



# wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 2, 2023 – 08:03 PM EDT

PDB ID : 3QU4  
Title : Crystal structure of pyrophosphatase from bacteroides thetaiotaomicron, asp13ala mutant  
Authors : Patskovsky, Y.; Huang, H.; Toro, R.; Gerlt, J.A.; Burley, S.K.; Dunaway-Mariano, D.; Almo, S.C.; New York SGX Research Center for Structural Genomics (NYSGXRC); Enzyme Function Initiative (EFI)  
Deposited on : 2011-02-23  
Resolution : 2.10 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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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)  
Xtrriage (Phenix) : 1.13  
EDS : 2.35  
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

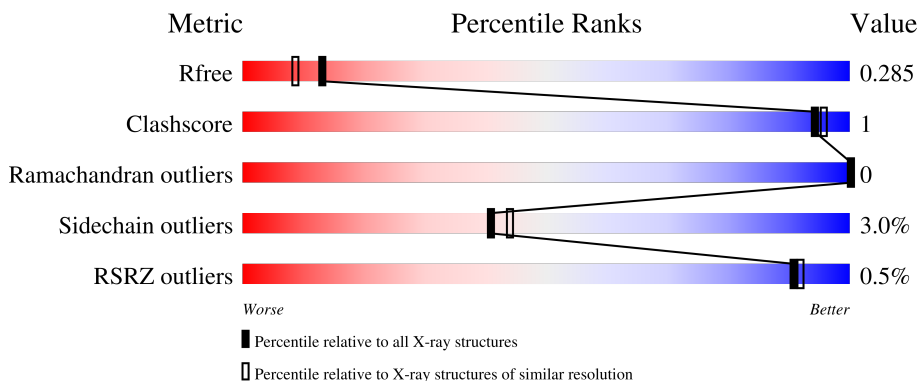
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	243	 86% 5% • 8%
1	B	243	 87% • 9%
1	C	243	 87% 5% 8%
1	D	243	 89% • 7%

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Mol	Chain	Length	Quality of chain
1	E	243	 88% 6% 7%
1	F	243	 88% 8%
1	G	243	 % 87% 5% 8%
1	H	243	 2% 85% 6% 8%

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 15199 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 INORGANIC PYROPHOSPHATASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	223	1773	1136	293	332	12	0	7	0
1	B	222	1781	1139	296	334	12	0	9	0
1	C	224	1779	1140	293	333	13	0	7	0
1	D	226	1775	1133	294	335	13	0	3	0
1	E	227	1792	1146	295	338	13	0	6	0
1	F	223	1754	1121	290	331	12	0	4	0
1	G	224	1759	1125	291	330	13	0	3	0
1	H	224	1776	1138	293	332	13	0	5	0

There are 160 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-18	GLY	-	expression tag	UNP Q8A5V9
A	-17	SER	-	expression tag	UNP Q8A5V9
A	-16	SER	-	expression tag	UNP Q8A5V9
A	-15	HIS	-	expression tag	UNP Q8A5V9
A	-14	HIS	-	expression tag	UNP Q8A5V9
A	-13	HIS	-	expression tag	UNP Q8A5V9
A	-12	HIS	-	expression tag	UNP Q8A5V9
A	-11	HIS	-	expression tag	UNP Q8A5V9
A	-10	HIS	-	expression tag	UNP Q8A5V9
A	-9	SER	-	expression tag	UNP Q8A5V9
A	-8	SER	-	expression tag	UNP Q8A5V9
A	-7	GLY	-	expression tag	UNP Q8A5V9
A	-6	LEU	-	expression tag	UNP Q8A5V9

