Full wwPDB X-ray Structure Validation Report ⓘ

Jun 24, 2025 – 04:02 pm BST

PDB ID	:	4BKA / pdb_00004bka
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 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:

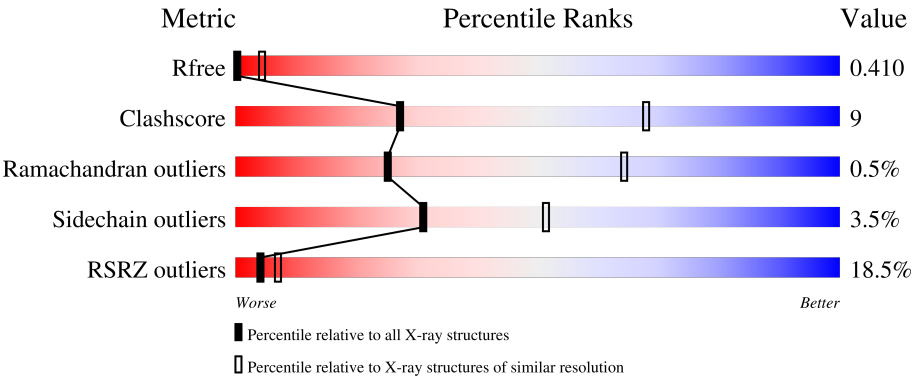
MolProbity	:	4-5-2 with Phenix2.0rc1
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.44

1 Overall quality at a glance (i)

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}	164625	1003 (6.62-3.98)
Clashscore	180529	1024 (6.60-4.00)
Ramachandran outliers	177936	1010 (6.64-3.92)
Sidechain outliers	177891	1123 (6.70-3.90)
RSRZ outliers	164620	1034 (6.64-3.96)

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 <=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	17% 70% 18% • 11%
2	C	180	11% 66% 10% • 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
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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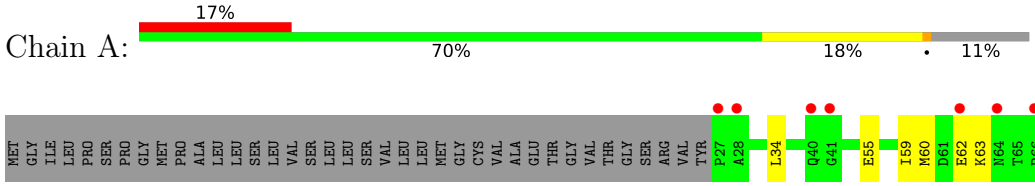
Chain	Residue	Modelled	Actual	Comment	Reference
C	19	SER	-	expression tag	UNP P52803
C	20	VAL	-	expression tag	UNP P52803
C	21	LEU	-	expression tag	UNP P52803
C	22	LEU	-	expression tag	UNP P52803
C	23	MET	-	expression tag	UNP P52803
C	24	GLY	-	expression tag	UNP P52803
C	25	CYS	-	expression tag	UNP P52803
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

