



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 01:19 AM UTC

PDB ID : 7W3O / pdb_00007w3o
Title : Crystal structure of human CYB5R3
Authors : Noda, N.N.
Deposited on : 2021-11-25
Resolution : 2.46 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

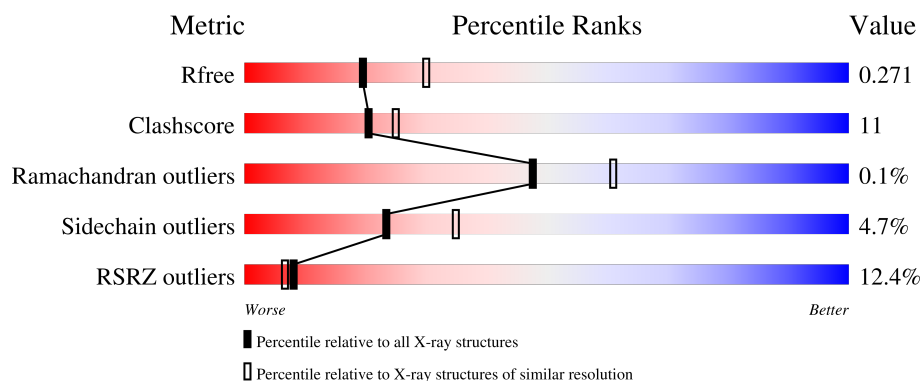
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.46 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	1190 (2.46-2.46)
Clashscore	190562	1229 (2.46-2.46)
Ramachandran outliers	187476	1218 (2.46-2.46)
Sidechain outliers	187428	1218 (2.46-2.46)
RSRZ outliers	180081	1190 (2.46-2.46)

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	278	3% 74% 22% • •
1	B	278	5% 74% 24% •
1	C	278	8% 74% 21% • •
1	D	278	9% 71% 25% • •
1	E	278	35% 68% 25% • 5%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11245 atoms, of which 80 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.

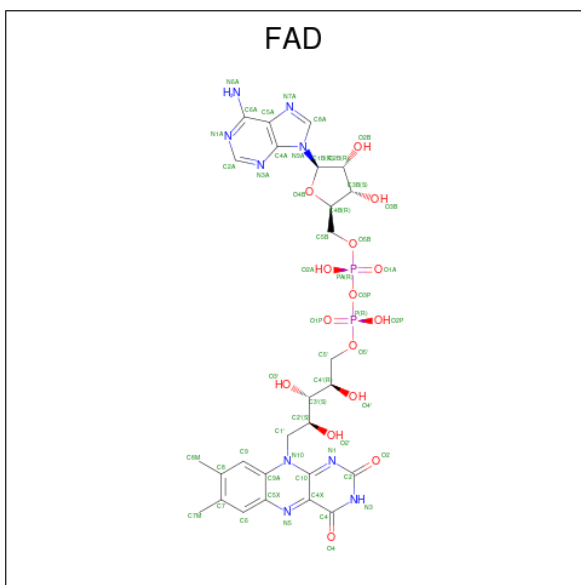
- Molecule 1 is a protein called NADH-cytochrome b5 reductase 3 soluble form.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	272	Total	C	N	O	S	0	0	0
			2171	1393	375	391	12			
1	B	272	Total	C	N	O	S	0	0	0
			2170	1393	375	390	12			
1	C	272	Total	C	N	O	S	0	0	0
			2170	1393	375	390	12			
1	D	270	Total	C	N	O	S	0	0	0
			2152	1383	371	386	12			
1	E	264	Total	C	N	O	S	0	0	0
			2098	1347	362	377	12			

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP P00387
A	-1	PRO	-	expression tag	UNP P00387
A	0	MET	-	expression tag	UNP P00387
B	-2	GLY	-	expression tag	UNP P00387
B	-1	PRO	-	expression tag	UNP P00387
B	0	MET	-	expression tag	UNP P00387
C	-2	GLY	-	expression tag	UNP P00387
C	-1	PRO	-	expression tag	UNP P00387
C	0	MET	-	expression tag	UNP P00387
D	-2	GLY	-	expression tag	UNP P00387
D	-1	PRO	-	expression tag	UNP P00387
D	0	MET	-	expression tag	UNP P00387
E	-2	GLY	-	expression tag	UNP P00387
E	-1	PRO	-	expression tag	UNP P00387
E	0	MET	-	expression tag	UNP P00387

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total 73	C 27	H 20	N 9	O 15	P 2	0	1
2	B	1	Total 73	C 27	H 20	N 9	O 15	P 2	0	1
2	C	1	Total 73	C 27	H 20	N 9	O 15	P 2	0	1
2	D	1	Total 73	C 27	H 20	N 9	O 15	P 2	0	1

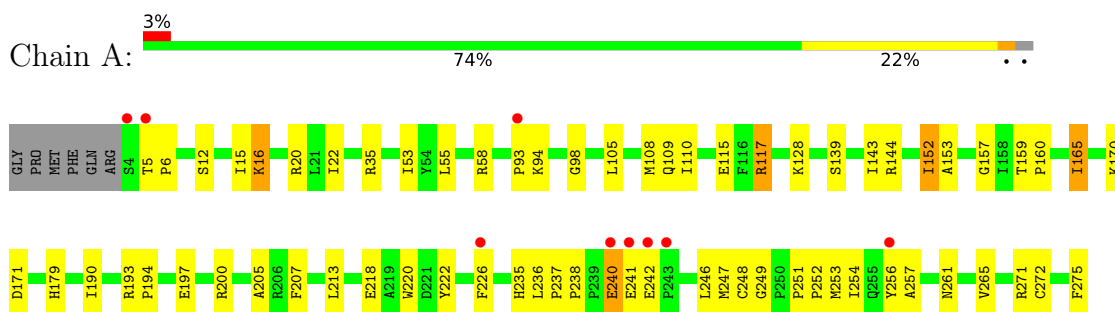
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	81	Total O 81 81	0	0
3	B	36	Total O 36 36	0	0
3	C	37	Total O 37 37	0	0
3	D	21	Total O 21 21	0	0
3	E	17	Total O 17 17	0	0

