



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:49 AM UTC

PDB ID : 3HLI / pdb_00003hli
Title : diisopropyl fluorophosphatase (DFPase), active site mutants
Authors : Chen, J.C.-H.; Blum, M.-M.
Deposited on : 2009-05-27
Resolution : 1.40 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
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

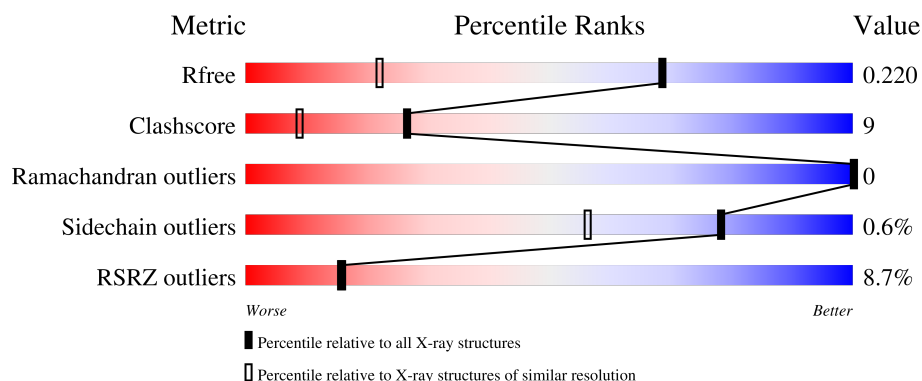
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.40 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	2563 (1.40-1.40)
Clashscore	190562	2660 (1.40-1.40)
Ramachandran outliers	187476	2611 (1.40-1.40)
Sidechain outliers	187428	2610 (1.40-1.40)
RSRZ outliers	180081	2561 (1.40-1.40)

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	314	6% 80% 18% .
1	B	314	10% 78% 21% ..
1	C	314	7% 82% 16% ..
1	D	314	11% 79% 19% ..

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10803 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 Diisopropyl-fluorophosphatase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	313	Total	C	N	O	S	0	0	0
			2443	1551	414	462	16			
1	B	312	Total	C	N	O	S	0	0	0
			2438	1548	413	461	16			
1	C	312	Total	C	N	O	S	0	0	0
			2438	1548	413	461	16			
1	D	312	Total	C	N	O	S	0	0	0
			2438	1548	413	461	16			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	37	ASP	GLU	engineered mutation	UNP Q7SIG4
A	144	ALA	TYR	engineered mutation	UNP Q7SIG4
A	146	ALA	ARG	engineered mutation	UNP Q7SIG4
A	195	MET	THR	engineered mutation	UNP Q7SIG4
B	37	ASP	GLU	engineered mutation	UNP Q7SIG4
B	144	ALA	TYR	engineered mutation	UNP Q7SIG4
B	146	ALA	ARG	engineered mutation	UNP Q7SIG4
B	195	MET	THR	engineered mutation	UNP Q7SIG4
C	37	ASP	GLU	engineered mutation	UNP Q7SIG4
C	144	ALA	TYR	engineered mutation	UNP Q7SIG4
C	146	ALA	ARG	engineered mutation	UNP Q7SIG4
C	195	MET	THR	engineered mutation	UNP Q7SIG4
D	37	ASP	GLU	engineered mutation	UNP Q7SIG4
D	144	ALA	TYR	engineered mutation	UNP Q7SIG4
D	146	ALA	ARG	engineered mutation	UNP Q7SIG4
D	195	MET	THR	engineered mutation	UNP Q7SIG4

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total 2	Ca 2	0	0
2	B	2	Total 2	Ca 2	0	0
2	C	2	Total 2	Ca 2	0	0
2	D	2	Total 2	Ca 2	0	0

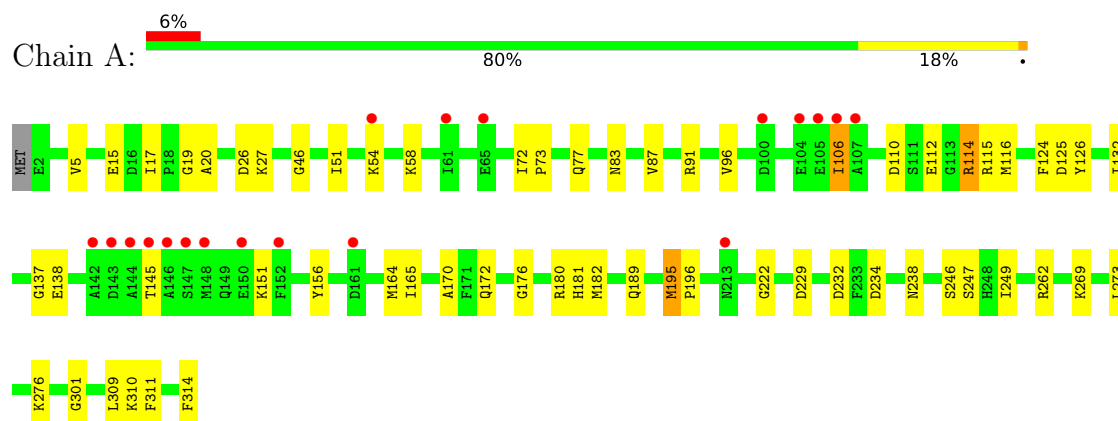
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	250	Total 250	O 250	0	0
3	B	273	Total 273	O 273	0	0
3	C	270	Total 270	O 270	0	0
3	D	245	Total 245	O 245	0	0

