



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 11:13 AM UTC

PDB ID : 6E2Q / pdb_00006e2q
Title : Structure of human JAK2 FERM/SH2 in complex with Erythropoietin Receptor
Authors : Ferrao, R.; Lupardus, P.J.
Deposited on : 2018-07-11
Resolution : 2.65 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

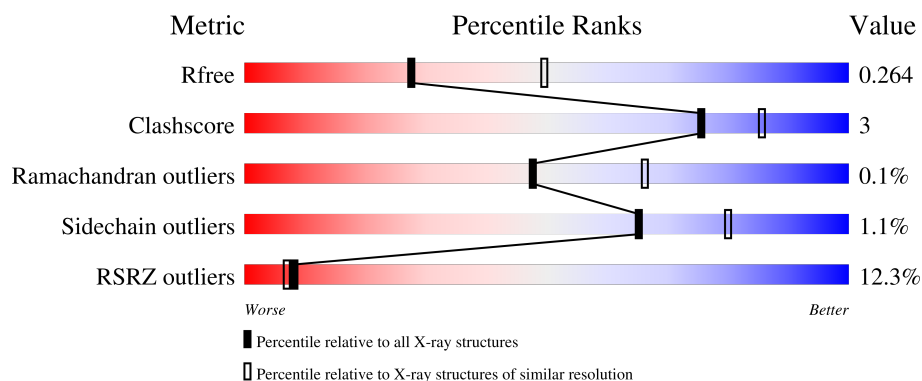
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 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	1110 (2.66-2.66)
Clashscore	190562	1141 (2.66-2.66)
Ramachandran outliers	187476	1126 (2.66-2.66)
Sidechain outliers	187428	1126 (2.66-2.66)
RSRZ outliers	180081	1110 (2.66-2.66)

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	483	6% 90% 8% .
1	B	483	8% 90% 7% .
1	C	483	13% 85% 11% .
1	D	483	16% 80% 10% 11%
2	M	83	12% 45% 7% . 47%

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Mol	Chain	Length	Quality of chain
2	N	83	13%63%31%
2	O	83	11%59%37%
2	P	83	14%54%43%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 16599 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 Tyrosine-protein kinase JAK2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	473	Total	C	N	O	S	0	0	0
			3840	2457	660	702	21			
1	B	470	Total	C	N	O	S	0	0	0
			3809	2440	652	695	22			
1	C	463	Total	C	N	O	S	0	0	0
			3705	2378	630	676	21			
1	D	431	Total	C	N	O	S	0	0	0
			3493	2248	595	632	18			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	34	GLY	-	expression tag	UNP O60674
A	35	SER	-	expression tag	UNP O60674
A	515	GLY	-	expression tag	UNP O60674
A	516	SER	-	expression tag	UNP O60674
B	34	GLY	-	expression tag	UNP O60674
B	35	SER	-	expression tag	UNP O60674
B	515	GLY	-	expression tag	UNP O60674
B	516	SER	-	expression tag	UNP O60674
C	34	GLY	-	expression tag	UNP O60674
C	35	SER	-	expression tag	UNP O60674
C	515	GLY	-	expression tag	UNP O60674
C	516	SER	-	expression tag	UNP O60674
D	34	GLY	-	expression tag	UNP O60674
D	35	SER	-	expression tag	UNP O60674
D	515	GLY	-	expression tag	UNP O60674
D	516	SER	-	expression tag	UNP O60674

- Molecule 2 is a protein called Erythropoietin receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	M	44	Total	C	N	O	S	0	0	0
			362	239	57	64	2			
2	N	57	Total	C	N	O	S	0	0	0
			454	296	70	86	2			
2	O	52	Total	C	N	O	S	0	0	0
			417	273	64	79	1			
2	P	47	Total	C	N	O	S	0	0	0
			374	247	59	66	2			

