



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 06:55 AM UTC

PDB ID : 7MBF / pdb_00007mbf
Title : codeinone reductase isoform 1.3 Apo form
Authors : Carr, S.C.; Ng, K.K.S.
Deposited on : 2021-03-31
Resolution : 2.40 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

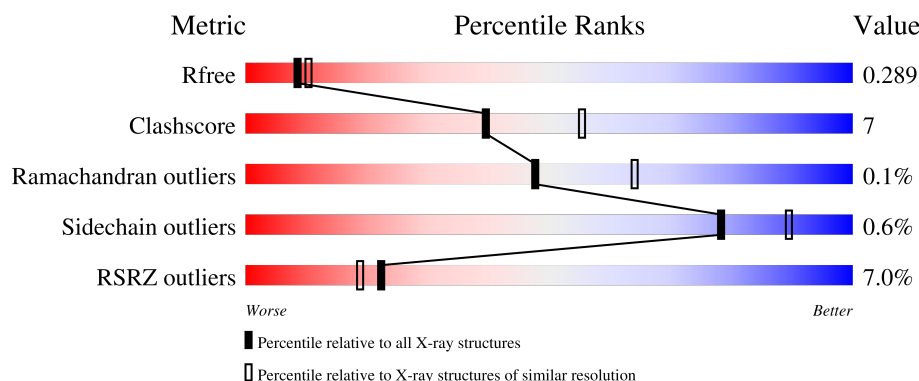
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	326	7% 82% 13% 5%
1	B	326	6% 76% 19% 5%
1	C	326	11% 73% 19% 8%
1	D	326	3% 83% 12% 5%
1	E	326	4% 81% 13% 5%

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Mol	Chain	Length	Quality of chain
1	F	326	9% 77% 17% 6%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 14524 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 NADPH-dependent codeinone reductase 1-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	310	Total	C	N	O	S	0	0	0
			2409	1533	408	448	20			
1	B	310	Total	C	N	O	S	0	0	0
			2419	1539	410	451	19			
1	C	301	Total	C	N	O	S	0	0	0
			2343	1491	399	433	20			
1	D	309	Total	C	N	O	S	0	0	0
			2410	1535	408	447	20			
1	E	309	Total	C	N	O	S	0	0	1
			2404	1530	407	447	20			
1	F	305	Total	C	N	O	S	0	0	0
			2375	1515	400	440	20			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	GLY	-	expression tag	UNP Q9SQ68
A	-3	PRO	-	expression tag	UNP Q9SQ68
A	-2	GLY	-	expression tag	UNP Q9SQ68
A	-1	TYR	-	expression tag	UNP Q9SQ68
A	0	GLN	-	expression tag	UNP Q9SQ68
B	-4	GLY	-	expression tag	UNP Q9SQ68
B	-3	PRO	-	expression tag	UNP Q9SQ68
B	-2	GLY	-	expression tag	UNP Q9SQ68
B	-1	TYR	-	expression tag	UNP Q9SQ68
B	0	GLN	-	expression tag	UNP Q9SQ68
C	-4	GLY	-	expression tag	UNP Q9SQ68
C	-3	PRO	-	expression tag	UNP Q9SQ68
C	-2	GLY	-	expression tag	UNP Q9SQ68
C	-1	TYR	-	expression tag	UNP Q9SQ68
C	0	GLN	-	expression tag	UNP Q9SQ68
D	-4	GLY	-	expression tag	UNP Q9SQ68
D	-3	PRO	-	expression tag	UNP Q9SQ68

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-2	GLY	-	expression tag	UNP Q9SQ68
D	-1	TYR	-	expression tag	UNP Q9SQ68
D	0	GLN	-	expression tag	UNP Q9SQ68
E	-4	GLY	-	expression tag	UNP Q9SQ68
E	-3	PRO	-	expression tag	UNP Q9SQ68
E	-2	GLY	-	expression tag	UNP Q9SQ68
E	-1	TYR	-	expression tag	UNP Q9SQ68
E	0	GLN	-	expression tag	UNP Q9SQ68
F	-4	GLY	-	expression tag	UNP Q9SQ68
F	-3	PRO	-	expression tag	UNP Q9SQ68
F	-2	GLY	-	expression tag	UNP Q9SQ68
F	-1	TYR	-	expression tag	UNP Q9SQ68
F	0	GLN	-	expression tag	UNP Q9SQ68

