



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 10:22 PM UTC

PDB ID : 3HEI / pdb_00003hei
Title : Ligand Recognition by A-Class Eph Receptors: Crystal Structures of the EphA2 Ligand-Binding Domain and the EphA2/ephrin-A1 Complex
Authors : Himanen, J.P.; Goldgur, Y.; Miao, H.; Myshkin, E.; Guo, H.; Buck, M.; Nguyen, M.; Rajashankar, K.R.; Wang, B.; Nikolov, D.B.
Deposited on : 2009-05-08
Resolution : 2.00 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

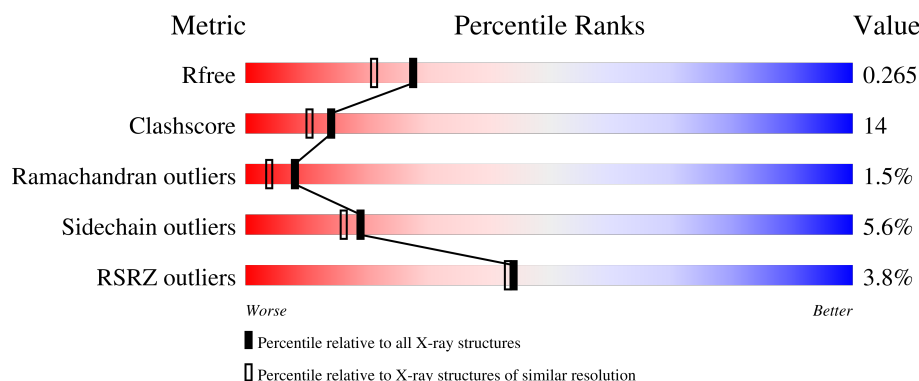
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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.



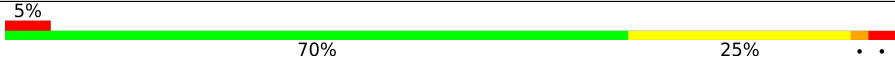
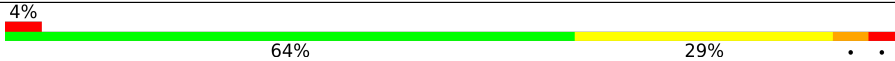
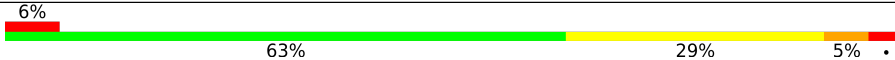
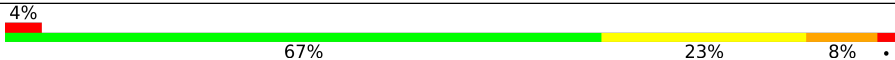
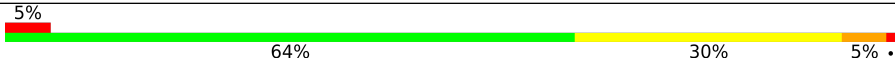
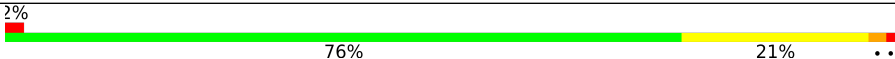
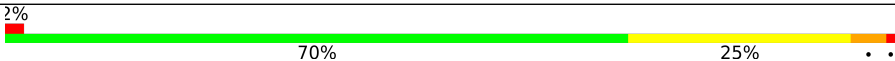
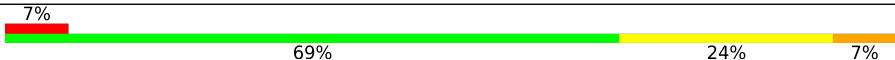
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	174	3% 79% 18% .
1	C	174	2% 78% 20% ..
1	E	174	2% 80% 17% .
1	G	174	% 77% 18% ..
1	I	174	6% 78% 20% .

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	K	174	
1	M	174	
1	O	174	
2	B	132	
2	D	132	
2	F	132	
2	H	132	
2	J	132	
2	L	132	
2	N	132	
2	P	132	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 22908 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 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	174	Total	C	N	O	S	0	0	0
			1399	896	231	262	10			
1	C	174	Total	C	N	O	S	0	0	0
			1399	896	231	262	10			
1	E	174	Total	C	N	O	S	0	0	0
			1399	896	231	262	10			
1	G	174	Total	C	N	O	S	0	0	0
			1399	896	231	262	10			
1	I	174	Total	C	N	O	S	0	0	0
			1399	896	231	262	10			
1	K	174	Total	C	N	O	S	0	0	0
			1399	896	231	262	10			
1	M	174	Total	C	N	O	S	0	0	0
			1399	896	231	262	10			
1	O	174	Total	C	N	O	S	0	0	0
			1399	896	231	262	10			

- Molecule 2 is a protein called Ephrin-A1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	132	Total	C	N	O	S	0	0	0
			1120	712	197	206	5			
2	D	132	Total	C	N	O	S	0	0	0
			1120	712	197	206	5			
2	F	132	Total	C	N	O	S	0	0	0
			1120	712	197	206	5			
2	H	132	Total	C	N	O	S	0	0	0
			1120	712	197	206	5			
2	J	132	Total	C	N	O	S	0	0	0
			1120	712	197	206	5			
2	L	132	Total	C	N	O	S	0	0	0
			1120	712	197	206	5			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	N	132	Total	C	N	O	S	0	0	0
			1120	712	197	206	5			
2	P	132	Total	C	N	O	S	0	0	0
			1120	712	197	206	5			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	148	LYS	-	expression tag	UNP P20827
B	149	ILE	-	expression tag	UNP P20827
D	148	LYS	-	expression tag	UNP P20827
D	149	ILE	-	expression tag	UNP P20827
F	148	LYS	-	expression tag	UNP P20827
F	149	ILE	-	expression tag	UNP P20827
H	148	LYS	-	expression tag	UNP P20827
H	149	ILE	-	expression tag	UNP P20827
J	148	LYS	-	expression tag	UNP P20827
J	149	ILE	-	expression tag	UNP P20827
L	148	LYS	-	expression tag	UNP P20827
L	149	ILE	-	expression tag	UNP P20827
N	148	LYS	-	expression tag	UNP P20827
N	149	ILE	-	expression tag	UNP P20827
P	148	LYS	-	expression tag	UNP P20827
P	149	ILE	-	expression tag	UNP P20827

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	200	Total	O	0	0
			200	200		
3	B	226	Total	O	0	0
			226	226		
3	C	225	Total	O	0	0
			225	225		
3	D	171	Total	O	0	0
			171	171		
3	E	178	Total	O	0	0
			178	178		
3	F	179	Total	O	0	0
			179	179		
3	G	219	Total	O	0	0
			219	219		

Continued on next page...