There are 68 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	259	GLY	-	expression tag	UNP P19235
M	260	SER	-	expression tag	UNP P19235
M	261	GLY	-	expression tag	UNP P19235
M	262	SER	-	expression tag	UNP P19235
M	263	GLY	-	expression tag	UNP P19235
M	264	SER	-	expression tag	UNP P19235
M	265	GLY	-	expression tag	UNP P19235
M	266	SER	-	expression tag	UNP P19235
M	267	GLY	-	expression tag	UNP P19235
M	268	SER	-	expression tag	UNP P19235
M	269	GLY	-	expression tag	UNP P19235
M	270	SER	-	expression tag	UNP P19235
M	271	GLY	-	expression tag	UNP P19235
M	272	SER	-	expression tag	UNP P19235
M	339	GLY	-	expression tag	UNP P19235
M	340	ASN	-	expression tag	UNP P19235
M	341	SER	-	expression tag	UNP P19235
N	259	GLY	-	expression tag	UNP P19235
N	260	SER	-	expression tag	UNP P19235
N	261	GLY	-	expression tag	UNP P19235
N	262	SER	-	expression tag	UNP P19235
N	263	GLY	-	expression tag	UNP P19235
N	264	SER	-	expression tag	UNP P19235
N	265	GLY	-	expression tag	UNP P19235
N	266	SER	-	expression tag	UNP P19235
N	267	GLY	-	expression tag	UNP P19235
N	268	SER	-	expression tag	UNP P19235
N	269	GLY	-	expression tag	UNP P19235
N	270	SER	-	expression tag	UNP P19235
N	271	GLY	-	expression tag	UNP P19235
N	272	SER	-	expression tag	UNP P19235

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Chain	Residue	Modelled	Actual	Comment	Reference
N	339	GLY	-	expression tag	UNP P19235
N	340	ASN	-	expression tag	UNP P19235
N	341	SER	-	expression tag	UNP P19235
O	259	GLY	-	expression tag	UNP P19235
O	260	SER	-	expression tag	UNP P19235
O	261	GLY	-	expression tag	UNP P19235
O	262	SER	-	expression tag	UNP P19235
O	263	GLY	-	expression tag	UNP P19235
O	264	SER	-	expression tag	UNP P19235
O	265	GLY	-	expression tag	UNP P19235
O	266	SER	-	expression tag	UNP P19235
O	267	GLY	-	expression tag	UNP P19235
O	268	SER	-	expression tag	UNP P19235
O	269	GLY	-	expression tag	UNP P19235
O	270	SER	-	expression tag	UNP P19235
O	271	GLY	-	expression tag	UNP P19235
O	272	SER	-	expression tag	UNP P19235
O	339	GLY	-	expression tag	UNP P19235
O	340	ASN	-	expression tag	UNP P19235
O	341	SER	-	expression tag	UNP P19235
P	259	GLY	-	expression tag	UNP P19235
P	260	SER	-	expression tag	UNP P19235
P	261	GLY	-	expression tag	UNP P19235
P	262	SER	-	expression tag	UNP P19235
P	263	GLY	-	expression tag	UNP P19235
P	264	SER	-	expression tag	UNP P19235
P	265	GLY	-	expression tag	UNP P19235
P	266	SER	-	expression tag	UNP P19235
P	267	GLY	-	expression tag	UNP P19235
P	268	SER	-	expression tag	UNP P19235
P	269	GLY	-	expression tag	UNP P19235
P	270	SER	-	expression tag	UNP P19235
P	271	GLY	-	expression tag	UNP P19235
P	272	SER	-	expression tag	UNP P19235
P	339	GLY	-	expression tag	UNP P19235
P	340	ASN	-	expression tag	UNP P19235
P	341	SER	-	expression tag	UNP P19235

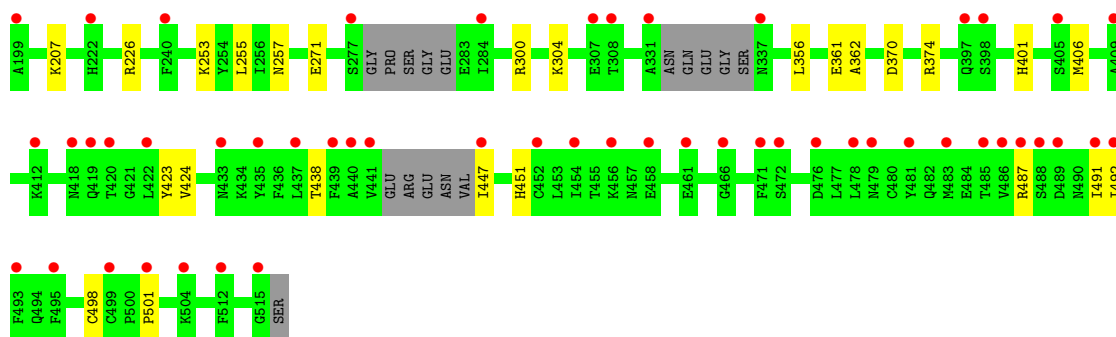
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	55	Total O 55 55	0	0

