



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 03:06 PM GMT

PDB ID : 4BKA
Title : crystal structure of the human EphA4 ectodomain in complex with human ephrin A5
Authors : Seiradake, E.; Schaupp, A.; del Toro Ruiz, D.; Kaufmann, R.; Mitakidis, N.; Harlos, K.; Aricescu, A.R.; Klein, R.; Jones, E.Y.
Deposited on : 2013-04-23
Resolution : 5.30 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

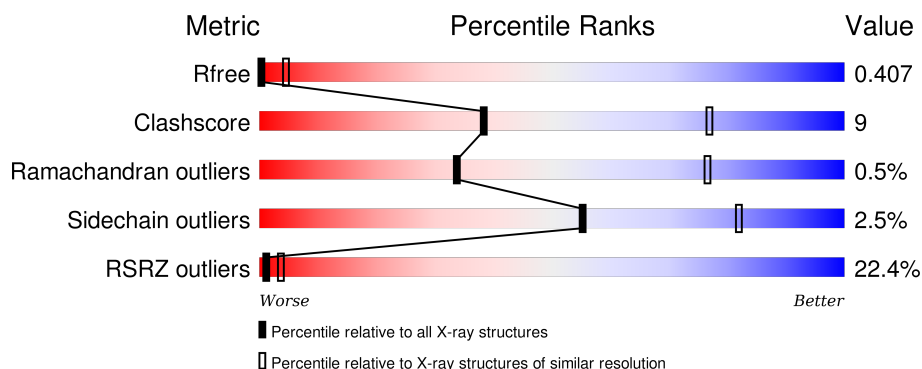
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 5.30 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}	91344	1162 (7.00-3.60)
Clashscore	102246	1007 (6.92-3.68)
Ramachandran outliers	100387	1018 (6.98-3.62)
Sidechain outliers	100360	1174 (7.00-3.60)
RSRZ outliers	91569	1163 (7.00-3.60)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	568	<div> <div>16%</div> <div> <div></div> <div>72%</div> <div>17%</div> <div>•</div> <div>11%</div> </div> </div>
2	C	180	<div> <div>29%</div> <div> <div></div> <div>67%</div> <div>9%</div> <div>•</div> <div>24%</div> </div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5087 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 EPHRIN TYPE-A RECEPTOR 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	507	3948	2461	682	779	26	0	0	0

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	MET	-	EXPRESSION TAG	UNP P54764
A	-10	GLY	-	EXPRESSION TAG	UNP P54764
A	-9	ILE	-	EXPRESSION TAG	UNP P54764
A	-8	LEU	-	EXPRESSION TAG	UNP P54764
A	-7	PRO	-	EXPRESSION TAG	UNP P54764
A	-6	SER	-	EXPRESSION TAG	UNP P54764
A	-5	PRO	-	EXPRESSION TAG	UNP P54764
A	-4	GLY	-	EXPRESSION TAG	UNP P54764
A	-3	MET	-	EXPRESSION TAG	UNP P54764
A	-2	PRO	-	EXPRESSION TAG	UNP P54764
A	-1	ALA	-	EXPRESSION TAG	UNP P54764
A	0	LEU	-	EXPRESSION TAG	UNP P54764
A	1	LEU	-	EXPRESSION TAG	UNP P54764
A	2	SER	-	EXPRESSION TAG	UNP P54764
A	3	LEU	-	EXPRESSION TAG	UNP P54764
A	4	VAL	-	EXPRESSION TAG	UNP P54764
A	5	SER	-	EXPRESSION TAG	UNP P54764
A	6	LEU	-	EXPRESSION TAG	UNP P54764
A	7	LEU	-	EXPRESSION TAG	UNP P54764
A	8	SER	-	EXPRESSION TAG	UNP P54764
A	9	VAL	-	EXPRESSION TAG	UNP P54764
A	10	LEU	-	EXPRESSION TAG	UNP P54764
A	11	LEU	-	EXPRESSION TAG	UNP P54764
A	12	MET	-	EXPRESSION TAG	UNP P54764
A	13	GLY	-	EXPRESSION TAG	UNP P54764
A	14	CYS	-	EXPRESSION TAG	UNP P54764
A	15	VAL	-	EXPRESSION TAG	UNP P54764

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Chain	Residue	Modelled	Actual	Comment	Reference
A	16	ALA	-	EXPRESSION TAG	UNP P54764
A	17	GLU	-	EXPRESSION TAG	UNP P54764
A	18	THR	-	EXPRESSION TAG	UNP P54764
A	19	GLY	-	EXPRESSION TAG	UNP P54764
A	548	GLY	-	EXPRESSION TAG	UNP P54764
A	549	THR	-	EXPRESSION TAG	UNP P54764
A	550	LYS	-	EXPRESSION TAG	UNP P54764
A	551	HIS	-	EXPRESSION TAG	UNP P54764
A	552	HIS	-	EXPRESSION TAG	UNP P54764
A	553	HIS	-	EXPRESSION TAG	UNP P54764
A	554	HIS	-	EXPRESSION TAG	UNP P54764
A	555	HIS	-	EXPRESSION TAG	UNP P54764
A	556	HIS	-	EXPRESSION TAG	UNP P54764

