



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 10:59 PM UTC

PDB ID : 3C8N / pdb_00003c8n
Title : Crystal structure of apo-FGD1 from Mycobacterium tuberculosis
Authors : Bashiri, G.; Squire, C.J.; Moreland, N.J.; Baker, E.N.
Deposited on : 2008-02-12
Resolution : 1.90 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

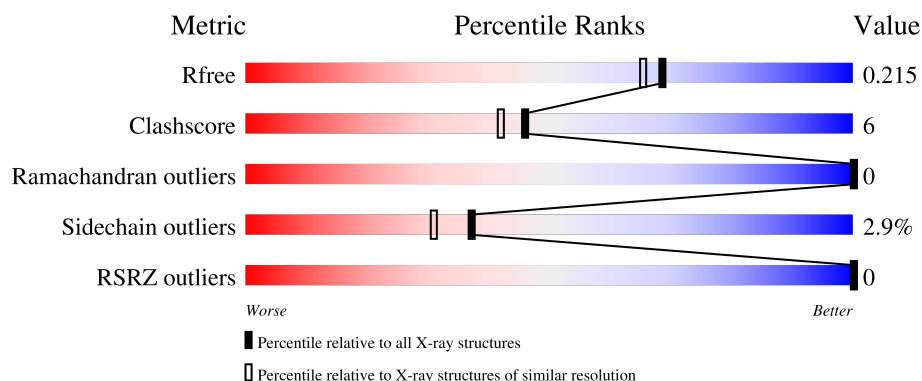
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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}	180053	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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	356	
1	B	356	
1	C	356	
1	D	356	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 10741 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 Probable F420-dependent glucose-6-phosphate dehydrogenase FGD1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	343	Total	C	N	O	S	Se	0	1	0
			2667	1693	472	491	2	9			
1	B	332	Total	C	N	O	S	Se	0	2	0
			2577	1637	449	481	2	8			
1	C	332	Total	C	N	O	S	Se	0	2	0
			2567	1632	452	473	2	8			
1	D	330	Total	C	N	O	S	Se	0	2	0
			2559	1630	451	468	2	8			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MSE	-	expression tag	UNP P96253
A	-18	GLY	-	expression tag	UNP P96253
A	-17	SER	-	expression tag	UNP P96253
A	-16	SER	-	expression tag	UNP P96253
A	-15	HIS	-	expression tag	UNP P96253
A	-14	HIS	-	expression tag	UNP P96253
A	-13	HIS	-	expression tag	UNP P96253
A	-12	HIS	-	expression tag	UNP P96253
A	-11	HIS	-	expression tag	UNP P96253
A	-10	HIS	-	expression tag	UNP P96253
A	-9	SER	-	expression tag	UNP P96253
A	-8	SER	-	expression tag	UNP P96253
A	-7	GLY	-	expression tag	UNP P96253
A	-6	LEU	-	expression tag	UNP P96253
A	-5	VAL	-	expression tag	UNP P96253
A	-4	PRO	-	expression tag	UNP P96253
A	-3	ARG	-	expression tag	UNP P96253
A	-2	GLY	-	expression tag	UNP P96253
A	-1	SER	-	expression tag	UNP P96253
A	0	HIS	-	expression tag	UNP P96253

