



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 23, 2023 – 04:32 PM EDT

PDB ID : 5TI1
Title : Crystal Structure of Fumarylacetoacetate hydrolase from Burkholderia xenovorans LB400
Authors : Seattle Structural Genomics Center for Infectious Disease; SSGCID; Seattle Structural Genomics Center for Infectious Disease (SSGCID)
Deposited on : 2016-09-30
Resolution : 2.00 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

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

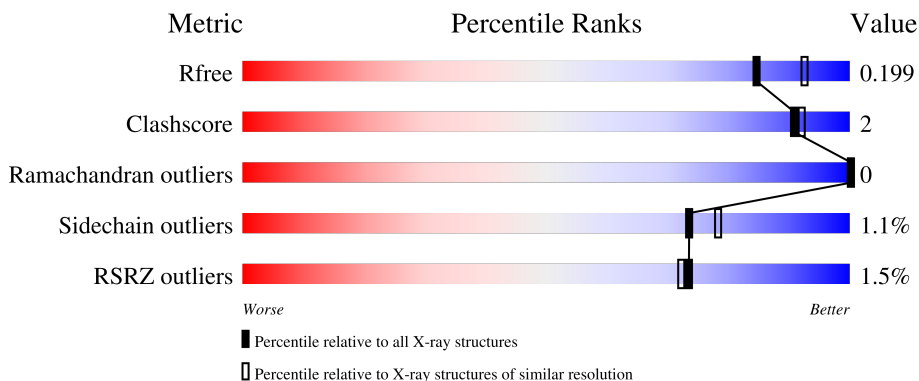
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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.



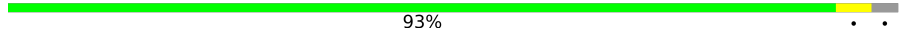


Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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 $\leq 5\%$. 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	444	 4% 90% 6%
1	B	444	 % 93%
1	C	444	 5% 91% 6%
1	D	444	 92%
1	E	444	 91% 6%

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Mol	Chain	Length	Quality of chain
1	F	444	 93%
1	G	444	%  91% 5%
1	H	444	%  93%

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 29129 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 Fumarylacetoacetate hydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	426	3304	2081	582	630	11	0	12	0
1	B	429	3289	2072	578	627	12	0	4	0
1	C	429	3251	2050	572	618	11	0	2	0
1	D	429	3278	2060	579	628	11	0	3	0
1	E	429	3319	2095	582	630	12	0	8	0
1	F	429	3297	2075	579	632	11	0	5	0
1	G	429	3348	2112	587	638	11	0	14	0
1	H	430	3318	2092	584	631	11	0	7	0

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	MET	-	initiating methionine	UNP Q144Z1
A	-6	ALA	-	expression tag	UNP Q144Z1
A	-5	HIS	-	expression tag	UNP Q144Z1
A	-4	HIS	-	expression tag	UNP Q144Z1
A	-3	HIS	-	expression tag	UNP Q144Z1
A	-2	HIS	-	expression tag	UNP Q144Z1
A	-1	HIS	-	expression tag	UNP Q144Z1
A	0	HIS	-	expression tag	UNP Q144Z1
B	-7	MET	-	initiating methionine	UNP Q144Z1
B	-6	ALA	-	expression tag	UNP Q144Z1
B	-5	HIS	-	expression tag	UNP Q144Z1
B	-4	HIS	-	expression tag	UNP Q144Z1
B	-3	HIS	-	expression tag	UNP Q144Z1