- Molecule 2 is a protein called EPHRIN-A5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	137	Total	C	N	O	S	0	0	1
			1139	728	197	206	8			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	0	MET	-	EXPRESSION TAG	UNP P52803
C	1	GLY	-	EXPRESSION TAG	UNP P52803
C	2	ILE	-	EXPRESSION TAG	UNP P52803
C	3	LEU	-	EXPRESSION TAG	UNP P52803
C	4	PRO	-	EXPRESSION TAG	UNP P52803
C	5	SER	-	EXPRESSION TAG	UNP P52803
C	6	PRO	-	EXPRESSION TAG	UNP P52803
C	7	GLY	-	EXPRESSION TAG	UNP P52803
C	8	MET	-	EXPRESSION TAG	UNP P52803
C	9	PRO	-	EXPRESSION TAG	UNP P52803
C	10	ALA	-	EXPRESSION TAG	UNP P52803
C	11	LEU	-	EXPRESSION TAG	UNP P52803
C	12	LEU	-	EXPRESSION TAG	UNP P52803
C	13	SER	-	EXPRESSION TAG	UNP P52803
C	14	LEU	-	EXPRESSION TAG	UNP P52803
C	15	VAL	-	EXPRESSION TAG	UNP P52803
C	16	SER	-	EXPRESSION TAG	UNP P52803
C	17	LEU	-	EXPRESSION TAG	UNP P52803
C	18	LEU	-	EXPRESSION TAG	UNP P52803

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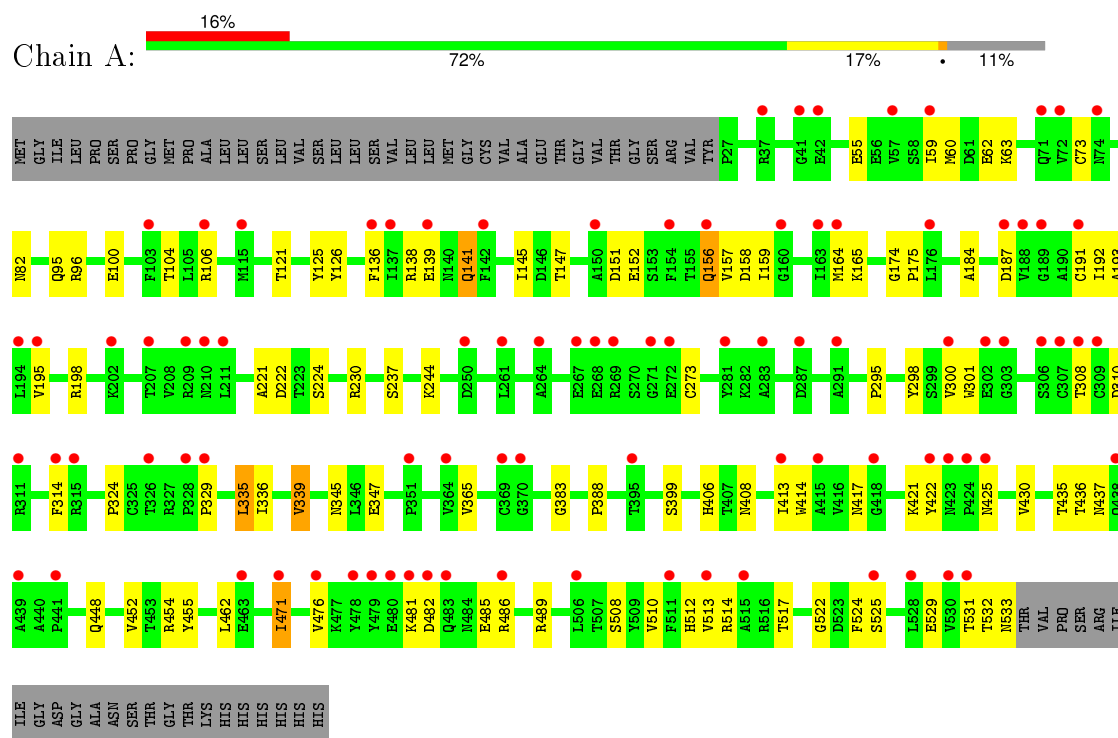
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Chain	Residue	Modelled	Actual	Comment	Reference
C	19	SER	-	EXPRESSION TAG	UNP P52803
C	20	VAL	-	EXPRESSION TAG	UNP P52803
C	21	LEU	-	EXPRESSION TAG	UNP P52803
C	22	LEU	-	EXPRESSION TAG	UNP P52803
C	23	MET	-	EXPRESSION TAG	UNP P52803
C	24	GLY	-	EXPRESSION TAG	UNP P52803
C	25	CYS	-	EXPRESSION TAG	UNP P52803
C	26	VAL	-	EXPRESSION TAG	UNP P52803
C	27	ALA	-	EXPRESSION TAG	UNP P52803
C	28	GLU	-	EXPRESSION TAG	UNP P52803
C	29	THR	-	EXPRESSION TAG	UNP P52803
C	30	GLY	-	EXPRESSION TAG	UNP P52803
C	172	GLY	-	EXPRESSION TAG	UNP P52803
C	173	THR	-	EXPRESSION TAG	UNP P52803
C	174	LYS	-	EXPRESSION TAG	UNP P52803
C	175	HIS	-	EXPRESSION TAG	UNP P52803
C	176	HIS	-	EXPRESSION TAG	UNP P52803
C	177	HIS	-	EXPRESSION TAG	UNP P52803
C	178	HIS	-	EXPRESSION TAG	UNP P52803
C	179	HIS	-	EXPRESSION TAG	UNP P52803
C	180	HIS	-	EXPRESSION TAG	UNP P52803