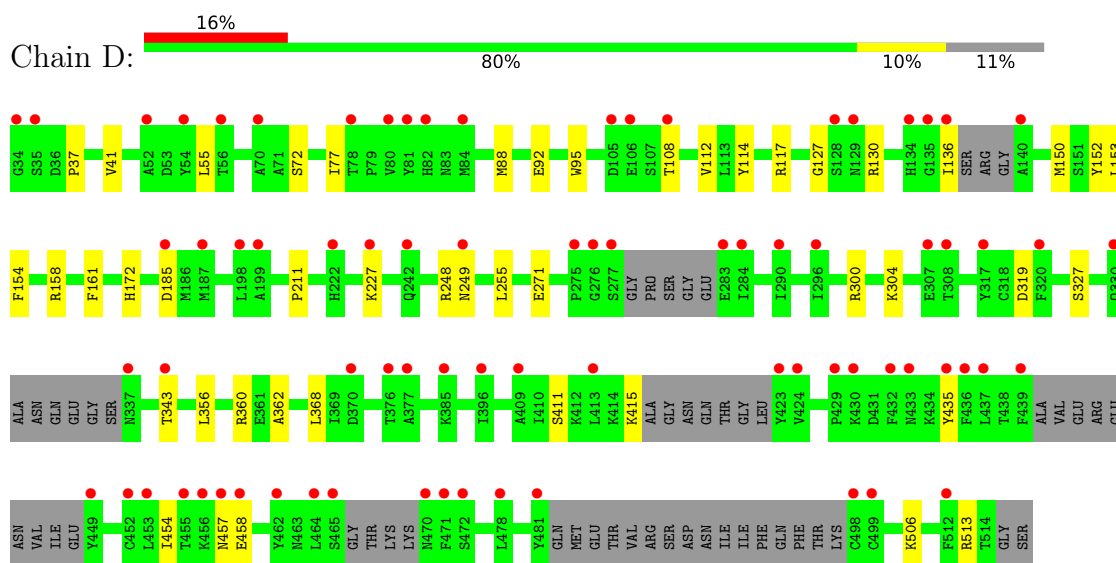
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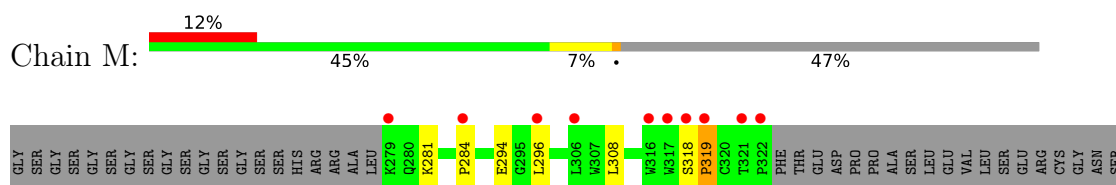
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	38	Total 38	O 38	0	0
3	C	31	Total 31	O 31	0	0
3	D	11	Total 11	O 11	0	0
3	M	3	Total 3	O 3	0	0
3	N	4	Total 4	O 4	0	0
3	O	2	Total 2	O 2	0	0
3	P	1	Total 1	O 1	0	0



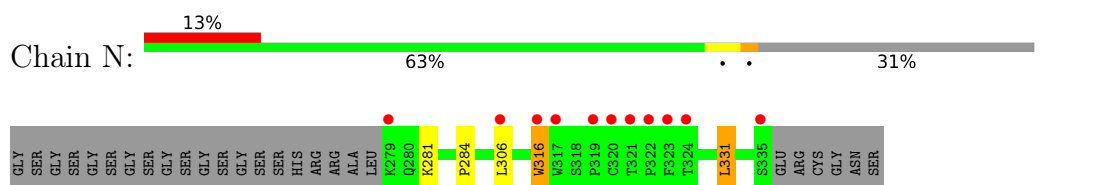
• Molecule 1: Tyrosine-protein kinase JAK2