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	HIS	-	expression tag	UNP Q144Z1
B	-1	HIS	-	expression tag	UNP Q144Z1
B	0	HIS	-	expression tag	UNP Q144Z1
C	-7	MET	-	initiating methionine	UNP Q144Z1
C	-6	ALA	-	expression tag	UNP Q144Z1
C	-5	HIS	-	expression tag	UNP Q144Z1
C	-4	HIS	-	expression tag	UNP Q144Z1
C	-3	HIS	-	expression tag	UNP Q144Z1
C	-2	HIS	-	expression tag	UNP Q144Z1
C	-1	HIS	-	expression tag	UNP Q144Z1
C	0	HIS	-	expression tag	UNP Q144Z1
D	-7	MET	-	initiating methionine	UNP Q144Z1
D	-6	ALA	-	expression tag	UNP Q144Z1
D	-5	HIS	-	expression tag	UNP Q144Z1
D	-4	HIS	-	expression tag	UNP Q144Z1
D	-3	HIS	-	expression tag	UNP Q144Z1
D	-2	HIS	-	expression tag	UNP Q144Z1
D	-1	HIS	-	expression tag	UNP Q144Z1
D	0	HIS	-	expression tag	UNP Q144Z1
E	-7	MET	-	initiating methionine	UNP Q144Z1
E	-6	ALA	-	expression tag	UNP Q144Z1
E	-5	HIS	-	expression tag	UNP Q144Z1
E	-4	HIS	-	expression tag	UNP Q144Z1
E	-3	HIS	-	expression tag	UNP Q144Z1
E	-2	HIS	-	expression tag	UNP Q144Z1
E	-1	HIS	-	expression tag	UNP Q144Z1
E	0	HIS	-	expression tag	UNP Q144Z1
F	-7	MET	-	initiating methionine	UNP Q144Z1
F	-6	ALA	-	expression tag	UNP Q144Z1
F	-5	HIS	-	expression tag	UNP Q144Z1
F	-4	HIS	-	expression tag	UNP Q144Z1
F	-3	HIS	-	expression tag	UNP Q144Z1
F	-2	HIS	-	expression tag	UNP Q144Z1
F	-1	HIS	-	expression tag	UNP Q144Z1
F	0	HIS	-	expression tag	UNP Q144Z1
G	-7	MET	-	initiating methionine	UNP Q144Z1
G	-6	ALA	-	expression tag	UNP Q144Z1
G	-5	HIS	-	expression tag	UNP Q144Z1
G	-4	HIS	-	expression tag	UNP Q144Z1
G	-3	HIS	-	expression tag	UNP Q144Z1
G	-2	HIS	-	expression tag	UNP Q144Z1
G	-1	HIS	-	expression tag	UNP Q144Z1

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Chain	Residue	Modelled	Actual	Comment	Reference
G	0	HIS	-	expression tag	UNP Q144Z1
H	-7	MET	-	initiating methionine	UNP Q144Z1
H	-6	ALA	-	expression tag	UNP Q144Z1
H	-5	HIS	-	expression tag	UNP Q144Z1
H	-4	HIS	-	expression tag	UNP Q144Z1
H	-3	HIS	-	expression tag	UNP Q144Z1
H	-2	HIS	-	expression tag	UNP Q144Z1
H	-1	HIS	-	expression tag	UNP Q144Z1
H	0	HIS	-	expression tag	UNP Q144Z1

- 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 SODIUM ION (three-letter code: NA) (formula: Na).

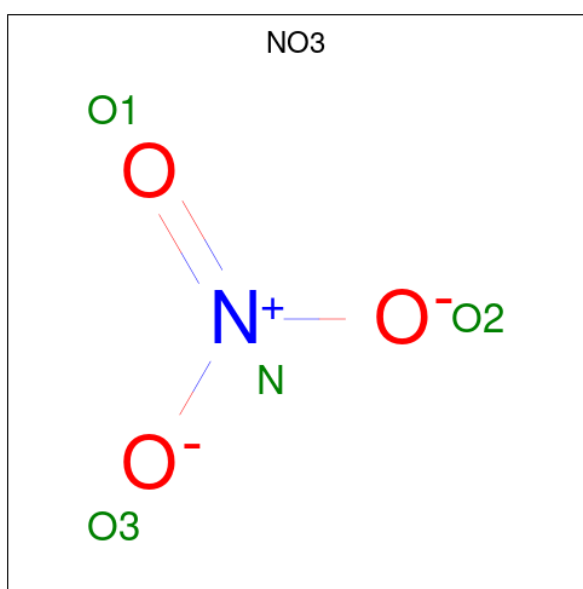
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Na 1 1	0	0
3	B	1	Total Na 1 1	0	0
3	C	1	Total Na 1 1	0	0
3	D	1	Total Na 1 1	0	0