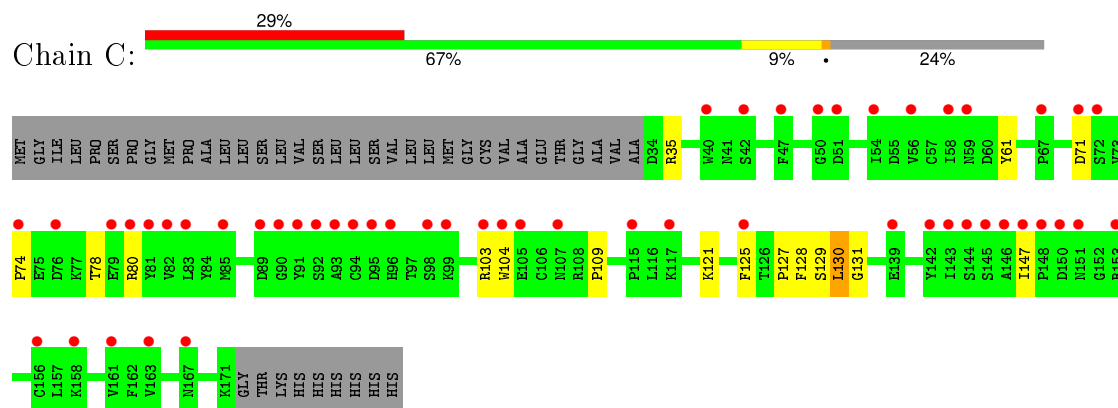
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: EPHRIN TYPE-A RECEPTOR 4



• Molecule 2: EPHRIN-A5



4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	202.63 Å 202.63 Å 326.23 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	84.87 – 5.30 84.73 – 5.30	Depositor EDS
% Data completeness (in resolution range)	96.3 (84.87-5.30) 96.4 (84.73-5.30)	Depositor EDS
R_{merge}	0.74	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.67 (at 5.41 Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.383 , 0.408 0.383 , 0.407	Depositor DCC
R_{free} test set	449 reflections (5.09%)	DCC
Wilson B-factor (Å ²)	155.3	Xtriage
Anisotropy	0.356	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 217.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.31$, $\langle L^2 \rangle = 0.15$	Xtriage
Outliers	0 of 9268 reflections	Xtriage
F_o, F_c correlation	0.73	EDS
Total number of atoms	5087	wwPDB-VP
Average B, all atoms (Å ²)	243.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.86% 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, 0.375 respectively for untwinned datasets, and 0.333, 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	0.31	0/4032	0.56	0/5484
2	C	0.33	0/1177	0.50	0/1592
All	All	0.32	0/5209	0.55	0/7076

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	3948	0	3801	87	104
2	C	1139	0	1053	62	8
All	All	5087	0	4854	90	104

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (90) 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:195:VAL:HG22	2:C:128:PHE:CE1	1.46	1.46
1:A:195:VAL:CG2	2:C:128:PHE:HE1	1.31	1.39