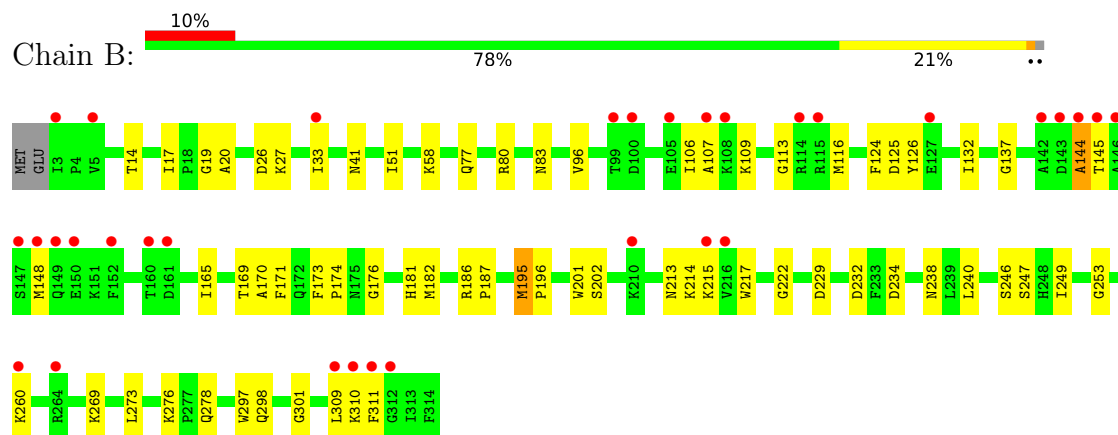
3 Residue-property plots [i](#)

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.

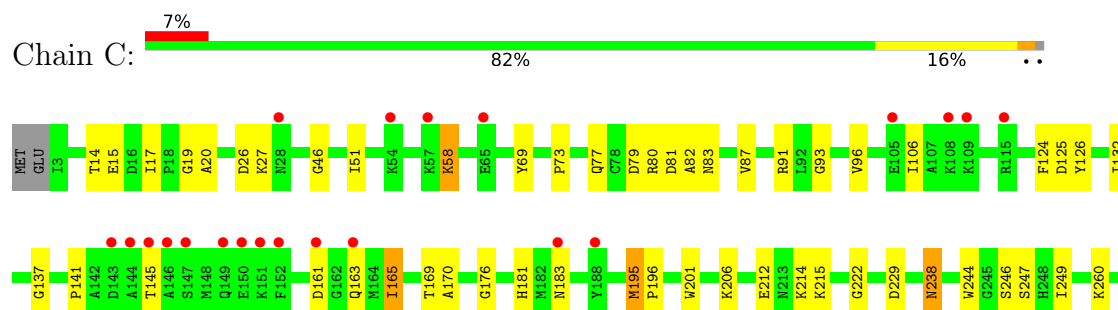
• Molecule 1: Diisopropyl-fluorophosphatase