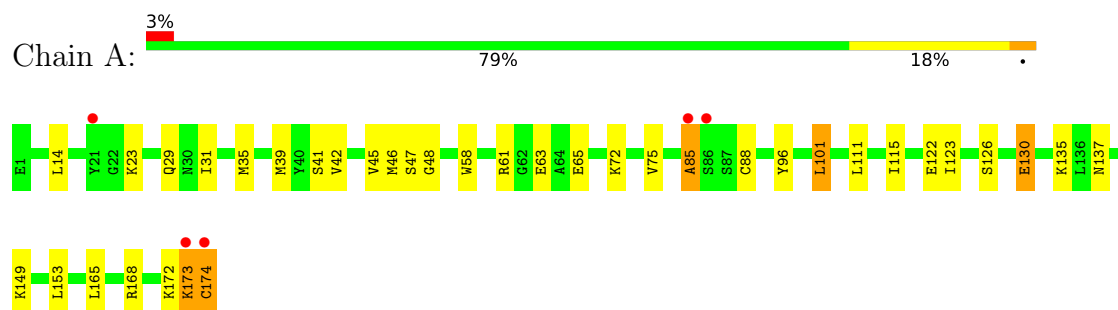
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	H	203	Total 203	O 203	0	0
3	I	115	Total 115	O 115	0	0
3	J	145	Total 145	O 145	0	0
3	K	173	Total 173	O 173	0	0
3	L	149	Total 149	O 149	0	0
3	M	157	Total 157	O 157	0	0
3	N	173	Total 173	O 173	0	0
3	O	99	Total 99	O 99	0	0
3	P	144	Total 144	O 144	0	0

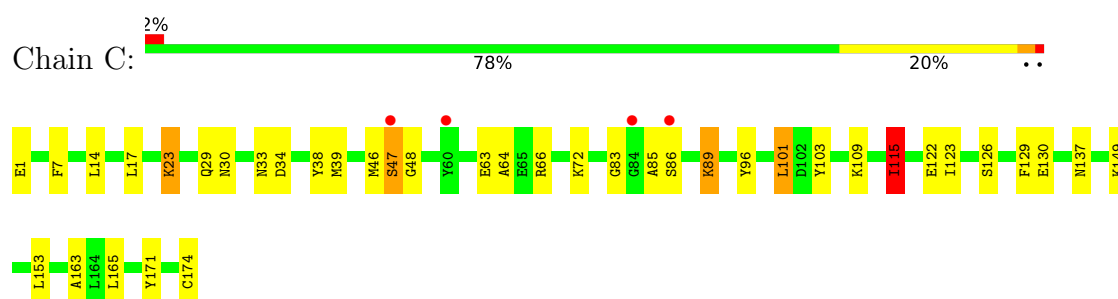
3 Residue-property plots [i](#)

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.

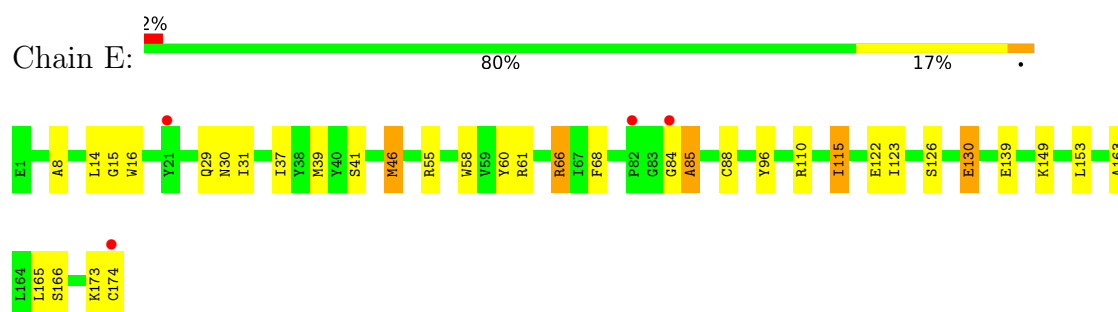
- Molecule 1: Ephrin type-A receptor 2



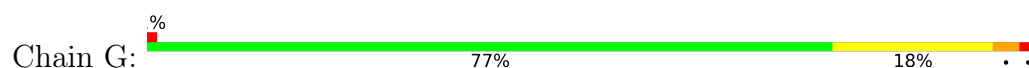
- Molecule 1: Ephrin type-A receptor 2

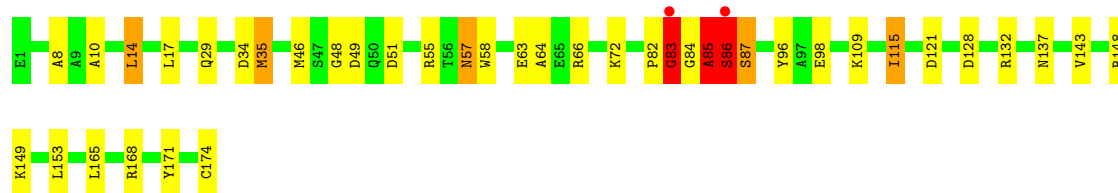


- Molecule 1: Ephrin type-A receptor 2

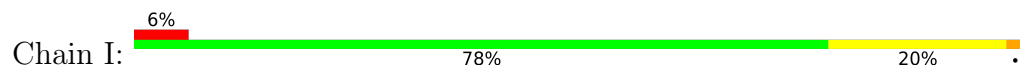


- Molecule 1: Ephrin type-A receptor 2

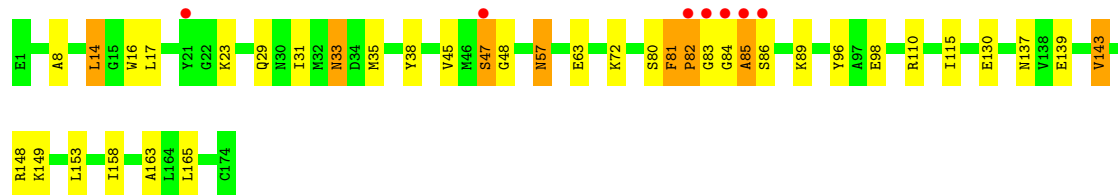
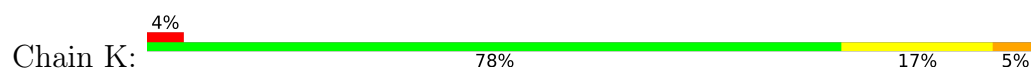