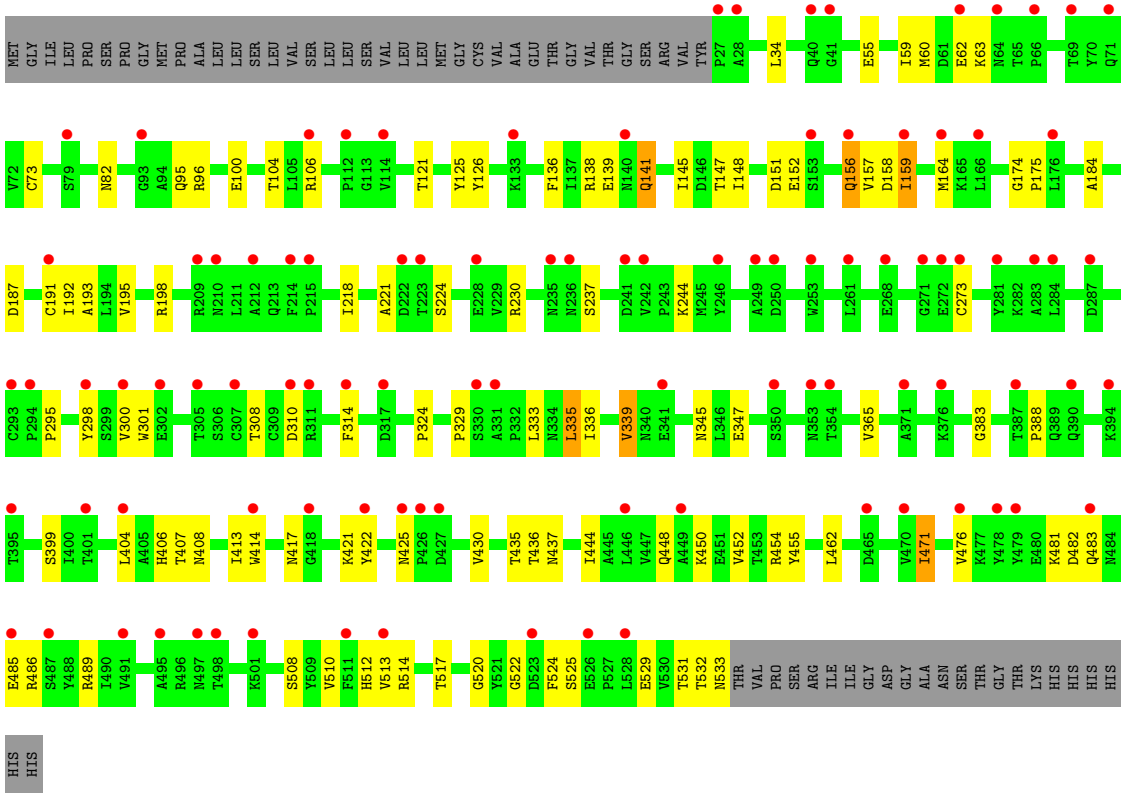
3 Residue-property plots (i)

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: EPHRIN TYPE-A RECEPTOR 4

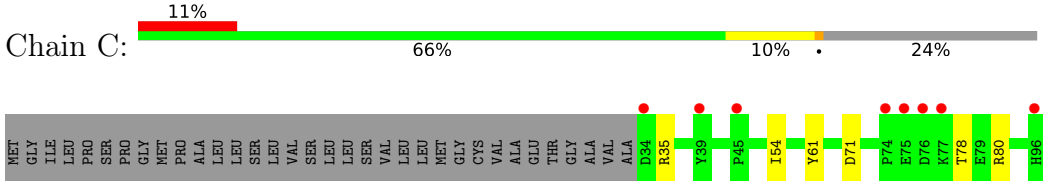
Chain A:

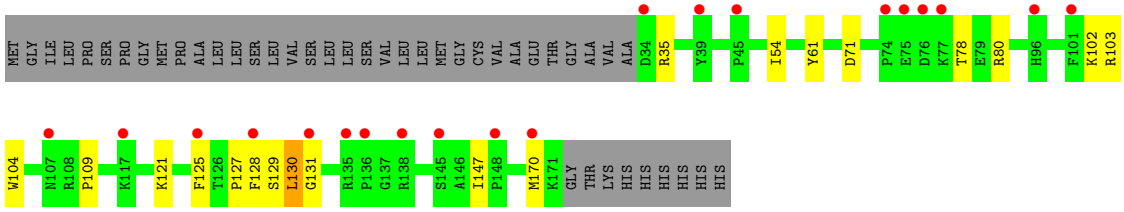




• Molecule 2: EPHRIN-A5

Chain C:





4 Data and refinement statistics (i)

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 84.87 – 5.30	Depositor EDS
% Data completeness (in resolution range)	96.3 (84.87-5.30) 96.3 (84.87-5.30)	Depositor EDS
R_{merge}	0.74	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.67 (at 5.41Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.383 , 0.408 0.384 , 0.410	Depositor DCC
R_{free} test set	449 reflections (4.82%)	wwPDB-VP
Wilson B-factor (Å^2)	155.3	Xtriage
Anisotropy	0.356	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 244.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.31$, $< L^2 > = 0.15$	Xtriage
Estimated twinning fraction	No twinning to report.	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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

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	0.66	0/4032	1.15	4/5484 (0.1%)
2	C	0.63	1/1177 (0.1%)	1.03	0/1592
All	All	0.65	1/5209 (0.0%)	1.13	4/7076 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	170	MET	C-N	-5.73	1.25	1.33

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	333	LEU	N-CA-C	7.81	119.79	111.28
1	A	159	ILE	N-CA-C	5.23	116.00	110.72
1	A	156	GLN	N-CA-C	5.10	117.97	111.69
1	A	520	GLY	N-CA-C	5.09	117.45	110.58

There are no chirality outliers.