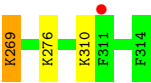


• Molecule 1: Diisopropyl-fluorophosphatase

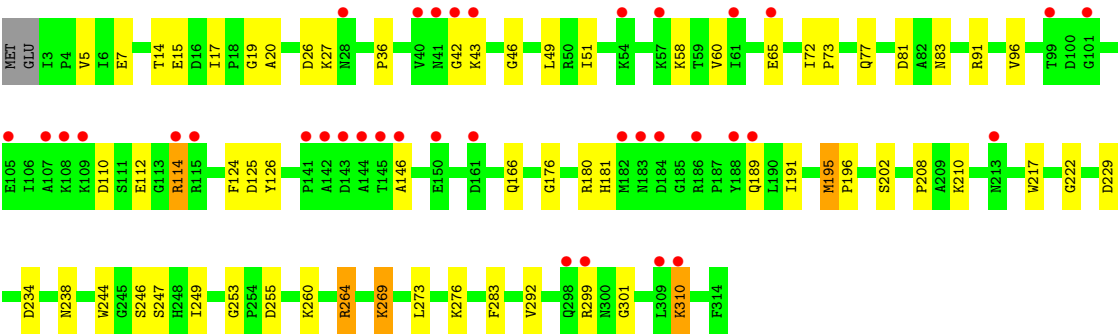
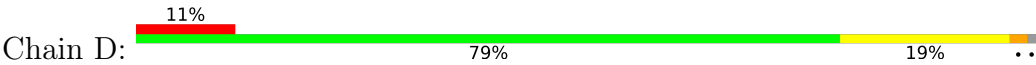


• Molecule 1: Diisopropyl-fluorophosphatase





● Molecule 1: Diisopropyl-fluorophosphatase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	66.95Å 74.49Å 118.95Å 90.00° 100.00° 90.00°	Depositor
Resolution (Å)	24.82 – 1.40 24.82 – 1.40	Depositor EDS
% Data completeness (in resolution range)	94.5 (24.82-1.40) 94.4 (24.82-1.40)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.85 (at 1.40Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.205 , 0.221 0.203 , 0.220	Depositor DCC
R_{free} test set	10622 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	8.9	Xtriage
Anisotropy	0.178	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.42 , 42.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	10803	wwPDB-VP
Average B, all atoms (Å ²)	12.0	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 22.49 % 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 5.6378e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

5.1 Standard geometry

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

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	0.31	0/2505	0.92	12/3390 (0.4%)
1	B	0.31	0/2500	0.93	11/3383 (0.3%)
1	C	0.30	0/2500	0.92	10/3383 (0.3%)
1	D	0.31	0/2500	0.92	7/3383 (0.2%)
All	All	0.31	0/10005	0.92	40/13539 (0.3%)

There are no bond length outliers.

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	276	LYS	N-CA-C	-6.97	100.86	109.65
1	C	222	GLY	N-CA-C	6.95	120.07	112.29
1	B	276	LYS	N-CA-C	-6.68	101.37	109.72
1	A	269	LYS	N-CA-C	6.63	121.03	108.97
1	C	276	LYS	N-CA-C	-6.62	101.44	109.72
1	B	269	LYS	N-CA-C	6.61	121.00	108.97
1	C	269	LYS	N-CA-C	6.51	120.82	108.97
1	D	249	ILE	N-CA-C	-6.50	99.07	108.17
1	D	269	LYS	N-CA-C	6.30	121.24	110.02
1	D	276	LYS	N-CA-C	-6.30	101.85	109.72
1	A	238	ASN	N-CA-C	-6.20	100.40	110.20
1	D	222	GLY	N-CA-C	6.18	120.47	112.68
1	B	238	ASN	N-CA-C	-6.04	100.66	110.20
1	C	238	ASN	N-CA-C	-6.01	100.70	110.20
1	B	125	ASP	N-CA-C	-5.92	101.70	110.46
1	D	238	ASN	N-CA-C	-5.84	100.14	109.96
1	D	195	MET	N-CA-C	5.84	122.71	109.81
1	A	195	MET	N-CA-C	5.79	122.61	109.81
1	A	222	GLY	N-CA-C	5.79	119.94	112.18
1	B	182	MET	N-CA-C	-5.62	103.28	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	249	ILE	N-CA-C	-5.62	99.66	107.80
1	C	195	MET	N-CA-C	5.58	122.15	109.81
1	A	249	ILE	N-CA-C	-5.56	99.74	107.80
1	A	132	ILE	N-CA-C	5.48	116.63	108.46
1	C	249	ILE	N-CA-C	-5.45	99.89	107.80
1	A	125	ASP	N-CA-C	-5.44	102.70	110.59
1	A	182	MET	N-CA-C	-5.44	103.52	110.53
1	B	132	ILE	N-CA-C	5.38	116.47	108.46
1	B	165	ILE	N-CA-C	5.37	115.69	108.17
1	D	125	ASP	N-CA-C	-5.36	102.53	110.46
1	B	195	MET	N-CA-C	5.33	121.59	109.81
1	B	222	GLY	N-CA-C	5.33	119.39	112.68
1	A	106	ILE	N-CA-C	5.23	116.00	110.72
1	C	132	ILE	N-CA-C	5.19	116.20	108.46
1	B	144	ALA	N-CA-C	5.18	117.02	110.33
1	A	165	ILE	N-CA-C	5.18	115.76	108.36
1	A	87	VAL	N-CA-C	5.16	115.28	107.75
1	C	165	ILE	N-CA-C	5.12	115.34	108.17
1	C	125	ASP	N-CA-C	-5.03	103.29	110.59
1	C	87	VAL	N-CA-C	5.02	115.14	108.11

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	2443	0	2362	45	0
1	B	2438	0	2360	53	0
1	C	2438	0	2360	38	0
1	D	2438	0	2360	53	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
3	A	250	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	273	0	0	3	0
3	C	270	0	0	5	0
3	D	245	0	0	3	0
All	All	10803	0	9442	179	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 9.