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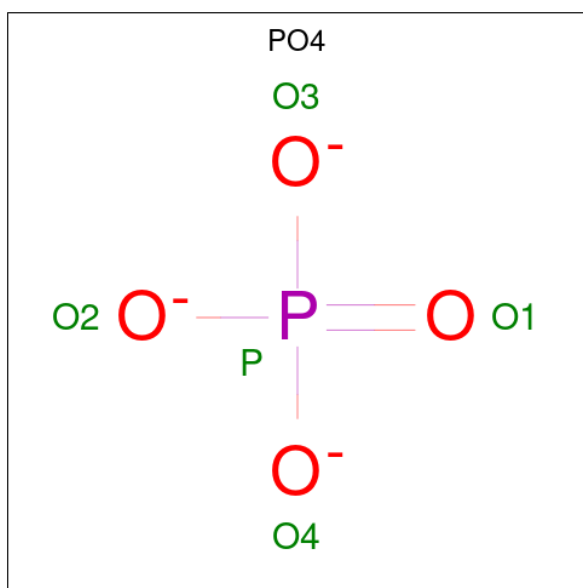
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	1	Total	Na	0	0
			1	1		
3	F	1	Total	Na	0	0
			1	1		
3	G	1	Total	Na	0	0
			1	1		
3	H	1	Total	Na	0	0
			1	1		

- Molecule 4 is NITRATE ION (three-letter code: NO3) (formula: NO₃).



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

- Molecule 5 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	F	1	Total	O	P	0	0
			5	4	1		

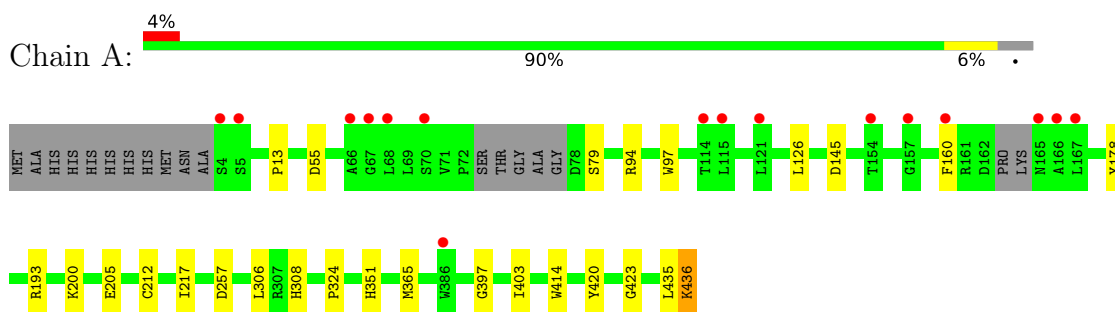
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	269	Total	O	0	2
			271	271		
6	B	263	Total	O	0	4
			267	267		
6	C	227	Total	O	0	4
			231	231		
6	D	320	Total	O	0	4
			324	324		
6	E	381	Total	O	0	4
			385	385		
6	F	385	Total	O	0	6
			391	391		
6	G	373	Total	O	0	1
			374	374		
6	H	426	Total	O	0	7
			433	433		

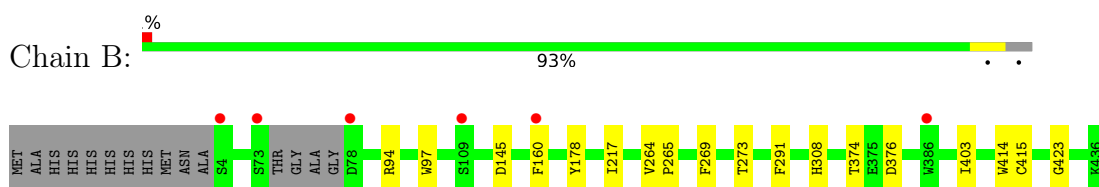
3 Residue-property plots [i](#)

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.