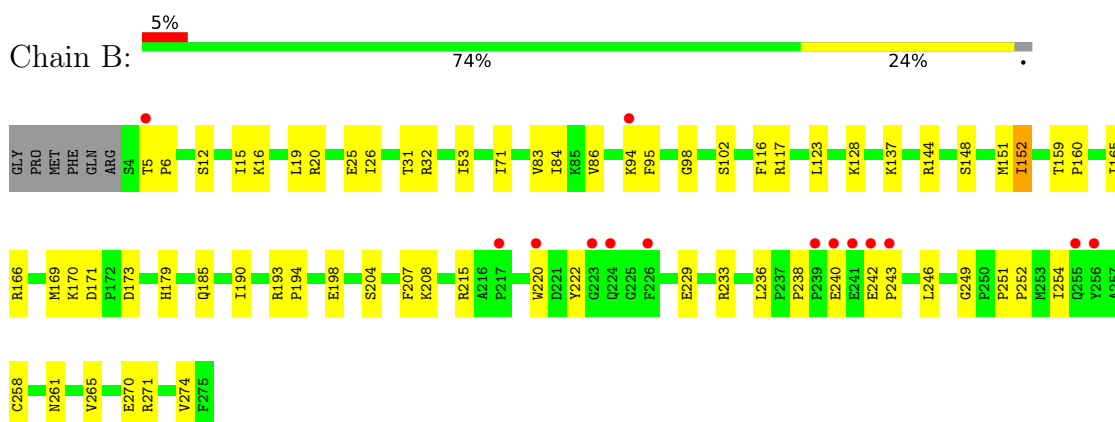
3 Residue-property plots [i](#)

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.

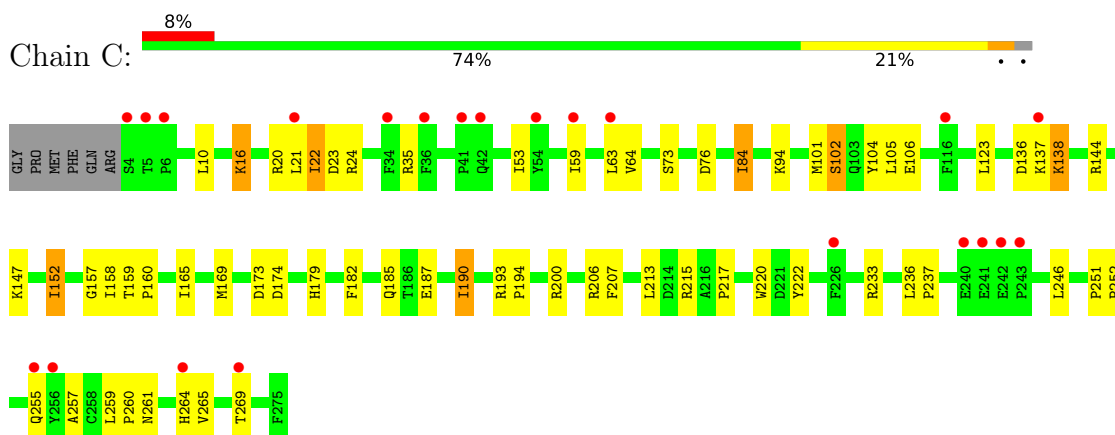
- Molecule 1: NADH-cytochrome b5 reductase 3 soluble form



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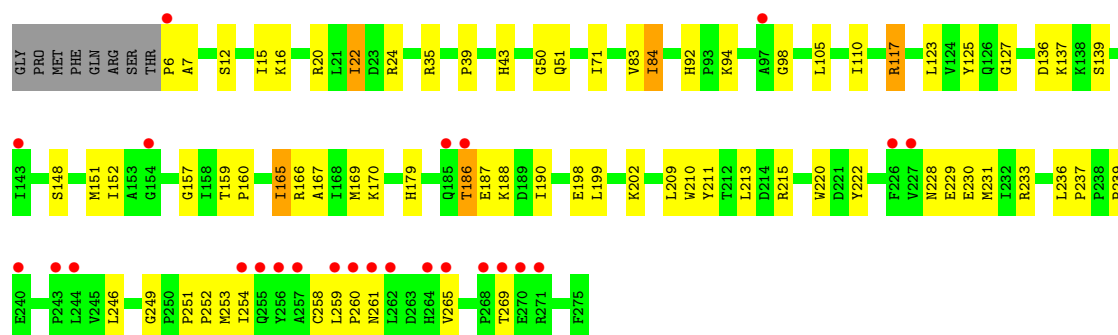