There are no planarity outliers.

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	3948	0	3801	86	104
2	C	1139	0	1053	61	8
All	All	5087	0	4854	89	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 (89) 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
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:55:GLU:OE1	2:C:121:LYS:HD2	1.56	1.04
1:A:55:GLU:CD	2:C:61:TYR:HH	1.65	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:OH	2.01	1.03
1:A:164:MET:HE2	2:C:130:LEU:CG	1.90	1.01
1:A:164:MET:HE2	2:C:130:LEU:HG	1.01	1.00
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:191:CYS:C	2:C:127:PRO:HB3	1.92	0.94
1:A:195:VAL:CG2	2:C:128:PHE:CE1	2.24	0.89
1:A:164:MET:SD	2:C:130:LEU:HB2	2.17	0.84
1:A:164:MET:CE	2:C:130:LEU:CG	2.53	0.80
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:73:CYS:HB2	2:C:127:PRO:HG3	1.73	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: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
1:A:164:MET:HE1	2:C:130:LEU:HG	1.81	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:GLU:OE1	2:C:121:LYS:NZ	2.37	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:164:MET:HE1	2:C:130:LEU:CB	2.35	0.55
1:A:336:ILE:HB	1:A:347:GLU:HB3	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: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:192:ILE:C	2:C:127:PRO:HB2	2.40	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:192:ILE:N	2:C:127:PRO:HB3	2.27	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:HG3	2:C:104:TRP:HA	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:MET:HG2	2:C:103:ARG:O	2.17	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: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:164:MET:HE1	2:C:130:LEU:CG	2.41	0.40
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:301:TRP:CE2	1:A:414:TRP:CD2[5_675]	0.97	1.23
1:A:454:ARG:NH1	1:A:482:ASP:OD1[16_454]	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:158:ASP:OD2	1:A:455:TYR:OH[8_565]	1.11	1.09
1:A:301:TRP:CH2	1:A:414:TRP:CE2[5_675]	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:158:ASP:CG	1:A:455:TYR:OH[8_565]	1.37	0.83
1:A:301:TRP:CZ3	1:A:365:VAL:CG2[5_675]	1.37	0.83
1:A:152:GLU:OE2	1:A:512:HIS:CE1[6_555]	1.39	0.81
1:A:531:THR:CB	1:A:531:THR:CB[16_454]	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:224:SER:OG	1:A:345:ASN:OD1[6_555]	1.61	0.59
1:A:422:TYR:CG	1:A:422:TYR:OH[5_675]	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:301:TRP:CH2	1:A:414:TRP:CZ2[5_675]	1.98	0.22
1:A:454:ARG:CZ	1:A:482:ASP:OD1[16_454]	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:152:GLU:CG	1:A:512:HIS:CE1[6_555]	2.13	0.07
1:A:301:TRP:CD2	1:A:414:TRP:CD2[5_675]	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:158:ASP:CB	1:A:455:TYR:OH[8_565]	2.18	0.02
1:A:481:LYS:CE	1:A:533:ASN:CB[16_454]	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%)	22 60
2	C	133/180 (74%)	124 (93%)	9 (7%)	0	100 100
All	All	636/748 (85%)	601 (94%)	32 (5%)	3 (0%)	25 64

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%)	422 (96%)	17 (4%)	27 48
2	C	126/161 (78%)	123 (98%)	3 (2%)	44 62
All	All	565/650 (87%)	545 (96%)	20 (4%)	31 51

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

Mol	Chain	Res	Type
1	A	34	LEU
1	A	95	GLN
1	A	141	GLN

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Mol	Chain	Res	Type
1	A	148	ILE
1	A	218	ILE
1	A	300	VAL
1	A	335	LEU
1	A	339	VAL
1	A	404	LEU
1	A	407	THR
1	A	408	ASN
1	A	435	THR
1	A	444	ILE
1	A	450	LYS
1	A	462	LEU
1	A	471	ILE
1	A	483	GLN
2	C	54	ILE
2	C	102	LYS
2	C	130	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	29	ASN
1	A	40	GLN
1	A	64	ASN
1	A	109	ASN
1	A	123	ASN
1	A	131	ASN
1	A	213	GLN
1	A	259	ASN
1	A	266	HIS
1	A	296	HIS
1	A	391	ASN
1	A	438	GLN
1	A	483	GLN
2	C	53	HIS
2	C	59	ASN
2	C	68	HIS
2	C	123	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	C	1
1	A	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, 95^{th} 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%)	1.10	99 (19%) 4 7	43, 211, 428, 500	0
2	C	137/180 (76%)	0.78	20 (14%) 7 10	119, 287, 458, 500	0
All	All	644/748 (86%)	1.03	119 (18%) 4 7	43, 230, 433, 500	0