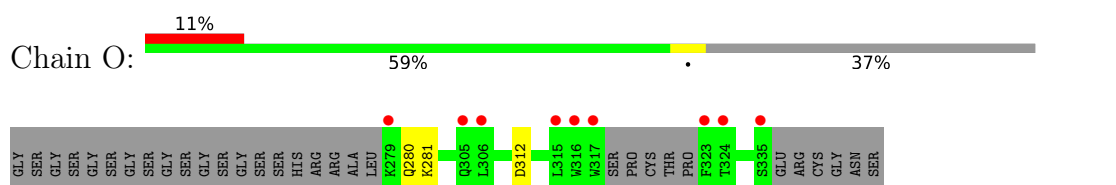
• Molecule 2: Erythropoietin receptor



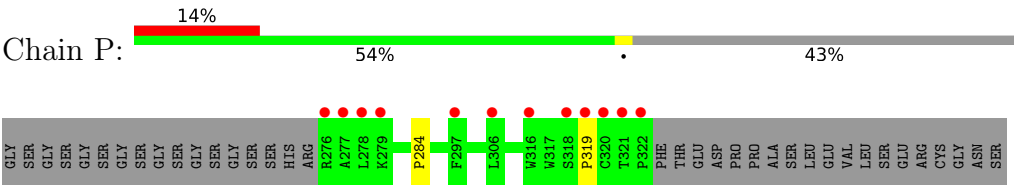
• Molecule 2: Erythropoietin receptor



• Molecule 2: Erythropoietin receptor



● Molecule 2: Erythropoietin receptor



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	178.49Å 114.88Å 179.82Å 90.00° 93.21° 90.00°	Depositor
Resolution (Å)	48.44 – 2.65 48.44 – 2.65	Depositor EDS
% Data completeness (in resolution range)	99.6 (48.44-2.65) 92.0 (48.44-2.65)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.95 (at 2.65Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.225 , 0.263 0.228 , 0.264	Depositor DCC
R_{free} test set	1997 reflections (1.90%)	wwPDB-VP
Wilson B-factor (Å ²)	54.0	Xtriage
Anisotropy	0.519	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 36.7	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	16599	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.33% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.08	0/3933	0.25	0/5319
1	B	0.08	0/3902	0.25	0/5277
1	C	0.07	0/3795	0.24	0/5141
1	D	0.07	0/3578	0.23	0/4839
2	M	0.09	0/379	0.22	0/520
2	N	0.08	0/473	0.25	0/651
2	O	0.06	0/433	0.19	0/594
2	P	0.08	0/391	0.22	0/538
All	All	0.08	0/16884	0.24	0/22879

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 [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	3840	0	3769	22	0
1	B	3809	0	3736	20	0
1	C	3705	0	3582	28	0
1	D	3493	0	3403	26	0
2	M	362	0	327	5	0
2	N	454	0	412	4	0
2	O	417	0	369	2	0
2	P	374	0	329	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	55	0	0	0	0
3	B	38	0	0	1	0
3	C	31	0	0	1	0
3	D	11	0	0	0	0
3	M	3	0	0	0	0
3	N	4	0	0	0	0
3	O	2	0	0	0	0
3	P	1	0	0	0	0
All	All	16599	0	15927	97	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 3.

