



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:49 AM UTC

PDB ID : 2DYB / pdb_00002dyb
Title : The crystal structure of human p40(phox)
Authors : Honbou, K.
Deposited on : 2006-09-08
Resolution : 3.15 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

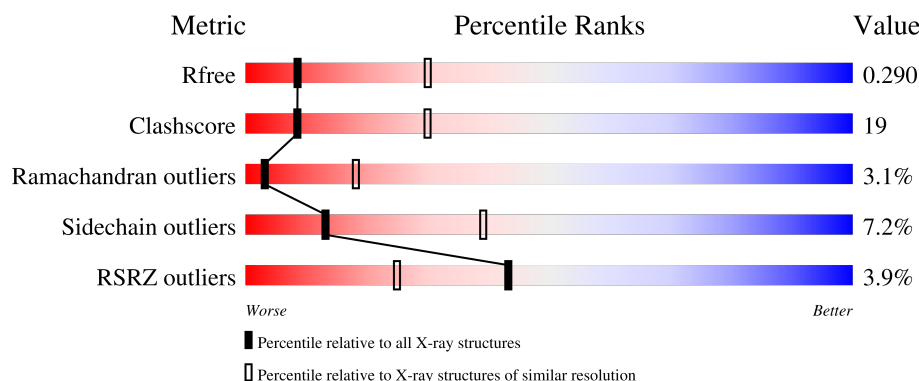
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.15 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	2361 (3.20-3.12)
Clashscore	190562	2486 (3.20-3.12)
Ramachandran outliers	187476	2405 (3.20-3.12)
Sidechain outliers	187428	2404 (3.20-3.12)
RSRZ outliers	180081	2361 (3.20-3.12)

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	341	5% 54% 32% • 13%
1	B	341	5% 46% 27% 7% 20%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	CAF	A	84	-	-	-	X

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 4252 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 Neutrophil cytosol factor 4.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	298	Total	As	C	N	O	S	0	0	0
			2273	1	1463	377	425	7			
1	B	273	Total	As	C	N	O	S	0	0	0
			1979	1	1270	329	374	5			

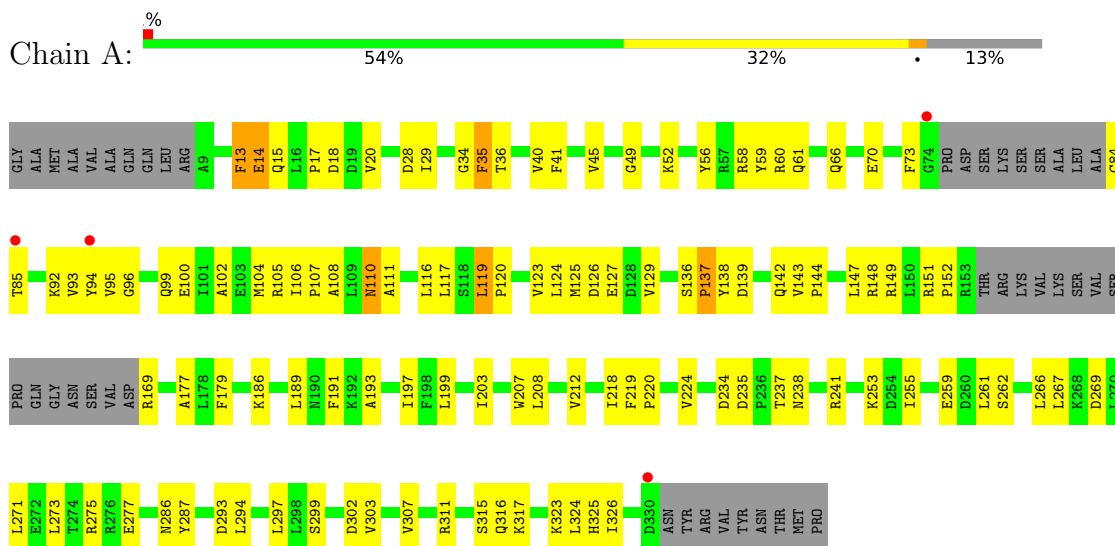
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	cloning artifact	UNP Q15080
A	0	ALA	-	cloning artifact	UNP Q15080
B	-1	GLY	-	cloning artifact	UNP Q15080
B	0	ALA	-	cloning artifact	UNP Q15080