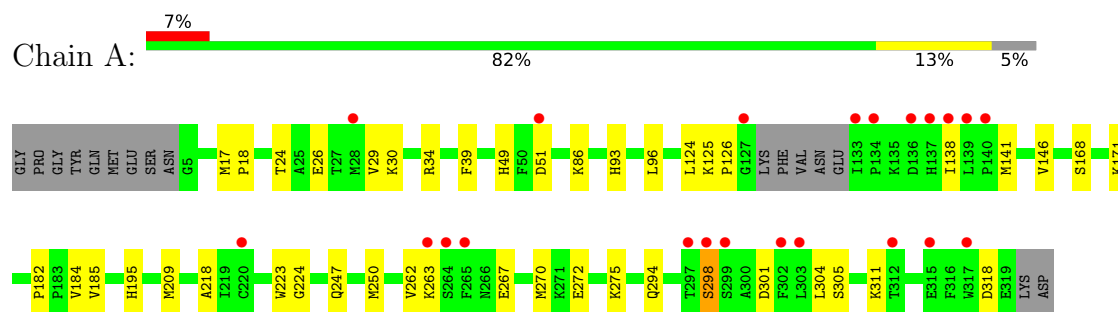
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	38	Total O 38 38	0	0
2	B	22	Total O 22 22	0	0
2	C	15	Total O 15 15	0	0
2	D	41	Total O 41 41	0	0
2	E	28	Total O 28 28	0	0
2	F	20	Total O 20 20	0	0

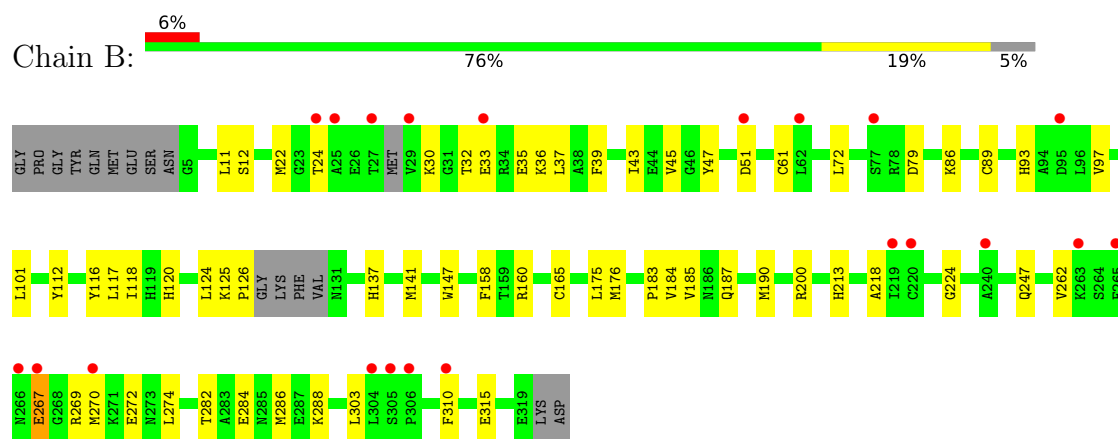
3 Residue-property plots [i](#)

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.

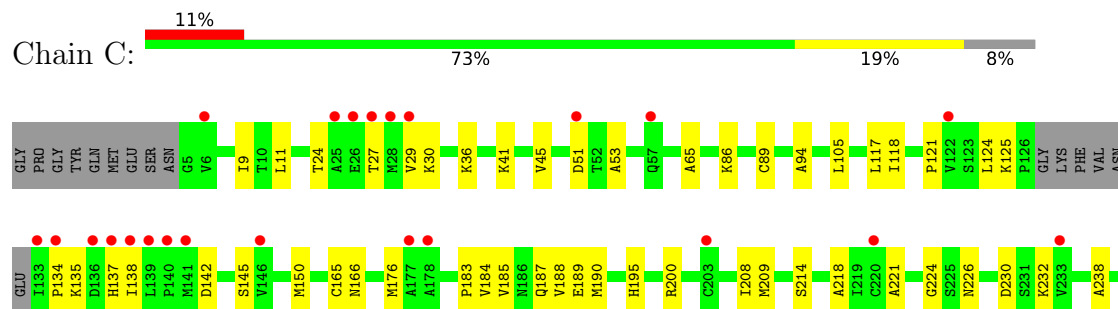
- Molecule 1: NADPH-dependent codeinone reductase 1-3

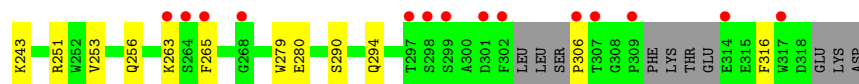


- Molecule 1: NADPH-dependent codeinone reductase 1-3

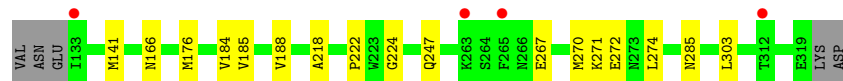
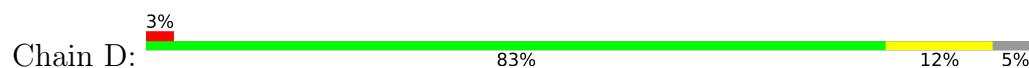