All (97) 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:300:ARG:NH2	2:M:281:LYS:O	2.25	0.69
1:A:122:ARG:NH1	1:A:125:CYS:SG	2.74	0.60
1:A:248:ARG:NH2	2:N:316:TRP:O	2.35	0.60
1:B:78:THR:HG22	1:B:80:VAL:H	1.68	0.59
1:C:300:ARG:NH2	2:N:281:LYS:O	2.36	0.57
1:C:122:ARG:NH1	1:C:128:SER:O	2.38	0.56
1:D:300:ARG:NH2	2:O:281:LYS:O	2.38	0.56
1:C:38:VAL:HG23	1:C:56:THR:HG23	1.87	0.56
1:B:271:GLU:HG3	1:B:304:LYS:HB2	1.88	0.55
1:D:457:ASN:OD1	1:D:458:GLU:N	2.40	0.55
1:A:167:LYS:O	1:A:262:GLN:NE2	2.35	0.54
1:B:51:GLU:HG3	1:B:52:ALA:H	1.72	0.54
1:B:138:ARG:NH1	2:M:294:GLU:OE2	2.41	0.54
1:D:435:TYR:HB2	1:D:454:ILE:HB	1.90	0.54
1:C:401:HIS:HD1	1:C:501:PRO:HG3	1.71	0.53
1:B:154:PHE:HA	1:B:255:LEU:HD21	1.90	0.53
1:D:41:VAL:HB	1:D:55:LEU:HB2	1.89	0.53
1:C:370:ASP:OD2	1:C:374:ARG:NH2	2.39	0.52
1:B:117:ARG:NH1	3:B:604:HOH:O	2.38	0.52
1:A:38:VAL:HG23	1:A:56:THR:HG23	1.91	0.52
1:C:356:LEU:HD23	1:C:361:GLU:HG2	1.91	0.52
1:C:487:ARG:HA	1:C:492:ILE:HA	1.91	0.52
1:B:253:LYS:HE3	1:B:257:ASN:HD21	1.75	0.51
1:D:114:TYR:O	1:D:152:TYR:OH	2.24	0.51
1:D:271:GLU:HG3	1:D:304:LYS:HB2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:PHE:HA	1:A:255:LEU:HD21	1.93	0.50
1:C:51:GLU:HG3	1:C:52:ALA:H	1.76	0.50
1:C:154:PHE:HA	1:C:255:LEU:HD21	1.92	0.50
1:A:181:MET:HE2	1:A:257:ASN:HB3	1.93	0.50
1:C:153:LEU:HD23	1:C:255:LEU:HD13	1.92	0.50
1:C:356:LEU:HD22	1:C:362:ALA:HA	1.94	0.50
1:D:154:PHE:HA	1:D:255:LEU:HD21	1.94	0.50
1:C:423:TYR:CZ	1:C:498:CYS:HB3	2.46	0.49
1:A:41:VAL:HB	1:A:55:LEU:HB2	1.94	0.49
1:D:172:HIS:CE1	2:P:284:PRO:HB2	2.49	0.48
1:C:122:ARG:NH2	3:C:603:HOH:O	2.47	0.47
1:D:127:GLY:O	1:D:130:ARG:NH1	2.46	0.47
1:A:300:ARG:HH21	2:M:284:PRO:HD3	1.80	0.47
1:C:187:MET:SD	1:C:197:PRO:HB3	2.54	0.47
1:C:271:GLU:HG3	1:C:304:LYS:HB2	1.96	0.47
1:B:167:LYS:O	1:B:262:GLN:NE2	2.43	0.47
1:D:37:PRO:HB3	1:D:108:THR:H	1.80	0.47
1:A:172:HIS:CE1	2:N:284:PRO:HB2	2.49	0.47
1:D:356:LEU:HD22	1:D:362:ALA:HA	1.96	0.47
1:B:356:LEU:HD22	1:B:362:ALA:HA	1.97	0.47
1:C:406:MET:SD	1:C:451:HIS:NE2	2.89	0.46
1:A:51:GLU:HG3	1:A:52:ALA:H	1.81	0.46
1:D:117:ARG:NH2	1:D:368:LEU:HB2	2.30	0.46
1:B:117:ARG:NH2	1:B:368:LEU:HB2	2.31	0.46
1:D:327:SER:OG	1:D:343:THR:OG1	2.34	0.46
1:C:253:LYS:HE3	1:C:257:ASN:HD21	1.81	0.46
1:A:114:TYR:O	1:A:152:TYR:OH	2.23	0.45
1:A:133:ARG:HB2	1:A:142:ALA:HB3	1.99	0.45
2:M:318:SER:OG	2:M:319:PRO:HD3	2.18	0.44
1:D:227:LYS:HE2	1:D:227:LYS:HB3	1.88	0.44
1:D:150:MET:HE1	1:D:248:ARG:HG3	2.00	0.44
1:A:435:TYR:HB2	1:A:454:ILE:HB	1.99	0.44
1:C:401:HIS:ND1	1:C:501:PRO:HG3	2.33	0.44
1:A:356:LEU:HD22	1:A:362:ALA:HA	1.99	0.43
1:C:253:LYS:HB2	2:M:308:LEU:HD21	1.99	0.43
1:D:319:ASP:OD2	1:D:513:ARG:NH2	2.48	0.43
1:B:412:LYS:NZ	1:B:500:PRO:O	2.51	0.43
1:D:506:LYS:HD3	1:D:506:LYS:HA	1.83	0.43
1:B:356:LEU:HD23	1:B:361:GLU:HG2	2.01	0.43
1:D:153:LEU:HD23	1:D:255:LEU:HD13	1.99	0.43
1:A:136:ILE:HD13	1:A:407:ASP:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:421:GLY:HA3	1:B:496:THR:HG22	2.01	0.43
1:A:147:ASP:OD1	1:A:248:ARG:NH1	2.51	0.43
1:A:452:CYS:SG	2:N:331:LEU:HD23	2.59	0.43
1:C:181:MET:HE2	1:C:257:ASN:HB3	2.00	0.43
1:A:290:ILE:HD11	1:A:365:PHE:HE1	1.83	0.43
1:B:153:LEU:HD23	1:B:255:LEU:HD13	2.00	0.43
1:A:433:ASN:OD1	1:A:456:LYS:NZ	2.52	0.42
1:C:145:LEU:HB2	1:C:149:VAL:HB	2.00	0.42
1:C:39:LEU:HB2	1:C:104:ILE:HG13	2.01	0.42
1:B:277:SER:O	1:B:281:GLY:N	2.52	0.42
1:D:161:PHE:CZ	1:D:211:PRO:HG3	2.53	0.42
1:D:249:ASN:ND2	2:P:319:PRO:O	2.52	0.42
1:B:506:LYS:HA	1:B:506:LYS:HD3	1.86	0.42
1:D:88:MET:HE3	1:D:95:TRP:CE2	2.55	0.42
1:D:411:SER:O	1:D:415:LYS:HG2	2.20	0.42
1:B:435:TYR:HB2	1:B:454:ILE:HB	2.02	0.41
1:C:78:THR:OG1	1:C:80:VAL:HG12	2.20	0.41
1:A:506:LYS:HA	1:A:506:LYS:HD3	1.92	0.41
1:B:456:LYS:HD2	1:B:462:TYR:CE1	2.55	0.41
1:C:169:PRO:HG2	1:C:174:THR:HG21	2.02	0.41
1:D:92:GLU:OE1	1:D:360:ARG:NH1	2.53	0.41
1:C:207:LYS:HZ1	1:C:226:ARG:HD2	1.86	0.41
1:D:72:SER:HB3	1:D:77:ILE:HB	2.03	0.41
1:A:118:PHE:CZ	1:A:371:GLY:HA3	2.56	0.41
1:B:253:LYS:NZ	2:O:312:ASP:OD2	2.50	0.41
1:C:105:ASP:N	1:C:108:THR:OG1	2.54	0.40
1:C:424:VAL:N	1:C:438:THR:O	2.54	0.40
1:C:41:VAL:HB	1:C:55:LEU:HB2	2.03	0.40
1:D:158:ARG:NE	1:D:185:ASP:OD2	2.54	0.40
1:B:370:ASP:OD2	1:B:374:ARG:NH2	2.49	0.40
1:D:435:TYR:N	1:D:454:ILE:O	2.50	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	467/483 (97%)	455 (97%)	12 (3%)	0	100	100
1	B	464/483 (96%)	446 (96%)	18 (4%)	0	100	100
1	C	453/483 (94%)	440 (97%)	13 (3%)	0	100	100
1	D	415/483 (86%)	399 (96%)	16 (4%)	0	100	100
2	M	42/83 (51%)	39 (93%)	2 (5%)	1 (2%)	4	7
2	N	55/83 (66%)	51 (93%)	4 (7%)	0	100	100
2	O	48/83 (58%)	46 (96%)	2 (4%)	0	100	100
2	P	45/83 (54%)	41 (91%)	4 (9%)	0	100	100
All	All	1989/2264 (88%)	1917 (96%)	71 (4%)	1 (0%)	48	66