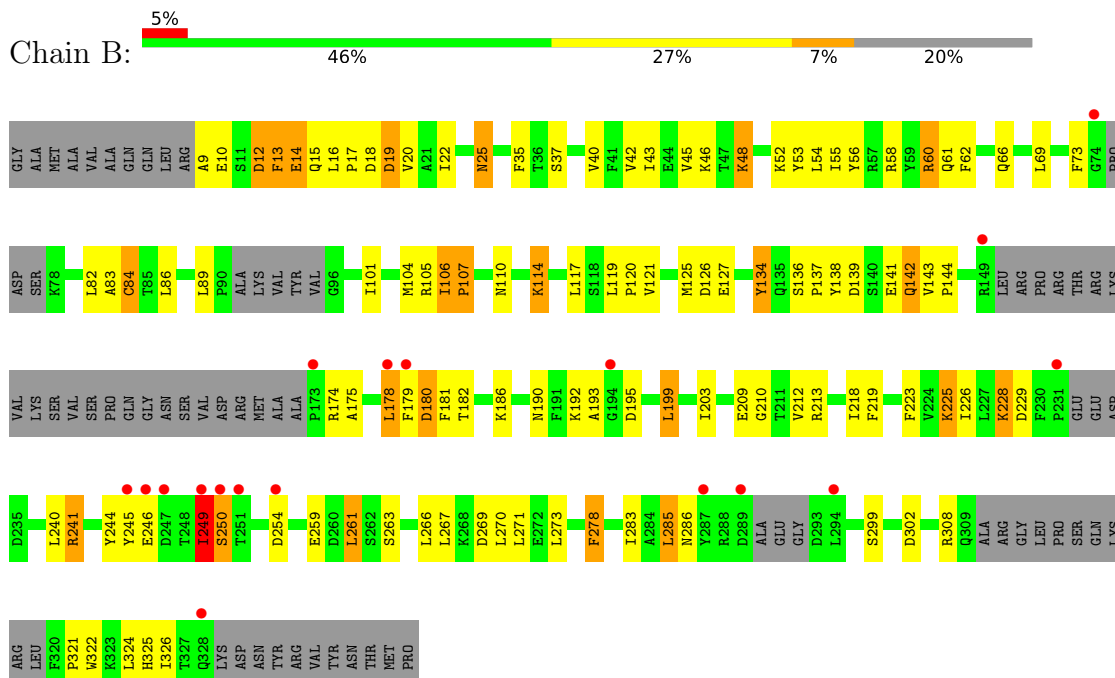
3 Residue-property plots [i](#)

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: Neutrophil cytosol factor 4



• Molecule 1: Neutrophil cytosol factor 4



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	146.27Å 189.81Å 79.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.80 – 3.15 40.80 – 3.15	Depositor EDS
% Data completeness (in resolution range)	97.7 (40.80-3.15) 97.6 (40.80-3.15)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.51 (at 3.01Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.263 , 0.302 0.245 , 0.290	Depositor DCC
R_{free} test set	2155 reflections (9.54%)	wwPDB-VP
Wilson B-factor (Å ²)	93.6	Xtriage
Anisotropy	0.541	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 62.6	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	0.91	EDS
Total number of atoms	4252	wwPDB-VP
Average B, all atoms (Å ²)	82.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.26% 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

5.1 Standard geometry

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

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	0.64	0/2314	1.05	11/3155 (0.3%)
1	B	0.65	2/2008 (0.1%)	1.11	19/2735 (0.7%)
All	All	0.65	2/4322 (0.0%)	1.08	30/5890 (0.5%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	246	GLU	CA-C	7.97	1.56	1.52
1	B	37	SER	CA-CB	5.27	1.60	1.52

