



Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 11:14 pm BST

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

<https://www.wwpdb.org/validation/2017/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
Xtriage (Phenix) : 1.13
EDS : 2.11
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

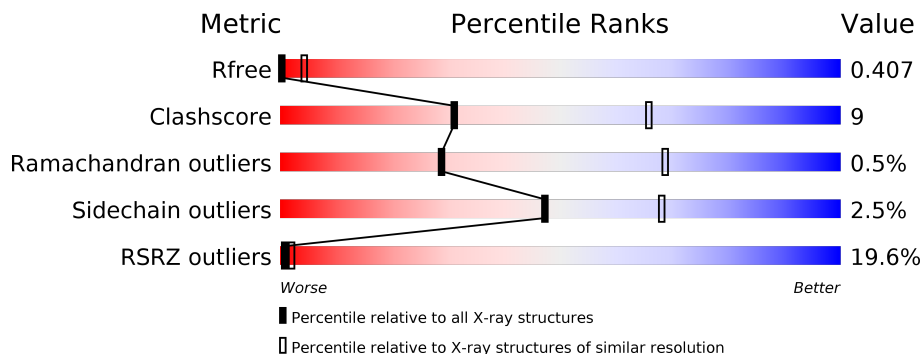
1 Overall quality at a glance

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}	130704	1181 (6.80-3.80)
Clashscore	141614	1006 (6.74-3.86)
Ramachandran outliers	138981	1185 (6.80-3.80)
Sidechain outliers	138945	1159 (6.80-3.80)
RSRZ outliers	127900	1003 (6.80-3.76)

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 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	568	 15% 72% 17% • 11%
2	C	180	 24% 67% 9% • 24%

2 Entry composition i

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
			Total	C	N	O	S			
2	C	137	1139	728	197	206	8	0	0	1

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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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

4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	202.63Å 202.63Å 326.23Å 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 5.41Å)	Xtrriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.383 , 0.408 0.383 , 0.407	Depositor DCC
R_{free} test set	447 reflections (4.82%)	wwPDB-VP
Wilson B-factor (Å ²)	155.3	Xtrriage
Anisotropy	0.356	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 218.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.31$, $\langle L^2 \rangle = 0.15$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
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

Xtrriage'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, 0.333 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	0.31	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:329:PRO:HD3	1:A:417:ASN:HB2	1.86	0.56
1:A:55:GLU:OE1	2:C:121:LYS:NZ	2.37	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:335:LEU:HD12	1:A:430:VAL:HG12	2.02	0.42
1:A:476:VAL:HG22	1:A:513:VAL:HG22	2.01	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:96:ARG:HG3	1:A:174:GLY:HA3	2.02	0.41
1:A:193:ALA:CB	2:C:128:PHE:CA	2.99	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 [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	503/568 (89%)	477 (95%)	23 (5%)	3 (1%)	25	65
2	C	133/180 (74%)	124 (93%)	9 (7%)	0	100	100
All	All	636/748 (85%)	601 (94%)	32 (5%)	3 (0%)	29	69

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 [i](#)

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%)	44	65
2	C	126/161 (78%)	124 (98%)	2 (2%)	62	79
All	All	565/650 (87%)	551 (98%)	14 (2%)	47	68

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1
2	C	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	148:PRO	C	150:ASP	N	3.28
1	A	202:LYS	C	203:LYS	N	3.25

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%)	0.93	83 (16%) 1 3	43, 211, 428, 500	0
2	C	137/180 (76%)	1.48	43 (31%) 0 1	119, 287, 458, 500	0
All	All	644/748 (86%)	1.05	126 (19%) 1 2	43, 230, 433, 500	0