- Molecule 1: NADPH-dependent codeinone reductase 1-3

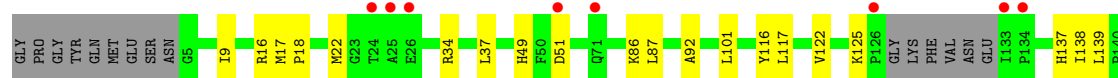
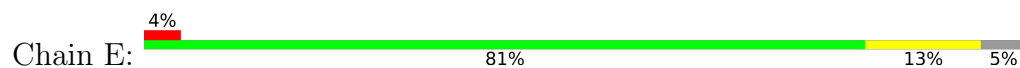




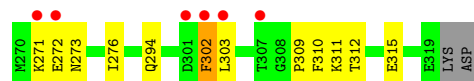
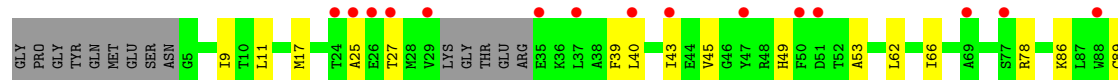
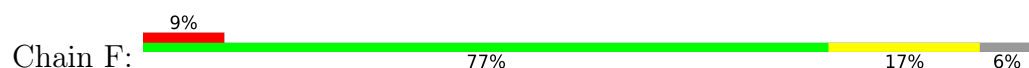
- Molecule 1: NADPH-dependent codeinone reductase 1-3



- Molecule 1: NADPH-dependent codeinone reductase 1-3



- Molecule 1: NADPH-dependent codeinone reductase 1-3



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	78.94Å 90.94Å 144.80Å 90.00° 93.53° 90.00°	Depositor
Resolution (Å)	43.37 – 2.40 43.37 – 2.40	Depositor EDS
% Data completeness (in resolution range)	84.3 (43.37-2.40) 73.4 (43.37-2.40)	Depositor EDS
R_{merge}	0.21	Depositor
R_{sym}	0.21	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.90 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.8.0230, PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.219 , 0.277 0.235 , 0.289	Depositor DCC
R_{free} test set	2005 reflections (2.98%)	wwPDB-VP
Wilson B-factor (Å ²)	28.1	Xtriage
Anisotropy	0.322	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 45.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	14524	wwPDB-VP
Average B, all atoms (Å ²)	50.0	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 30.95 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.2007e-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

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	0.11	0/2458	0.28	0/3324
1	B	0.11	0/2467	0.30	0/3336
1	C	0.12	0/2389	0.31	0/3228
1	D	0.10	0/2459	0.28	0/3326
1	E	0.11	0/2453	0.29	0/3317
1	F	0.12	0/2423	0.29	0/3278
All	All	0.11	0/14649	0.29	0/19809

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

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	2409	0	2422	28	0
1	B	2419	0	2431	37	0
1	C	2343	0	2360	42	0
1	D	2410	0	2429	24	0
1	E	2404	0	2419	31	0
1	F	2375	0	2388	38	0
2	A	38	0	0	0	0
2	B	22	0	0	0	0
2	C	15	0	0	0	0
2	D	41	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	28	0	0	1	0
2	F	20	0	0	0	0
All	All	14524	0	14449	194	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 7.