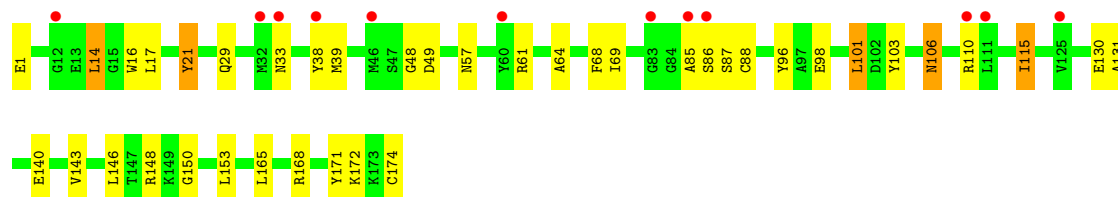
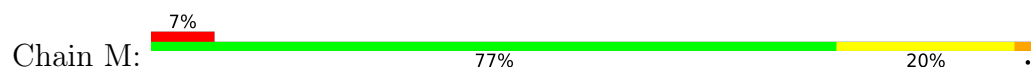
- Molecule 1: Ephrin type-A receptor 2



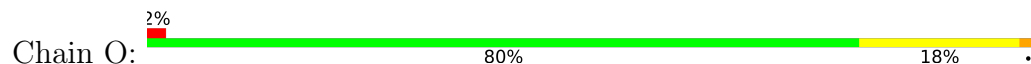
- Molecule 1: Ephrin type-A receptor 2



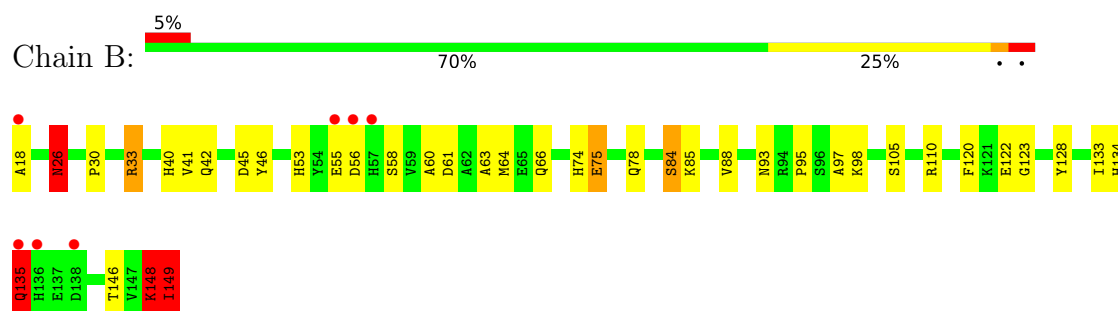
- Molecule 1: Ephrin type-A receptor 2



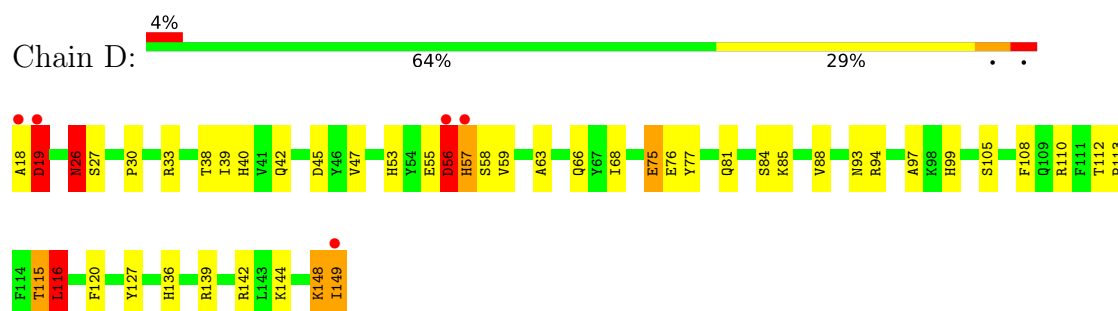
- Molecule 1: Ephrin type-A receptor 2



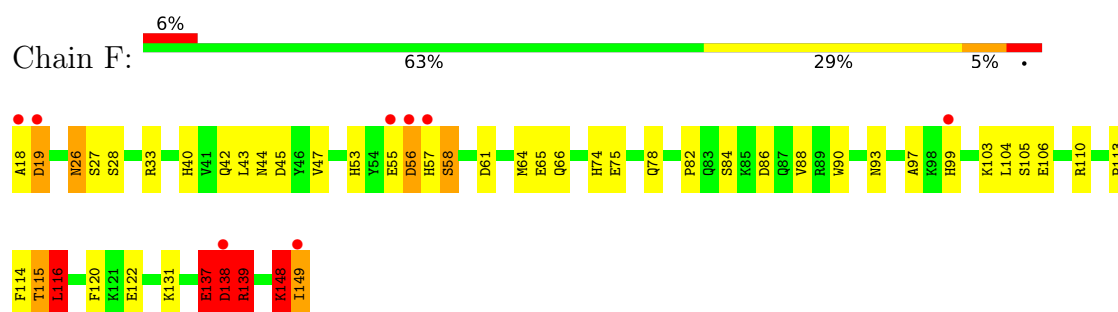
- Molecule 2: Ephrin-A1



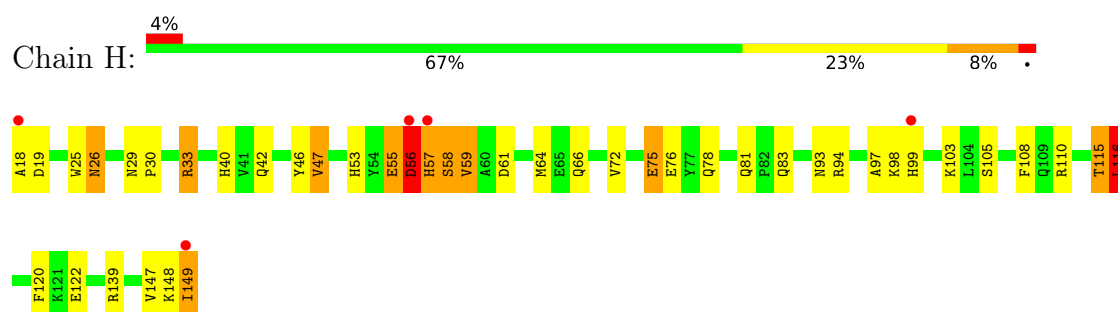
- Molecule 2: Ephrin-A1



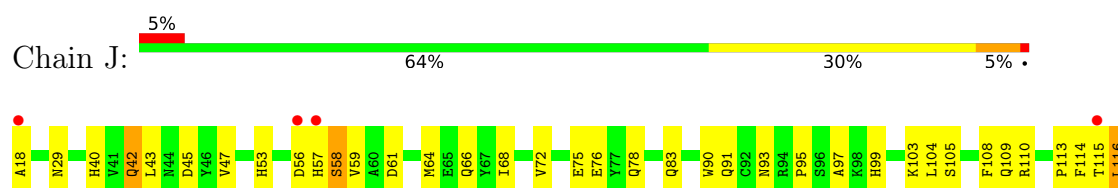
- Molecule 2: Ephrin-A1

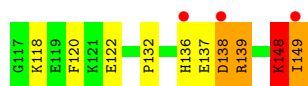


- Molecule 2: Ephrin-A1

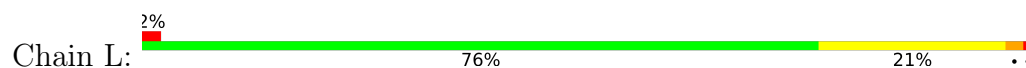


- Molecule 2: Ephrin-A1

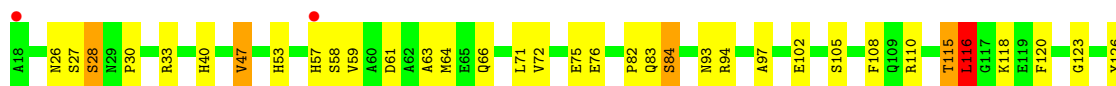




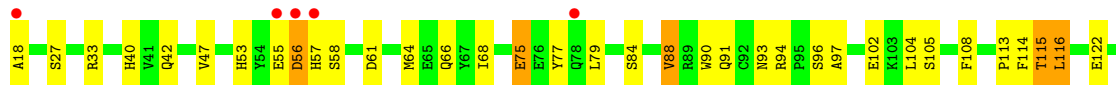
• Molecule 2: Ephrin-A1



• Molecule 2: Ephrin-A1



• Molecule 2: Ephrin-A1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	58.48Å 102.11Å 135.25Å 84.25° 79.77° 73.94°	Depositor
Resolution (Å)	50.00 – 2.00 50.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	96.0 (50.00-2.00) 96.1 (50.00-2.00)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.40 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.172 , 0.233 0.209 , 0.265	Depositor DCC
R_{free} test set	9696 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	21.6	Xtriage
Anisotropy	0.193	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 34.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.019 for h,h-k,h-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	22908	wwPDB-VP
Average B, all atoms (Å ²)	10.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.47% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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	1.48	5/1433 (0.3%)	1.26	6/1940 (0.3%)
1	C	1.41	3/1433 (0.2%)	1.26	6/1940 (0.3%)
1	E	1.26	6/1433 (0.4%)	1.14	1/1940 (0.1%)
1	G	1.47	11/1433 (0.8%)	1.23	6/1940 (0.3%)
1	I	1.06	0/1433	1.01	1/1940 (0.1%)
1	K	1.33	3/1433 (0.2%)	1.22	5/1940 (0.3%)
1	M	1.11	1/1433 (0.1%)	1.09	0/1940
1	O	1.03	1/1433 (0.1%)	1.09	0/1940
2	B	1.49	5/1154 (0.4%)	1.35	12/1562 (0.8%)
2	D	1.50	10/1154 (0.9%)	1.29	10/1562 (0.6%)
2	F	1.45	4/1154 (0.3%)	1.36	9/1562 (0.6%)
2	H	1.63	10/1154 (0.9%)	1.35	8/1562 (0.5%)
2	J	1.29	0/1154	1.21	8/1562 (0.5%)
2	L	1.31	2/1154 (0.2%)	1.19	3/1562 (0.2%)
2	N	1.41	3/1154 (0.3%)	1.22	5/1562 (0.3%)