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:164:MET:CE	2:C:130:LEU:HG	1.72	1.17
1:A:55:GLU:HG2	2:C:61:TYR:OH	1.46	1.13
1:A:55:GLU:OE1	2:C:61:TYR:OH	1.64	1.13
1:A:55:GLU:CG	2:C:61:TYR:OH	1.98	1.11
1:A:164:MET:HE2	2:C:130:LEU:HG	1.14	1.07
1:A:55:GLU:OE1	2:C:121:LYS:HD2	1.56	1.04
1:A:59:ILE:HG12	2:C:103:ARG:HH22	1.17	1.03
1:A:55:GLU:CD	2:C:61:TYR:HH	1.65	0.99
1:A:55:GLU:CD	2:C:61:TYR:OH	2.01	0.98
1:A:59:ILE:HG12	2:C:103:ARG:NH2	1.79	0.97
1:A:104:THR:HG21	2:C:129:SER:N	1.79	0.97
1:A:59:ILE:CG1	2:C:103:ARG:HH22	1.77	0.96
1:A:104:THR:HG21	2:C:129:SER:H	1.32	0.94
1:A:195:VAL:CG2	2:C:128:PHE:CE1	2.24	0.89
1:A:191:CYS:C	2:C:127:PRO:HB3	1.92	0.89
1:A:164:MET:CE	2:C:130:LEU:CG	2.53	0.85
1:A:164:MET:HE2	2:C:130:LEU:CG	2.04	0.85
1:A:164:MET:SD	2:C:130:LEU:HB2	2.17	0.84
1:A:55:GLU:OE1	2:C:121:LYS:CD	2.34	0.75
1:A:195:VAL:HG22	2:C:128:PHE:HE1	0.60	0.75
1:A:164:MET:CE	2:C:130:LEU:HB2	2.17	0.75
1:A:164:MET:HE1	2:C:130:LEU:HG	1.68	0.72
1:A:73:CYS:HB2	2:C:127:PRO:HG3	1.73	0.70
1:A:164:MET:HE1	2:C:130:LEU:CB	2.21	0.70
1:A:193:ALA:CB	2:C:128:PHE:HB2	2.21	0.70
1:A:59:ILE:HG23	2:C:103:ARG:HH12	1.57	0.69
1:A:164:MET:CE	2:C:130:LEU:CB	2.71	0.69
1:A:59:ILE:HG12	2:C:103:ARG:CZ	2.24	0.67
1:A:106:ARG:HH21	2:C:125:PHE:HB3	1.60	0.66
1:A:164:MET:HE1	2:C:130:LEU:CG	2.26	0.63
1:A:60:MET:CG	2:C:103:ARG:O	2.46	0.63
1:A:193:ALA:HB1	2:C:128:PHE:HB2	1.81	0.62
1:A:59:ILE:HG23	2:C:103:ARG:NH1	2.15	0.61
1:A:195:VAL:HG21	2:C:128:PHE:CE1	2.34	0.61
1:A:59:ILE:HG12	2:C:103:ARG:NH1	2.15	0.60
1:A:59:ILE:HG12	2:C:103:ARG:HH12	1.66	0.59
1:A:138:ARG:HB3	1:A:141:GLN:HB2	1.85	0.57
2:C:35:ARG:HG2	2:C:61:TYR:HB2	1.86	0.57
1:A:55:GLU:OE1	2:C:121:LYS:NZ	2.37	0.56
1:A:329:PRO:HD3	1:A:417:ASN:HB2	1.86	0.56
1:A:336:ILE:HB	1:A:347:GLU:HB3	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:164:MET:HE1	2:C:130:LEU:HB2	1.87	0.55
1:A:471:ILE:HA	1:A:517:THR:HG22	1.87	0.55
1:A:100:GLU:HB3	1:A:198:ARG:HB2	1.88	0.55
1:A:106:ARG:HD3	1:A:157:VAL:HG23	1.90	0.54
1:A:59:ILE:HD13	2:C:131:GLY:HA2	1.89	0.54
1:A:125:TYR:HB2	1:A:184:ALA:HB3	1.90	0.53
2:C:80:ARG:HB3	2:C:147:ILE:HD12	1.90	0.53
1:A:104:THR:HB	2:C:128:PHE:HA	1.90	0.53
1:A:55:GLU:OE1	2:C:121:LYS:CE	2.58	0.51
1:A:298:TYR:HB2	1:A:310:ASP:HB3	1.93	0.51
1:A:193:ALA:CB	2:C:128:PHE:CB	2.88	0.50
1:A:513:VAL:H	1:A:525:SER:HB2	1.76	0.50
1:A:192:ILE:N	2:C:127:PRO:HB3	2.27	0.49
1:A:126:TYR:HB3	1:A:145:ILE:HD11	1.94	0.49
1:A:106:ARG:HB2	1:A:191:CYS:HB3	1.95	0.49
1:A:82:ASN:HB2	1:A:187:ASP:HB3	1.94	0.49
1:A:59:ILE:CG2	2:C:103:ARG:HH12	2.24	0.49
1:A:104:THR:HG21	2:C:129:SER:CA	2.43	0.47
1:A:406:HIS:H	1:A:437:ASN:HB2	1.79	0.47
1:A:104:THR:HG21	2:C:129:SER:CB	2.44	0.47
2:C:78:THR:HG21	2:C:109:PRO:HG3	1.97	0.47
1:A:191:CYS:SG	2:C:127:PRO:HG3	2.54	0.47
1:A:295:PRO:HD2	1:A:324:PRO:HB3	1.97	0.46
1:A:59:ILE:HG13	2:C:103:ARG:HH22	1.74	0.46
1:A:486:ARG:HD3	1:A:489:ARG:HH12	1.81	0.46
1:A:193:ALA:HB3	2:C:128:PHE:HA	1.98	0.45
1:A:339:VAL:HG21	1:A:436:THR:HA	1.98	0.45
1:A:514:ARG:HH11	1:A:522:GLY:H	1.65	0.45
1:A:60:MET:HG3	2:C:103:ARG:O	2.17	0.45
1:A:191:CYS:O	2:C:127:PRO:HB3	2.15	0.44
1:A:175:PRO:HB3	1:A:221:ALA:HB1	1.99	0.44
1:A:230:ARG:HG2	1:A:244:LYS:HB3	2.00	0.44
1:A:237:SER:HB2	1:A:273:CYS:SG	2.58	0.44
1:A:335:LEU:HD11	1:A:413:ILE:HD12	1.99	0.44
1:A:104:THR:CG2	2:C:129:SER:HB3	2.49	0.43
1:A:60:MET:HG2	2:C:103:ARG:O	2.17	0.42
1:A:60:MET:HG3	2:C:104:TRP:HA	2.00	0.42
1:A:121:THR:HB	1:A:147:THR:HG22	2.00	0.42
1:A:476:VAL:HG22	1:A:513:VAL:HG22	2.01	0.42
1:A:335:LEU:HD12	1:A:430:VAL:HG12	2.02	0.42
1:A:192:ILE:C	2:C:127:PRO:HB2	2.40	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:62:GLU:HA	1:A:63:LYS:HA	1.76	0.41
1:A:159:ILE:H	1:A:159:ILE:HG13	1.75	0.41
1:A:193:ALA:CB	2:C:128:PHE:CA	2.99	0.41
1:A:96:ARG:HG3	1:A:174:GLY:HA3	2.02	0.41
1:A:156:GLN:N	1:A:157:VAL:HA	2.36	0.41
1:A:55:GLU:OE1	2:C:61:TYR:CZ	2.66	0.40