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Chain	Residue	Modelled	Actual	Comment	Reference
A	243	MSE	LEU	engineered mutation	UNP P96253
B	-19	MSE	-	expression tag	UNP P96253
B	-18	GLY	-	expression tag	UNP P96253
B	-17	SER	-	expression tag	UNP P96253
B	-16	SER	-	expression tag	UNP P96253
B	-15	HIS	-	expression tag	UNP P96253
B	-14	HIS	-	expression tag	UNP P96253
B	-13	HIS	-	expression tag	UNP P96253
B	-12	HIS	-	expression tag	UNP P96253
B	-11	HIS	-	expression tag	UNP P96253
B	-10	HIS	-	expression tag	UNP P96253
B	-9	SER	-	expression tag	UNP P96253
B	-8	SER	-	expression tag	UNP P96253
B	-7	GLY	-	expression tag	UNP P96253
B	-6	LEU	-	expression tag	UNP P96253
B	-5	VAL	-	expression tag	UNP P96253
B	-4	PRO	-	expression tag	UNP P96253
B	-3	ARG	-	expression tag	UNP P96253
B	-2	GLY	-	expression tag	UNP P96253
B	-1	SER	-	expression tag	UNP P96253
B	0	HIS	-	expression tag	UNP P96253
B	243	MSE	LEU	engineered mutation	UNP P96253
C	-19	MSE	-	expression tag	UNP P96253
C	-18	GLY	-	expression tag	UNP P96253
C	-17	SER	-	expression tag	UNP P96253
C	-16	SER	-	expression tag	UNP P96253
C	-15	HIS	-	expression tag	UNP P96253
C	-14	HIS	-	expression tag	UNP P96253
C	-13	HIS	-	expression tag	UNP P96253
C	-12	HIS	-	expression tag	UNP P96253
C	-11	HIS	-	expression tag	UNP P96253
C	-10	HIS	-	expression tag	UNP P96253
C	-9	SER	-	expression tag	UNP P96253
C	-8	SER	-	expression tag	UNP P96253
C	-7	GLY	-	expression tag	UNP P96253
C	-6	LEU	-	expression tag	UNP P96253
C	-5	VAL	-	expression tag	UNP P96253
C	-4	PRO	-	expression tag	UNP P96253
C	-3	ARG	-	expression tag	UNP P96253
C	-2	GLY	-	expression tag	UNP P96253
C	-1	SER	-	expression tag	UNP P96253
C	0	HIS	-	expression tag	UNP P96253

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Chain	Residue	Modelled	Actual	Comment	Reference
C	243	MSE	LEU	engineered mutation	UNP P96253
D	-19	MSE	-	expression tag	UNP P96253
D	-18	GLY	-	expression tag	UNP P96253
D	-17	SER	-	expression tag	UNP P96253
D	-16	SER	-	expression tag	UNP P96253
D	-15	HIS	-	expression tag	UNP P96253
D	-14	HIS	-	expression tag	UNP P96253
D	-13	HIS	-	expression tag	UNP P96253
D	-12	HIS	-	expression tag	UNP P96253
D	-11	HIS	-	expression tag	UNP P96253
D	-10	HIS	-	expression tag	UNP P96253
D	-9	SER	-	expression tag	UNP P96253
D	-8	SER	-	expression tag	UNP P96253
D	-7	GLY	-	expression tag	UNP P96253
D	-6	LEU	-	expression tag	UNP P96253
D	-5	VAL	-	expression tag	UNP P96253
D	-4	PRO	-	expression tag	UNP P96253
D	-3	ARG	-	expression tag	UNP P96253
D	-2	GLY	-	expression tag	UNP P96253
D	-1	SER	-	expression tag	UNP P96253
D	0	HIS	-	expression tag	UNP P96253
D	243	MSE	LEU	engineered mutation	UNP P96253

- Molecule 2 is water.

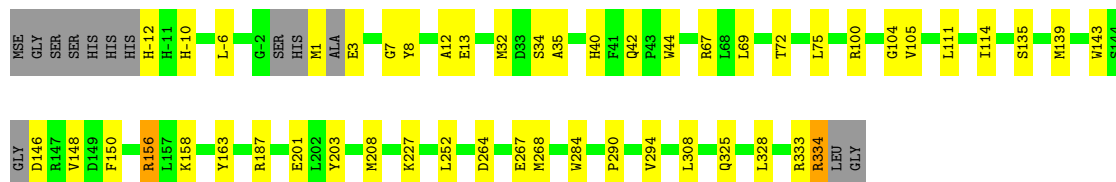
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	124	Total O 124 124	0	0
2	B	111	Total O 111 111	0	0
2	C	78	Total O 78 78	0	0
2	D	58	Total O 58 58	0	0

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.

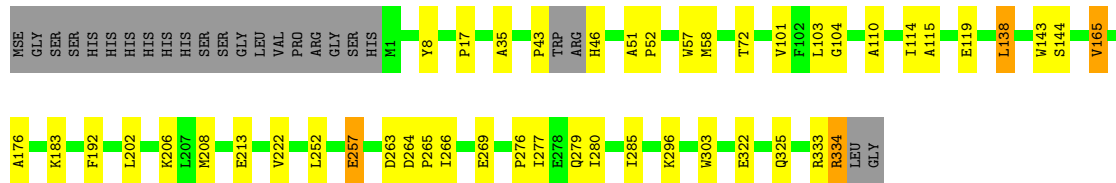
- Molecule 1: Probable F420-dependent glucose-6-phosphate dehydrogenase FGD1