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	226	ILE	N-CA-C	12.86	126.61	108.23
1	A	317	LYS	N-CA-C	10.02	121.79	111.07
1	A	316	GLN	N-CA-C	-9.36	95.91	110.42
1	B	249	ILE	N-CA-C	7.70	125.36	109.34
1	B	228	LYS	N-CA-C	7.12	125.98	110.80
1	A	151	ARG	CA-C-N	6.82	126.78	120.03
1	A	151	ARG	C-N-CA	6.82	126.78	120.03
1	B	179	PHE	N-CA-C	-6.72	99.16	109.65
1	A	36	THR	N-CA-C	-6.52	98.77	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	186	LYS	N-CA-C	-6.52	105.29	113.18
1	B	181	PHE	N-CA-C	6.42	119.37	108.90
1	B	250	SER	N-CA-C	6.21	119.31	109.50
1	A	92	LYS	N-CA-C	5.92	118.83	109.96
1	B	10	GLU	N-CA-C	-5.91	104.97	111.82
1	B	225	LYS	CA-C-N	-5.89	115.10	123.17
1	B	225	LYS	C-N-CA	-5.89	115.10	123.17
1	B	19	ASP	N-CA-C	5.84	120.11	113.15
1	B	142	GLN	N-CA-C	5.80	118.85	109.40
1	B	35	PHE	N-CA-C	-5.76	105.36	112.38
1	A	96	GLY	N-CA-C	-5.68	99.71	113.18
1	B	246	GLU	N-CA-C	5.67	117.14	108.12
1	B	62	PHE	N-CA-C	-5.60	104.57	111.40
1	B	308	ARG	N-CA-C	-5.48	105.39	111.36
1	B	174	ARG	N-CA-C	5.47	115.77	108.38
1	B	203	ILE	N-CA-C	-5.25	106.68	111.67
1	A	234	ASP	N-CA-C	5.23	119.64	113.16
1	B	73	PHE	N-CA-C	5.18	119.75	113.38
1	A	315	SER	N-CA-C	5.17	117.94	110.28
1	A	186	LYS	N-CA-C	-5.09	105.92	111.82
1	A	35	PHE	N-CA-C	-5.08	105.74	111.28

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	134	TYR	Sidechain

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	2273	0	2095	77	0
1	B	1979	0	1697	81	0
All	All	4252	0	3792	153	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 19.