All (179) 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:D:264:ARG:HB2	1:D:264:ARG:HH11	1.33	0.93
1:A:17:ILE:HD11	1:A:58:LYS:HD2	1.56	0.86
1:A:26:ASP:HB2	1:A:83:ASN:HD21	1.42	0.84
1:B:17:ILE:HD13	1:B:33:ILE:HD12	1.60	0.82
1:D:126:TYR:H	1:D:181:HIS:CE1	1.99	0.80
1:A:126:TYR:H	1:A:181:HIS:CE1	2.01	0.78
1:D:126:TYR:H	1:D:181:HIS:HE1	1.30	0.78
1:B:126:TYR:H	1:B:181:HIS:CE1	2.02	0.78
1:C:126:TYR:H	1:C:181:HIS:CE1	2.01	0.77
1:D:5:VAL:HG11	1:D:264:ARG:HH12	1.49	0.77
1:B:41:ASN:HD21	1:D:7:GLU:H	1.34	0.76
1:A:180:ARG:HE	1:A:189:GLN:NE2	1.82	0.76
1:C:77:GLN:HE21	1:C:124:PHE:H	1.33	0.76
1:C:126:TYR:H	1:C:181:HIS:HE1	1.33	0.75
1:A:77:GLN:HE21	1:A:124:PHE:H	1.33	0.75
1:A:310:LYS:NZ	1:B:144:ALA:HB3	2.03	0.74
1:D:26:ASP:HB2	1:D:83:ASN:HD21	1.53	0.74
1:B:17:ILE:HD13	1:B:33:ILE:CD1	2.17	0.74
1:B:26:ASP:HB2	1:B:83:ASN:HD21	1.54	0.72
1:A:17:ILE:HD11	1:A:58:LYS:CD	2.20	0.71
1:C:96:VAL:CG2	1:C:106:ILE:HD11	2.22	0.70
1:B:126:TYR:H	1:B:181:HIS:HE1	1.39	0.70
1:A:126:TYR:H	1:A:181:HIS:HE1	1.38	0.69
1:D:77:GLN:HE21	1:D:124:PHE:H	1.40	0.69
1:C:26:ASP:HB2	1:C:83:ASN:HD21	1.57	0.68
1:B:77:GLN:HE21	1:B:124:PHE:H	1.42	0.67
1:C:96:VAL:HG21	1:C:106:ILE:HD11	1.76	0.67
1:B:310:LYS:HZ2	1:B:311:PHE:HE2	1.41	0.66
1:D:112:GLU:HB2	1:D:114:ARG:HD2	1.79	0.64
1:D:43:LYS:N	1:D:43:LYS:HD2	2.13	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:17:ILE:CD1	1:A:58:LYS:HD2	2.25	0.63
1:D:264:ARG:HB2	1:D:264:ARG:NH1	2.09	0.62
1:B:96:VAL:CG2	1:B:106:ILE:HD11	2.31	0.61
1:B:41:ASN:ND2	1:D:7:GLU:H	1.97	0.61
1:A:116:MET:HE1	1:A:164:MET:SD	2.41	0.59
1:B:253:GLY:CA	1:B:260:LYS:HE3	2.32	0.59
1:B:311:PHE:CE1	1:C:91:ARG:HD3	2.37	0.59
1:A:112:GLU:HB2	1:A:114:ARG:HD2	1.85	0.58
1:A:151:LYS:HE3	1:A:172:GLN:OE1	2.04	0.58
1:A:110:ASP:OD2	1:A:114:ARG:HD3	2.04	0.58
1:B:96:VAL:HG23	1:B:106:ILE:HD11	1.87	0.57
1:C:15:GLU:C	1:C:17:ILE:HD12	2.30	0.57
1:A:151:LYS:N	1:A:151:LYS:HD2	2.19	0.57
1:A:54:LYS:NZ	1:D:180:ARG:HH22	2.03	0.56
1:D:202:SER:HB3	1:D:217:TRP:HB2	1.87	0.56
1:B:27:LYS:H	1:B:83:ASN:ND2	2.03	0.56
1:D:5:VAL:HG11	1:D:264:ARG:NH1	2.19	0.56
1:C:51:ILE:HD12	1:C:58:LYS:HG2	1.86	0.56
1:C:80:ARG:NH2	1:C:310:LYS:HG3	2.20	0.56
1:A:96:VAL:CG2	1:A:106:ILE:HD11	2.36	0.56
1:B:51:ILE:HD12	1:B:58:LYS:HG2	1.88	0.55
1:C:81:ASP:OD1	1:C:310:LYS:HD2	2.07	0.54
1:D:15:GLU:C	1:D:17:ILE:HD12	2.33	0.54
1:B:201:TRP:CE3	1:B:214:LYS:HE2	2.43	0.53
1:A:15:GLU:HB2	3:A:803:HOH:O	2.07	0.53
1:C:58:LYS:HB2	1:C:58:LYS:NZ	2.24	0.53
1:A:54:LYS:HZ1	1:D:180:ARG:HH22	1.57	0.53
1:C:163:GLN:HE21	1:C:165:ILE:HD11	1.73	0.53
1:D:27:LYS:H	1:D:83:ASN:ND2	2.05	0.53
1:C:93:GLY:HA3	3:C:779:HOH:O	2.09	0.52
1:B:202:SER:HB3	1:B:217:TRP:HB2	1.92	0.52
1:C:215:LYS:HG2	3:C:340:HOH:O	2.09	0.52
1:C:201:TRP:CE3	1:C:214:LYS:HE2	2.45	0.52