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	M	319	PRO

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	419/432 (97%)	416 (99%)	3 (1%)	76	86
1	B	415/432 (96%)	411 (99%)	4 (1%)	68	81
1	C	395/432 (91%)	389 (98%)	6 (2%)	57	75
1	D	377/432 (87%)	375 (100%)	2 (0%)	81	91
2	M	39/69 (56%)	38 (97%)	1 (3%)	40	63
2	N	50/69 (72%)	47 (94%)	3 (6%)	17	30
2	O	44/69 (64%)	43 (98%)	1 (2%)	44	66
2	P	38/69 (55%)	38 (100%)	0	100	100
All	All	1777/2004 (89%)	1757 (99%)	20 (1%)	65	80

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	112	VAL
1	A	240	PHE
1	A	456	LYS
1	B	112	VAL
1	B	217	LYS
1	B	441	VAL
1	B	491	ILE
1	C	109	ARG
1	C	112	VAL
1	C	136	ILE
1	C	170	VAL
1	C	447	ILE
1	C	491	ILE
1	D	112	VAL
1	D	136	ILE
2	M	296	LEU
2	N	306	LEU
2	N	316	TRP
2	N	331	LEU
2	O	280	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	103	HIS
1	A	175	GLN
1	A	195	GLN
1	A	293	ASN
1	A	297	GLN
1	B	40	GLN
1	B	459	ASN
1	C	40	GLN
1	C	103	HIS
1	C	202	ASN
1	C	463	ASN
1	D	100	HIS
1	D	159	HIS
1	D	202	ASN
1	D	293	ASN
1	D	303	HIS
1	D	345	HIS

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Mol	Chain	Res	Type
1	D	470	ASN
2	N	311	ASN