All (153) 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:B:22:ILE:HD11	1:B:46:LYS:HE3	1.51	0.93
1:A:58:ARG:HG2	1:A:61:GLN:HG3	1.54	0.87
1:B:40:VAL:HG11	1:B:56:TYR:HB3	1.55	0.86
1:A:106:ILE:HB	1:A:107:PRO:HD3	1.55	0.86
1:A:299:SER:O	1:A:302:ASP:HB2	1.82	0.79
1:B:244:TYR:O	1:B:250:SER:HA	1.82	0.79
1:B:175:ALA:HB2	1:B:199:LEU:HD21	1.68	0.76
1:A:126:ASP:HB3	1:A:129:VAL:HG23	1.68	0.75
1:B:83:ALA:O	1:B:84:CAF:HB3	1.88	0.72
1:A:143:VAL:HB	1:A:144:PRO:HD3	1.71	0.72
1:A:241:ARG:HB3	1:A:323:LYS:HG2	1.73	0.71
1:A:110:ASN:H	1:A:110:ASN:HD22	1.39	0.70
1:A:120:PRO:O	1:A:123:VAL:HG12	1.92	0.70
1:A:149:ARG:O	1:A:152:PRO:HD3	1.91	0.70
1:B:105:ARG:C	1:B:107:PRO:HD2	2.16	0.70
1:B:175:ALA:HA	1:B:225:LYS:O	1.93	0.69
1:A:119:LEU:HB3	1:A:123:VAL:HG11	1.77	0.67
1:A:266:LEU:O	1:A:269:ASP:N	2.27	0.66
1:A:34:GLY:O	1:A:169:ARG:NH2	2.28	0.66
1:B:114:LYS:HE3	1:B:114:LYS:HA	1.78	0.65
1:A:253:LYS:NZ	1:A:277:GLU:OE1	2.25	0.65
1:A:108:ALA:O	1:A:111:ALA:HB3	1.98	0.64
1:B:240:LEU:HD21	1:B:324:LEU:HD12	1.79	0.64
1:A:28:ASP:OD1	1:A:29:ILE:N	2.33	0.62
1:A:147:LEU:HD21	1:B:144:PRO:CB	2.30	0.61
1:B:43:ILE:HB	1:B:55:ILE:HG13	1.81	0.61
1:A:286:ASN:HB3	1:A:294:LEU:HD11	1.82	0.60
1:A:287:TYR:CD2	1:A:297:LEU:HD21	2.37	0.60
1:B:119:LEU:HB3	1:B:120:PRO:HD2	1.84	0.60
1:B:241:ARG:HB2	1:B:254:ASP:OD1	2.01	0.59
1:B:16:LEU:HD11	1:B:121:VAL:HB	1.84	0.59
1:B:245:TYR:HA	1:B:249:ILE:O	2.03	0.58
1:A:177:ALA:HA	1:A:224:VAL:HG12	1.87	0.57
1:B:42:VAL:HG12	1:B:54:LEU:HD23	1.87	0.56
1:B:283:ILE:HD12	1:B:283:ILE:O	2.06	0.56
1:A:17:PRO:O	1:A:20:VAL:HG12	2.06	0.56
1:B:17:PRO:HG2	1:B:20:VAL:HG23	1.88	0.55
1:A:119:LEU:HB3	1:A:123:VAL:CG1	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:199:LEU:HD22	1:A:208:LEU:HD23	1.90	0.54
1:A:35:PHE:HA	1:A:273:LEU:HD12	1.90	0.54
1:B:286:ASN:O	1:B:325:HIS:HB2	2.07	0.54
1:A:13:PHE:O	1:A:15:GLN:N	2.40	0.54
1:A:267:LEU:O	1:A:271:LEU:HG	2.08	0.53
1:A:58:ARG:CG	1:A:61:GLN:HG3	2.32	0.53
1:A:126:ASP:HB3	1:A:129:VAL:CG2	2.36	0.53
1:A:212:VAL:O	1:A:212:VAL:HG13	2.07	0.53
1:A:207:TRP:O	1:A:208:LEU:HD12	2.08	0.53
1:A:267:LEU:HD11	1:A:271:LEU:HD11	1.90	0.53
1:B:285:LEU:CD2	1:B:285:LEU:N	2.72	0.53
1:A:238:ASN:OD1	1:A:261:LEU:HD13	2.09	0.52
1:B:13:PHE:O	1:B:16:LEU:N	2.36	0.52
1:B:244:TYR:O	1:B:250:SER:CA	2.56	0.52
1:B:285:LEU:HD12	1:B:324:LEU:HD22	1.92	0.52
1:A:106:ILE:HB	1:A:107:PRO:CD	2.35	0.52
1:A:119:LEU:HD12	1:A:123:VAL:HG11	1.91	0.52
1:B:299:SER:H	1:B:302:ASP:CG	2.18	0.52
1:B:209:GLU:HG2	1:B:210:GLY:N	2.25	0.52
1:A:148:ARG:HH22	1:B:25:ASN:HB3	1.75	0.51
1:B:114:LYS:HE3	1:B:114:LYS:CA	2.41	0.51
1:B:119:LEU:HB3	1:B:120:PRO:CD	2.40	0.51
1:A:117:LEU:HA	1:A:124:LEU:HD11	1.92	0.50
1:A:267:LEU:HD13	1:A:267:LEU:C	2.36	0.50
1:B:13:PHE:O	1:B:14:GLU:C	2.55	0.50
1:A:40:VAL:HG11	1:A:56:TYR:HB3	1.93	0.50
1:A:286:ASN:O	1:A:325:HIS:N	2.42	0.50
1:A:271:LEU:O	1:A:275:ARG:HG3	2.12	0.49
1:A:106:ILE:CB	1:A:107:PRO:HD3	2.36	0.49
1:A:66:GLN:O	1:A:70:GLU:HG3	2.12	0.49
1:B:105:ARG:O	1:B:107:PRO:N	2.45	0.49
1:B:175:ALA:CA	1:B:225:LYS:O	2.60	0.49
1:B:13:PHE:O	1:B:16:LEU:HB2	2.12	0.49
1:B:266:LEU:O	1:B:267:LEU:C	2.56	0.49
1:B:285:LEU:HD13	1:B:326:ILE:HD12	1.95	0.49
1:B:261:LEU:O	1:B:261:LEU:HD23	2.12	0.49
1:A:255:ILE:HD13	1:A:277:GLU:HG3	1.94	0.49
1:A:136:SER:O	1:A:137:PRO:C	2.56	0.48
1:B:278:PHE:CD1	1:B:278:PHE:N	2.81	0.48
1:A:266:LEU:O	1:A:267:LEU:C	2.57	0.48