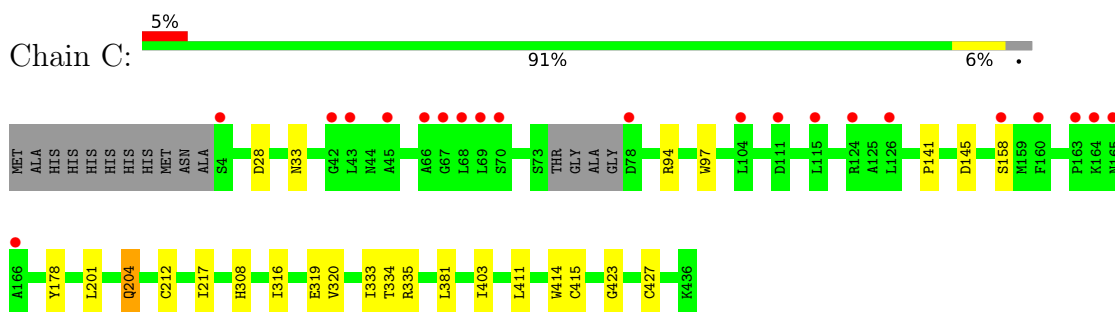
- Molecule 1: Fumarylacetoacetate hydrolase



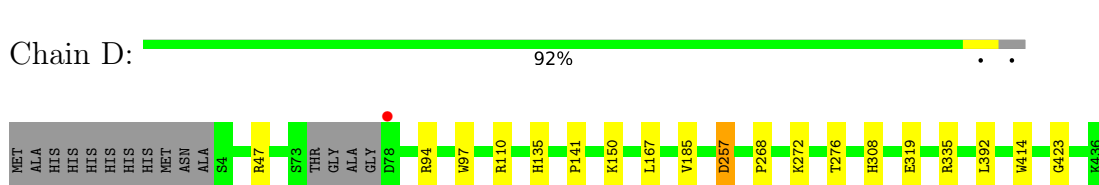
- Molecule 1: Fumarylacetoacetate hydrolase



- Molecule 1: Fumarylacetoacetate hydrolase



- Molecule 1: Fumarylacetoacetate hydrolase



- Molecule 1: Fumarylacetoacetate hydrolase

Chain E:  91% 6%

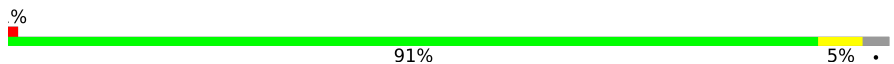


• Molecule 1: Fumarylacetoacetate hydrolase

Chain F:  93%

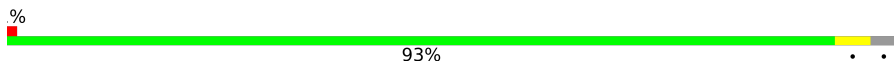


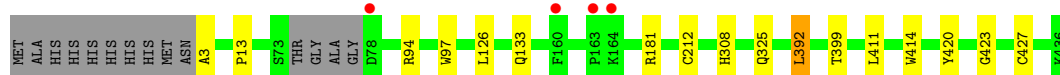
• Molecule 1: Fumarylacetoacetate hydrolase

Chain G:  91% 5%



• Molecule 1: Fumarylacetoacetate hydrolase

Chain H:  93%



4 Data and refinement statistics i

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	65.90Å 83.10Å 186.29Å 101.63° 91.17° 113.81°	Depositor
Resolution (Å)	40.31 – 2.00 48.70 – 2.00	Depositor EDS
% Data completeness (in resolution range)	95.5 (40.31-2.00) 95.6 (48.70-2.00)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.44 (at 2.00Å)	Xtrriage
Refinement program	PHENIX (dev_2499: ???)	Depositor
R, R_{free}	0.154 , 0.199 0.154 , 0.199	Depositor DCC
R_{free} test set	2001 reflections (0.88%)	wwPDB-VP
Wilson B-factor (Å ²)	22.9	Xtrriage
Anisotropy	0.747	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 58.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.027 for h,-h-k,-l	Xtrriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	29129	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 19.61% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NA, NO3, PO4, MG