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	VAL	-	expression tag	UNP Q8A5V9
A	-4	PRO	-	expression tag	UNP Q8A5V9
A	-3	ARG	-	expression tag	UNP Q8A5V9
A	-2	GLY	-	expression tag	UNP Q8A5V9
A	-1	SER	-	expression tag	UNP Q8A5V9
A	0	HIS	-	expression tag	UNP Q8A5V9
A	13	ALA	ASP	engineered mutation	UNP Q8A5V9
B	-18	GLY	-	expression tag	UNP Q8A5V9
B	-17	SER	-	expression tag	UNP Q8A5V9
B	-16	SER	-	expression tag	UNP Q8A5V9
B	-15	HIS	-	expression tag	UNP Q8A5V9
B	-14	HIS	-	expression tag	UNP Q8A5V9
B	-13	HIS	-	expression tag	UNP Q8A5V9
B	-12	HIS	-	expression tag	UNP Q8A5V9
B	-11	HIS	-	expression tag	UNP Q8A5V9
B	-10	HIS	-	expression tag	UNP Q8A5V9
B	-9	SER	-	expression tag	UNP Q8A5V9
B	-8	SER	-	expression tag	UNP Q8A5V9
B	-7	GLY	-	expression tag	UNP Q8A5V9
B	-6	LEU	-	expression tag	UNP Q8A5V9
B	-5	VAL	-	expression tag	UNP Q8A5V9
B	-4	PRO	-	expression tag	UNP Q8A5V9
B	-3	ARG	-	expression tag	UNP Q8A5V9
B	-2	GLY	-	expression tag	UNP Q8A5V9
B	-1	SER	-	expression tag	UNP Q8A5V9
B	0	HIS	-	expression tag	UNP Q8A5V9
B	13	ALA	ASP	engineered mutation	UNP Q8A5V9
C	-18	GLY	-	expression tag	UNP Q8A5V9
C	-17	SER	-	expression tag	UNP Q8A5V9
C	-16	SER	-	expression tag	UNP Q8A5V9
C	-15	HIS	-	expression tag	UNP Q8A5V9
C	-14	HIS	-	expression tag	UNP Q8A5V9
C	-13	HIS	-	expression tag	UNP Q8A5V9
C	-12	HIS	-	expression tag	UNP Q8A5V9
C	-11	HIS	-	expression tag	UNP Q8A5V9
C	-10	HIS	-	expression tag	UNP Q8A5V9
C	-9	SER	-	expression tag	UNP Q8A5V9
C	-8	SER	-	expression tag	UNP Q8A5V9
C	-7	GLY	-	expression tag	UNP Q8A5V9
C	-6	LEU	-	expression tag	UNP Q8A5V9
C	-5	VAL	-	expression tag	UNP Q8A5V9
C	-4	PRO	-	expression tag	UNP Q8A5V9

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-3	ARG	-	expression tag	UNP Q8A5V9
C	-2	GLY	-	expression tag	UNP Q8A5V9
C	-1	SER	-	expression tag	UNP Q8A5V9
C	0	HIS	-	expression tag	UNP Q8A5V9
C	13	ALA	ASP	engineered mutation	UNP Q8A5V9
D	-18	GLY	-	expression tag	UNP Q8A5V9
D	-17	SER	-	expression tag	UNP Q8A5V9
D	-16	SER	-	expression tag	UNP Q8A5V9
D	-15	HIS	-	expression tag	UNP Q8A5V9
D	-14	HIS	-	expression tag	UNP Q8A5V9
D	-13	HIS	-	expression tag	UNP Q8A5V9
D	-12	HIS	-	expression tag	UNP Q8A5V9
D	-11	HIS	-	expression tag	UNP Q8A5V9
D	-10	HIS	-	expression tag	UNP Q8A5V9
D	-9	SER	-	expression tag	UNP Q8A5V9
D	-8	SER	-	expression tag	UNP Q8A5V9
D	-7	GLY	-	expression tag	UNP Q8A5V9
D	-6	LEU	-	expression tag	UNP Q8A5V9
D	-5	VAL	-	expression tag	UNP Q8A5V9
D	-4	PRO	-	expression tag	UNP Q8A5V9
D	-3	ARG	-	expression tag	UNP Q8A5V9
D	-2	GLY	-	expression tag	UNP Q8A5V9
D	-1	SER	-	expression tag	UNP Q8A5V9
D	0	HIS	-	expression tag	UNP Q8A5V9
D	13	ALA	ASP	engineered mutation	UNP Q8A5V9
E	-18	GLY	-	expression tag	UNP Q8A5V9
E	-17	SER	-	expression tag	UNP Q8A5V9
E	-16	SER	-	expression tag	UNP Q8A5V9
E	-15	HIS	-	expression tag	UNP Q8A5V9
E	-14	HIS	-	expression tag	UNP Q8A5V9
E	-13	HIS	-	expression tag	UNP Q8A5V9
E	-12	HIS	-	expression tag	UNP Q8A5V9
E	-11	HIS	-	expression tag	UNP Q8A5V9
E	-10	HIS	-	expression tag	UNP Q8A5V9
E	-9	SER	-	expression tag	UNP Q8A5V9
E	-8	SER	-	expression tag	UNP Q8A5V9
E	-7	GLY	-	expression tag	UNP Q8A5V9
E	-6	LEU	-	expression tag	UNP Q8A5V9
E	-5	VAL	-	expression tag	UNP Q8A5V9
E	-4	PRO	-	expression tag	UNP Q8A5V9
E	-3	ARG	-	expression tag	UNP Q8A5V9
E	-2	GLY	-	expression tag	UNP Q8A5V9