1:A:286:ASN:CB	1:A:294:LEU:HD11	2.42	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:303:VAL:O	1:A:307:VAL:HG23	2.13	0.48
1:A:147:LEU:HD21	1:B:144:PRO:HB2	1.95	0.48
1:B:105:ARG:C	1:B:107:PRO:CD	2.85	0.48
1:B:106:ILE:O	1:B:110:ASN:ND2	2.47	0.47
1:A:99:GLN:O	1:A:102:ALA:HB3	2.13	0.47
1:B:285:LEU:N	1:B:285:LEU:HD22	2.29	0.47
1:A:40:VAL:HG12	1:A:41:PHE:N	2.30	0.47
1:B:278:PHE:N	1:B:278:PHE:HD1	2.12	0.47
1:A:147:LEU:HD21	1:B:144:PRO:HB3	1.97	0.47
1:A:138:TYR:O	1:A:142:GLN:HG3	2.14	0.46
1:B:283:ILE:HD12	1:B:283:ILE:C	2.41	0.46
1:A:238:ASN:ND2	1:A:259:GLU:O	2.48	0.46
1:B:137:PRO:O	1:B:141:GLU:HG3	2.16	0.46
1:A:100:GLU:C	1:A:102:ALA:N	2.74	0.46
1:B:126:ASP:O	1:B:127:GLU:C	2.58	0.46
1:B:60:ARG:NH2	1:B:269:ASP:OD2	2.49	0.46
1:B:66:GLN:OE1	1:B:89:LEU:HB2	2.16	0.45
1:B:180:ASP:OD1	1:B:193:ALA:N	2.47	0.45
1:A:59:TYR:CD1	1:A:105:ARG:HD3	2.51	0.45
1:A:326:ILE:N	1:A:326:ILE:HD12	2.30	0.45
1:B:16:LEU:HG	1:B:125:MET:HE1	1.97	0.45
1:A:110:ASN:H	1:A:110:ASN:ND2	2.08	0.45
1:A:287:TYR:CE2	1:A:297:LEU:HD21	2.52	0.45
1:A:179:PHE:CA	1:A:193:ALA:HB2	2.46	0.45
1:B:58:ARG:O	1:B:61:GLN:HB2	2.16	0.45
1:B:13:PHE:O	1:B:15:GLN:N	2.50	0.45
1:B:82:LEU:O	1:B:83:ALA:HB3	2.17	0.45
1:B:101:ILE:O	1:B:104:MET:HB3	2.18	0.44
1:B:101:ILE:O	1:B:104:MET:N	2.51	0.44
1:A:189:LEU:HD11	1:A:212:VAL:HG12	1.99	0.43
1:B:42:VAL:CG1	1:B:54:LEU:HD23	2.47	0.43
1:B:178:LEU:HB2	1:B:223:PHE:O	2.17	0.43
1:B:9:ALA:N	1:B:12:ASP:HB2	2.33	0.43
1:B:244:TYR:CD1	1:B:278:PHE:CD2	3.07	0.43
1:A:179:PHE:C	1:A:193:ALA:HB2	2.43	0.43
1:B:45:VAL:HB	1:B:53:TYR:CE1	2.54	0.43
1:A:20:VAL:HG13	1:A:20:VAL:O	2.18	0.43
1:B:43:ILE:HB	1:B:55:ILE:CG1	2.47	0.43
1:B:270:LEU:O	1:B:273:LEU:HB3	2.19	0.43
1:B:53:TYR:CD1	1:B:53:TYR:C	2.95	0.43
1:A:179:PHE:HA	1:A:193:ALA:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:18:ASP:HA	1:B:48:LYS:HE2	1.99	0.43
1:A:119:LEU:HB3	1:A:120:PRO:HD2	2.00	0.43
1:B:69:LEU:HA	1:B:69:LEU:HD23	1.72	0.43
1:A:235:ASP:OD1	1:A:237:THR:HB	2.19	0.42
1:B:199:LEU:H	1:B:199:LEU:HG	1.48	0.42
1:B:270:LEU:HD22	1:B:324:LEU:HD11	2.01	0.42
1:A:56:TYR:CD1	1:A:56:TYR:N	2.88	0.42
1:A:84:CAF:SG	1:A:85:THR:N	2.91	0.42
1:B:9:ALA:CA	1:B:12:ASP:HB2	2.49	0.42
1:A:45:VAL:O	1:A:52:LYS:HA	2.20	0.42
1:A:219:PHE:HB2	1:A:220:PRO:HD2	2.01	0.42
1:B:182:THR:HA	1:B:190:ASN:OD1	2.19	0.42
1:A:59:TYR:O	1:A:61:GLN:N	2.53	0.42
1:A:138:TYR:CE1	1:A:142:GLN:NE2	2.88	0.42
1:B:9:ALA:HA	1:B:12:ASP:HB2	2.01	0.42
1:B:136:SER:O	1:B:139:ASP:HB2	2.20	0.42
1:B:322:TRP:H	1:B:322:TRP:CD1	2.36	0.42
1:B:138:TYR:CE2	1:B:142:GLN:NE2	2.88	0.41
1:B:218:ILE:O	1:B:219:PHE:HB3	2.21	0.41
1:A:267:LEU:CD1	1:A:271:LEU:HD11	2.50	0.41
1:B:19:ASP:OD1	1:B:19:ASP:C	2.64	0.41
1:A:191:PHE:CD2	1:A:197:ILE:HD11	2.55	0.41
1:A:18:ASP:HB3	1:A:49:GLY:HA3	2.02	0.41
1:B:195:ASP:OD2	1:B:213:ARG:NH2	2.53	0.41
1:B:86:LEU:HD23	1:B:86:LEU:HA	1.91	0.41
1:A:136:SER:HG	1:A:139:ASP:CG	2.27	0.40
1:B:192:LYS:O	1:B:195:ASP:HB2	2.20	0.40
1:A:147:LEU:HD12	1:B:54:LEU:HD21	2.02	0.40
1:B:143:VAL:O	1:B:144:PRO:C	2.63	0.40
1:A:203:ILE:HD11	1:A:218:ILE:HG22	2.03	0.40
1:B:114:LYS:HE3	1:B:114:LYS:O	2.21	0.40
1:A:126:ASP:O	1:A:127:GLU:C	2.65	0.40
1:B:241:ARG:NH2	1:B:254:ASP:OD2	2.55	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	292/341 (86%)	262 (90%)	23 (8%)	7 (2%)	4	23
1	B	258/341 (76%)	227 (88%)	21 (8%)	10 (4%)	2	14
All	All	550/682 (81%)	489 (89%)	44 (8%)	17 (3%)	3	18