2	P	1.26	2/1154 (0.2%)	1.16	6/1562 (0.4%)
All	All	1.35	66/20696 (0.3%)	1.21	86/28016 (0.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	G	0	1
2	B	0	2
2	F	0	1
2	J	0	1
All	All	0	6

All (66) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	N	26	ASN	N-CA	13.29	1.62	1.46
2	H	26	ASN	CA-CB	11.76	1.77	1.53
2	B	26	ASN	CG-ND2	11.14	1.56	1.33
2	H	26	ASN	N-CA	10.95	1.59	1.46
2	D	116	LEU	N-CA	10.72	1.60	1.46
2	D	26	ASN	CG-ND2	10.20	1.54	1.33
2	N	26	ASN	CA-CB	9.04	1.72	1.53
2	H	26	ASN	CG-OD1	8.90	1.40	1.23
1	G	14	LEU	C-O	8.66	1.34	1.24
2	H	115	THR	C-O	-8.50	1.12	1.23
1	G	86	SER	C-O	8.17	1.34	1.24
2	B	26	ASN	CB-CG	7.98	1.72	1.52
2	F	116	LEU	N-CA	7.95	1.56	1.46
2	D	68	ILE	CA-CB	6.97	1.62	1.54
2	H	116	LEU	N-CA	6.88	1.55	1.46
1	A	42	VAL	N-CA	6.87	1.54	1.46
2	D	115	THR	C-N	-6.76	1.24	1.33
1	G	57	ASN	CB-CG	6.70	1.68	1.52
1	K	47	SER	C-O	6.58	1.31	1.23
2	D	26	ASN	CB-CG	6.54	1.68	1.52
1	G	83	GLY	N-CA	6.32	1.54	1.45
1	A	31	ILE	CA-CB	-6.23	1.47	1.54
2	F	26	ASN	CA-CB	6.22	1.67	1.54
2	L	78	GLN	N-CA	6.18	1.53	1.46
1	G	85	ALA	N-CA	6.14	1.54	1.46
2	D	19	ASP	CA-CB	-6.12	1.43	1.53
1	C	47	SER	C-O	6.04	1.31	1.23
2	D	19	ASP	C-O	-5.93	1.16	1.24
2	L	116	LEU	N-CA	5.87	1.53	1.46
1	E	61	ARG	CA-C	5.87	1.60	1.52
1	K	143	VAL	CA-C	-5.86	1.45	1.52
1	G	57	ASN	CG-ND2	5.86	1.45	1.33
1	E	115	ILE	CA-CB	5.80	1.61	1.55
2	H	59	VAL	CA-C	5.77	1.59	1.52
2	B	146	THR	CA-C	5.76	1.59	1.52
1	A	61	ARG	CA-C	5.75	1.60	1.52
2	H	29	ASN	CA-C	5.73	1.59	1.52
2	B	63	ALA	CA-C	5.71	1.60	1.52
2	H	115	THR	C-N	-5.65	1.25	1.33
1	K	8	ALA	CA-CB	5.60	1.62	1.53
1	G	115	ILE	CA-CB	5.59	1.61	1.54
2	P	55	GLU	CA-C	5.57	1.59	1.52
2	P	56	ASP	N-CA	5.46	1.53	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	115	ILE	CG1-CD1	-5.42	1.30	1.51
1	C	7	PHE	C-O	5.42	1.30	1.24
1	G	55	ARG	N-CA	5.41	1.52	1.46
1	E	166	SER	C-O	5.37	1.30	1.23
2	H	147	VAL	CA-CB	5.37	1.60	1.54
2	H	26	ASN	CA-C	5.37	1.59	1.52
1	E	55	ARG	N-CA	5.33	1.52	1.46
2	B	128	TYR	N-CA	5.32	1.52	1.46
1	M	150	GLY	N-CA	5.30	1.51	1.45
2	N	26	ASN	CG-OD1	5.29	1.33	1.23
2	D	115	THR	C-O	-5.28	1.16	1.23
1	A	135	LYS	CA-CB	5.24	1.59	1.53
1	O	57	ASN	CB-CG	5.20	1.65	1.52
1	G	8	ALA	CA-CB	5.14	1.62	1.53
1	G	87	SER	CA-C	-5.14	1.47	1.53
2	F	88	VAL	N-CA	5.12	1.52	1.46
2	D	112	THR	CA-CB	5.10	1.61	1.54
2	D	26	ASN	CA-CB	5.08	1.62	1.53
1	E	8	ALA	N-CA	5.08	1.52	1.46
1	A	75	VAL	N-CA	5.05	1.52	1.46
1	E	31	ILE	CA-CB	-5.04	1.48	1.54
1	G	83	GLY	CA-C	5.02	1.58	1.51
2	F	137	GLU	CA-C	-5.00	1.47	1.52