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	0.34	0/3397	0.54	0/4623
1	B	0.33	0/3377	0.54	0/4601
1	C	0.33	0/3333	0.52	0/4545
1	D	0.35	0/3361	0.54	0/4579
1	E	0.37	0/3419	0.57	0/4656
1	F	0.38	0/3386	0.56	0/4612
1	G	0.36	0/3451	0.55	0/4700
1	H	0.40	0/3415	0.58	1/4651 (0.0%)
All	All	0.36	0/27139	0.55	1/36967 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	181	ARG	NE-CZ-NH2	-5.49	117.56	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3304	0	3202	14	0
1	B	3289	0	3181	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	3251	0	3124	13	0
1	D	3278	0	3167	11	0
1	E	3319	0	3235	14	0
1	F	3297	0	3199	8	0
1	G	3348	0	3251	11	0
1	H	3318	0	3226	9	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	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
4	C	4	0	0	0	0
4	D	8	0	0	0	0
4	E	4	0	0	0	0
4	F	4	0	0	0	0
4	G	4	0	0	0	0
4	H	4	0	0	0	0
5	F	5	0	0	0	0
6	A	271	0	0	2	0
6	B	267	0	0	0	0
6	C	231	0	0	1	0
6	D	324	0	0	1	0
6	E	385	0	0	1	0
6	F	391	0	0	1	0
6	G	374	0	0	1	0
6	H	433	0	0	3	0
All	All	29129	0	25585	88	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 2.