All (194) 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:125:LYS:HE3	1:E:139:LEU:HD11	1.67	0.76
1:A:247:GLN:HE22	1:A:275:LYS:HB2	1.51	0.75
1:C:53:ALA:HB2	1:C:86:LYS:HE2	1.69	0.75
1:C:89:CYS:HB2	1:C:124:LEU:HG	1.70	0.74
1:F:247:GLN:HB2	1:F:276:ILE:HG22	1.70	0.73
1:A:171:LYS:NZ	1:A:318:ASP:OD2	2.21	0.73
1:A:247:GLN:NE2	1:A:272:GLU:O	2.21	0.72
1:B:184:VAL:HG12	1:B:185:VAL:HG23	1.71	0.72
1:A:184:VAL:HG12	1:A:185:VAL:HG23	1.72	0.71
1:B:284:GLU:OE1	1:B:288:LYS:NZ	2.24	0.70
1:C:195:HIS:HE1	1:C:290:SER:HA	1.57	0.70
1:A:250:MET:HE3	1:A:262:VAL:HG11	1.74	0.70
1:A:93:HIS:HB2	1:A:96:LEU:HD23	1.78	0.66
1:A:24:THR:O	1:A:263:LYS:NZ	2.27	0.65
1:D:51:ASP:OD2	1:D:86:LYS:NZ	2.30	0.65
1:A:24:THR:HG22	1:A:39:PHE:HZ	1.63	0.64
1:C:124:LEU:HA	1:C:125:LYS:NZ	2.13	0.63
1:D:89:CYS:HB2	1:D:124:LEU:HD12	1.78	0.63
1:F:138:ILE:HG22	1:F:309:PRO:HD2	1.81	0.63
1:F:53:ALA:HB2	1:F:86:LYS:HE2	1.80	0.62
1:F:195:HIS:H	1:F:294:GLN:HE22	1.48	0.62
1:A:185:VAL:HG22	1:A:209:MET:HB3	1.81	0.61
1:C:24:THR:O	1:C:263:LYS:NZ	2.34	0.61
1:C:135:LYS:HB3	1:C:306:PRO:HG2	1.82	0.61
1:C:138:ILE:HD11	1:C:306:PRO:HD2	1.83	0.60
1:C:27:THR:HG22	1:C:29:VAL:HG23	1.83	0.60
1:D:184:VAL:HG12	1:D:185:VAL:HG23	1.84	0.60
1:E:122:VAL:HG21	1:E:303:LEU:HD22	1.83	0.59
1:D:17:MET:HE2	1:D:49:HIS:CE1	2.37	0.59
1:B:267:GLU:HA	1:B:270:MET:HG2	1.85	0.58
1:D:122:VAL:HG21	1:D:303:LEU:HD22	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:51:ASP:OD1	1:C:86:LYS:NZ	2.36	0.58
1:D:60:GLU:HG2	1:D:107:ASN:HB3	1.86	0.57
1:C:176:MET:HE2	1:C:208:ILE:HD11	1.85	0.57
1:B:101:LEU:HD21	1:B:158:PHE:HB3	1.86	0.57
1:B:247:GLN:NE2	1:B:272:GLU:O	2.38	0.57
1:E:101:LEU:HB2	1:E:116:TYR:HE1	1.69	0.57
1:F:122:VAL:HG21	1:F:303:LEU:HD22	1.87	0.56
1:B:24:THR:HG22	1:B:39:PHE:HZ	1.70	0.56
1:C:189:GLU:HG3	1:C:214:SER:HB2	1.86	0.56
1:A:34:ARG:HD2	1:D:222:PRO:HB2	1.87	0.56
1:D:247:GLN:NE2	1:D:272:GLU:O	2.39	0.56
1:F:9:ILE:HG21	1:F:209:MET:HE2	1.87	0.55
1:A:125:LYS:HD3	1:A:126:PRO:HD2	1.88	0.55
1:A:168:SER:OG	1:A:318:ASP:OD2	2.20	0.54
1:A:223:TRP:HD1	1:A:298:SER:HA	1.72	0.54
1:F:311:LYS:HG3	1:F:312:THR:HG23	1.90	0.54
1:C:185:VAL:HG22	1:C:209:MET:HB3	1.89	0.53
1:C:218:ALA:HB1	1:C:221:ALA:HB3	1.90	0.53
1:E:18:PRO:HB2	1:E:49:HIS:HB2	1.90	0.53
1:C:195:HIS:H	1:C:294:GLN:HE22	1.55	0.53
1:E:125:LYS:HA	1:E:125:LYS:HE2	1.89	0.53
1:B:79:ASP:OD1	1:B:79:ASP:N	2.39	0.53
1:F:243:LYS:HD2	1:F:247:GLN:HE21	1.73	0.52
1:D:17:MET:HE2	1:D:49:HIS:HE1	1.74	0.51
1:B:51:ASP:OD2	1:B:86:LYS:NZ	2.42	0.51
1:C:125:LYS:HZ2	1:C:138:ILE:CA	2.23	0.51
1:F:62:LEU:O	1:F:66:ILE:HG13	2.10	0.51
1:B:269:ARG:NH1	1:C:230:ASP:OD1	2.38	0.50
1:D:92:ALA:HB1	1:D:141:MET:HE2	1.94	0.50
1:F:9:ILE:HD13	1:F:209:MET:HE2	1.92	0.50
1:F:39:PHE:O	1:F:43:ILE:HG13	2.12	0.50
1:B:11:LEU:HD13	1:B:184:VAL:HG11	1.93	0.50
1:E:17:MET:HE2	1:E:49:HIS:NE2	2.27	0.50
1:C:226:ASN:HB2	1:C:230:ASP:OD2	2.10	0.50
1:C:195:HIS:H	1:C:294:GLN:NE2	2.10	0.50
1:F:302:PHE:N	1:F:302:PHE:CD2	2.79	0.50