All (86) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	26	ASN	N-CA-C	-11.69	89.19	109.06
2	N	26	ASN	N-CA-C	-10.68	90.90	109.06
2	D	115	THR	O-C-N	-10.40	110.93	122.79
2	D	19	ASP	N-CA-C	9.87	131.81	110.80
2	H	115	THR	O-C-N	-9.14	112.37	122.79
2	F	115	THR	N-CA-C	-9.10	99.22	110.41
2	D	115	THR	N-CA-C	-9.09	98.53	110.53
1	K	81	PHE	CA-C-N	8.48	130.44	119.84
1	K	81	PHE	C-N-CA	8.48	130.44	119.84
2	H	116	LEU	N-CA-CB	8.40	124.69	110.49
2	F	138	ASP	N-CA-C	-8.15	97.78	110.42
2	D	19	ASP	CA-CB-CG	-7.89	104.71	112.60
2	P	115	THR	N-CA-C	-7.78	98.77	110.28
1	C	66	ARG	NE-CZ-NH2	-7.78	112.20	119.20
2	N	115	THR	N-CA-C	-7.77	99.54	110.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	84	SER	N-CA-C	7.61	119.71	108.60
2	F	26	ASN	CA-CB-CG	7.53	120.13	112.60
2	D	115	THR	CA-C-N	-7.41	107.39	121.54
2	D	115	THR	C-N-CA	-7.41	107.39	121.54
2	F	149	ILE	N-CA-CB	7.14	123.63	111.50
1	G	14	LEU	N-CA-C	-7.00	97.31	108.73
2	B	134	HIS	CA-C-N	6.99	134.90	121.54
2	B	134	HIS	C-N-CA	6.99	134.90	121.54
2	L	28	SER	CB-CA-C	6.91	121.86	110.17
1	A	47	SER	CA-C-N	-6.83	112.19	121.06
1	A	47	SER	C-N-CA	-6.83	112.19	121.06
1	A	23	LYS	N-CA-C	-6.63	99.11	109.72
2	H	115	THR	N-CA-C	-6.61	101.81	110.53
2	B	148	LYS	CA-C-N	-6.52	109.97	121.70
2	B	148	LYS	C-N-CA	-6.52	109.97	121.70
1	G	85	ALA	CA-C-N	-6.41	109.31	121.54
1	G	85	ALA	C-N-CA	-6.41	109.31	121.54
2	D	116	LEU	N-CA-CB	6.33	121.19	110.49
2	J	148	LYS	CA-C-N	-6.22	110.50	121.70
2	J	148	LYS	C-N-CA	-6.22	110.50	121.70
1	I	2	VAL	N-CA-C	-6.18	98.83	107.80
2	P	138	ASP	N-CA-C	-6.18	101.05	110.14
2	F	33	ARG	N-CA-C	6.18	118.80	111.33
2	H	26	ASN	N-CA-CB	6.13	122.11	111.13
2	P	96	SER	N-CA-C	6.12	120.06	111.30
1	K	57	ASN	N-CA-C	-6.11	102.42	110.43
2	B	95	PRO	CA-C-N	-6.08	112.97	123.25
2	B	95	PRO	C-N-CA	-6.08	112.97	123.25
2	B	135	GLN	N-CA-C	6.04	123.66	110.80
2	H	26	ASN	CB-CA-C	-5.99	97.22	109.38
2	J	95	PRO	CA-C-N	-5.94	113.21	123.25
2	J	95	PRO	C-N-CA	-5.94	113.21	123.25
2	P	27	SER	CA-C-N	-5.94	112.35	122.56
2	P	27	SER	C-N-CA	-5.94	112.35	122.56
1	K	143	VAL	CB-CA-C	-5.90	100.38	111.30
2	B	149	ILE	N-CA-CB	5.89	121.52	111.50
2	B	26	ASN	CA-CB-CG	5.71	118.31	112.60
1	G	14	LEU	O-C-N	5.66	129.67	123.22
2	B	88	VAL	N-CA-CB	5.63	117.68	110.13
2	D	127	TYR	N-CA-C	5.57	118.18	108.76
2	F	148	LYS	CA-C-N	-5.57	111.68	121.70
2	F	148	LYS	C-N-CA	-5.57	111.68	121.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	34	ASP	N-CA-C	5.56	119.64	112.86
1	C	174	CYS	CA-C-O	-5.53	111.40	120.80
2	H	57	HIS	CB-CA-C	5.44	121.24	110.42
2	L	137	GLU	CA-C-N	5.43	128.57	120.31
2	L	137	GLU	C-N-CA	5.43	128.57	120.31
2	N	26	ASN	CB-CA-C	-5.40	98.41	109.38
2	J	149	ILE	N-CA-CB	5.40	120.67	111.50
2	J	138	ASP	N-CA-C	-5.39	101.48	110.17
1	E	115	ILE	CB-CA-C	-5.33	105.51	111.80
1	K	23	LYS	N-CA-C	-5.30	101.92	110.14
2	B	58	SER	N-CA-C	5.22	116.97	111.28
2	P	88	VAL	N-CA-CB	5.18	116.89	110.05
1	C	109	LYS	CB-CG-CD	-5.14	99.47	111.30
2	F	115	THR	O-C-N	-5.13	116.39	122.65
1	A	172	LYS	CA-C-N	-5.10	115.91	123.05
1	A	172	LYS	C-N-CA	-5.10	115.91	123.05
2	N	126	TYR	CA-CB-CG	-5.10	104.73	113.90
1	A	41	SER	N-CA-CB	-5.07	102.14	111.37
1	C	23	LYS	N-CA-C	-5.06	101.85	109.85
2	B	123	GLY	N-CA-C	-5.04	108.36	115.32
1	C	109	LYS	CB-CA-C	-5.02	101.34	110.63
1	G	86	SER	CA-CB-OG	-5.02	101.07	111.10
2	D	26	ASN	CA-CB-CG	5.02	117.62	112.60
1	G	66	ARG	CG-CD-NE	-5.01	100.97	112.00
2	J	29	ASN	CA-C-N	5.01	125.28	119.47
2	J	29	ASN	C-N-CA	5.01	125.28	119.47
2	H	25	TRP	CA-C-O	-5.01	116.35	122.41
2	D	57	HIS	N-CA-C	-5.00	102.67	110.42
2	F	116	LEU	N-CA-CB	5.00	118.94	110.49