All (104) 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)
1:A:301:TRP:CE2	1:A:414:TRP:CE3[5_675]	0.50	1.70
1:A:448:GLN:OE1	1:A:448:GLN:OE1[16_454]	0.67	1.53
1:A:481:LYS:CD	1:A:533:ASN:CG[16_454]	0.68	1.52
1:A:301:TRP:CZ2	1:A:414:TRP:CD2[5_675]	0.69	1.51
1:A:481:LYS:CE	1:A:533:ASN:OD1[16_454]	0.73	1.47
1:A:301:TRP:CZ2	1:A:414:TRP:CE2[5_675]	0.74	1.46
1:A:298:TYR:CD2	1:A:425:ASN:ND2[5_675]	0.76	1.44
1:A:152:GLU:OE2	1:A:512:HIS:NE2[6_555]	0.82	1.38
1:A:308:THR:OG1	1:A:421:LYS:O[5_675]	0.95	1.25
1:A:454:ARG:NH1	1:A:482:ASP:OD1[16_454]	0.97	1.23
1:A:301:TRP:CE2	1:A:414:TRP:CD2[5_675]	0.97	1.23
1:A:481:LYS:CD	1:A:533:ASN:ND2[16_454]	0.98	1.22
1:A:508:SER:OG	1:A:532:THR:O[16_454]	1.01	1.19
1:A:531:THR:O	1:A:531:THR:OG1[16_454]	1.01	1.19
1:A:301:TRP:NE1	1:A:414:TRP:CE3[5_675]	1.04	1.16
1:A:481:LYS:CE	1:A:533:ASN:CG[16_454]	1.06	1.14
1:A:301:TRP:CH2	1:A:414:TRP:CE2[5_675]	1.11	1.09
1:A:158:ASP:OD2	1:A:455:TYR:OH[8_565]	1.11	1.09
1:A:139:GLU:OE2	2:C:71:ASP:O[3_465]	1.13	1.07
1:A:531:THR:CG2	1:A:531:THR:CG2[16_454]	1.14	1.06
1:A:136:PHE:CE1	2:C:71:ASP:OD1[3_465]	1.15	1.05
1:A:531:THR:C	1:A:531:THR:OG1[16_454]	1.21	0.99
1:A:422:TYR:CZ	1:A:422:TYR:OH[5_675]	1.29	0.91
1:A:422:TYR:CE1	1:A:422:TYR:OH[5_675]	1.29	0.91
1:A:301:TRP:CD2	1:A:414:TRP:CE3[5_675]	1.30	0.90
1:A:422:TYR:CE2	1:A:422:TYR:CZ[5_675]	1.32	0.88
1:A:301:TRP:CZ3	1:A:365:VAL:CG2[5_675]	1.37	0.83
1:A:158:ASP:CG	1:A:455:TYR:OH[8_565]	1.37	0.83
1:A:531:THR:CB	1:A:531:THR:CB[16_454]	1.39	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:152:GLU:OE2	1:A:512:HIS:CE1[6_555]	1.39	0.81
1:A:481:LYS:CG	1:A:533:ASN:ND2[16_454]	1.41	0.79
1:A:531:THR:CA	1:A:531:THR:CB[16_454]	1.42	0.78
1:A:422:TYR:CE2	1:A:422:TYR:OH[5_675]	1.43	0.77
1:A:531:THR:C	1:A:531:THR:CB[16_454]	1.43	0.77
1:A:422:TYR:CD1	1:A:422:TYR:OH[5_675]	1.44	0.76
1:A:448:GLN:NE2	1:A:448:GLN:NE2[16_454]	1.45	0.75
1:A:452:VAL:O	1:A:529:GLU:OE1[16_454]	1.47	0.73
1:A:481:LYS:CD	1:A:533:ASN:OD1[16_454]	1.47	0.73
1:A:301:TRP:CD2	1:A:414:TRP:CZ3[5_675]	1.49	0.71
1:A:301:TRP:CH2	1:A:414:TRP:NE1[5_675]	1.50	0.70
1:A:301:TRP:CE2	1:A:414:TRP:CZ3[5_675]	1.51	0.69
1:A:422:TYR:CD2	1:A:422:TYR:OH[5_675]	1.57	0.63
1:A:422:TYR:CE1	1:A:422:TYR:CZ[5_675]	1.57	0.63
1:A:422:TYR:CG	1:A:422:TYR:OH[5_675]	1.61	0.59
1:A:224:SER:OG	1:A:345:ASN:OD1[6_555]	1.61	0.59
1:A:298:TYR:CE2	1:A:425:ASN:ND2[5_675]	1.62	0.58
1:A:482:ASP:OD2	1:A:533:ASN:C[16_454]	1.62	0.58
1:A:448:GLN:CD	1:A:448:GLN:OE1[16_454]	1.65	0.55
1:A:152:GLU:CD	1:A:512:HIS:NE2[6_555]	1.66	0.54
1:A:301:TRP:CZ2	1:A:414:TRP:NE1[5_675]	1.67	0.53
1:A:139:GLU:CD	2:C:71:ASP:O[3_465]	1.68	0.52
1:A:301:TRP:CE3	1:A:365:VAL:CG2[5_675]	1.69	0.51
1:A:301:TRP:CZ2	1:A:414:TRP:CG[5_675]	1.69	0.51
1:A:481:LYS:NZ	1:A:533:ASN:CB[16_454]	1.69	0.51
1:A:139:GLU:OE2	2:C:71:ASP:C[3_465]	1.72	0.48
1:A:301:TRP:CD1	1:A:414:TRP:CE3[5_675]	1.74	0.46
1:A:308:THR:CB	1:A:421:LYS:O[5_675]	1.74	0.46
1:A:152:GLU:OE2	1:A:512:HIS:CD2[6_555]	1.77	0.43
1:A:151:ASP:OD1	1:A:524:PHE:CZ[6_555]	1.78	0.42
1:A:481:LYS:NZ	1:A:533:ASN:OD1[16_454]	1.79	0.41
1:A:314:PHE:CZ	1:A:314:PHE:CZ[5_675]	1.81	0.39
1:A:481:LYS:NZ	1:A:533:ASN:CG[16_454]	1.81	0.39
1:A:301:TRP:CH2	1:A:414:TRP:CD2[5_675]	1.82	0.38
1:A:314:PHE:CE1	1:A:314:PHE:CE1[5_675]	1.83	0.37
1:A:301:TRP:NE1	1:A:414:TRP:CZ3[5_675]	1.84	0.36
1:A:301:TRP:CG	1:A:414:TRP:CZ3[5_675]	1.85	0.35
1:A:422:TYR:CE2	1:A:422:TYR:CE2[5_675]	1.85	0.35
1:A:508:SER:OG	1:A:532:THR:C[16_454]	1.87	0.33
1:A:301:TRP:CG	1:A:414:TRP:CE3[5_675]	1.88	0.32
1:A:298:TYR:CG	1:A:425:ASN:ND2[5_675]	1.89	0.31