All (126) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	268	GLU	6.9
1	A	422	TYR	5.6
1	A	515	ALA	5.4
2	C	92	SER	5.3
1	A	530	VAL	5.0
1	A	513	VAL	4.9
1	A	314	PHE	4.8
2	C	105	GLU	4.4
1	A	271	GLY	4.2
1	A	483	GLN	4.1
2	C	95	ASP	4.1
1	A	303	GLY	3.9
1	A	106	ARG	3.9
2	C	51	ASP	3.9
1	A	160	GLY	3.8
2	C	145	SER	3.7
1	A	211	LEU	3.7
1	A	425	ASN	3.6
2	C	139	GLU	3.5
1	A	511	PHE	3.5
2	C	40	TRP	3.5
1	A	272	GLU	3.5
1	A	137	ILE	3.3
2	C	79	GLU	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	441	PRO	3.3
1	A	189	GLY	3.2
1	A	307	CYS	3.2
2	C	83	LEU	3.2
1	A	202	LYS	3.2
2	C	143	ILE	3.1
1	A	71	GLN	3.0
1	A	306	SER	3.0
2	C	156	CYS	3.0
1	A	395	THR	3.0
1	A	191	CYS	2.9
2	C	76	ASP	2.9
1	A	370	GLY	2.9
1	A	369	CYS	2.8
1	A	188	VAL	2.8
1	A	283	ALA	2.8
2	C	94	CYS	2.8
1	A	413	ILE	2.8
2	C	71	ASP	2.8
1	A	302	GLU	2.8
2	C	144	SER	2.7
2	C	89	ASP	2.7
1	A	486	ARG	2.7
1	A	291	ALA	2.7
1	A	194	LEU	2.7
1	A	163	ILE	2.7
2	C	54	ILE	2.7
1	A	41	GLY	2.6
1	A	209	ARG	2.6
2	C	146	ALA	2.6
2	C	151	ASN	2.6
1	A	531	THR	2.6
1	A	210	ASN	2.6
1	A	311	ARG	2.6
2	C	107	ASN	2.6
1	A	136	PHE	2.6
1	A	269	ARG	2.6
2	C	158	LYS	2.6
1	A	267	GLU	2.6
1	A	264	ALA	2.6
2	C	90	GLY	2.6
1	A	438	GLN	2.6

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Mol	Chain	Res	Type	RSRZ
2	C	80	ARG	2.6
1	A	315	ARG	2.5
1	A	478	TYR	2.5
1	A	351	PRO	2.5
1	A	463	GLU	2.5
1	A	195	VAL	2.5
1	A	418	GLY	2.5
2	C	99	LYS	2.5
1	A	187	ASP	2.5
1	A	139	GLU	2.5
2	C	67	PRO	2.5
1	A	261	LEU	2.5
1	A	309	CYS	2.4
1	A	59	ILE	2.4
1	A	281	TYR	2.4
1	A	207	THR	2.4
1	A	528	LEU	2.4
1	A	74	ASN	2.4
1	A	57	VAL	2.4
1	A	480	GLU	2.4
1	A	115	MET	2.4
2	C	125	PHE	2.4
1	A	287	ASP	2.3
1	A	423	ASN	2.3
2	C	163	VAL	2.3
1	A	42	GLU	2.3
1	A	176	LEU	2.3
2	C	150	ASP	2.3
1	A	328	PRO	2.3
1	A	525	SER	2.2
2	C	47	PHE	2.2
2	C	104	TRP	2.2
2	C	81	TYR	2.2
2	C	96	HIS	2.2
2	C	58	ILE	2.2
2	C	142	TYR	2.2
2	C	93	ALA	2.2
1	A	156	GLN	2.1
1	A	142	PHE	2.1
2	C	42	SER	2.1
1	A	150	ALA	2.1
1	A	326	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	424	PRO	2.1
2	C	153	ARG	2.1
1	A	154	PHE	2.1
1	A	506	LEU	2.1
2	C	161	VAL	2.1
1	A	72	VAL	2.1
1	A	329	PRO	2.1
2	C	56	VAL	2.1
1	A	476	VAL	2.1
1	A	481	LYS	2.1
2	C	115	PRO	2.1
1	A	308	THR	2.0
1	A	364	VAL	2.0
2	C	167	ASN	2.0
1	A	479	TYR	2.0
2	C	103	ARG	2.0
1	A	37	ARG	2.0
2	C	91	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 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.