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	48	GLY	Peptide
2	B	135	GLN	Peptide
2	B	148	LYS	Peptide
2	F	148	LYS	Peptide
1	G	83	GLY	Peptide
2	J	148	LYS	Peptide

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	1399	0	1348	25	0
1	C	1399	0	1348	32	0
1	E	1399	0	1348	35	0
1	G	1399	0	1348	31	0
1	I	1399	0	1348	33	0
1	K	1399	0	1348	28	0
1	M	1399	0	1348	45	0
1	O	1399	0	1348	27	0
2	B	1120	0	1058	34	0
2	D	1120	0	1058	39	0
2	F	1120	0	1058	63	0
2	H	1120	0	1058	54	0
2	J	1120	0	1058	47	0
2	L	1120	0	1058	35	0
2	N	1120	0	1058	31	0
2	P	1120	0	1058	40	0
3	A	200	0	0	8	0
3	B	226	0	0	11	1
3	C	225	0	0	13	0
3	D	171	0	0	8	0
3	E	178	0	0	10	0
3	F	179	0	0	20	0
3	G	219	0	0	11	0
3	H	203	0	0	20	1
3	I	115	0	0	7	0
3	J	145	0	0	12	0
3	K	173	0	0	8	1
3	L	149	0	0	7	0
3	M	157	0	0	13	1
3	N	173	0	0	8	0
3	O	99	0	0	10	0
3	P	144	0	0	6	0
All	All	22908	0	19248	562	2

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 14.

All (562) 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)
2:H:26:ASN:CA	2:H:26:ASN:CB	1.77	1.57
2:F:47:VAL:HB	3:F:1187:HOH:O	1.27	1.30
2:H:18:ALA:HB3	3:H:720:HOH:O	1.18	1.27
2:H:139:ARG:HD3	3:H:1411:HOH:O	1.29	1.23
2:P:18:ALA:O	3:P:1057:HOH:O	1.58	1.19
1:K:35:MET:HG3	3:K:1839:HOH:O	1.42	1.16
2:D:18:ALA:N	3:D:2672:HOH:O	1.79	1.15
1:C:89:LYS:HE2	3:C:245:HOH:O	1.42	1.15
2:P:40:HIS:CE1	2:P:148:LYS:HB3	1.85	1.12
1:G:86:SER:HB3	3:G:1220:HOH:O	1.50	1.11
2:J:99:HIS:HE1	3:J:1893:HOH:O	1.30	1.11
1:M:1:GLU:N	3:M:2241:HOH:O	1.77	1.11
1:C:96:TYR:HD2	1:C:115:ILE:HD11	1.14	1.08
2:N:28:SER:HB2	3:N:2112:HOH:O	0.92	1.08
1:O:30:ASN:HB3	3:O:604:HOH:O	1.52	1.05
1:C:96:TYR:CD2	1:C:115:ILE:HD11	1.90	1.05
2:B:149:ILE:HG22	3:B:1383:HOH:O	1.56	1.04
1:G:174:CYS:C	3:G:1254:HOH:O	2.00	1.03
1:K:96:TYR:CD2	1:K:115:ILE:HD11	1.93	1.03
2:P:40:HIS:HE1	2:P:148:LYS:HB3	1.15	1.03
2:J:40:HIS:CE1	2:J:148:LYS:HB3	1.94	1.02
1:E:30:ASN:HB3	3:E:687:HOH:O	1.59	1.00
2:D:81:GLN:NE2	1:O:35:MET:SD	2.33	1.00
1:C:86:SER:HB3	3:C:1168:HOH:O	1.60	0.99
1:M:168:ARG:HD3	3:M:1104:HOH:O	1.63	0.98
1:C:63:GLU:HB3	3:C:1747:HOH:O	1.63	0.97
1:A:39:MET:HE2	1:A:165:LEU:HD11	1.45	0.96
2:F:148:LYS:HD2	2:F:149:ILE:C	1.91	0.96
2:D:19:ASP:OD2	2:D:45:ASP:OD1	1.84	0.95
1:G:46:MET:SD	3:G:2602:HOH:O	2.22	0.95
2:P:114:PHE:HB3	3:P:1231:HOH:O	1.66	0.95
2:J:40:HIS:HE1	2:J:148:LYS:HB3	1.25	0.95
2:H:18:ALA:N	3:H:925:HOH:O	1.98	0.95
1:A:122:GLU:HG3	3:A:1801:HOH:O	1.67	0.95
1:C:149:LYS:HD3	3:C:1959:HOH:O	1.68	0.94
2:F:18:ALA:HB3	3:F:2722:HOH:O	0.77	0.94
2:B:98:LYS:HE2	3:B:2361:HOH:O	1.65	0.94
2:F:18:ALA:N	3:F:2185:HOH:O	1.98	0.94
2:P:61:ASP:HA	2:P:64:MET:HE2	1.47	0.94
2:N:148:LYS:HD2	3:N:1611:HOH:O	1.69	0.93
1:I:30:ASN:HB3	3:I:370:HOH:O	1.69	0.92