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:301:TRP:CZ2	1:A:414:TRP:CE3[5_675]	1.89	0.31
1:A:151:ASP:OD1	1:A:524:PHE:CE2[6_555]	1.90	0.30
1:A:136:PHE:CZ	2:C:71:ASP:OD1[3_465]	1.91	0.29
1:A:301:TRP:CE2	1:A:414:TRP:CE2[5_675]	1.93	0.27
1:A:454:ARG:NH1	1:A:482:ASP:CG[16_454]	1.93	0.27
1:A:224:SER:CB	1:A:399:SER:OG[6_555]	1.94	0.26
1:A:152:GLU:CD	1:A:512:HIS:CE1[6_555]	1.95	0.25
1:A:301:TRP:CZ2	1:A:414:TRP:CZ2[5_675]	1.95	0.25
1:A:136:PHE:CE1	2:C:71:ASP:CG[3_465]	1.96	0.24
1:A:139:GLU:OE1	2:C:71:ASP:O[3_465]	1.97	0.23
1:A:531:THR:CB	1:A:531:THR:CG2[16_454]	1.97	0.23
1:A:454:ARG:CZ	1:A:482:ASP:OD1[16_454]	1.98	0.22
1:A:301:TRP:CH2	1:A:414:TRP:CZ2[5_675]	1.98	0.22
1:A:481:LYS:CD	1:A:533:ASN:CB[16_454]	1.99	0.21
1:A:298:TYR:CD2	1:A:425:ASN:CG[5_675]	2.00	0.20
1:A:531:THR:O	1:A:531:THR:CB[16_454]	2.00	0.20
1:A:301:TRP:CD1	1:A:414:TRP:CZ3[5_675]	2.01	0.19
1:A:481:LYS:CE	1:A:533:ASN:ND2[16_454]	2.01	0.19
1:A:301:TRP:NE1	1:A:414:TRP:CD2[5_675]	2.03	0.17
1:A:301:TRP:CZ2	1:A:414:TRP:CD1[5_675]	2.04	0.16
1:A:452:VAL:O	1:A:529:GLU:CD[16_454]	2.04	0.16
1:A:139:GLU:OE2	2:C:71:ASP:CA[3_465]	2.07	0.13
1:A:314:PHE:CE1	1:A:314:PHE:CZ[5_675]	2.09	0.11
1:A:152:GLU:OE1	1:A:510:VAL:CG1[6_555]	2.11	0.09
1:A:448:GLN:CD	1:A:448:GLN:NE2[16_454]	2.11	0.09
1:A:481:LYS:CG	1:A:533:ASN:CG[16_454]	2.12	0.08
1:A:301:TRP:CD2	1:A:414:TRP:CD2[5_675]	2.13	0.07
1:A:152:GLU:CG	1:A:512:HIS:CE1[6_555]	2.13	0.07
1:A:448:GLN:CD	1:A:448:GLN:CD[16_454]	2.13	0.07
1:A:298:TYR:CE2	1:A:425:ASN:CG[5_675]	2.14	0.06
1:A:308:THR:OG1	1:A:421:LYS:C[5_675]	2.15	0.05
1:A:301:TRP:CZ3	1:A:365:VAL:CB[5_675]	2.17	0.03
1:A:481:LYS:CE	1:A:533:ASN:CB[16_454]	2.18	0.02
1:A:158:ASP:CB	1:A:455:TYR:OH[8_565]	2.18	0.02