1:A:26:ASP:HB2	1:A:83:ASN:ND2	2.20	0.52
1:C:96:VAL:HG23	1:C:106:ILE:HD11	1.91	0.52
1:B:213:ASN:OD1	1:B:215:LYS:HE3	2.10	0.51
1:A:5:VAL:HG22	1:A:262:ARG:HB2	1.91	0.51
1:C:51:ILE:CD1	1:C:58:LYS:HG2	2.40	0.51
1:A:96:VAL:HG21	1:A:106:ILE:HD11	1.94	0.50
1:B:27:LYS:H	1:B:83:ASN:HD21	1.60	0.50
1:D:114:ARG:NH1	1:D:166:GLN:OE1	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:189:GLN:HE21	1:D:191:ILE:HD11	1.77	0.49
1:A:180:ARG:HE	1:A:189:GLN:HE21	1.59	0.49
1:C:246:SER:O	1:C:247:SER:HB2	2.13	0.49
1:D:72:ILE:HD12	1:D:91:ARG:HG2	1.93	0.49
1:B:33:ILE:HD11	1:B:51:ILE:HD11	1.93	0.49
1:A:51:ILE:HD12	1:A:58:LYS:HG2	1.94	0.49
1:B:144:ALA:HA	3:B:504:HOH:O	2.12	0.49
1:C:215:LYS:HE2	3:C:340:HOH:O	2.11	0.49
1:B:310:LYS:NZ	1:B:311:PHE:HE2	2.09	0.49
1:B:253:GLY:HA3	1:B:260:LYS:HE3	1.94	0.48
1:D:27:LYS:H	1:D:83:ASN:HD21	1.61	0.48
1:A:46:GLY:HA3	1:A:73:PRO:HD2	1.95	0.48
1:C:27:LYS:H	1:C:83:ASN:ND2	2.11	0.48
1:A:54:LYS:HD3	1:D:255:ASP:OD2	2.14	0.48
1:B:26:ASP:HB2	1:B:83:ASN:ND2	2.27	0.48
1:D:42:GLY:C	1:D:43:LYS:HD2	2.39	0.48
1:D:180:ARG:HB3	1:D:189:GLN:HG2	1.95	0.48
1:C:137:GLY:HA3	1:C:145:THR:HG23	1.96	0.48
1:A:309:LEU:HA	3:A:678:HOH:O	2.14	0.47
1:B:148:MET:HG2	1:B:173:PHE:CD2	2.49	0.47
1:D:110:ASP:OD2	1:D:114:ARG:HD3	2.15	0.47
1:A:246:SER:O	1:A:247:SER:HB2	2.15	0.47
1:D:310:LYS:H	1:D:310:LYS:HG2	1.52	0.47
1:B:51:ILE:CD1	1:B:58:LYS:HG2	2.44	0.46
1:B:309:LEU:HB3	3:B:366:HOH:O	2.15	0.46
1:B:246:SER:O	1:B:247:SER:HB2	2.15	0.46
1:D:26:ASP:HB2	1:D:83:ASN:ND2	2.27	0.46
1:A:116:MET:HE3	1:A:156:TYR:CE1	2.50	0.46
1:D:181:HIS:HD2	3:D:349:HOH:O	1.99	0.46
1:A:311:PHE:HE1	1:B:144:ALA:CB	2.29	0.46
1:A:19:GLY:O	1:A:20:ALA:C	2.59	0.45
1:D:19:GLY:O	1:D:20:ALA:C	2.59	0.45
1:B:19:GLY:O	1:B:20:ALA:C	2.60	0.45
1:C:161:ASP:OD2	1:C:163:GLN:HG3	2.16	0.45
1:D:246:SER:O	1:D:247:SER:HB2	2.16	0.45
1:D:51:ILE:HD12	1:D:58:LYS:HG2	1.97	0.45
1:D:234:ASP:HA	1:D:301:GLY:HA2	1.98	0.45
1:C:69:TYR:CE2	1:C:141:PRO:HB3	2.52	0.45
1:D:180:ARG:HD2	3:D:716:HOH:O	2.17	0.45
1:B:169:THR:O	1:B:170:ALA:HB3	2.16	0.45
1:B:176:GLY:HA3	1:B:229:ASP:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:19:GLY:O	1:C:20:ALA:C	2.59	0.45
1:D:46:GLY:HA3	1:D:73:PRO:HD2	2.00	0.44
1:D:112:GLU:CB	1:D:114:ARG:HD2	2.47	0.44
1:B:14:THR:HG23	1:B:17:ILE:HD11	2.00	0.44
1:B:273:LEU:HD12	1:B:273:LEU:C	2.43	0.44
1:A:176:GLY:HA3	1:A:229:ASP:O	2.17	0.44
1:C:238:ASN:HD21	1:C:260:LYS:NZ	2.15	0.44
1:D:14:THR:HG23	1:D:17:ILE:HD11	2.00	0.44
1:C:79:ASP:HB3	1:C:82:ALA:O	2.18	0.44
1:B:234:ASP:HA	1:B:301:GLY:HA2	1.99	0.44
1:D:195:MET:HB3	1:D:196:PRO:CD	2.48	0.44
1:A:151:LYS:O	1:A:170:ALA:HA	2.18	0.43
1:B:96:VAL:HG21	1:B:106:ILE:HD11	2.00	0.43
1:C:195:MET:HB3	1:C:196:PRO:CD	2.48	0.43
1:A:72:ILE:HD12	1:A:91:ARG:HG2	1.99	0.43