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-1	SER	-	expression tag	UNP Q8A5V9
E	0	HIS	-	expression tag	UNP Q8A5V9
E	13	ALA	ASP	engineered mutation	UNP Q8A5V9
F	-18	GLY	-	expression tag	UNP Q8A5V9
F	-17	SER	-	expression tag	UNP Q8A5V9
F	-16	SER	-	expression tag	UNP Q8A5V9
F	-15	HIS	-	expression tag	UNP Q8A5V9
F	-14	HIS	-	expression tag	UNP Q8A5V9
F	-13	HIS	-	expression tag	UNP Q8A5V9
F	-12	HIS	-	expression tag	UNP Q8A5V9
F	-11	HIS	-	expression tag	UNP Q8A5V9
F	-10	HIS	-	expression tag	UNP Q8A5V9
F	-9	SER	-	expression tag	UNP Q8A5V9
F	-8	SER	-	expression tag	UNP Q8A5V9
F	-7	GLY	-	expression tag	UNP Q8A5V9
F	-6	LEU	-	expression tag	UNP Q8A5V9
F	-5	VAL	-	expression tag	UNP Q8A5V9
F	-4	PRO	-	expression tag	UNP Q8A5V9
F	-3	ARG	-	expression tag	UNP Q8A5V9
F	-2	GLY	-	expression tag	UNP Q8A5V9
F	-1	SER	-	expression tag	UNP Q8A5V9
F	0	HIS	-	expression tag	UNP Q8A5V9
F	13	ALA	ASP	engineered mutation	UNP Q8A5V9
G	-18	GLY	-	expression tag	UNP Q8A5V9
G	-17	SER	-	expression tag	UNP Q8A5V9
G	-16	SER	-	expression tag	UNP Q8A5V9
G	-15	HIS	-	expression tag	UNP Q8A5V9
G	-14	HIS	-	expression tag	UNP Q8A5V9
G	-13	HIS	-	expression tag	UNP Q8A5V9
G	-12	HIS	-	expression tag	UNP Q8A5V9
G	-11	HIS	-	expression tag	UNP Q8A5V9
G	-10	HIS	-	expression tag	UNP Q8A5V9
G	-9	SER	-	expression tag	UNP Q8A5V9
G	-8	SER	-	expression tag	UNP Q8A5V9
G	-7	GLY	-	expression tag	UNP Q8A5V9
G	-6	LEU	-	expression tag	UNP Q8A5V9
G	-5	VAL	-	expression tag	UNP Q8A5V9
G	-4	PRO	-	expression tag	UNP Q8A5V9
G	-3	ARG	-	expression tag	UNP Q8A5V9
G	-2	GLY	-	expression tag	UNP Q8A5V9
G	-1	SER	-	expression tag	UNP Q8A5V9
G	0	HIS	-	expression tag	UNP Q8A5V9