All (119) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	268	GLU	7.0
1	A	465	ASP	5.5
1	A	223	THR	5.1
1	A	153	SER	4.8
1	A	27	PRO	4.7
1	A	156	GLN	4.7
1	A	235	ASN	4.4
1	A	422	TYR	4.3
1	A	283	ALA	4.2
1	A	497	ASN	4.2
1	A	371	ALA	4.1
1	A	176	LEU	4.1
1	A	66	PRO	3.9
1	A	485	GLU	3.8
1	A	305	THR	3.8
1	A	311	ARG	3.8
1	A	41	GLY	3.7
1	A	164	MET	3.7
2	C	39	TYR	3.6
1	A	166	LEU	3.6
1	A	476	VAL	3.6
1	A	271	GLY	3.5
1	A	317	ASP	3.5
1	A	214	PHE	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	159	ILE	3.4
1	A	242	VAL	3.4
1	A	341	GLU	3.4
1	A	511	PHE	3.3
1	A	222	ASP	3.3
1	A	501	LYS	3.3
1	A	261	LEU	3.3
1	A	302	GLU	3.3
1	A	114	VAL	3.2
2	C	76	ASP	3.2
2	C	74	PRO	3.2
1	A	314	PHE	3.2
1	A	246	TYR	3.1
1	A	133	LYS	3.1
1	A	191	CYS	3.1
1	A	479	TYR	3.0
1	A	241	ASP	3.0
1	A	425	ASN	2.9
1	A	40	GLN	2.9
1	A	401	THR	2.9
1	A	215	PRO	2.9
1	A	426	PRO	2.9
1	A	513	VAL	2.9
2	C	148	PRO	2.9
1	A	69	THR	2.8
1	A	273	CYS	2.8
1	A	331	ALA	2.8
1	A	495	ALA	2.8
1	A	330	SER	2.8
1	A	387	THR	2.8
1	A	478	TYR	2.7
1	A	210	ASN	2.7
1	A	376	LYS	2.7
2	C	131	GLY	2.7
1	A	470	VAL	2.7
1	A	28	ALA	2.7
2	C	75	GLU	2.7
2	C	170	MET	2.6
1	A	449	ALA	2.6
1	A	418	GLY	2.6
1	A	487	SER	2.6
1	A	253	TRP	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	236	ASN	2.6
1	A	300	VAL	2.6
1	A	112	PRO	2.6
1	A	353	ASN	2.5
1	A	281	TYR	2.5
1	A	395	THR	2.5
1	A	528	LEU	2.5
2	C	77	LYS	2.5
2	C	45	PRO	2.5
1	A	79	SER	2.4
1	A	71	GLN	2.4
1	A	298	TYR	2.4
2	C	136	PRO	2.4
1	A	209	ARG	2.4
1	A	390	GLN	2.4
1	A	106	ARG	2.4
2	C	107	ASN	2.4
1	A	93	GLY	2.4
1	A	62	GLU	2.4
1	A	250	ASP	2.4
1	A	446	LEU	2.3
1	A	140	ASN	2.3
2	C	145	SER	2.3
2	C	101	PHE	2.3
2	C	125	PHE	2.3
1	A	394	LYS	2.3
1	A	212	ALA	2.3
2	C	138	ARG	2.2
1	A	523	ASP	2.2
1	A	483	GLN	2.2
1	A	284	LEU	2.2
2	C	96	HIS	2.2
1	A	427	ASP	2.2
1	A	272	GLU	2.2
1	A	526	GLU	2.2
1	A	294	PRO	2.2
1	A	491	VAL	2.2
1	A	310	ASP	2.2
1	A	64	ASN	2.1
1	A	404	LEU	2.1
2	C	34	ASP	2.1
1	A	307	CYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	287	ASP	2.1
1	A	249	ALA	2.1
2	C	117	LYS	2.1
1	A	498	THR	2.1
1	A	293	CYS	2.1
1	A	414	TRP	2.1
2	C	128	PHE	2.1
2	C	135	ARG	2.0
1	A	228	GLU	2.0
1	A	350	SER	2.0
1	A	354	THR	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.