1:C:86:LYS:HG2	1:C:117:LEU:HB2	1.93	0.50
1:E:51:ASP:OD1	1:E:86:LYS:NZ	2.40	0.49
1:E:171:LYS:NZ	1:E:318:ASP:OD2	2.45	0.49
1:A:29:VAL:HG22	1:A:30:LYS:H	1.78	0.49
1:C:190:MET:HE2	1:C:253:VAL:HG13	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:17:MET:HE2	1:A:49:HIS:CE1	2.48	0.49
1:C:29:VAL:HG12	1:C:30:LYS:H	1.78	0.49
1:C:218:ALA:O	1:C:224:GLY:HA3	2.13	0.49
1:D:8:MET:HE1	1:D:18:PRO:HG3	1.95	0.49
1:B:190:MET:SD	1:B:200:ARG:HD2	2.53	0.48
1:E:101:LEU:HB2	1:E:116:TYR:CE1	2.48	0.48
1:E:138:ILE:HD13	1:E:303:LEU:HA	1.95	0.48
1:C:176:MET:SD	1:C:183:PRO:HD2	2.52	0.48
1:E:92:ALA:HB1	1:E:141:MET:HE2	1.95	0.48
1:D:218:ALA:O	1:D:224:GLY:HA3	2.13	0.48
1:B:176:MET:SD	1:B:183:PRO:HD2	2.54	0.48
1:D:119:HIS:HD2	1:D:120:HIS:CE1	2.32	0.48
1:C:243:LYS:HE2	1:C:279:TRP:CG	2.48	0.48
1:F:269:ARG:HA	1:F:272:GLU:HB3	1.96	0.48
1:C:124:LEU:HA	1:C:125:LYS:HZ3	1.76	0.47
1:D:271:LYS:NZ	2:D:403:HOH:O	2.46	0.47
1:A:311:LYS:HE2	1:E:282:THR:HG21	1.95	0.47
1:B:39:PHE:O	1:B:43:ILE:HG13	2.14	0.47
1:F:93:HIS:HB2	1:F:96:LEU:HD13	1.96	0.47
1:A:24:THR:HG22	1:A:39:PHE:CZ	2.47	0.47
1:F:45:VAL:HG13	1:F:271:LYS:HE2	1.96	0.47
1:D:267:GLU:HB2	1:D:271:LYS:HE3	1.96	0.47
1:E:116:TYR:HD2	1:E:117:LEU:H	1.63	0.47
1:E:302:PHE:CD2	1:E:303:LEU:HG	2.50	0.47
1:C:124:LEU:HA	1:C:125:LYS:HZ1	1.79	0.47
1:E:176:MET:HE1	1:E:206:ASN:HB3	1.97	0.47
1:F:86:LYS:HG2	1:F:117:LEU:HB2	1.97	0.47
1:F:310:PHE:HD1	1:F:315:GLU:HG2	1.79	0.47
1:F:302:PHE:CD2	1:F:303:LEU:HG	2.51	0.46
1:C:36:LYS:HG3	1:C:65:ALA:HB2	1.97	0.46
1:C:166:ASN:HA	1:C:188:VAL:HG12	1.98	0.46
1:E:22:MET:HE2	1:E:264:SER:HB3	1.97	0.46
1:B:89:CYS:HB2	1:B:124:LEU:HG	1.97	0.46
1:E:185:VAL:HG22	1:E:209:MET:HB3	1.97	0.46
1:D:39:PHE:O	1:D:43:ILE:HG13	2.15	0.46
1:C:232:LYS:HA	1:C:232:LYS:HD3	1.79	0.45
1:A:305:SER:O	1:A:311:LYS:HG2	2.17	0.45
1:C:9:ILE:HD13	1:C:209:MET:HE2	1.98	0.45
1:B:165:CYS:SG	1:B:187:GLN:HB3	2.57	0.45
1:C:41:LYS:O	1:C:45:VAL:HG23	2.16	0.45
1:A:18:PRO:HB2	1:A:49:HIS:HB2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:121:PRO:HD2	1:C:316:PHE:CZ	2.51	0.45
1:D:267:GLU:HA	1:D:270:MET:HB2	1.99	0.44
1:E:9:ILE:HD13	1:E:209:MET:HE2	1.98	0.44
1:C:200:ARG:NH2	1:C:256:GLN:OE1	2.50	0.44
1:E:125:LYS:HB2	1:E:137:HIS:HB3	1.99	0.44
1:B:86:LYS:HG2	1:B:117:LEU:HB2	1.99	0.44
1:B:118:ILE:HD13	1:B:141:MET:HE1	1.99	0.44
1:C:165:CYS:SG	1:C:187:GLN:HB3	2.57	0.44
1:D:20:LEU:HD23	1:D:274:LEU:HD23	1.98	0.44
1:F:185:VAL:HG22	1:F:209:MET:HB3	1.99	0.44
1:A:141:MET:HE2	1:A:146:VAL:HG11	1.99	0.44
1:B:218:ALA:O	1:B:224:GLY:HA3	2.18	0.44
1:E:34:ARG:HA	1:E:37:LEU:HD12	1.99	0.44
1:A:26:GLU:OE2	1:A:263:LYS:HE3	2.18	0.44
1:A:124:LEU:HD23	1:A:138:ILE:HA	2.00	0.44
1:C:134:PRO:HB2	1:C:137:HIS:HB2	2.00	0.44
1:E:16:ARG:NH1	2:E:403:HOH:O	2.51	0.44
1:F:17:MET:HE2	1:F:49:HIS:HE1	1.81	0.44
1:F:218:ALA:O	1:F:224:GLY:HA3	2.18	0.43
1:A:182:PRO:HD2	1:B:12:SER:O	2.17	0.43
1:C:118:ILE:HG13	1:C:150:MET:HE2	2.00	0.43