- Molecule 1: NADH-cytochrome b5 reductase 3 soluble form



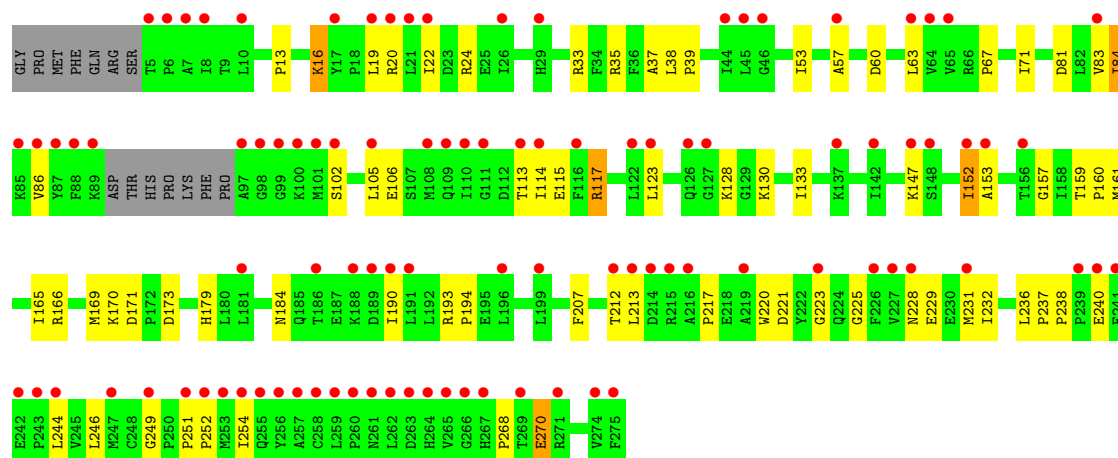
● Molecule 1: NADH-cytochrome b5 reductase 3 soluble form

Chain D:  9% 71% 25% ..



● Molecule 1: NADH-cytochrome b5 reductase 3 soluble form

Chain E:  35% 68% 25% 5%



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	163.36Å 79.92Å 169.40Å 90.00° 98.72° 90.00°	Depositor
Resolution (Å)	49.57 – 2.46 49.57 – 2.46	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.57-2.46) 100.0 (49.57-2.46)	Depositor EDS
R_{merge}	0.26	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.17 (at 2.45Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.231 , 0.260 (Not available) , 0.271	Depositor DCC
R_{free} test set	4017 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å ²)	52.4	Xtriage
Anisotropy	0.175	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 53.2	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	0.93	EDS
Total number of atoms	11245	wwPDB-VP
Average B, all atoms (Å ²)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.57% 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: FAD

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	0.79	1/2231 (0.0%)	0.82	0/3028
1	B	0.60	0/2230	0.65	0/3026
1	C	0.58	0/2230	0.67	2/3026 (0.1%)
1	D	0.44	0/2211	0.51	0/2999
1	E	0.39	0/2152	0.49	0/2917
All	All	0.58	1/11054 (0.0%)	0.64	2/14996 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	242	GLU	C-O	-8.96	1.19	1.23

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	206	ARG	NE-CZ-NH2	5.25	123.92	119.20
1	C	206	ARG	NE-CZ-NH1	-5.03	116.47	121.50

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	2171	0	2178	50	0
1	B	2170	0	2177	42	0
1	C	2170	0	2177	54	0
1	D	2152	0	2161	53	0
1	E	2098	0	2107	60	0
2	A	53	20	0	0	0
2	B	53	20	0	0	0
2	C	53	20	0	0	0
2	D	53	20	0	0	0
3	A	81	0	0	7	0
3	B	36	0	0	3	1
3	C	37	0	0	12	1
3	D	21	0	0	12	0
3	E	17	0	0	3	0
All	All	11165	80	10800	246	1

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 11.