All (88) 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:E:25:PRO:O	6:E:601:HOH:O	1.80	0.99
1:A:324:PRO:HG2	1:A:397[B]:GLY:HA3	1.82	0.62
1:E:20:GLU:OE2	1:E:110[B]:ARG:NH2	2.35	0.60
1:B:414:TRP:HA	1:B:423:GLY:HA2	1.86	0.57
1:A:94:ARG:NH1	6:A:608:HOH:O	2.36	0.56
1:C:201:LEU:HB2	1:C:204:GLN:HG3	1.87	0.56
1:D:319:GLU:HG2	1:D:335:ARG:HG2	1.87	0.56
1:A:414:TRP:HA	1:A:423:GLY:HA2	1.88	0.56
1:A:193[B]:ARG:HD3	1:A:435:LEU:HG	1.87	0.55
1:A:217:ILE:HG23	1:A:403:ILE:HD11	1.88	0.55
1:F:411:LEU:HB2	1:F:427:CYS:HB3	1.90	0.53
1:A:55:ASP:HB2	6:A:741:HOH:O	2.08	0.53
1:C:28:ASP:OD1	1:C:423:GLY:HA3	2.09	0.52
1:B:217:ILE:HG23	1:B:403:ILE:HD11	1.91	0.52
1:D:94:ARG:HA	1:D:97:TRP:CD2	2.45	0.51
1:G:324:PRO:HG2	1:G:397[A]:GLY:HA3	1.92	0.51
1:H:13:PRO:HB3	1:H:420:TYR:CE1	2.46	0.51
1:C:145:ASP:HB3	1:C:178:TYR:CE1	2.46	0.51
1:E:94:ARG:HA	1:E:97:TRP:CE3	2.46	0.50
1:A:94:ARG:HA	1:A:97:TRP:CD2	2.47	0.50
1:G:217:ILE:HG23	1:G:403:ILE:HD11	1.94	0.49
1:E:414:TRP:HA	1:E:423:GLY:HA2	1.95	0.49
1:F:414:TRP:HA	1:F:423:GLY:HA2	1.95	0.49
1:A:145:ASP:HB3	1:A:178:TYR:CE1	2.48	0.49
1:C:414:TRP:HA	1:C:423:GLY:HA2	1.94	0.49
1:D:257:ASP:OD1	1:D:257:ASP:N	2.47	0.48
1:G:147:TYR:CD2	1:G:176:ILE:HD11	2.49	0.48
1:H:94:ARG:HA	1:H:97:TRP:CD2	2.48	0.48
1:D:414:TRP:HA	1:D:423:GLY:HA2	1.96	0.48
1:C:217:ILE:HG23	1:C:403:ILE:HD11	1.96	0.48
1:G:411:LEU:HB2	1:G:427:CYS:HB3	1.95	0.48
1:H:94:ARG:HA	1:H:97:TRP:CE3	2.49	0.47
1:F:94:ARG:HA	1:F:97:TRP:CD2	2.49	0.47
1:D:47[B]:ARG:HG2	1:D:135:HIS:CD2	2.49	0.47
1:G:94:ARG:HA	1:G:97:TRP:CE3	2.49	0.47
1:H:411:LEU:HB2	1:H:427:CYS:HB3	1.97	0.46
1:E:94:ARG:HA	1:E:97:TRP:CD2	2.50	0.46
1:E:160:PHE:HE2	1:E:260:GLN:HE22	1.62	0.46
1:A:306:LEU:HD21	1:A:351:HIS:HB2	1.97	0.46
1:G:84[B]:ASP:OD1	1:G:139[B]:GLN:NE2	2.48	0.46
1:C:319:GLU:HG2	1:C:335:ARG:HG2	1.98	0.46
1:A:13:PRO:HB3	1:A:420:TYR:CE1	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:94:ARG:HA	1:B:97:TRP:CD2	2.51	0.46
1:E:411:LEU:HB2	1:E:427:CYS:HB3	1.97	0.45
1:D:268:PRO:HB2	1:D:272:LYS:HG3	1.98	0.45
1:C:320:VAL:HB	1:C:334:THR:HG22	1.99	0.45
1:B:145:ASP:HB3	1:B:178:TYR:CE1	2.52	0.45
1:H:3:ALA:N	6:H:616:HOH:O	2.50	0.45
1:E:269:PHE:O	1:E:273:THR:HG23	2.17	0.44
1:D:94:ARG:HA	1:D:97:TRP:CE3	2.53	0.44
1:D:150:LYS:HG3	1:D:167:LEU:HD11	1.99	0.44
1:A:200:LYS:HE2	1:A:205:GLU:O	2.18	0.43
1:C:33:ASN:HB3	6:C:611:HOH:O	2.18	0.43
1:C:411:LEU:HB2	1:C:427:CYS:HB3	2.00	0.43
1:G:185:VAL:HA	1:G:276:THR:O	2.19	0.43
1:F:198:GLN:HG3	6:F:715:HOH:O	2.17	0.43
1:E:41:ASP:OD2	1:E:48:ARG:NH2	2.43	0.43
1:F:145:ASP:HB3	1:F:178:TYR:CE1	2.54	0.43
1:B:374:THR:OG1	1:B:376:ASP:OD1	2.20	0.43
1:F:94:ARG:HA	1:F:97:TRP:CE3	2.54	0.43
1:C:94:ARG:HA	1:C:97:TRP:CD2	2.54	0.42
1:C:316:ILE:HG12	1:C:415:CYS:SG	2.59	0.42
1:E:257:ASP:OD1	1:E:257:ASP:N	2.52	0.42
1:A:436:LYS:HB2	1:A:436:LYS:HE2	1.78	0.42
1:F:324:PRO:HG2	1:F:397:GLY:HA3	2.02	0.42
1:H:414:TRP:HA	1:H:423:GLY:HA2	2.02	0.42
1:B:264:VAL:HA	1:B:265:PRO:HA	1.81	0.42
1:D:110:ARG:HD3	6:D:856:HOH:O	2.20	0.41
1:G:6:ASP:O	1:G:10:THR:HG23	2.19	0.41
1:A:257:ASP:OD1	1:A:257:ASP:N	2.53	0.41
1:A:145:ASP:HB3	1:A:178:TYR:CZ	2.56	0.41
1:H:325:GLN:HG3	6:H:830:HOH:O	2.20	0.41
1:B:291:PHE:CD1	1:B:415:CYS:HB3	2.54	0.41
1:G:145:ASP:HB3	1:G:178:TYR:CE1	2.55	0.41
1:H:392:LEU:O	1:H:399:THR:HA	2.20	0.41
1:E:145:ASP:HB3	1:E:178:TYR:CE1	2.56	0.41
1:E:200:LYS:HE2	1:E:205:GLU:O	2.20	0.41
1:B:269:PHE:O	1:B:273:THR:HG23	2.21	0.41
1:E:320:VAL:HB	1:E:334:THR:HG22	2.02	0.41
1:G:414:TRP:HA	1:G:423:GLY:HA2	2.04	0.40
1:C:333:ILE:HD12	1:C:381:LEU:HD21	2.02	0.40
1:D:185:VAL:HA	1:D:276:THR:O	2.22	0.40
1:E:147:TYR:CD2	1:E:176:ILE:HD11	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:133[B]:GLN:HG3	6:H:919:HOH:O	2.22	0.40
1:F:185:VAL:HA	1:F:276:THR:O	2.21	0.40
1:G:293[A]:VAL:HG21	6:G:728:HOH:O	2.20	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	432/444 (97%)	415 (96%)	17 (4%)	0	100	100
1	B	429/444 (97%)	415 (97%)	14 (3%)	0	100	100
1	C	427/444 (96%)	413 (97%)	14 (3%)	0	100	100
1	D	428/444 (96%)	413 (96%)	15 (4%)	0	100	100
1	E	433/444 (98%)	418 (96%)	15 (4%)	0	100	100
1	F	430/444 (97%)	415 (96%)	15 (4%)	0	100	100
1	G	439/444 (99%)	419 (95%)	20 (5%)	0	100	100
1	H	433/444 (98%)	416 (96%)	17 (4%)	0	100	100
All	All	3451/3552 (97%)	3324 (96%)	127 (4%)	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	346/362 (96%)	339 (98%)	7 (2%)	55	58
1	B	346/362 (96%)	344 (99%)	2 (1%)	86	90
1	C	337/362 (93%)	333 (99%)	4 (1%)	71	76
1	D	345/362 (95%)	342 (99%)	3 (1%)	78	83
1	E	351/362 (97%)	348 (99%)	3 (1%)	78	83
1	F	349/362 (96%)	346 (99%)	3 (1%)	78	83
1	G	352/362 (97%)	349 (99%)	3 (1%)	78	83
1	H	350/362 (97%)	346 (99%)	4 (1%)	73	78
All	All	2776/2896 (96%)	2747 (99%)	29 (1%)	73	81