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:61:ASP:HA	2:H:64:MET:HE2	1.52	0.90
2:D:40:HIS:CE1	2:D:148:LYS:HB3	2.07	0.90
2:L:149:ILE:HG23	3:L:1626:HOH:O	1.70	0.90
2:P:114:PHE:HD2	3:P:1231:HOH:O	1.56	0.89
1:A:96:TYR:CD2	1:A:115:ILE:HD11	2.07	0.89
3:I:2496:HOH:O	2:L:85:LYS:HD2	1.73	0.87
2:H:47:VAL:HG12	2:H:108:PHE:HE1	1.39	0.87
1:M:174:CYS:HA	3:M:910:HOH:O	1.73	0.87
1:E:96:TYR:CD2	1:E:115:ILE:HD11	2.09	0.87
1:C:1:GLU:N	3:C:2424:HOH:O	2.08	0.87
2:D:57:HIS:HD2	3:D:2611:HOH:O	1.56	0.87
2:L:149:ILE:CG2	3:L:1626:HOH:O	2.22	0.86
1:I:15:GLY:N	3:I:2053:HOH:O	2.05	0.86
1:E:84:GLY:HA2	1:M:86:SER:OG	1.76	0.85
2:P:114:PHE:CD2	3:P:1231:HOH:O	2.28	0.85
1:E:85:ALA:HB1	1:E:88:CYS:HB2	1.59	0.85
1:G:168:ARG:CD	3:G:1511:HOH:O	2.25	0.85
1:A:39:MET:HB3	1:A:165:LEU:HD13	1.58	0.84
2:D:26:ASN:OD1	3:D:1452:HOH:O	1.95	0.84
2:L:31:LYS:HZ1	2:P:149:ILE:HD12	1.42	0.84
1:K:96:TYR:HD2	1:K:115:ILE:HD11	1.42	0.84
2:H:26:ASN:ND2	3:H:154:HOH:O	2.11	0.84
1:I:96:TYR:CD2	1:I:115:ILE:HD11	2.13	0.83
2:J:122:GLU:CB	2:J:149:ILE:HG12	2.08	0.83
2:H:98:LYS:O	1:I:110:ARG:HD2	1.79	0.83
1:I:35:MET:SD	2:L:81:GLN:NE2	2.49	0.83
2:D:30:PRO:O	2:D:33:ARG:HG2	1.78	0.83
1:C:122:GLU:HG3	3:C:1086:HOH:O	1.79	0.82
1:G:168:ARG:HD2	3:G:1511:HOH:O	1.80	0.82
2:D:115:THR:O	2:D:116:LEU:CB	2.19	0.82
2:H:26:ASN:CB	2:H:26:ASN:C	2.52	0.82
1:M:68:PHE:CE1	1:M:172:LYS:HD2	2.15	0.82
1:E:66:ARG:HD2	3:E:906:HOH:O	1.79	0.82
1:K:110:ARG:HD3	3:K:2020:HOH:O	1.80	0.81
1:E:46:MET:HE1	1:E:84:GLY:H	1.45	0.81
2:J:149:ILE:HB	3:J:1904:HOH:O	1.78	0.81
1:M:96:TYR:CD2	1:M:115:ILE:HD11	2.14	0.81
1:M:174:CYS:C	3:M:910:HOH:O	2.23	0.81
2:B:40:HIS:CE1	2:B:148:LYS:HB3	2.15	0.81
2:J:122:GLU:HB3	2:J:149:ILE:HG12	1.63	0.80
1:M:174:CYS:CA	3:M:910:HOH:O	2.28	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:40:HIS:HE1	2:B:148:LYS:HB3	1.47	0.79
1:G:96:TYR:CD2	1:G:115:ILE:HD11	2.17	0.79
2:F:18:ALA:HB1	3:F:819:HOH:O	1.82	0.79
2:J:138:ASP:O	2:J:139:ARG:HB2	1.80	0.79
2:D:33:ARG:HD3	3:D:1836:HOH:O	1.82	0.79
2:N:123:GLY:HA3	2:N:149:ILE:HD12	1.64	0.79
2:H:57:HIS:O	2:H:58:SER:CB	2.27	0.79
1:M:101:LEU:N	1:M:101:LEU:HD23	1.96	0.78
2:D:19:ASP:CG	3:D:1471:HOH:O	2.25	0.78
2:J:99:HIS:CE1	3:J:1893:HOH:O	2.17	0.78
1:E:66:ARG:HG3	1:E:66:ARG:HH11	1.48	0.78
1:O:57:ASN:HB3	3:O:1100:HOH:O	1.84	0.78
2:H:47:VAL:CG1	2:H:108:PHE:HE1	1.96	0.78
2:B:75:GLU:HG3	3:B:2665:HOH:O	1.83	0.77
1:G:29:GLN:HE22	2:H:105:SER:H	1.30	0.77
1:M:29:GLN:HE22	2:N:105:SER:H	1.33	0.77
1:K:81:PHE:O	1:K:84:GLY:N	2.15	0.77
1:A:39:MET:HB3	1:A:165:LEU:CD1	2.15	0.77
1:E:84:GLY:O	1:E:85:ALA:HB3	1.85	0.77
1:O:30:ASN:CB	3:O:604:HOH:O	2.20	0.77
2:H:103:LYS:HE3	3:H:1158:HOH:O	1.83	0.77
1:K:29:GLN:HE22	2:L:105:SER:H	1.32	0.76
2:L:47:VAL:HG12	2:L:108:PHE:HE1	1.51	0.76
2:P:47:VAL:HG12	2:P:108:PHE:HE1	1.51	0.76
2:F:40:HIS:HE1	2:F:148:LYS:HB3	1.51	0.76
1:K:33:ASN:O	1:K:35:MET:SD	2.45	0.75
2:F:40:HIS:CE1	2:F:148:LYS:HB3	2.22	0.75
1:E:39:MET:HB3	1:E:165:LEU:HD13	1.68	0.75
2:D:115:THR:O	2:D:116:LEU:HB2	1.85	0.74
2:B:64:MET:CE	3:B:798:HOH:O	2.34	0.74
2:B:133:ILE:C	2:B:135:GLN:H	1.96	0.74
1:C:115:ILE:N	1:C:115:ILE:HD13	2.01	0.74
2:H:47:VAL:HG12	2:H:108:PHE:CE1	2.22	0.73
1:E:29:GLN:HE22	2:F:105:SER:H	1.34	0.73
2:L:42:GLN:HE22	2:L:148:LYS:HE2	1.53	0.72