All (246) 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:5:THR:HB	1:A:6:PRO:HD3	1.33	1.07
1:D:20:ARG:NH1	3:D:1401:HOH:O	1.84	0.97
1:B:152:ILE:HD11	1:B:236:LEU:HD11	1.49	0.93
1:D:50:GLY:O	3:D:1403:HOH:O	1.92	0.88
1:C:174:ASP:OD2	3:C:1401:HOH:O	1.92	0.86
1:E:270:GLU:OE2	1:E:270:GLU:N	2.09	0.85
1:D:190:ILE:HD11	1:D:213:LEU:HD21	1.58	0.85
1:C:73:SER:OG	3:C:1402:HOH:O	1.95	0.84
1:D:152:ILE:HD11	1:D:236:LEU:HD11	1.60	0.84
1:E:228:ASN:HB2	3:E:302:HOH:O	1.79	0.83
1:A:115:GLU:OE1	3:A:1401:HOH:O	1.97	0.82
1:C:16:LYS:NZ	3:C:1403:HOH:O	2.01	0.81
1:D:22:ILE:HD11	1:D:35:ARG:HG2	1.63	0.81
1:E:221:ASP:OD1	3:E:301:HOH:O	1.99	0.80
1:A:94:LYS:HG3	1:C:264:HIS:NE2	1.97	0.80
1:A:271:ARG:HH22	1:B:198:GLU:CD	1.90	0.79
1:E:229:GLU:N	3:E:302:HOH:O	2.12	0.79
1:C:24:ARG:NH2	1:C:106:GLU:OE2	2.16	0.79
1:E:190:ILE:HD11	1:E:213:LEU:HD21	1.63	0.78
1:E:13:PRO:O	1:E:117:ARG:NH2	2.16	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:23:ASP:OD2	1:E:130:LYS:NZ	2.17	0.78
1:E:161:MET:O	1:E:165:ILE:HG12	1.83	0.78
1:E:166:ARG:O	1:E:170:LYS:HG2	1.83	0.78
1:E:16:LYS:HG3	1:E:117:ARG:HG3	1.65	0.76
1:C:152:ILE:HD11	1:C:236:LEU:HD11	1.66	0.76
1:D:84:ILE:HD13	1:D:105:LEU:HD13	1.68	0.75
1:A:94:LYS:HE3	1:C:264:HIS:HE1	1.53	0.74
1:C:173:ASP:OD1	3:C:1404:HOH:O	2.05	0.73
1:A:94:LYS:HE3	1:C:264:HIS:CE1	2.24	0.72
1:A:5:THR:HB	1:A:6:PRO:CD	2.15	0.71
1:A:275:PHE:O	3:A:1402:HOH:O	2.09	0.70
1:A:152:ILE:HD11	1:A:236:LEU:HD11	1.74	0.69
1:E:213:LEU:O	1:E:225:GLY:N	2.24	0.69
1:C:23:ASP:HB2	1:E:128:LYS:HD2	1.73	0.69
1:A:205:ALA:O	3:A:1403:HOH:O	2.11	0.68
1:A:256:TYR:CE2	1:C:259:LEU:HD22	2.29	0.68
1:B:173:ASP:OD1	3:B:1401:HOH:O	2.12	0.68
1:E:33:ARG:HH12	1:E:35:ARG:HD2	1.59	0.67
1:B:229:GLU:HG2	1:B:233:ARG:NH1	2.09	0.67
1:E:128:LYS:NZ	1:E:171:ASP:OD2	2.28	0.67
1:D:233:ARG:NH1	1:D:265:VAL:HG22	2.10	0.66
1:B:159:THR:OG1	1:B:160:PRO:HD3	1.95	0.65
1:A:5:THR:CB	1:A:6:PRO:HD3	2.20	0.65
1:A:226:PHE:CG	1:C:255:GLN:HG2	2.32	0.65
1:A:256:TYR:HD2	1:C:259:LEU:HD13	1.60	0.64
1:D:229:GLU:N	1:D:261:ASN:HD22	1.95	0.64
1:A:251:PRO:HB2	1:C:269:THR:HG21	1.79	0.64
1:E:33:ARG:NH1	1:E:35:ARG:HD2	2.13	0.64
1:E:71:ILE:HD13	1:E:83:VAL:HG23	1.80	0.63
1:E:249:GLY:H	1:E:254:ILE:HD11	1.62	0.63
1:A:58:ARG:NH1	3:A:1407:HOH:O	2.31	0.63
1:D:166:ARG:NE	3:D:1405:HOH:O	2.14	0.63
1:A:256:TYR:CD2	1:C:259:LEU:HD13	2.35	0.62
1:A:249:GLY:H	1:A:254:ILE:HD11	1.64	0.62
1:B:185:GLN:OE1	1:B:215:ARG:NH2	2.34	0.61
1:D:261:ASN:O	1:D:265:VAL:HG23	2.00	0.61
1:B:25:GLU:OE2	3:B:1402:HOH:O	2.16	0.61
1:B:166:ARG:O	1:B:170:LYS:HG3	2.00	0.61
1:D:125:TYR:CZ	1:D:127:GLY:HA2	2.35	0.60
1:D:71:ILE:HD13	1:D:83:VAL:HG23	1.83	0.60
1:C:190:ILE:HD11	1:C:213:LEU:HD21	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:128:LYS:NZ	1:A:171:ASP:OD2	2.34	0.60
1:C:233:ARG:NH1	1:C:265:VAL:HG22	2.16	0.60
1:D:159:THR:OG1	1:D:160:PRO:HD3	2.01	0.60
1:C:169:MET:HE3	1:C:207:PHE:HB2	1.83	0.60
1:A:249:GLY:N	1:A:254:ILE:HD11	2.16	0.59
1:C:10:LEU:O	3:C:1406:HOH:O	2.16	0.59
1:B:251:PRO:N	1:B:252:PRO:HD2	2.17	0.59
1:D:6:PRO:HA	3:D:1406:HOH:O	2.00	0.59
1:E:38:LEU:HB3	1:E:39:PRO:HD2	1.85	0.59
1:B:151:MET:SD	1:B:165:ILE:HD11	2.43	0.59
1:D:51:GLN:HA	3:D:1403:HOH:O	2.03	0.58
1:C:159:THR:OG1	1:C:160:PRO:HD3	2.02	0.58
1:B:229:GLU:HG2	1:B:233:ARG:HH12	1.67	0.58
1:E:179:HIS:CG	1:E:237:PRO:HD3	2.38	0.58
1:E:157:GLY:O	1:E:160:PRO:HD2	2.03	0.57
1:A:251:PRO:N	1:A:252:PRO:HD2	2.19	0.57
1:D:92:HIS:N	3:D:1402:HOH:O	1.91	0.57
1:C:76:ASP:OD1	3:C:1407:HOH:O	2.18	0.57
1:B:95:PHE:HB3	3:B:1424:HOH:O	2.05	0.56