1:F:269:ARG:O	1:F:273:ASN:N	2.37	0.43
1:A:51:ASP:OD2	1:A:86:LYS:NZ	2.51	0.43
1:B:32:THR:HG23	1:B:35:GLU:H	1.83	0.43
1:B:36:LYS:HB2	1:B:61:CYS:HB3	2.00	0.43
1:B:45:VAL:HG12	1:B:274:LEU:HD11	2.01	0.43
1:C:142:ASP:OD2	1:C:145:SER:OG	2.18	0.43
1:E:302:PHE:HD2	1:E:303:LEU:H	1.66	0.43
1:A:195:HIS:CE1	1:A:294:GLN:HE22	2.37	0.43
1:F:165:CYS:SG	1:F:187:GLN:HB3	2.59	0.43
1:F:172:LEU:O	1:F:176:MET:HG2	2.17	0.43
1:F:302:PHE:N	1:F:302:PHE:HD2	2.16	0.43
1:E:218:ALA:O	1:E:224:GLY:HA3	2.19	0.43
1:F:86:LYS:HD3	1:F:165:CYS:SG	2.59	0.42
1:B:24:THR:HG22	1:B:39:PHE:CZ	2.52	0.42
1:D:166:ASN:HA	1:D:188:VAL:HG12	2.01	0.42
1:E:170:LYS:HD3	1:E:174:GLU:OE2	2.19	0.42
1:C:195:HIS:CE1	1:C:290:SER:HA	2.46	0.42
1:D:285:ASN:ND2	2:D:406:HOH:O	2.50	0.42
1:F:11:LEU:HB3	1:F:184:VAL:CG2	2.49	0.42
1:F:78:ARG:HE	1:F:110:LEU:HD22	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:108:LEU:HB3	1:F:110:LEU:HD12	2.00	0.42
1:A:218:ALA:O	1:A:224:GLY:HA3	2.20	0.42
1:B:101:LEU:HD12	1:B:116:TYR:CD2	2.54	0.42
1:B:147:TRP:HB2	1:B:175:LEU:HD11	2.02	0.42
1:D:59:GLU:HB3	1:D:108:LEU:HG	2.00	0.42
1:A:267:GLU:HA	1:A:270:MET:HG2	2.02	0.42
1:B:30:LYS:HE3	1:B:30:LYS:HB3	1.75	0.42
1:F:89:CYS:HB2	1:F:124:LEU:HD12	2.01	0.42
1:B:310:PHE:HD2	1:B:315:GLU:HG3	1.85	0.41
1:C:238:ALA:HB1	1:C:243:LYS:O	2.21	0.41
1:E:87:LEU:HB2	1:E:116:TYR:CE2	2.56	0.41
1:F:125:LYS:HA	1:F:126:PRO:HD2	1.90	0.41
1:B:187:GLN:HG2	1:B:213:HIS:HD2	1.85	0.41
1:D:125:LYS:HE2	1:D:125:LYS:HB3	1.86	0.41
1:E:282:THR:O	1:E:286:MET:HG2	2.20	0.41
1:F:11:LEU:HB3	1:F:184:VAL:HG22	2.03	0.41
1:B:22:MET:HA	1:B:262:VAL:O	2.20	0.41
1:C:11:LEU:HB3	1:C:184:VAL:CG1	2.51	0.41
1:C:251:ARG:NH2	1:C:280:GLU:HG2	2.36	0.41
1:F:86:LYS:HD2	1:F:119:HIS:CD2	2.56	0.41
1:B:124:LEU:HA	1:B:137:HIS:O	2.20	0.41
1:B:125:LYS:HA	1:B:126:PRO:HD3	1.96	0.41
1:D:53:ALA:HB2	1:D:86:LYS:HD2	2.01	0.41
1:F:25:ALA:C	1:F:27:THR:H	2.29	0.41
1:B:89:CYS:SG	1:B:120:HIS:HB2	2.61	0.41
1:E:222:PRO:HA	1:F:265:PHE:O	2.21	0.41
1:E:251:ARG:HD3	1:E:276:ILE:O	2.21	0.41
1:B:47:TYR:CE1	1:B:270:MET:HB2	2.56	0.40
1:B:282:THR:O	1:B:286:MET:HG2	2.22	0.40
1:D:176:MET:HE3	1:D:176:MET:HB3	1.92	0.40
1:E:230:ASP:OD1	1:F:269:ARG:NH1	2.52	0.40
1:B:32:THR:OG1	1:B:33:GLU:N	2.54	0.40
1:F:250:MET:HE1	1:F:273:ASN:OD1	2.21	0.40
1:A:301:ASP:HA	1:A:304:LEU:HG	2.02	0.40
1:B:93:HIS:O	1:B:97:VAL:HG23	2.22	0.40
1:E:243:LYS:HD2	1:E:247:GLN:HE21	1.85	0.40
1:F:243:LYS:HD2	1:F:247:GLN:NE2	2.37	0.40
1:B:112:TYR:CE2	1:B:160:ARG:HD2	2.57	0.40
1:C:105:LEU:HD23	1:C:105:LEU:HA	1.88	0.40
1:E:166:ASN:HA	1:E:188:VAL:HG12	2.04	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	306/326 (94%)	296 (97%)	9 (3%)	1 (0%)	36	50
1	B	304/326 (93%)	297 (98%)	7 (2%)	0	100	100
1	C	293/326 (90%)	280 (96%)	12 (4%)	1 (0%)	36	50
1	D	305/326 (94%)	293 (96%)	12 (4%)	0	100	100
1	E	305/326 (94%)	296 (97%)	9 (3%)	0	100	100
1	F	299/326 (92%)	290 (97%)	9 (3%)	0	100	100
All	All	1812/1956 (93%)	1752 (97%)	58 (3%)	2 (0%)	48	64