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Chain	Residue	Modelled	Actual	Comment	Reference
G	13	ALA	ASP	engineered mutation	UNP Q8A5V9
H	-18	GLY	-	expression tag	UNP Q8A5V9
H	-17	SER	-	expression tag	UNP Q8A5V9
H	-16	SER	-	expression tag	UNP Q8A5V9
H	-15	HIS	-	expression tag	UNP Q8A5V9
H	-14	HIS	-	expression tag	UNP Q8A5V9
H	-13	HIS	-	expression tag	UNP Q8A5V9
H	-12	HIS	-	expression tag	UNP Q8A5V9
H	-11	HIS	-	expression tag	UNP Q8A5V9
H	-10	HIS	-	expression tag	UNP Q8A5V9
H	-9	SER	-	expression tag	UNP Q8A5V9
H	-8	SER	-	expression tag	UNP Q8A5V9
H	-7	GLY	-	expression tag	UNP Q8A5V9
H	-6	LEU	-	expression tag	UNP Q8A5V9
H	-5	VAL	-	expression tag	UNP Q8A5V9
H	-4	PRO	-	expression tag	UNP Q8A5V9
H	-3	ARG	-	expression tag	UNP Q8A5V9
H	-2	GLY	-	expression tag	UNP Q8A5V9
H	-1	SER	-	expression tag	UNP Q8A5V9
H	0	HIS	-	expression tag	UNP Q8A5V9
H	13	ALA	ASP	engineered mutation	UNP Q8A5V9

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Mg 1 1	0	0
2	B	1	Total Mg 1 1	0	0
2	C	1	Total Mg 1 1	0	0
2	D	1	Total Mg 1 1	0	0
2	E	1	Total Mg 1 1	0	0
2	F	1	Total Mg 1 1	0	0
2	G	1	Total Mg 1 1	0	0
2	H	1	Total Mg 1 1	0	0

- Molecule 3 is ACETATE ION (three-letter code: ACT) (formula: C<sub>2</sub>H<sub>3</sub>O<sub>2</sub>).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 4 2 2	0	0
3	D	1	Total C O 4 2 2	0	0
3	H	1	Total C O 4 2 2	0	0

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Cl 1 1	0	0
4	B	1	Total Cl 1 1	0	0
4	C	1	Total Cl 1 1	0	0
4	D	1	Total Cl 1 1	0	0
4	E	1	Total Cl 1 1	0	0
4	F	1	Total Cl 1 1	0	0
4	G	1	Total Cl 1 1	0	0
4	H	1	Total Cl 1 1	0	0


- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	133	Total 133	O 133	0	0
5	B	132	Total 132	O 132	0	0
5	C	128	Total 128	O 128	0	0
5	D	123	Total 123	O 123	0	0
5	E	112	Total 112	O 112	0	0
5	F	116	Total 116	O 116	0	0
5	G	126	Total 126	O 126	0	0
5	H	112	Total 112	O 112	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: INORGANIC PYROPHOSPHATASE

Chain A: 




- Molecule 1: INORGANIC PYROPHOSPHATASE

Chain B: 



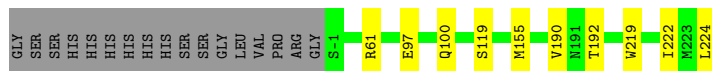
- Molecule 1: INORGANIC PYROPHOSPHATASE

Chain C: 



- Molecule 1: INORGANIC PYROPHOSPHATASE

Chain D: 




- Molecule 1: INORGANIC PYROPHOSPHATASE

Chain E: 

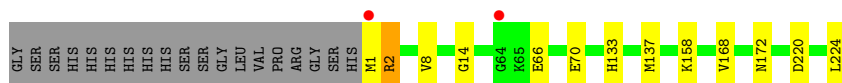
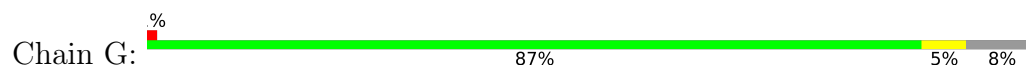