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	79	SER
1	A	126	LEU
1	A	160	PHE
1	A	212	CYS
1	A	308	HIS
1	A	365	MET
1	A	436	LYS
1	B	160	PHE
1	B	308	HIS
1	C	158	SER
1	C	204	GLN
1	C	212	CYS
1	C	308	HIS
1	D	257	ASP
1	D	308	HIS
1	D	392	LEU
1	E	71	VAL
1	E	308	HIS
1	E	365	MET
1	F	4	SER
1	F	212	CYS
1	F	308	HIS
1	G	71	VAL
1	G	212	CYS
1	G	308	HIS
1	H	126	LEU
1	H	212	CYS

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Mol	Chain	Res	Type
1	H	308	HIS
1	H	392	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	204	GLN
1	F	165	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](#)

Of 24 ligands modelled in this entry, 16 are monoatomic - leaving 8 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	$\# Z > 2$
4	NO3	G	503	-	1,3,3	0.66	0	0,3,3	-	-
4	NO3	H	503	-	1,3,3	0.76	0	0,3,3	-	-
4	NO3	E	503	-	1,3,3	0.79	0	0,3,3	-	-
4	NO3	C	503	-	1,3,3	0.73	0	0,3,3	-	-
4	NO3	D	503	-	1,3,3	0.73	0	0,3,3	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NO3	F	504	-	1,3,3	0.66	0	0,3,3	-	-
5	PO4	F	503	-	4,4,4	0.90	0	6,6,6	0.46	0
4	NO3	D	504	-	1,3,3	0.78	0	0,3,3	-	-