1:B:233:ARG:NH1	1:B:265:VAL:HG22	2.21	0.56
1:A:170:LYS:NZ	3:A:1410:HOH:O	2.38	0.56
1:D:7:ALA:N	3:D:1406:HOH:O	2.38	0.56
1:D:166:ARG:NH2	3:D:1405:HOH:O	2.29	0.56
1:C:22:ILE:O	1:E:128:LYS:HE3	2.05	0.56
1:D:187:GLU:O	1:D:190:ILE:HG12	2.05	0.56
1:A:271:ARG:NH2	1:B:198:GLU:OE2	2.39	0.55
1:B:169:MET:HE3	1:B:207:PHE:HB2	1.89	0.55
1:E:212:THR:OG1	1:E:231:MET:HE1	2.07	0.55
1:E:249:GLY:N	1:E:254:ILE:HD11	2.20	0.55
1:E:169:MET:HE3	1:E:207:PHE:HB2	1.88	0.55
1:C:157:GLY:O	1:C:160:PRO:HD2	2.07	0.55
1:C:200:ARG:NH2	3:C:1409:HOH:O	2.20	0.54
1:C:59:ILE:HG12	1:C:104:TYR:CD1	2.42	0.54
1:D:251:PRO:N	1:D:252:PRO:HD2	2.22	0.54
1:C:136:ASP:OD1	1:C:138:LYS:N	2.41	0.54
1:D:157:GLY:O	1:D:160:PRO:HD2	2.07	0.54
1:E:251:PRO:N	1:E:252:PRO:HD2	2.22	0.54
1:D:71:ILE:HD13	1:D:83:VAL:CG2	2.37	0.54
1:E:193:ARG:HB3	1:E:194:PRO:HD3	1.89	0.54
1:A:20:ARG:NH2	3:A:1404:HOH:O	2.38	0.53
1:D:117:ARG:HG2	3:D:1410:HOH:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:71:ILE:HD13	1:E:83:VAL:CG2	2.38	0.53
1:D:123:LEU:HD23	1:D:123:LEU:C	2.34	0.53
1:D:228:ASN:C	1:D:261:ASN:HD22	2.16	0.53
1:B:233:ARG:HH12	1:B:265:VAL:HG22	1.73	0.53
1:B:242:GLU:O	1:B:271:ARG:NH1	2.41	0.53
1:E:152:ILE:O	1:E:161:MET:HE3	2.09	0.53
1:C:220:TRP:CZ2	1:C:222:TYR:HB2	2.44	0.52
1:A:93:PRO:HG2	1:A:94:LYS:HD3	1.91	0.52
1:D:12:SER:HB3	1:D:15:ILE:HD12	1.92	0.52
1:A:159:THR:OG1	1:A:160:PRO:HD3	2.10	0.51
1:C:187:GLU:OE1	1:C:217:PRO:HG3	2.10	0.51
1:B:19:LEU:HD12	1:B:116:PHE:CD1	2.45	0.51
1:C:179:HIS:CG	1:C:237:PRO:HD3	2.45	0.51
1:C:251:PRO:N	1:C:252:PRO:HD2	2.24	0.51
1:A:247:MET:HE1	1:A:272:CYS:HB3	1.93	0.51
1:D:198:GLU:HG2	1:D:202:LYS:HE3	1.92	0.51
1:E:232:ILE:O	1:E:236:LEU:HB2	2.10	0.51
1:B:220:TRP:CE2	1:B:222:TYR:HB2	2.46	0.51
1:E:57:ALA:O	1:E:63:LEU:HD12	2.10	0.51
1:C:73:SER:CB	3:C:1402:HOH:O	2.57	0.51
1:D:233:ARG:HH12	1:D:265:VAL:HG22	1.73	0.51
1:E:114:ILE:HG12	1:E:115:GLU:H	1.76	0.51
1:B:144:ARG:NH1	1:B:270:GLU:O	2.44	0.50
1:C:158:ILE:HB	1:C:182:PHE:CZ	2.47	0.50
1:E:240:GLU:CD	1:E:240:GLU:H	2.19	0.50
1:B:254:ILE:HD13	1:B:274:VAL:HG13	1.94	0.50
1:D:179:HIS:CG	1:D:237:PRO:HD3	2.46	0.50
1:E:35:ARG:HG3	1:E:81:ASP:OD1	2.12	0.49
1:E:159:THR:OG1	1:E:160:PRO:HD3	2.11	0.49
1:A:235:HIS:O	1:A:236:LEU:HD23	2.12	0.49
1:C:23:ASP:OD1	1:C:24:ARG:N	2.42	0.49
1:C:259:LEU:O	3:C:1408:HOH:O	2.18	0.49
1:D:167:ALA:HA	1:D:170:LYS:HE2	1.94	0.49
1:C:22:ILE:HD11	1:C:35:ARG:HG2	1.94	0.49
1:E:153:ALA:HB2	1:E:161:MET:HG3	1.95	0.49
1:D:165:ILE:O	1:D:169:MET:HG2	2.13	0.49
1:E:38:LEU:HB3	1:E:39:PRO:CD	2.43	0.49
1:E:184:ASN:O	1:E:213:LEU:HA	2.13	0.48
1:A:20:ARG:NE	3:A:1404:HOH:O	2.19	0.48
1:D:239:PRO:CG	1:D:265:VAL:HG12	2.44	0.48
1:C:185:GLN:OE1	1:C:215:ARG:NH2	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:220:TRP:CE2	1:C:222:TYR:HB2	2.49	0.48
1:E:16:LYS:HG3	1:E:117:ARG:CG	2.41	0.48
1:E:86:VAL:HA	1:E:102:SER:HB2	1.94	0.48
1:D:228:ASN:HA	1:D:261:ASN:ND2	2.29	0.47
1:A:197:GLU:HG2	1:A:200:ARG:NH2	2.29	0.47
1:B:31:THR:C	1:B:32:ARG:HG2	2.39	0.47
1:B:128:LYS:NZ	1:B:171:ASP:OD2	2.47	0.47
1:A:165:ILE:HD12	1:A:207:PHE:CE1	2.50	0.47
1:A:236:LEU:HB3	1:A:237:PRO:HD2	1.96	0.47
1:E:24:ARG:NH2	1:E:106:GLU:OE2	2.45	0.47
1:D:136:ASP:OD2	1:D:139:SER:OG	2.31	0.46
1:D:117:ARG:NH1	3:D:1410:HOH:O	2.47	0.46
1:A:190:ILE:HD11	1:A:213:LEU:HD21	1.97	0.46
1:C:257:ALA:O	1:C:261:ASN:ND2	2.39	0.46
1:A:256:TYR:CD2	1:C:259:LEU:CD1	2.98	0.46
1:B:12:SER:HB3	1:B:15:ILE:HD12	1.97	0.46
1:D:251:PRO:CD	1:D:252:PRO:HD2	2.46	0.46
1:E:228:ASN:OD1	1:E:231:MET:HG3	2.15	0.46