Chain A: 



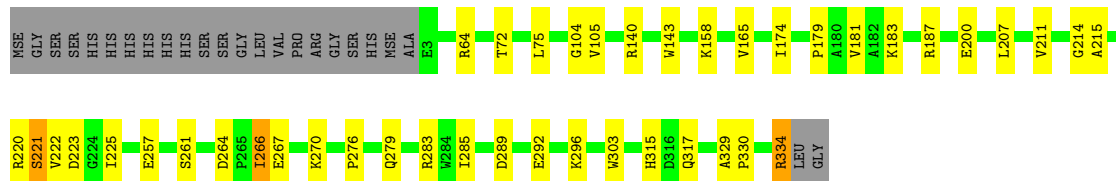
- Molecule 1: Probable F420-dependent glucose-6-phosphate dehydrogenase FGD1

Chain B: 



- Molecule 1: Probable F420-dependent glucose-6-phosphate dehydrogenase FGD1

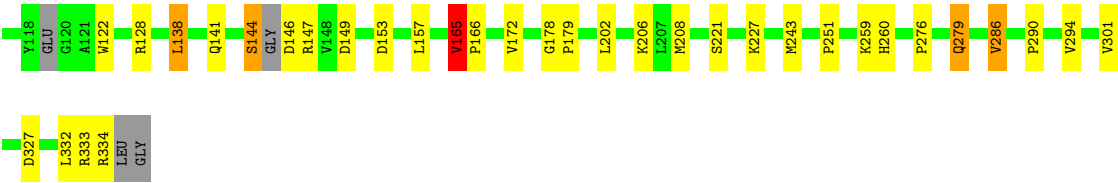
Chain C: 



- Molecule 1: Probable F420-dependent glucose-6-phosphate dehydrogenase FGD1

Chain D: 





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	80.95Å 89.13Å 90.86Å 90.00° 91.64° 90.00°	Depositor
Resolution (Å)	40.10 – 1.90 40.10 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.7 (40.10-1.90) 91.7 (40.10-1.90)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.74 (at 1.89Å)	Xtriage
Refinement program	REFMAC 5.3.0008	Depositor
R, R_{free}	0.212 , 0.255 (Not available) , 0.215	Depositor DCC
R_{free} test set	5067 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	28.3	Xtriage
Anisotropy	0.123	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 25.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.030 for -h,l,k 0.035 for -h,-l,-k 0.099 for h,-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	10741	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.58% 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](#)

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	1.01	1/2730 (0.0%)	1.05	2/3689 (0.1%)
1	B	1.01	3/2639 (0.1%)	1.08	2/3569 (0.1%)
1	C	0.89	1/2633 (0.0%)	1.06	3/3567 (0.1%)
1	D	0.85	3/2623 (0.1%)	1.02	3/3548 (0.1%)
All	All	0.94	8/10625 (0.1%)	1.05	10/14373 (0.1%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	165[A]	VAL	CA-CB	6.55	1.59	1.54
1	B	165[B]	VAL	CA-CB	6.55	1.59	1.54
1	A	114	ILE	CA-CB	6.10	1.61	1.54
1	C	165	VAL	CA-CB	5.66	1.61	1.54
1	B	57	TRP	C-O	-5.59	1.17	1.24
1	D	21	VAL	CA-CB	5.50	1.60	1.54
1	D	172	VAL	CA-CB	5.29	1.60	1.54
1	D	165	VAL	CA-CB	5.12	1.60	1.54

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	178	GLY	CA-C-N	6.60	126.84	119.32
1	D	178	GLY	C-N-CA	6.60	126.84	119.32
1	B	51	ALA	CA-C-N	-5.61	114.15	119.76
1	B	51	ALA	C-N-CA	-5.61	114.15	119.76
1	C	289	ASP	CA-C-N	5.55	125.38	119.28
1	C	289	ASP	C-N-CA	5.55	125.38	119.28
1	A	143	TRP	CA-C-N	-5.39	112.00	121.70
1	A	143	TRP	C-N-CA	-5.39	112.00	121.70
1	C	317	GLN	N-CA-C	5.38	117.90	111.71
1	D	25	VAL	N-CA-C	-5.08	105.59	110.72

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	2667	0	2582	35	0
1	B	2577	0	2507	35	0
1	C	2567	0	2470	26	0
1	D	2559	0	2477	30	0
2	A	124	0	0	4	0
2	B	111	0	0	10	0
2	C	78	0	0	4	0
2	D	58	0	0	5	0
All	All	10741	0	10036	119	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 6.