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	94	ALA
1	A	298	SER

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	261/276 (95%)	261 (100%)	0	100	100
1	B	263/276 (95%)	259 (98%)	4 (2%)	57	77
1	C	254/276 (92%)	253 (100%)	1 (0%)	84	92
1	D	262/276 (95%)	262 (100%)	0	100	100
1	E	261/276 (95%)	260 (100%)	1 (0%)	84	92

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	F	258/276 (94%)	255 (99%)	3 (1%)	63 81
All	All	1559/1656 (94%)	1550 (99%)	9 (1%)	78 89

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	37	LEU
1	B	72	LEU
1	B	267	GLU
1	B	303	LEU
1	C	265	PHE
1	E	302	PHE
1	F	40	LEU
1	F	133	ILE
1	F	302	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	GLN
1	A	187	GLN
1	A	247	GLN
1	B	49	HIS
1	B	107	ASN
1	B	187	GLN
1	B	213	HIS
1	C	103	ASN
1	C	195	HIS
1	C	207	ASN
1	C	266	ASN
1	D	49	HIS
1	D	119	HIS
1	D	195	HIS
1	E	173	GLN
1	E	247	GLN
1	F	49	HIS
1	F	93	HIS
1	F	206	ASN
1	F	247	GLN
1	F	294	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](#)

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

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	310/326 (95%)	0.38	22 (7%) 22 18	18, 38, 82, 100	0
1	B	310/326 (95%)	0.77	21 (6%) 23 20	26, 52, 81, 100	0
1	C	301/326 (92%)	0.94	37 (12%) 8 6	31, 53, 89, 117	0
1	D	309/326 (94%)	0.36	9 (2%) 53 50	18, 41, 72, 96	0
1	E	309/326 (94%)	0.40	13 (4%) 40 36	23, 40, 76, 100	0
1	F	305/326 (93%)	0.87	28 (9%) 14 12	25, 53, 86, 98	0
All	All	1844/1956 (94%)	0.62	130 (7%) 22 19	18, 47, 84, 117	0