1:B:171:PHE:HB3	1:B:174:PRO:HD3	1.99	0.43
1:D:176:GLY:HA3	1:D:229:ASP:O	2.17	0.43
1:B:240:LEU:HD12	1:B:240:LEU:N	2.33	0.43
1:A:27:LYS:H	1:A:83:ASN:ND2	2.16	0.43
1:B:297:TRP:CG	1:B:298:GLN:N	2.87	0.43
1:C:181:HIS:HD2	3:C:338:HOH:O	2.02	0.43
1:C:244:TRP:CZ2	1:C:269:LYS:HD3	2.54	0.43
1:A:96:VAL:HG23	1:A:106:ILE:HD11	2.00	0.43
1:A:314:PHE:HA	3:A:1055:HOH:O	2.19	0.42
1:A:310:LYS:HZ1	1:B:144:ALA:HB3	1.80	0.42
1:C:46:GLY:HA3	1:C:73:PRO:HD2	2.01	0.42
1:D:244:TRP:CH2	1:D:269:LYS:HE3	2.54	0.42
1:D:253:GLY:CA	1:D:260:LYS:HE3	2.50	0.42
1:C:15:GLU:HB2	3:C:376:HOH:O	2.19	0.42
1:A:195:MET:HB3	1:A:196:PRO:CD	2.50	0.42
1:A:310:LYS:HZ2	1:B:144:ALA:HB3	1.79	0.42
1:B:201:TRP:CZ3	1:B:214:LYS:HE2	2.55	0.42
1:D:81:ASP:OD1	1:D:310:LYS:HD2	2.19	0.42
1:D:299:ARG:HG2	1:D:299:ARG:HH11	1.84	0.42
1:A:234:ASP:HA	1:A:301:GLY:HA2	2.02	0.42
1:B:181:HIS:HD2	3:B:392:HOH:O	2.03	0.42
1:C:14:THR:HG23	1:C:17:ILE:HD11	2.02	0.42
1:D:49:LEU:CD2	1:D:60:VAL:HG22	2.50	0.42
1:D:180:ARG:HB3	1:D:189:GLN:CG	2.50	0.42
1:C:169:THR:O	1:C:170:ALA:HB3	2.20	0.42
1:D:65:GLU:CD	1:D:65:GLU:C	2.88	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:208:PRO:O	1:D:210:LYS:HG3	2.20	0.42
1:B:137:GLY:HA3	1:B:145:THR:HG22	2.01	0.41
1:B:186:ARG:HA	1:B:187:PRO:HD3	1.97	0.41
1:D:43:LYS:N	1:D:43:LYS:CD	2.83	0.41
1:C:206:LYS:HE3	1:C:212:GLU:OE1	2.19	0.41
1:D:96:VAL:O	1:D:96:VAL:HG13	2.20	0.41
1:A:115:ARG:HE	1:A:138:GLU:CD	2.27	0.41
1:A:181:HIS:HD2	3:A:348:HOH:O	2.02	0.41
1:B:195:MET:HB3	1:B:196:PRO:CD	2.50	0.41
1:C:176:GLY:HA3	1:C:229:ASP:O	2.20	0.41
1:B:297:TRP:CG	1:B:298:GLN:H	2.38	0.41
1:C:201:TRP:CZ3	1:C:214:LYS:HE2	2.56	0.41
1:A:273:LEU:C	1:A:273:LEU:HD12	2.46	0.41
1:B:107:ALA:O	1:B:116:MET:HG3	2.21	0.41
1:B:278:GLN:HE21	1:B:278:GLN:HA	1.86	0.41
1:B:80:ARG:CZ	1:B:310:LYS:HB3	2.51	0.40
1:B:109:LYS:HD3	1:B:113:GLY:O	2.21	0.40
1:C:77:GLN:NE2	1:C:124:PHE:H	2.11	0.40
1:D:36:PRO:HB3	1:D:73:PRO:O	2.21	0.40
1:A:137:GLY:HA3	1:A:145:THR:CG2	2.52	0.40
1:A:232:ASP:HB2	1:A:273:LEU:CD1	2.51	0.40
1:D:110:ASP:OD1	1:D:114:ARG:HD3	2.21	0.40
1:D:146:ALA:HB3	3:D:1025:HOH:O	2.21	0.40
1:D:273:LEU:HA	1:D:283:PHE:O	2.22	0.40
1:B:232:ASP:HB2	1:B:273:LEU:HD11	2.03	0.40
1:D:14:THR:HG22	1:D:292:VAL:HB	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	311/314 (99%)	301 (97%)	10 (3%)	0	100	100
1	B	310/314 (99%)	297 (96%)	13 (4%)	0	100	100
1	C	310/314 (99%)	299 (96%)	11 (4%)	0	100	100
1	D	310/314 (99%)	298 (96%)	12 (4%)	0	100	100
All	All	1241/1256 (99%)	1195 (96%)	46 (4%)	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	259/261 (99%)	258 (100%)	1 (0%)	84	67
1	B	259/261 (99%)	259 (100%)	0	100	100
1	C	259/261 (99%)	257 (99%)	2 (1%)	73	48
1	D	259/261 (99%)	256 (99%)	3 (1%)	63	34
All	All	1036/1044 (99%)	1030 (99%)	6 (1%)	78	56