All (119) 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:A:150:PHE:O	1:A:156:ARG:HG3	1.51	1.09
1:D:55:LEU:HD13	2:D:378:HOH:O	1.68	0.90
1:B:285:ILE:HG23	1:B:296:LYS:HD3	1.54	0.89
1:B:144:SER:HB3	2:B:358:HOH:O	1.74	0.88
1:B:269:GLU:HB3	2:B:364:HOH:O	1.76	0.83
1:B:257:GLU:H	1:B:257:GLU:CD	1.89	0.79
1:D:144:SER:HB2	1:D:146:ASP:HB2	1.68	0.74
1:B:114:ILE:HD13	1:B:263:ASP:CB	2.18	0.74
1:B:266:ILE:HA	2:B:364:HOH:O	1.89	0.71
1:A:150:PHE:O	1:A:156:ARG:CG	2.37	0.70
1:A:69:LEU:HD12	1:A:100:ARG:O	1.91	0.70
1:B:103:LEU:HD22	2:B:434:HOH:O	1.93	0.69
1:C:264:ASP:HB3	1:C:267:GLU:HG2	1.73	0.69
1:B:114:ILE:HD13	1:B:263:ASP:HB3	1.74	0.68
1:D:128:ARG:HH12	1:D:260:HIS:HB3	1.58	0.68
1:C:200:GLU:HG3	1:C:303:TRP:CZ2	2.29	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:243:MSE:HE2	1:D:286:VAL:HG11	1.75	0.66
1:D:165:VAL:HG23	1:D:166:PRO:HD2	1.79	0.64
1:B:143:TRP:HZ2	2:B:434:HOH:O	1.81	0.64
1:B:183:LYS:HE3	1:B:213:GLU:HG2	1.80	0.63
1:D:333:ARG:O	1:D:334:ARG:HB2	2.00	0.62
1:B:17:PRO:HG3	1:B:52:PRO:HB3	1.81	0.61
1:B:119:GLU:O	2:B:427:HOH:O	2.15	0.61
1:D:141:GLN:O	1:D:144:SER:OG	2.19	0.61
1:A:111:LEU:HD22	1:A:268:MSE:HE3	1.83	0.61
1:C:72:THR:O	1:C:104:GLY:HA3	2.01	0.60
1:D:110:ALA:HB1	1:D:114:ILE:HD13	1.83	0.60
1:A:1:MSE:O	1:A:3:GLU:N	2.34	0.60
1:B:333:ARG:O	1:B:334:ARG:HB2	2.00	0.60
1:A:334:ARG:NH2	2:A:355:HOH:O	2.35	0.59
1:B:208:MSE:HG3	1:B:303:TRP:O	2.03	0.58
1:C:292:GLU:HG2	1:C:296:LYS:HE2	1.85	0.58
1:A:333:ARG:O	1:A:334:ARG:HB2	2.03	0.58
1:B:114:ILE:HD13	1:B:263:ASP:HB2	1.85	0.57
1:A:67:ARG:HD2	2:C:355:HOH:O	2.05	0.57
1:A:13:GLU:HG3	1:A:40[B]:HIS:CE1	2.41	0.56
1:B:138:LEU:C	1:B:138:LEU:HD23	2.31	0.56
1:B:202:LEU:HA	1:B:206:LYS:HD2	1.90	0.54
1:A:111:LEU:HD22	1:A:268:MSE:CE	2.38	0.54
1:D:3:GLU:N	2:D:369:HOH:O	2.40	0.54
1:A:69:LEU:HD12	1:A:100:ARG:C	2.33	0.54
1:A:208:MSE:HE1	1:A:227:LYS:CD	2.38	0.54
1:A:325:GLN:NE2	2:A:394:HOH:O	2.40	0.54
1:C:220:ARG:NH2	1:C:225:ILE:HG12	2.24	0.53
1:D:301:VAL:HG11	1:D:334:ARG:NH1	2.24	0.52
1:A:12:ALA:HB3	1:A:40[B]:HIS:CE1	2.45	0.52
1:B:192:PHE:CE2	1:B:208:MSE:HE1	2.44	0.52
1:B:322:GLU:CG	2:B:391:HOH:O	2.57	0.52
1:A:-10:HIS:NE2	1:C:315[A]:HIS:CD2	2.78	0.52
1:D:27:ALA:HB1	1:D:32:MSE:HG3	1.92	0.52
1:A:13:GLU:HG2	1:A:44:TRP:CD1	2.45	0.51
1:C:215:ALA:CB	1:C:222:VAL:HG13	2.40	0.51
1:A:-12:HIS:HB3	1:C:315[A]:HIS:CD2	2.46	0.51
1:D:276:PRO:HG2	1:D:279:GLN:HB2	1.93	0.51
1:D:103:LEU:HG	1:D:105:VAL:HG13	1.92	0.51
1:D:89:ALA:CB	2:D:378:HOH:O	2.59	0.50
1:D:40[B]:HIS:HE1	1:D:50:HIS:O	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:257:GLU:CD	1:B:257:GLU:N	2.62	0.50
1:A:284:TRP:O	2:A:437:HOH:O	2.19	0.49
1:C:257:GLU:O	1:C:261:SER:HB2	2.13	0.49
1:A:135:SER:O	1:A:139:MSE:HG3	2.13	0.49
1:C:276:PRO:HG2	1:C:279:GLN:HB2	1.95	0.49
1:C:221:SER:HB2	1:C:223:ASP:OD1	2.13	0.48
1:D:84:ALA:HB2	1:D:157:LEU:HD21	1.95	0.48
1:D:89:ALA:HB1	2:D:378:HOH:O	2.13	0.48
1:A:333:ARG:O	1:A:334:ARG:CB	2.61	0.48