All (130) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	24	THR	5.5
1	E	51	ASP	4.8
1	B	265	PHE	4.1
1	C	122	VAL	4.1
1	F	29	VAL	3.8
1	F	47	TYR	3.8
1	C	220	CYS	3.7
1	F	51	ASP	3.7
1	A	133	ILE	3.6
1	A	297	THR	3.4
1	D	265	PHE	3.4
1	A	136	ASP	3.3
1	A	303	LEU	3.3
1	C	265	PHE	3.2
1	D	29	VAL	3.2
1	C	302	PHE	3.2
1	F	43	ILE	3.2
1	D	26	GLU	3.2
1	B	263	LYS	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	306	PRO	3.1
1	E	134	PRO	3.1
1	B	219	ILE	3.0
1	F	303	LEU	3.0
1	F	26	GLU	3.0
1	C	137	HIS	3.0
1	A	139	LEU	3.0
1	F	133	ILE	2.9
1	C	26	GLU	2.9
1	A	134	PRO	2.9
1	F	50	PHE	2.9
1	D	263	LYS	2.9
1	A	265	PHE	2.9
1	C	297	THR	2.9
1	B	27	THR	2.8
1	C	29	VAL	2.8
1	E	24	THR	2.8
1	B	33	GLU	2.7
1	C	140	PRO	2.7
1	A	299	SER	2.7
1	F	35	GLU	2.7
1	C	27	THR	2.7
1	F	69	ALA	2.7
1	C	136	ASP	2.6
1	F	37	LEU	2.6
1	C	309	PRO	2.6
1	F	88	TRP	2.6
1	E	133	ILE	2.6
1	F	302	PHE	2.6
1	C	233	VAL	2.6
1	C	307	THR	2.6
1	C	141	MET	2.6
1	C	138	ILE	2.6
1	E	26	GLU	2.6
1	F	40	LEU	2.6
1	B	29	VAL	2.6
1	C	139	LEU	2.5
1	A	137	HIS	2.5
1	A	263	LYS	2.5
1	C	298	SER	2.5
1	C	133	ILE	2.5
1	A	312	THR	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	27	THR	2.5
1	F	263	LYS	2.5
1	A	264	SER	2.5
1	B	305	SER	2.5
1	A	220	CYS	2.4
1	B	95	ASP	2.4
1	D	24	THR	2.4
1	D	133	ILE	2.4
1	E	302	PHE	2.4
1	F	265	PHE	2.4
1	B	24	THR	2.4
1	C	134	PRO	2.4
1	C	299	SER	2.4
1	F	271	LYS	2.4
1	C	57	GLN	2.4
1	A	302	PHE	2.4
1	B	62	LEU	2.4
1	B	220	CYS	2.4
1	C	28	MET	2.4
1	C	264	SER	2.3
1	C	146	VAL	2.3
1	C	263	LYS	2.3
1	F	132	GLU	2.3
1	E	126	PRO	2.3
1	E	297	THR	2.3
1	B	304	LEU	2.3
1	B	51	ASP	2.3
1	C	51	ASP	2.3
1	B	310	PHE	2.3
1	B	270	MET	2.3
1	F	122	VAL	2.3
1	B	25	ALA	2.2
1	E	25	ALA	2.2
1	F	77	SER	2.2
1	A	315	GLU	2.2
1	B	306	PRO	2.2
1	C	178	ALA	2.2
1	C	203	CYS	2.2
1	A	28	MET	2.2
1	A	127	GLY	2.2
1	D	77	SER	2.2
1	A	51	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	6	VAL	2.2
1	B	240	ALA	2.2
1	E	263	LYS	2.2
1	F	25	ALA	2.2
1	C	268	GLY	2.2
1	A	298	SER	2.2
1	F	185	VAL	2.1
1	B	266	ASN	2.1
1	C	25	ALA	2.1
1	E	220	CYS	2.1
1	C	301	ASP	2.1
1	A	138	ILE	2.1
1	C	314	GLU	2.1
1	B	77	SER	2.1
1	A	317	TRP	2.1
1	F	27	THR	2.1
1	B	267	GLU	2.1
1	F	272	GLU	2.1
1	E	305	SER	2.1
1	F	301	ASP	2.1
1	A	140	PRO	2.1
1	C	317	TRP	2.1
1	F	307	THR	2.1
1	F	135	LYS	2.0
1	E	71	GLN	2.0
1	C	177	ALA	2.0
1	D	312	THR	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.