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	473/483 (97%)	0.44	30 (6%)	26 19	34, 57, 96, 118	0
1	B	470/483 (97%)	0.65	39 (8%)	17 12	39, 64, 102, 125	0
1	C	463/483 (95%)	0.99	63 (13%)	7 5	38, 68, 118, 159	0
1	D	431/483 (89%)	1.19	77 (17%)	3 2	45, 78, 121, 135	0
2	M	44/83 (53%)	1.26	10 (22%)	2 1	48, 64, 100, 129	0
2	N	57/83 (68%)	1.21	11 (19%)	3 2	53, 78, 155, 168	0
2	O	52/83 (62%)	1.11	9 (17%)	4 3	64, 81, 115, 140	0
2	P	47/83 (56%)	1.56	12 (25%)	1 1	53, 73, 127, 135	0
All	All	2037/2264 (89%)	0.85	251 (12%)	8 7	34, 68, 113, 168	0

All (251) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	136	ILE	7.4
2	P	322	PRO	7.1
2	M	322	PRO	6.6
1	D	136	ILE	6.0
1	D	439	PHE	5.8
2	P	321	THR	5.5
1	C	337	ASN	5.5
1	D	140	ALA	5.4
1	B	277	SER	5.3
1	B	224	LEU	5.2
1	D	277	SER	5.2
2	O	317	TRP	5.2
2	O	323	PHE	5.0
1	C	140	ALA	4.9
2	N	317	TRP	4.8
2	P	278	LEU	4.7