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	114	ARG
1	C	58	LYS
1	C	183	ASN
1	D	114	ARG
1	D	264	ARG
1	D	310	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	77	GLN

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Mol	Chain	Res	Type
1	A	83	ASN
1	A	181	HIS
1	A	189	GLN
1	A	237	ASN
1	A	238	ASN
1	A	243	ASN
1	A	258	GLN
1	A	278	GLN
1	A	304	GLN
1	B	41	ASN
1	B	77	GLN
1	B	83	ASN
1	B	181	HIS
1	B	238	ASN
1	B	243	ASN
1	B	258	GLN
1	B	278	GLN
1	B	300	ASN
1	B	304	GLN
1	C	77	GLN
1	C	83	ASN
1	C	163	GLN
1	C	181	HIS
1	C	238	ASN
1	C	243	ASN
1	C	258	GLN
1	C	298	GLN
1	C	304	GLN
1	D	41	ASN
1	D	77	GLN
1	D	83	ASN
1	D	163	GLN
1	D	181	HIS
1	D	189	GLN
1	D	238	ASN
1	D	243	ASN
1	D	258	GLN
1	D	278	GLN
1	D	304	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 8 are monoatomic - leaving 0 for Mogul analysis.

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	313/314 (99%)	0.36	19 (6%) 27 28	4, 10, 21, 32	0
1	B	312/314 (99%)	0.53	32 (10%) 12 11	4, 10, 22, 33	0
1	C	312/314 (99%)	0.34	22 (7%) 22 23	4, 9, 20, 30	0
1	D	312/314 (99%)	0.44	36 (11%) 9 10	4, 9, 21, 30	0
All	All	1249/1256 (99%)	0.42	109 (8%) 16 16	4, 10, 21, 33	0