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

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, 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	426/444 (95%)	-0.18	16 (3%) 40 39	17, 38, 69, 90	0
1	B	429/444 (96%)	-0.31	6 (1%) 75 74	20, 40, 65, 86	0
1	C	429/444 (96%)	-0.07	21 (4%) 29 28	20, 41, 75, 92	0
1	D	429/444 (96%)	-0.43	1 (0%) 95 94	19, 32, 53, 77	0
1	E	429/444 (96%)	-0.50	1 (0%) 95 94	13, 26, 49, 69	0
1	F	429/444 (96%)	-0.56	0 100 100	14, 26, 49, 78	0
1	G	429/444 (96%)	-0.47	4 (0%) 84 83	13, 28, 52, 83	0
1	H	430/444 (96%)	-0.49	4 (0%) 84 83	13, 24, 48, 86	0
All	All	3430/3552 (96%)	-0.38	53 (1%) 73 72	13, 31, 62, 92	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	115	LEU	4.0
1	C	126	LEU	3.9
1	A	160	PHE	3.9
1	C	166	ALA	3.8
1	C	4	SER	3.7
1	A	154	THR	3.7
1	H	160	PHE	3.6
1	C	66	ALA	3.5
1	C	158	SER	3.5
1	C	163	PRO	3.4
1	C	69	LEU	3.4
1	C	165	ASN	3.3
1	C	160	PHE	3.3
1	C	164	LYS	3.3
1	A	386	TRP	3.2
1	C	78	ASP	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	68	LEU	2.9
1	H	164	LYS	2.9
1	H	163	PRO	2.8
1	B	73	SER	2.8
1	A	67	GLY	2.7
1	A	68	LEU	2.7
1	C	104	LEU	2.6
1	A	66	ALA	2.6
1	A	121	LEU	2.6
1	B	109	SER	2.6
1	B	4	SER	2.6
1	C	124	ARG	2.6
1	C	111	ASP	2.5
1	C	115	LEU	2.6
1	A	5	SER	2.5
1	A	167	LEU	2.4
1	C	43	LEU	2.4
1	A	114	THR	2.4
1	G	4	SER	2.4
1	B	160	PHE	2.3
1	E	397	GLY	2.3
1	A	165	ASN	2.2
1	C	42	GLY	2.2
1	G	162	ASP	2.2
1	H	78	ASP	2.2
1	A	4	SER	2.2
1	A	166	ALA	2.1
1	C	67	GLY	2.1
1	B	386[A]	TRP	2.1
1	A	70	SER	2.1
1	C	70	SER	2.1
1	B	78	ASP	2.1
1	D	78	ASP	2.1
1	C	45	ALA	2.1
1	G	164	LYS	2.1
1	G	160	PHE	2.0
1	A	157	GLY	2.0

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

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
4	NO3	C	503	4/4	0.78	0.15	75,75,76,77	0
4	NO3	D	503	4/4	0.78	0.14	64,65,65,66	0
4	NO3	H	503	4/4	0.89	0.20	62,64,65,65	0
4	NO3	E	503	4/4	0.90	0.10	55,58,59,59	0
4	NO3	G	503	4/4	0.92	0.23	73,74,74,74	0
4	NO3	F	504	4/4	0.92	0.10	70,71,71,72	0
5	PO4	F	503	5/5	0.95	0.08	69,73,75,76	0
4	NO3	D	504	4/4	0.96	0.11	50,53,53,54	0
2	MG	D	501	1/1	0.97	0.06	34,34,34,34	0
3	NA	C	502	1/1	0.97	0.10	20,20,20,20	1
3	NA	D	502	1/1	0.99	0.11	20,20,20,20	0
3	NA	E	502	1/1	0.99	0.11	21,21,21,21	1
3	NA	F	502	1/1	0.99	0.10	18,18,18,18	0
3	NA	H	502	1/1	0.99	0.13	17,17,17,17	1
2	MG	C	501	1/1	0.99	0.03	32,32,32,32	0
2	MG	A	501	1/1	0.99	0.05	28,28,28,28	0
2	MG	E	501	1/1	0.99	0.04	23,23,23,23	0
2	MG	F	501	1/1	0.99	0.05	21,21,21,21	0
2	MG	H	501	1/1	0.99	0.04	22,22,22,22	0
3	NA	A	502	1/1	0.99	0.08	23,23,23,23	0
3	NA	B	502	1/1	0.99	0.06	22,22,22,22	1
2	MG	B	501	1/1	0.99	0.05	28,28,28,28	0
3	NA	G	502	1/1	1.00	0.11	18,18,18,18	0
2	MG	G	501	1/1	1.00	0.05	21,21,21,21	0

6.5 Other polymers [i](#)

There are no such residues in this entry.