1:C:75:LEU:O	1:C:105:VAL:HA	2.15	0.47
1:A:208:MSE:HE1	1:A:227:LYS:HD3	1.96	0.47
1:B:58:MSE:HE1	1:B:101:VAL:HG13	1.95	0.47
1:A:146:ASP:O	1:A:148:VAL:HG23	2.15	0.47
1:D:179:PRO:HG3	1:D:206:LYS:HB3	1.97	0.47
1:A:290:PRO:O	1:A:294:VAL:HG23	2.15	0.47
1:C:207:LEU:O	1:C:211:VAL:HG23	2.15	0.46
1:C:329:ALA:N	1:C:330:PRO:HD2	2.29	0.46
1:D:83:PRO:HB2	1:D:138:LEU:HD22	1.97	0.46
1:B:176:ALA:HB3	1:B:192:PHE:HE1	1.81	0.46
1:A:12:ALA:HB3	1:A:40[B]:HIS:HE1	1.80	0.46
1:A:75:LEU:O	1:A:105:VAL:HA	2.16	0.46
1:D:67:ARG:NH1	2:D:355:HOH:O	2.49	0.46
1:B:285:ILE:CG2	1:B:296:LYS:HD3	2.37	0.46
1:C:334:ARG:NE	1:C:334:ARG:HA	2.31	0.46
1:B:143:TRP:O	1:B:165[A]:VAL:HG21	2.16	0.46
1:D:138:LEU:C	1:D:138:LEU:HD23	2.41	0.46
1:D:202:LEU:HD12	1:D:206:LYS:HD2	1.97	0.46
1:B:322:GLU:HG3	2:B:391:HOH:O	2.16	0.45
1:B:325:GLN:NE2	2:B:362:HOH:O	2.48	0.45
1:C:266:ILE:HG22	1:C:270:LYS:HE3	1.98	0.45
1:A:8:TYR:O	1:A:35:ALA:HA	2.17	0.45
1:C:183:LYS:O	1:C:187:ARG:HG3	2.17	0.44
1:B:72:THR:O	1:B:104:GLY:HA3	2.18	0.44
1:C:187:ARG:HG2	1:C:214:GLY:O	2.17	0.44
1:C:285:ILE:HG23	1:C:296:LYS:HE3	1.99	0.44
1:C:140:ARG:HD3	2:C:366:HOH:O	2.16	0.44
1:C:179:PRO:HD2	2:C:344:HOH:O	2.18	0.44
1:C:181:VAL:HG23	2:C:399:HOH:O	2.16	0.44
1:A:163:TYR:CE2	1:B:43:PRO:HD2	2.53	0.43
1:B:276:PRO:HG2	1:B:279:GLN:CG	2.47	0.43
1:B:277:ILE:HA	1:B:280:ILE:HD12	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:-12:HIS:CE1	1:C:315[B]:HIS:CD2	3.07	0.43
1:D:208:MSE:HE1	1:D:227:LYS:HD3	2.00	0.42
1:D:122:TRP:CZ2	1:D:128:ARG:HD3	2.54	0.42
1:A:7:GLY:HA3	1:A:34:SER:OG	2.20	0.42
1:B:110:ALA:HB1	1:B:114:ILE:HD12	2.02	0.42
1:C:158:LYS:O	1:D:115:ALA:HA	2.20	0.41
1:C:140:ARG:HG2	1:C:143:TRP:CE3	2.56	0.41
1:D:290:PRO:HB3	1:D:327:ASP:HB3	2.02	0.41
1:C:64:ARG:HG2	1:D:63:GLU:HG3	2.02	0.41
1:A:203:TYR:O	1:A:208:MSE:HG2	2.20	0.41
1:A:264:ASP:HB3	1:A:267:GLU:HB3	2.02	0.41
1:B:264:ASP:HA	1:B:265:PRO:HD3	1.80	0.41
1:A:8:TYR:HB2	1:A:32:MSE:HG3	2.02	0.41
1:B:8:TYR:O	1:B:35:ALA:HA	2.21	0.41
1:D:294:VAL:HG22	1:D:332:LEU:HG	2.02	0.41
1:A:42:GLN:OE1	2:A:377:HOH:O	2.22	0.41
1:B:322:GLU:HG2	2:B:391:HOH:O	2.20	0.41
1:A:72:THR:O	1:A:104:GLY:HA3	2.21	0.41
1:D:75:LEU:O	1:D:105:VAL:HA	2.21	0.40
1:A:158:LYS:O	1:B:115:ALA:HA	2.21	0.40
1:D:251:PRO:O	1:D:259:LYS:HD2	2.22	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	337/356 (95%)	329 (98%)	8 (2%)	0	100	100
1	B	330/356 (93%)	324 (98%)	6 (2%)	0	100	100
1	C	332/356 (93%)	323 (97%)	9 (3%)	0	100	100
1	D	326/356 (92%)	320 (98%)	6 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1325/1424 (93%)	1296 (98%)	29 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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	268/270 (99%)	260 (97%)	8 (3%)	36	30
1	B	260/270 (96%)	254 (98%)	6 (2%)	44	40
1	C	255/270 (94%)	250 (98%)	5 (2%)	48	46
1	D	255/270 (94%)	244 (96%)	11 (4%)	26	18
All	All	1038/1080 (96%)	1008 (97%)	30 (3%)	37	31