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	503/568 (89%)	477 (95%)	23 (5%)	3 (1%)	30	73
2	C	133/180 (74%)	124 (93%)	9 (7%)	0	100	100
All	All	636/748 (85%)	601 (94%)	32 (5%)	3 (0%)	34	76

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	388	PRO
1	A	485	GLU
1	A	383	GLY

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	439/489 (90%)	427 (97%)	12 (3%)	52	80
2	C	126/161 (78%)	124 (98%)	2 (2%)	70	88
All	All	565/650 (87%)	551 (98%)	14 (2%)	55	82

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	95	GLN
1	A	141	GLN
1	A	156	GLN
1	A	165	LYS
1	A	222	ASP
1	A	300	VAL
1	A	335	LEU
1	A	339	VAL
1	A	408	ASN

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Mol	Chain	Res	Type
1	A	435	THR
1	A	462	LEU
1	A	471	ILE
2	C	74	PRO
2	C	130	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	40	GLN
1	A	64	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 carbohydrates 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	507/568 (89%)	1.02	91 (17%) 2 5	43, 211, 428, 500	0
2	C	137/180 (76%)	1.59	53 (38%) 0 3	119, 287, 458, 500	0
All	All	644/748 (86%)	1.14	144 (22%) 1 4	43, 230, 433, 500	0