1:A:193:ARG:HB3	1:A:194:PRO:HD3	1.97	0.46
1:D:239:PRO:HG3	1:D:265:VAL:HG12	1.98	0.46
1:E:152:ILE:HD11	1:E:236:LEU:HD11	1.98	0.46
1:B:53:ILE:HD12	1:B:53:ILE:C	2.41	0.45
1:A:16:LYS:HD2	1:A:117:ARG:HE	1.81	0.45
1:B:193:ARG:HB3	1:B:194:PRO:HD3	1.98	0.45
1:E:16:LYS:CD	1:E:117:ARG:HD3	2.47	0.45
1:A:220:TRP:CZ2	1:A:222:TYR:HB2	2.50	0.45
1:A:220:TRP:CE2	1:A:222:TYR:HB2	2.52	0.45
1:C:123:LEU:C	1:C:123:LEU:HD23	2.42	0.45
1:D:209:LEU:HD21	1:D:211:TYR:OH	2.17	0.45
1:C:84:ILE:HD13	1:C:105:LEU:HD13	1.98	0.45
1:D:186:THR:HG22	1:D:187:GLU:H	1.81	0.45
1:E:114:ILE:HG12	1:E:115:GLU:N	2.32	0.45
1:A:12:SER:HB3	1:A:15:ILE:HD12	1.99	0.44
1:D:24:ARG:NE	3:D:1408:HOH:O	2.43	0.44
1:D:249:GLY:HA3	1:D:253:MET:HE1	1.99	0.44
1:E:268:PRO:HB2	1:E:270:GLU:OE2	2.18	0.44
1:E:217:PRO:HG2	1:E:220:TRP:HB2	1.98	0.44
1:C:137:LYS:HE3	1:C:137:LYS:HB2	1.76	0.44
1:A:261:ASN:O	1:A:265:VAL:HG23	2.18	0.44
1:C:64:VAL:HG12	1:C:101:MET:HE2	1.99	0.44
1:A:153:ALA:HA	1:A:248:CYS:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:270:GLU:H	1:E:270:GLU:CD	2.05	0.44
1:A:22:ILE:HD11	1:A:35:ARG:HG2	2.00	0.43
1:B:238:PRO:HB2	1:B:240:GLU:OE1	2.17	0.43
1:C:259:LEU:HB2	1:C:260:PRO:HD3	1.99	0.43
1:A:108:MET:HB3	1:A:108:MET:HE2	1.87	0.43
1:E:165:ILE:O	1:E:169:MET:HG2	2.18	0.43
1:A:179:HIS:CG	1:A:237:PRO:HD3	2.53	0.43
1:D:220:TRP:HA	1:D:220:TRP:CE3	2.53	0.43
1:E:123:LEU:C	1:E:123:LEU:HD23	2.43	0.43
1:D:251:PRO:HD2	1:D:252:PRO:HD2	2.00	0.43
1:B:165:ILE:O	1:B:169:MET:HG2	2.19	0.43
1:B:190:ILE:HG22	1:B:193:ARG:HB2	2.00	0.43
1:D:179:HIS:CD2	1:D:237:PRO:HD3	2.53	0.43
1:E:84:ILE:HD13	1:E:105:LEU:HD13	2.01	0.43
1:B:249:GLY:N	1:B:254:ILE:HD11	2.34	0.43
1:C:63:LEU:HD12	1:C:63:LEU:HA	1.90	0.43
1:B:71:ILE:HD13	1:B:83:VAL:CG2	2.48	0.42
1:B:137:LYS:HB2	1:B:137:LYS:HE3	1.72	0.42
1:D:254:ILE:HA	1:D:258:CYS:SG	2.59	0.42
1:A:157:GLY:O	1:A:160:PRO:HD2	2.20	0.42
1:C:53:ILE:C	1:C:53:ILE:HD12	2.44	0.42
1:B:5:THR:HA	1:B:6:PRO:HD3	1.90	0.42
1:B:261:ASN:O	1:B:265:VAL:HG23	2.20	0.42
1:C:200:ARG:NE	3:C:1409:HOH:O	2.46	0.42
1:D:151:MET:SD	1:D:165:ILE:HD11	2.59	0.42
1:B:249:GLY:H	1:B:254:ILE:HD11	1.83	0.42
1:B:179:HIS:CE1	1:B:208:LYS:HG3	2.55	0.42
1:E:20:ARG:HH21	1:E:22:ILE:HG22	1.85	0.42
1:B:123:LEU:HD23	1:B:123:LEU:C	2.45	0.42
1:B:240:GLU:H	1:B:240:GLU:CD	2.28	0.42
1:E:212:THR:HA	1:E:223:GLY:O	2.19	0.42
1:D:259:LEU:HB2	1:D:260:PRO:HD3	2.02	0.41
1:B:86:VAL:HA	1:B:102:SER:HB2	2.02	0.41
1:A:238:PRO:HB2	1:A:240:GLU:HG2	2.02	0.41
1:C:20:ARG:HH21	1:E:173:ASP:CG	2.29	0.41
1:E:19:LEU:O	1:E:113:THR:HA	2.20	0.41
1:E:238:PRO:HB2	1:E:240:GLU:OE1	2.20	0.41
1:B:152:ILE:HG21	1:B:258:CYS:SG	2.61	0.41
1:A:53:ILE:C	1:A:53:ILE:HD12	2.45	0.41
1:D:210:TRP:CZ2	1:D:222:TYR:HA	2.55	0.41
1:B:242:GLU:N	1:B:243:PRO:HD3	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:228:ASN:OD1	1:D:231:MET:HG3	2.21	0.41
1:E:16:LYS:HD2	1:E:117:ARG:HD3	2.03	0.41
1:A:253:MET:O	1:A:257:ALA:HB3	2.20	0.41
1:C:200:ARG:CZ	3:C:1409:HOH:O	2.66	0.41
1:D:39:PRO:HB2	1:D:43:HIS:CE1	2.56	0.41
1:E:22:ILE:HG21	1:E:37:ALA:HB2	2.03	0.41
1:C:21:LEU:HD11	1:C:23:ASP:O	2.20	0.40
1:C:165:ILE:O	1:C:169:MET:HG2	2.21	0.40
1:D:199:LEU:HD23	1:D:199:LEU:HA	1.83	0.40
1:E:133:ILE:HD11	1:E:244:LEU:HD21	2.02	0.40
1:C:193:ARG:HB3	1:C:194:PRO:HD3	2.02	0.40
1:D:198:GLU:CG	1:D:202:LYS:HE3	2.51	0.40
1:A:55:LEU:HD13	1:A:105:LEU:HD21	2.03	0.40
1:E:16:LYS:HA	1:E:117:ARG:HG2	2.03	0.40
1:E:53:ILE:O	1:E:67:PRO:HA	2.22	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:1412:HOH:O	3:C:1434:HOH:O[3_545]	2.17	0.03