All (109) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	146	ALA	9.2
1	B	144	ALA	9.0
1	C	144	ALA	8.0
1	B	143	ASP	6.2
1	B	145	THR	5.9
1	B	147	SER	5.6
1	B	152	PHE	5.5
1	B	148	MET	5.3
1	D	144	ALA	5.2
1	C	146	ALA	5.1
1	A	146	ALA	4.8
1	B	310	LYS	4.5
1	A	145	THR	4.3
1	B	311	PHE	4.3
1	A	144	ALA	4.2
1	D	298	GLN	4.1
1	D	41	ASN	4.1
1	D	40	VAL	4.1
1	A	143	ASP	4.0
1	C	150	GLU	4.0
1	C	145	THR	3.9

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Mol	Chain	Res	Type	RSRZ
1	B	161	ASP	3.9
1	C	161	ASP	3.8
1	C	54	LYS	3.8
1	C	183	ASN	3.7
1	A	152	PHE	3.7
1	B	150	GLU	3.7
1	B	115	ARG	3.5
1	D	186	ARG	3.5
1	D	57	LYS	3.4
1	B	260	LYS	3.3
1	C	143	ASP	3.3
1	B	142	ALA	3.3
1	B	149	GLN	3.2
1	D	188	TYR	3.2
1	B	107	ALA	3.1
1	B	309	LEU	3.1
1	C	57	LYS	3.0
1	D	54	LYS	3.0
1	D	65	GLU	3.0
1	A	54	LYS	3.0
1	C	163	GLN	2.9
1	C	147	SER	2.9
1	A	142	ALA	2.9
1	A	148	MET	2.9
1	D	105	GLU	2.9
1	D	183	ASN	2.9
1	D	146	ALA	2.8
1	B	3	ILE	2.8
1	A	105	GLU	2.8
1	C	65	GLU	2.8
1	D	115	ARG	2.8
1	B	100	ASP	2.7
1	D	161	ASP	2.7
1	D	61	ILE	2.7
1	A	100	ASP	2.7
1	B	105	GLU	2.7
1	D	213	ASN	2.7
1	B	33	ILE	2.7
1	A	161	ASP	2.6
1	D	182	MET	2.6
1	D	107	ALA	2.6
1	C	108	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	114	ARG	2.6
1	C	311	PHE	2.5
1	D	43	LYS	2.5
1	C	149	GLN	2.5
1	D	189	GLN	2.5
1	D	28	ASN	2.5
1	D	142	ALA	2.5
1	D	143	ASP	2.5
1	A	147	SER	2.5
1	B	108	LYS	2.5
1	D	145	THR	2.5
1	A	107	ALA	2.4
1	D	150	GLU	2.4
1	A	150	GLU	2.4
1	C	152	PHE	2.4
1	C	109	LYS	2.4
1	D	101	GLY	2.4
1	A	213	ASN	2.4
1	A	65	GLU	2.4
1	D	114	ARG	2.3
1	D	141	PRO	2.3
1	D	310	LYS	2.3
1	D	309	LEU	2.3
1	B	210	LYS	2.3
1	D	99	THR	2.3
1	B	127	GLU	2.3
1	C	28	ASN	2.2
1	B	264	ARG	2.2
1	B	160	THR	2.2
1	D	42	GLY	2.2
1	A	104	GLU	2.2
1	A	61	ILE	2.2
1	C	188	TYR	2.2
1	D	108	LYS	2.2
1	D	109	LYS	2.2
1	B	99	THR	2.2
1	B	5	VAL	2.2
1	B	216	VAL	2.2
1	C	105	GLU	2.1
1	B	215	LYS	2.1
1	A	106	ILE	2.1
1	B	312	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	151	LYS	2.0
1	C	115	ARG	2.0
1	D	299	ARG	2.0
1	D	184	ASP	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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($\text{\AA}^2$)	Q<0.9
2	CA	A	315	1/1	1.00	0.01	4,4,4,4	0
2	CA	A	316	1/1	1.00	0.02	4,4,4,4	0
2	CA	B	315	1/1	1.00	0.01	3,3,3,3	0
2	CA	B	316	1/1	1.00	0.03	3,3,3,3	0
2	CA	C	315	1/1	1.00	0.01	4,4,4,4	0
2	CA	C	316	1/1	1.00	0.02	4,4,4,4	0
2	CA	D	315	1/1	1.00	0.01	3,3,3,3	0
2	CA	D	316	1/1	1.00	0.02	4,4,4,4	0

6.5 Other polymers [i](#)

There are no such residues in this entry.