All (144) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	268	GLU	7.2
1	A	422	TYR	6.1
1	A	515	ALA	6.0
2	C	92	SER	5.5
1	A	530	VAL	5.3
1	A	513	VAL	5.2
1	A	314	PHE	5.1
2	C	105	GLU	4.6
1	A	271	GLY	4.4
1	A	483	GLN	4.3
2	C	95	ASP	4.3
1	A	303	GLY	4.2
2	C	51	ASP	4.1
1	A	106	ARG	4.1
1	A	160	GLY	4.0
1	A	211	LEU	4.0
2	C	145	SER	3.9
2	C	40	TRP	3.8
1	A	425	ASN	3.7
1	A	511	PHE	3.7
2	C	139	GLU	3.7
1	A	272	GLU	3.6
1	A	137	ILE	3.6
2	C	79	GLU	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	189	GLY	3.4
2	C	83	LEU	3.4
2	C	143	ILE	3.3
1	A	441	PRO	3.3
1	A	307	CYS	3.3
1	A	202	LYS	3.2
1	A	395	THR	3.2
1	A	71	GLN	3.2
1	A	306	SER	3.1
1	A	283	ALA	3.1
1	A	370	GLY	3.1
2	C	76	ASP	3.0
2	C	156	CYS	3.0
1	A	413	ILE	3.0
1	A	188	VAL	3.0
1	A	291	ALA	3.0
1	A	191	CYS	3.0
2	C	71	ASP	2.9
1	A	369	CYS	2.9
2	C	146	ALA	2.9
1	A	194	LEU	2.9
1	A	302	GLU	2.9
1	A	163	ILE	2.9
2	C	89	ASP	2.9
2	C	94	CYS	2.9
2	C	144	SER	2.9
2	C	54	ILE	2.9
1	A	264	ALA	2.9
1	A	486	ARG	2.8
1	A	531	THR	2.8
1	A	478	TYR	2.8
1	A	41	GLY	2.8
1	A	136	PHE	2.8
1	A	209	ARG	2.7
2	C	90	GLY	2.7
1	A	267	GLU	2.7
2	C	151	ASN	2.7
1	A	281	TYR	2.7
1	A	311	ARG	2.7
1	A	210	ASN	2.7
1	A	269	ARG	2.7
2	C	107	ASN	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	438	GLN	2.7
1	A	261	LEU	2.7
2	C	80	ARG	2.7
1	A	195	VAL	2.7
1	A	418	GLY	2.7
1	A	59	ILE	2.7
2	C	158	LYS	2.7
1	A	315	ARG	2.7
1	A	463	GLU	2.6
1	A	187	ASP	2.6
1	A	139	GLU	2.6
1	A	528	LEU	2.6
1	A	207	THR	2.6
1	A	351	PRO	2.6
2	C	67	PRO	2.6
2	C	99	LYS	2.5
1	A	57	VAL	2.5
1	A	115	MET	2.5
2	C	125	PHE	2.5
1	A	309	CYS	2.5
1	A	176	LEU	2.5
1	A	480	GLU	2.5
1	A	74	ASN	2.5
2	C	81	TYR	2.5
1	A	287	ASP	2.5
2	C	163	VAL	2.5
2	C	104	TRP	2.4
1	A	42	GLU	2.4
2	C	142	TYR	2.4
2	C	47	PHE	2.4
1	A	423	ASN	2.4
2	C	93	ALA	2.4
2	C	150	ASP	2.4
1	A	150	ALA	2.4
2	C	58	ILE	2.4
1	A	525	SER	2.4
2	C	96	HIS	2.3
1	A	328	PRO	2.3
1	A	142	PHE	2.3
1	A	506	LEU	2.3
1	A	326	THR	2.3
1	A	154	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	479	TYR	2.3
1	A	156	GLN	2.3
2	C	91	TYR	2.3
2	C	42	SER	2.2
2	C	161	VAL	2.2
1	A	72	VAL	2.2
2	C	56	VAL	2.2
2	C	153	ARG	2.2
1	A	476	VAL	2.2
1	A	308	THR	2.2
1	A	364	VAL	2.2
1	A	424	PRO	2.2
1	A	103	PHE	2.2
1	A	329	PRO	2.1
1	A	481	LYS	2.1
2	C	147	ILE	2.1
2	C	115	PRO	2.1
2	C	167	ASN	2.1
1	A	300	VAL	2.1
2	C	103	ARG	2.1
1	A	37	ARG	2.1
1	A	164	MET	2.1
2	C	72	SER	2.1
2	C	85	MET	2.1
2	C	82	VAL	2.1
2	C	50	GLY	2.1
1	A	439	ALA	2.1
2	C	74	PRO	2.1
1	A	482	ASP	2.0
2	C	148	PRO	2.0
1	A	471	ILE	2.0
2	C	59	ASN	2.0
1	A	250	ASP	2.0
2	C	98	SER	2.0
1	A	415	ALA	2.0
2	C	117	LYS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates 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.