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	270/278 (97%)	259 (96%)	11 (4%)	0	100	100
1	B	270/278 (97%)	263 (97%)	7 (3%)	0	100	100
1	C	270/278 (97%)	262 (97%)	7 (3%)	1 (0%)	30	37
1	D	268/278 (96%)	261 (97%)	7 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	260/278 (94%)	254 (98%)	6 (2%)	0	100	100
All	All	1338/1390 (96%)	1299 (97%)	38 (3%)	1 (0%)	48	61

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	190	ILE

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	241/246 (98%)	228 (95%)	13 (5%)	20	29
1	B	241/246 (98%)	231 (96%)	10 (4%)	27	40
1	C	241/246 (98%)	231 (96%)	10 (4%)	27	40
1	D	238/246 (97%)	223 (94%)	15 (6%)	16	23
1	E	231/246 (94%)	223 (96%)	8 (4%)	32	46
All	All	1192/1230 (97%)	1136 (95%)	56 (5%)	23	35

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	LYS
1	A	109	GLN
1	A	110	ILE
1	A	117	ARG
1	A	139	SER
1	A	143	ILE
1	A	144	ARG
1	A	152	ILE
1	A	165	ILE
1	A	218	GLU
1	A	240	GLU

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Mol	Chain	Res	Type
1	A	241	GLU
1	A	246	LEU
1	B	16	LYS
1	B	20	ARG
1	B	26	ILE
1	B	84	ILE
1	B	94	LYS
1	B	117	ARG
1	B	148	SER
1	B	152	ILE
1	B	204	SER
1	B	246	LEU
1	C	16	LYS
1	C	22	ILE
1	C	84	ILE
1	C	94	LYS
1	C	102	SER
1	C	138	LYS
1	C	144	ARG
1	C	147	LYS
1	C	152	ILE
1	C	246	LEU
1	D	16	LYS
1	D	22	ILE
1	D	84	ILE
1	D	94	LYS
1	D	110	ILE
1	D	117	ARG
1	D	137	LYS
1	D	148	SER
1	D	165	ILE
1	D	186	THR
1	D	188	LYS
1	D	215	ARG
1	D	230	GLU
1	D	246	LEU
1	D	269	THR
1	E	16	LYS
1	E	60	ASP
1	E	84	ILE
1	E	117	ARG
1	E	147	LYS

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Mol	Chain	Res	Type
1	E	152	ILE
1	E	246	LEU
1	E	270	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	126	GLN
1	B	51	GLN
1	B	52	HIS
1	B	126	GLN
1	B	179	HIS
1	B	184	ASN
1	B	264	HIS
1	C	52	HIS
1	C	126	GLN
1	D	52	HIS
1	D	179	HIS
1	D	261	ASN
1	E	261	ASN

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 ⓘ

8 ligands are modelled in this entry.

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

There are no such residues in this entry.

5.8 Polymer linkage issues

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	272/278 (97%)	-0.11	9 (3%)	49	50	28, 43, 79, 133	0
1	B	272/278 (97%)	0.33	14 (5%)	33	31	32, 57, 97, 138	0
1	C	272/278 (97%)	0.58	22 (8%)	18	16	35, 63, 98, 129	0
1	D	270/278 (97%)	0.78	25 (9%)	14	12	45, 73, 113, 146	0
1	E	264/278 (94%)	1.71	98 (37%)	1	0	54, 97, 117, 138	0
All	All	1350/1390 (97%)	0.65	168 (12%)	8	7	28, 66, 112, 146	0

All (168) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	256	TYR	5.8
1	B	256	TYR	5.5
1	D	255	GLN	5.3
1	E	5	THR	5.1
1	C	241	GLU	4.9
1	E	256	TYR	4.9
1	E	156	THR	4.9
1	C	226	PHE	4.5
1	C	240	GLU	4.5
1	D	6	PRO	4.4
1	A	256	TYR	4.3
1	A	241	GLU	4.2
1	E	153	ALA	4.0
1	E	259	LEU	4.0
1	E	265	VAL	4.0
1	C	242	GLU	3.9
1	C	256	TYR	3.8
1	E	255	GLN	3.8
1	E	257	ALA	3.8
1	E	264	HIS	3.8