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Mol	Chain	Res	Type	RSRZ
2	P	277	ALA	4.6
1	C	277	SER	4.6
1	D	423	TYR	4.5
1	B	37	PRO	4.5
2	N	322	PRO	4.5
1	A	222	HIS	4.4
2	P	276	ARG	4.4
2	N	320	CYS	4.4
1	C	35	SER	4.4
1	D	128	SER	4.4
2	N	319	PRO	4.3
1	B	350	LYS	4.2
2	M	279	LYS	4.2
1	B	57	PHE	4.0
2	M	319	PRO	4.0
2	P	318	SER	4.0
2	P	279	LYS	3.9
1	D	465	SER	3.8
2	P	319	PRO	3.8
1	D	242	GLN	3.8
1	A	240	PHE	3.8
1	D	498	CYS	3.8
1	D	284	ILE	3.8
1	B	307	GLU	3.7
1	A	308	THR	3.6
1	D	452	CYS	3.6
2	N	323	PHE	3.6
1	D	307	GLU	3.6
1	C	491	ILE	3.6
1	D	499	CYS	3.6
2	O	279	LYS	3.6
1	D	433	ASN	3.5
1	C	433	ASN	3.5
1	C	458	GLU	3.5
1	A	493	PHE	3.5
1	D	317	TYR	3.4
1	B	222	HIS	3.4
1	A	284	ILE	3.3
2	N	306	LEU	3.3
2	N	321	THR	3.3
1	B	493	PHE	3.3
1	D	478	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	284	ILE	3.2
1	B	308	THR	3.2
1	B	281	GLY	3.2
2	O	306	LEU	3.2
1	B	347	GLN	3.2
1	D	330	GLN	3.2
1	D	455	THR	3.2
1	C	489	ASP	3.1
1	C	452	CYS	3.1
2	M	317	TRP	3.1
1	C	331	ALA	3.1
1	B	284	ILE	3.1
1	C	222	HIS	3.1
1	C	307	GLU	3.1
1	B	223	ILE	3.1
1	C	456	LYS	3.1
1	C	447	ILE	3.1
1	C	488	SER	3.1
1	D	222	HIS	3.1
2	N	324	THR	3.1
2	P	316	TRP	3.1
1	A	35	SER	3.1
1	D	472	SER	3.0
2	N	335	SER	3.0
1	C	493	PHE	3.0
2	O	335	SER	3.0
1	D	308	THR	3.0
1	C	471	PHE	3.0
1	C	435	TYR	3.0
1	D	187	MET	3.0
1	D	337	ASN	2.9
1	D	424	VAL	2.9
1	D	413	LEU	2.9
1	C	441	VAL	2.9
2	M	306	LEU	2.9
1	C	499	CYS	2.9
1	D	456	LYS	2.9
1	D	106	GLU	2.8
1	D	435	TYR	2.8
1	D	464	LEU	2.8
1	C	192	GLU	2.8
1	A	336	SER	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	36	ASP	2.8
1	A	224	LEU	2.8
1	D	78	THR	2.8
1	C	240	PHE	2.8
2	O	305	GLN	2.8
1	D	296	ILE	2.8
2	M	318	SER	2.8
1	B	348	ASP	2.8
1	C	461	GLU	2.8
1	C	504	LYS	2.8
1	C	483	MET	2.8
1	D	54	TYR	2.8
1	D	275	PRO	2.7
1	B	167	LYS	2.7
1	D	432	PHE	2.7
1	A	277	SER	2.7
1	B	317	TYR	2.7
1	C	454	ILE	2.6
1	A	283	GLU	2.6
1	C	472	SER	2.6
1	D	129	ASN	2.6
1	D	199	ALA	2.6
1	C	308	THR	2.6
1	D	376	THR	2.6
2	O	324	THR	2.6
1	C	481	TYR	2.6
1	A	483	MET	2.6
1	C	492	ILE	2.6
1	B	318	CYS	2.6
1	A	332	ASN	2.6
2	M	316	TRP	2.6
1	A	48	GLY	2.6
1	C	439	PHE	2.6
1	C	512	PHE	2.6
1	D	512	PHE	2.6
1	B	485	THR	2.6
1	D	108	THR	2.6
2	M	321	THR	2.6
1	A	51	GLU	2.6
2	N	316	TRP	2.5
1	D	105	ASP	2.5
1	D	471	PHE	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	293	ASN	2.5
1	A	420	THR	2.5
1	C	412	LYS	2.5
1	D	52	ALA	2.5
1	A	350	LYS	2.5
1	D	34	GLY	2.5
1	B	420	THR	2.5
1	D	385	LYS	2.4
1	D	134	HIS	2.4
1	D	370	ASP	2.4
1	D	409	ALA	2.4
1	B	204	ILE	2.4
1	B	458	GLU	2.4
1	B	515	GLY	2.4
1	C	422	LEU	2.4
2	P	306	LEU	2.4
1	C	405	SER	2.4
1	C	486	VAL	2.4
1	C	440	ALA	2.4
1	C	485	THR	2.4
1	B	337	ASN	2.4
1	C	479	ASN	2.4
2	P	320	CYS	2.4
1	C	466	GLY	2.4
1	B	38	VAL	2.4
1	C	478	LEU	2.3
1	C	420	THR	2.3
1	C	51	GLU	2.3
1	D	35	SER	2.3
1	B	102	PHE	2.3
1	D	343	THR	2.3
1	C	129	ASN	2.3
1	D	249	ASN	2.3
1	D	227	LYS	2.3
1	D	458	GLU	2.3
2	O	316	TRP	2.3
1	D	198	LEU	2.3
1	D	56	THR	2.3
1	C	197	PRO	2.3
1	C	476	ASP	2.3
1	C	419	GLN	2.3
1	D	320	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
2	M	296	LEU	2.3
2	P	297	PHE	2.3
1	D	396	ILE	2.3
1	A	78	THR	2.3
1	D	283	GLU	2.3
1	A	128	SER	2.3
1	C	487	ARG	2.3
1	B	170	VAL	2.3
1	D	430	LYS	2.2
1	B	225	THR	2.2
1	C	501	PRO	2.2
1	B	276	GLY	2.2
1	B	39	LEU	2.2
1	C	437	LEU	2.2
1	D	80	VAL	2.2
2	O	315	LEU	2.2
2	N	279	LYS	2.2
1	B	219	GLN	2.2
1	C	515	GLY	2.2
1	C	495	PHE	2.2
1	C	409	ALA	2.2
1	C	68	CYS	2.2
1	A	418	ASN	2.2
1	D	462	TYR	2.2
1	D	135	GLY	2.2
1	D	185	ASP	2.2
1	C	80	VAL	2.2
1	A	331	ALA	2.2
1	B	54	TYR	2.2
1	C	397	GLN	2.2
1	A	167	LYS	2.2
1	A	349	GLY	2.2
1	B	421	GLY	2.2
1	A	514	THR	2.1
1	B	56	THR	2.1
1	B	221	TYR	2.1
1	B	506	LYS	2.1
1	D	81	TYR	2.1
1	D	437	LEU	2.1
1	C	398	SER	2.1
1	D	70	ALA	2.1
1	C	108	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	129	ASN	2.1
1	D	457	ASN	2.1
1	A	223	ILE	2.1
1	D	84	MET	2.1
1	C	418	ASN	2.1
1	D	449	TYR	2.1
1	D	290	ILE	2.1
1	D	436	PHE	2.1
1	D	377	ALA	2.1
1	B	239	GLN	2.1
1	D	453	LEU	2.1
1	A	515	GLY	2.1
1	D	82	HIS	2.1
1	A	307	GLU	2.0
1	A	442	GLU	2.0
1	B	109	ARG	2.0
1	B	282	GLU	2.0
1	C	199	ALA	2.0
2	M	284	PRO	2.0
1	D	470	ASN	2.0
1	B	237	ILE	2.0
1	D	429	PRO	2.0
1	A	490	ASN	2.0
1	D	276	GLY	2.0
1	D	481	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.