- Molecule 1: INORGANIC PYROPHOSPHATASE

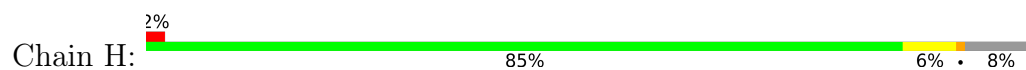
Chain F: 



- Molecule 1: INORGANIC PYROPHOSPHATASE



- Molecule 1: INORGANIC PYROPHOSPHATASE



## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	69.94Å 76.22Å 95.59Å 89.97° 89.97° 90.00°	Depositor
Resolution (Å)	20.00 – 2.10 45.35 – 2.00	Depositor EDS
% Data completeness (in resolution range)	93.4 (20.00-2.10) 91.8 (45.35-2.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.06 (at 2.00Å)	Xtrriage
Refinement program	REFMAC 5.5.0089	Depositor
R, $R_{free}$	0.216 , 0.286 0.219 , 0.285	Depositor DCC
$R_{free}$ test set	3721 reflections (3.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	30.0	Xtrriage
Anisotropy	0.438	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 23.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	0.227 for h,-k,-l 0.219 for -h,k,-l 0.440 for -h,-k,l	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	15199	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.09% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ACT, CL

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	0.45	0/1830	0.58	0/2469
1	B	0.43	0/1838	0.56	0/2480
1	C	0.44	0/1840	0.57	0/2483
1	D	0.45	0/1824	0.56	0/2462
1	E	0.43	0/1850	0.55	0/2498
1	F	0.45	0/1802	0.56	0/2435
1	G	0.44	0/1807	0.58	0/2438
1	H	0.44	0/1831	0.58	0/2471
All	All	0.44	0/14622	0.57	0/19736

There are no bond length outliers.

There are no bond angle outliers.

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	1773	0	1786	6	0
1	B	1781	0	1790	4	0
1	C	1779	0	1791	3	0
1	D	1775	0	1769	4	0
1	E	1792	0	1794	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	1754	0	1747	4	0
1	G	1759	0	1764	4	0
1	H	1776	0	1781	7	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
3	A	4	0	3	0	0
3	D	4	0	3	0	0
3	H	4	0	3	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
4	G	1	0	0	0	0
4	H	1	0	0	0	0
5	A	133	0	0	0	0
5	B	132	0	0	1	0
5	C	128	0	0	0	0
5	D	123	0	0	1	0
5	E	112	0	0	1	0
5	F	116	0	0	0	0
5	G	126	0	0	0	0
5	H	112	0	0	2	0
All	All	15199	0	14231	38	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 1.

The worst 5 of 38 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:147:LYS:HG2	1:C:176:GLY:HA2	1.71	0.73
1:E:20:MET:N	1:E:21:PRO:CD	2.56	0.69
1:F:190[A]:VAL:O	1:F:190[A]:VAL:HG13	1.92	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:147:LYS:HG2	1:B:176:GLY:HA2	1.80	0.62
1:F:190[A]:VAL:O	1:F:190[A]:VAL:CG1	2.49	0.60