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Mol	Chain	Res	Type	RSRZ
1	E	258	CYS	3.7
1	E	86	VAL	3.7
1	E	227	VAL	3.7
1	E	46	GLY	3.6
1	E	10	LEU	3.6
1	E	97	ALA	3.5
1	E	251	PRO	3.4
1	D	264	HIS	3.4
1	C	6	PRO	3.3
1	E	191	LEU	3.3
1	E	260	PRO	3.3
1	D	243	PRO	3.3
1	A	242	GLU	3.3
1	A	5	THR	3.3
1	E	242	GLU	3.2
1	C	137	LYS	3.2
1	C	4	SER	3.2
1	B	226	PHE	3.2
1	E	116	PHE	3.2
1	E	64	VAL	3.2
1	E	249	GLY	3.2
1	E	152	ILE	3.2
1	E	102	SER	3.1
1	B	241	GLU	3.1
1	A	226	PHE	3.1
1	D	259	LEU	3.1
1	C	34	PHE	3.1
1	E	63	LEU	3.1
1	E	223	GLY	3.1
1	E	239	PRO	3.0
1	C	116	PHE	3.0
1	D	185	GLN	3.0
1	E	262	LEU	2.9
1	E	114	ILE	2.9
1	E	253	MET	2.9
1	E	189	ASP	2.9
1	D	226	PHE	2.9
1	E	22	ILE	2.9
1	E	219	ALA	2.9
1	E	226	PHE	2.9
1	E	6	PRO	2.8
1	E	216	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	270	GLU	2.8
1	C	5	THR	2.8
1	E	99	GLY	2.8
1	C	63	LEU	2.8
1	C	264	HIS	2.8
1	D	97	ALA	2.8
1	E	87	TYR	2.7
1	C	269	THR	2.7
1	E	122	LEU	2.7
1	E	213	LEU	2.7
1	E	45	LEU	2.7
1	D	186	THR	2.7
1	E	186	THR	2.7
1	E	254	ILE	2.7
1	E	266	GLY	2.6
1	E	252	PRO	2.6
1	E	240	GLU	2.6
1	E	57	ALA	2.6
1	E	100	LYS	2.6
1	D	268	PRO	2.6
1	E	110	ILE	2.6
1	E	228	ASN	2.6
1	E	88	PHE	2.6
1	E	19	LEU	2.6
1	E	105	LEU	2.6
1	E	261	ASN	2.6
1	E	126	GLN	2.6
1	E	7	ALA	2.6
1	E	29	HIS	2.6
1	E	111	GLY	2.5
1	D	254	ILE	2.5
1	C	21	LEU	2.5
1	D	261	ASN	2.5
1	D	269	THR	2.5
1	E	21	LEU	2.5
1	E	274	VAL	2.5
1	E	148	SER	2.5
1	E	275	PHE	2.5
1	E	89	LYS	2.5
1	A	4	SER	2.5
1	B	217	PRO	2.4
1	C	243	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
1	E	243	PRO	2.4
1	D	143	ILE	2.4
1	E	263	ASP	2.4
1	B	255	GLN	2.4
1	E	137	LYS	2.4
1	C	59	ILE	2.4
1	B	5	THR	2.4
1	E	65	VAL	2.4
1	B	243	PRO	2.3
1	E	98	GLY	2.3
1	E	142	ILE	2.3
1	E	181	LEU	2.3
1	C	42	GLN	2.3
1	E	267	HIS	2.3
1	B	224	GLN	2.3
1	E	123	LEU	2.3
1	D	257	ALA	2.2
1	B	223	GLY	2.2
1	C	255	GLN	2.2
1	E	109	GLN	2.2
1	A	243	PRO	2.2
1	D	227	VAL	2.2
1	D	260	PRO	2.2
1	D	271	ARG	2.2
1	D	262	LEU	2.2
1	E	231	MET	2.2
1	E	26	ILE	2.2
1	B	240	GLU	2.2
1	A	93	PRO	2.2
1	C	41	PRO	2.2
1	E	83	VAL	2.2
1	E	247	MET	2.2
1	E	214	ASP	2.2
1	E	85	LYS	2.2
1	D	154	GLY	2.1
1	D	244	LEU	2.1
1	E	244	LEU	2.1
1	E	241	GLU	2.1
1	C	36	PHE	2.1
1	D	265	VAL	2.1
1	E	108	MET	2.1
1	E	196	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	199	LEU	2.1
1	E	8	ILE	2.1
1	E	17	TYR	2.1
1	B	94	LYS	2.1
1	E	147	LYS	2.1
1	B	239	PRO	2.1
1	E	101	MET	2.1
1	B	220	TRP	2.1
1	E	269	THR	2.1
1	A	240	GLU	2.1
1	E	44	ILE	2.1
1	E	127	GLY	2.1
1	E	215	ARG	2.1
1	E	271	ARG	2.1
1	E	212	THR	2.1
1	D	240	GLU	2.0
1	E	113	THR	2.0
1	E	188	LYS	2.0
1	E	190	ILE	2.0
1	E	20	ARG	2.0
1	B	242	GLU	2.0
1	C	54	TYR	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(Å ²)	Q<0.9
2	FAD	C	1301[A]	53/53	0.75	0.17	52,85,108,113	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	FAD	C	1301[B]	53/53	0.75	0.17	52,85,108,113	1
2	FAD	B	1301[A]	53/53	0.95	0.08	34,52,76,83	1
2	FAD	B	1301[B]	53/53	0.95	0.08	34,52,76,83	1
2	FAD	D	1301[A]	53/53	0.95	0.09	52,67,83,90	1
2	FAD	D	1301[B]	53/53	0.95	0.09	52,67,83,90	1
2	FAD	A	1301[A]	53/53	0.96	0.09	31,51,75,84	1
2	FAD	A	1301[B]	53/53	0.96	0.09	31,51,75,84	1

6.5 Other polymers [i](#)

There are no such residues in this entry.