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-6	LEU
1	A	156	ARG
1	A	187	ARG
1	A	201	GLU
1	A	252	LEU
1	A	308	LEU
1	A	328	LEU
1	A	334	ARG
1	B	46	HIS
1	B	138	LEU
1	B	222	VAL
1	B	252	LEU
1	B	257	GLU
1	B	334	ARG
1	C	174	ILE
1	C	221	SER
1	C	266	ILE

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Mol	Chain	Res	Type
1	C	283	ARG
1	C	334	ARG
1	D	38	SER
1	D	74	VAL
1	D	138	LEU
1	D	144	SER
1	D	147	ARG
1	D	149	ASP
1	D	153	ASP
1	D	165	VAL
1	D	221	SER
1	D	279	GLN
1	D	286	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	-12	HIS
1	A	299	GLN
1	D	279	GLN
1	D	299	GLN

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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

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	334/356 (93%)	-1.03	0 100 100	11, 23, 35, 43	1 (0%)
1	B	323/356 (90%)	-1.05	0 100 100	12, 23, 37, 48	2 (0%)
1	C	324/356 (91%)	-0.96	0 100 100	15, 26, 39, 45	2 (0%)
1	D	322/356 (90%)	-0.93	0 100 100	14, 28, 37, 42	2 (0%)
All	All	1303/1424 (91%)	-0.99	0 100 100	11, 25, 37, 48	7 (0%)

There are no RSRZ outliers to report.

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 oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.