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	14	GLU
1	B	14	GLU
1	B	106	ILE
1	B	212	VAL
1	B	259	GLU
1	A	60	ARG
1	B	228	LYS
1	B	263	SER
1	B	321	PRO
1	A	13	PHE
1	A	95	VAL
1	A	311	ARG
1	B	107	PRO
1	B	13	PHE
1	B	249	ILE
1	A	73	PHE
1	A	93	VAL

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	219/300 (73%)	208 (95%)	11 (5%)	22	50
1	B	170/300 (57%)	153 (90%)	17 (10%)	7	27
All	All	389/600 (65%)	361 (93%)	28 (7%)	13	39

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	GLU
1	A	94	TYR
1	A	104	MET
1	A	110	ASN
1	A	116	LEU
1	A	119	LEU
1	A	125	MET
1	A	137	PRO
1	A	262	SER
1	A	293	ASP
1	A	324	LEU
1	B	12	ASP
1	B	25	ASN
1	B	48	LYS
1	B	52	LYS
1	B	60	ARG
1	B	114	LYS
1	B	117	LEU
1	B	134	TYR
1	B	178	LEU
1	B	180	ASP
1	B	199	LEU
1	B	229	ASP
1	B	241	ARG
1	B	261	LEU
1	B	271	LEU
1	B	278	PHE
1	B	285	LEU

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	110	ASN
1	A	145	GLN
1	B	25	ASN
1	B	99	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

2 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	CAF	B	84	1	5,9,10	0.75	0	4,12,14	1.36	1 (25%)
1	CAF	A	84	1	5,9,10	0.75	0	4,12,14	0.92	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CAF	B	84	1	-	0/0/8/10	-
1	CAF	A	84	1	-	0/0/8/10	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	84	CAF	CA-CB-SG	2.12	117.36	112.49

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	84	CAF	1	0
1	A	84	CAF	1	0

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	297/341 (87%)	0.03	4 (1%) 75 55	45, 72, 109, 123	0
1	B	272/341 (79%)	0.49	18 (6%) 24 14	53, 100, 122, 129	0
All	All	569/682 (83%)	0.25	22 (3%) 43 25	45, 78, 120, 129	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	249	ILE	5.0
1	A	74	GLY	4.8
1	B	328	GLN	3.2
1	B	251	THR	3.0
1	A	330	ASP	2.9
1	B	194	GLY	2.9
1	B	179	PHE	2.9
1	B	245	TYR	2.9
1	B	250	SER	2.8
1	B	287	TYR	2.8
1	B	231	PRO	2.8
1	B	254	ASP	2.6
1	B	173	PRO	2.5
1	B	246	GLU	2.4
1	B	247	ASP	2.3
1	A	85	THR	2.2
1	B	294	LEU	2.2
1	A	94	TYR	2.2
1	B	178	LEU	2.2
1	B	149	ARG	2.1
1	B	74	GLY	2.1
1	B	289	ASP	2.1

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	CAF	A	84	10/11	0.79	0.48	105,106,108,108	10
1	CAF	B	84	10/11	0.97	0.12	81,84,88,89	0

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.