1%)	73	79
1	D	194/202 (96%)	190 (98%)	4 (2%)	53	59
1	E	184/202 (91%)	182 (99%)	2 (1%)	73	79
1	F	182/202 (90%)	179 (98%)	3 (2%)	62	69
All	All	1115/1212 (92%)	1097 (98%)	18 (2%)	62	69

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	LYS
1	A	71	GLU
1	A	146	ASP
1	A	228	GLU
1	B	23	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	146	ASP
1	B	247	ARG
1	C	77	GLU
1	C	146	ASP
1	D	20	LYS
1	D	71	GLU
1	D	146	ASP
1	D	247	ARG
1	E	146	ASP
1	E	237	PHE
1	F	20	LYS
1	F	146	ASP
1	F	247	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	96	ASN
1	A	235	ASN
1	C	235	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

2 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	MLT	E	302	-	8,8,8	0.89	0	10,10,10	1.36	1 (10%)
2	PG4	E	301	-	12,12,12	0.62	0	11,11,11	0.48	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
3	MLT	E	302	-	-	4/8/8/8	-
2	PG4	E	301	-	-	6/10/10/10	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	302	MLT	O2-C1-C2	2.45	118.11	112.72

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	302	MLT	O1-C1-C2-O3
3	E	302	MLT	O2-C1-C2-O3
2	E	301	PG4	O3-C5-C6-O4
2	E	301	PG4	O4-C7-C8-O5
3	E	302	MLT	O1-C1-C2-C3
3	E	302	MLT	O2-C1-C2-C3
2	E	301	PG4	C6-C5-O3-C4
2	E	301	PG4	C3-C4-O3-C5
2	E	301	PG4	C4-C3-O2-C2
2	E	301	PG4	C1-C2-O2-C3

There are no ring outliers.

No monomer is involved in short contacts.

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 (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	269/282 (95%)	-0.14	6 (2%)	62	66	22, 32, 59, 75	0
1	B	257/282 (91%)	-0.15	5 (1%)	66	71	21, 30, 51, 70	0
1	C	256/282 (90%)	0.02	6 (2%)	60	65	23, 32, 60, 75	0
1	D	269/282 (95%)	-0.22	1 (0%)	92	93	21, 28, 42, 54	0
1	E	256/282 (90%)	-0.12	8 (3%)	49	55	22, 31, 49, 65	0
1	F	258/282 (91%)	-0.08	10 (3%)	39	45	20, 28, 53, 81	0
All	All	1565/1692 (92%)	-0.11	36 (2%)	60	65	20, 30, 54, 81	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	58	ALA	7.0
1	C	74	TYR	5.5
1	C	70	PHE	4.7
1	E	59	GLY	4.6
1	F	72	THR	4.3
1	E	3	LEU	4.0
1	C	59	GLY	3.8
1	F	21	PRO	3.8
1	A	249	PHE	3.8
1	F	-1	GLN	3.6
1	E	2	THR	3.4
1	B	72	THR	3.3
1	F	65	ALA	3.1
1	D	-12	GLY	2.9
1	E	58	ALA	2.9
1	F	0	SER	2.8
1	F	73	ILE	2.8
1	E	249	PHE	2.5
1	A	77	GLU	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	70	PHE	2.4
1	F	78	ASP	2.4
1	E	23	ARG	2.4
1	C	250	LEU	2.3
1	E	250	LEU	2.3
1	F	2	THR	2.2
1	B	70	PHE	2.2
1	C	71	GLU	2.2
1	F	75	ALA	2.2
1	F	228	GLU	2.2
1	B	0	SER	2.1
1	A	242	PHE	2.1
1	A	237	PHE	2.1
1	B	224	ASP	2.1
1	A	254	PRO	2.1
1	A	228	GLU	2.0
1	B	65	ALA	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	PG4	E	301	13/13	0.51	0.21	64,68,69,69	0
3	MLT	E	302	9/9	0.61	0.27	61,64,65,66	0

6.5 Other polymers (i)

There are no such residues in this entry.