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	228/243 (94%)	224 (98%)	4 (2%)	0	100	100
1	B	229/243 (94%)	223 (97%)	6 (3%)	0	100	100
1	C	229/243 (94%)	225 (98%)	4 (2%)	0	100	100
1	D	227/243 (93%)	223 (98%)	4 (2%)	0	100	100
1	E	231/243 (95%)	228 (99%)	3 (1%)	0	100	100
1	F	225/243 (93%)	217 (96%)	8 (4%)	0	100	100
1	G	225/243 (93%)	219 (97%)	6 (3%)	0	100	100
1	H	227/243 (93%)	217 (96%)	10 (4%)	0	100	100
All	All	1821/1944 (94%)	1776 (98%)	45 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	193/203 (95%)	187 (97%)	6 (3%)	40	43
1	B	194/203 (96%)	187 (96%)	7 (4%)	35	36
1	C	194/203 (96%)	188 (97%)	6 (3%)	40	43
1	D	192/203 (95%)	189 (98%)	3 (2%)	62	69
1	E	195/203 (96%)	188 (96%)	7 (4%)	35	36
1	F	189/203 (93%)	183 (97%)	6 (3%)	39	41
1	G	190/203 (94%)	184 (97%)	6 (3%)	39	41
1	H	192/203 (95%)	184 (96%)	8 (4%)	30	30
All	All	1539/1624 (95%)	1490 (97%)	49 (3%)	41	41

5 of 49 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	223	MET
1	G	1	MET
1	F	60	GLN
1	F	155	MET
1	G	66	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	60	GLN
1	G	69	GLN
1	H	133	HIS
1	H	117	GLN
1	D	117	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 19 ligands modelled in this entry, 16 are monoatomic - leaving 3 for Mogul analysis.

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	ACT	D	226	-	3,3,3	0.78	0	3,3,3	1.30	0
3	ACT	A	226	-	3,3,3	0.83	0	3,3,3	1.38	0
3	ACT	H	226	-	3,3,3	0.72	0	3,3,3	1.41	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	223/243 (91%)	-0.39	1 (0%) 92 93	20, 34, 55, 89	0
1	B	222/243 (91%)	-0.36	1 (0%) 91 92	19, 35, 54, 78	0
1	C	224/243 (92%)	-0.41	1 (0%) 92 93	21, 33, 53, 69	0
1	D	226/243 (93%)	-0.41	0 100 100	20, 34, 50, 62	0
1	E	227/243 (93%)	-0.44	0 100 100	19, 33, 51, 64	0
1	F	223/243 (91%)	-0.37	0 100 100	21, 34, 55, 85	0
1	G	224/243 (92%)	-0.41	2 (0%) 84 86	16, 33, 52, 78	0
1	H	224/243 (92%)	-0.40	4 (1%) 68 72	21, 34, 56, 84	0
All	All	1793/1944 (92%)	-0.40	9 (0%) 91 92	16, 34, 54, 89	0

The worst 5 of 9 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	224	LEU	3.4
1	H	145	TYR	3.0
1	G	64	GLY	2.7
1	B	118	LEU	2.7
1	G	1	MET	2.7

### 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
3	ACT	H	226	4/4	0.87	0.12	38,40,43,45	0
3	ACT	A	226	4/4	0.95	0.13	37,43,44,45	0
4	CL	E	226	1/1	0.96	0.05	34,34,34,34	0
3	ACT	D	226	4/4	0.97	0.14	31,40,41,43	0
4	CL	A	227	1/1	0.98	0.04	31,31,31,31	0
4	CL	C	226	1/1	0.98	0.05	31,31,31,31	0
2	MG	B	225	1/1	0.98	0.09	13,13,13,13	0
4	CL	G	226	1/1	0.98	0.04	30,30,30,30	0
4	CL	H	227	1/1	0.98	0.09	35,35,35,35	0
2	MG	D	225	1/1	0.99	0.07	4,4,4,4	0
2	MG	E	225	1/1	0.99	0.11	9,9,9,9	0
4	CL	B	226	1/1	0.99	0.07	35,35,35,35	0
2	MG	G	225	1/1	0.99	0.11	6,6,6,6	0
4	CL	D	227	1/1	0.99	0.07	28,28,28,28	0
2	MG	H	225	1/1	0.99	0.14	18,18,18,18	0
4	CL	F	226	1/1	0.99	0.03	32,32,32,32	0
2	MG	A	225	1/1	0.99	0.12	10,10,10,10	0
2	MG	C	225	1/1	0.99	0.10	10,10,10,10	0
2	MG	F	225	1/1	1.00	0.10	12,12,12,12	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.