2:H:139:ARG:HB3	3:H:1411:HOH:O	1.88	0.72
1:E:122:GLU:HG3	3:E:2629:HOH:O	1.87	0.72
2:H:33:ARG:HG2	2:H:33:ARG:HH11	1.55	0.72
2:F:55:GLU:HG2	2:F:56:ASP:N	2.03	0.72
2:N:115:THR:O	2:N:116:LEU:HB2	1.89	0.72
1:E:60:TYR:HD2	3:K:2016:HOH:O	1.73	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:33:ARG:HH11	2:H:33:ARG:CG	2.02	0.72
2:F:138:ASP:O	2:F:139:ARG:HB2	1.89	0.71
2:H:53:HIS:HD2	3:H:619:HOH:O	1.74	0.71
1:I:101:LEU:N	1:I:101:LEU:HD23	2.05	0.71
2:D:47:VAL:CG1	2:D:108:PHE:HE1	2.02	0.71
1:I:29:GLN:HE22	2:J:105:SER:H	1.38	0.71
2:J:115:THR:O	2:J:116:LEU:HG	1.90	0.71
2:F:64:MET:CE	3:F:1420:HOH:O	2.39	0.70
1:E:39:MET:HE2	1:E:165:LEU:HD11	1.73	0.70
3:E:571:HOH:O	1:K:14:LEU:CD2	2.38	0.70
2:B:149:ILE:O	2:B:149:ILE:CG2	2.38	0.70
2:H:42:GLN:OE1	2:H:148:LYS:HD3	1.91	0.70
1:C:48:GLY:N	3:C:2451:HOH:O	2.24	0.70
2:P:18:ALA:C	3:P:1057:HOH:O	2.18	0.70
2:D:47:VAL:HG12	2:D:108:PHE:HE1	1.56	0.70
2:L:115:THR:O	2:L:116:LEU:CB	2.38	0.70
1:M:103:TYR:O	1:M:106:ASN:HB2	1.93	0.69
1:A:29:GLN:HE22	2:B:105:SER:H	1.39	0.69
2:B:84:SER:HB3	3:B:2286:HOH:O	1.92	0.69
2:N:115:THR:O	2:N:116:LEU:CB	2.37	0.69
2:J:66:GLN:HE21	2:J:93:ASN:HA	1.58	0.68
2:L:31:LYS:HZ1	2:P:149:ILE:CD1	2.05	0.68
2:P:66:GLN:HE21	2:P:93:ASN:HA	1.59	0.68
2:D:47:VAL:HG12	2:D:108:PHE:CE1	2.29	0.68
2:H:18:ALA:N	2:H:46:TYR:CE1	2.61	0.67
1:K:98:GLU:HB3	1:K:148:ARG:HG3	1.75	0.67
1:E:139:GLU:OE2	3:E:271:HOH:O	2.13	0.67
2:P:40:HIS:HE1	2:P:148:LYS:CB	2.00	0.67
2:B:26:ASN:OD1	3:B:1251:HOH:O	2.13	0.67
1:E:29:GLN:NE2	2:F:105:SER:H	1.93	0.66
2:L:53:HIS:HE1	2:L:97:ALA:O	1.78	0.66
2:J:40:HIS:HE1	2:J:148:LYS:CB	2.05	0.66
1:O:32:MET:HE1	1:O:134:VAL:HG11	1.77	0.66
2:P:138:ASP:OD1	2:P:139:ARG:N	2.28	0.66
1:K:29:GLN:NE2	2:L:105:SER:H	1.94	0.65
1:C:33:ASN:HB3	3:C:1649:HOH:O	1.97	0.65
2:J:47:VAL:HG12	2:J:108:PHE:HE1	1.59	0.65
2:N:33:ARG:HG2	3:N:1124:HOH:O	1.95	0.65
2:H:78:GLN:HG3	3:H:1637:HOH:O	1.96	0.65
1:G:29:GLN:NE2	2:H:105:SER:H	1.94	0.65
1:M:101:LEU:N	1:M:101:LEU:CD2	2.59	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:138:ASP:O	3:F:1466:HOH:O	2.15	0.65
2:N:27:SER:O	2:N:139:ARG:NH1	2.28	0.65
1:M:96:TYR:HD2	1:M:115:ILE:HD11	1.62	0.65
1:M:98:GLU:HB3	1:M:148:ARG:HG3	1.78	0.64
1:O:33:ASN:O	1:O:35:MET:HE2	1.97	0.64
2:L:47:VAL:CG1	2:L:108:PHE:HE1	2.11	0.64
1:C:96:TYR:HD2	1:C:115:ILE:CD1	2.00	0.64
2:H:53:HIS:HE1	2:H:97:ALA:O	1.80	0.64
2:J:122:GLU:HB2	2:J:149:ILE:HG12	1.78	0.64
2:H:57:HIS:O	2:H:58:SER:HB3	1.98	0.64
2:L:85:LYS:NZ	2:L:88:VAL:HG21	2.12	0.64
1:A:39:MET:CE	1:A:165:LEU:HD11	2.25	0.64
2:B:75:GLU:CG	3:B:2665:HOH:O	2.44	0.63
2:P:148:LYS:HD2	2:P:149:ILE:O	1.97	0.63
1:G:121:ASP:OD2	3:G:314:HOH:O	2.15	0.63
1:G:168:ARG:HD3	3:G:1511:HOH:O	1.94	0.63
2:N:59:VAL:HG12	2:N:63:ALA:HB3	1.78	0.63
1:E:174:CYS:SG	3:E:2217:HOH:O	1.99	0.63
2:N:47:VAL:CG1	2:N:108:PHE:HE1	2.12	0.63
2:P:53:HIS:HE1	2:P:97:ALA:O	1.82	0.63
1:I:58:TRP:HH2	1:I:149:LYS:HE2	1.64	0.63
1:M:14:LEU:HD22	1:M:16:TRP:NE1	2.14	0.63
2:F:40:HIS:HE1	2:F:148:LYS:CB	2.13	0.62
2:F:99:HIS:CE1	3:F:2244:HOH:O	2.52	0.62
2:F:137:GLU:HG3	3:F:1077:HOH:O	1.98	0.62
1:M:101:LEU:HD23	1:M:101:LEU:H	1.64	0.62
1:E:30:ASN:CB	3:E:687:HOH:O	2.28	0.62
2:F:55:GLU:CG	2:F:56:ASP:H	2.12	0.62
2:N:40:HIS:HE1	3:N:2682:HOH:O	1.82	0.62
2:N:47:VAL:HG12	2:N:108:PHE:CE1	2.35	0.61
2:N:118:LYS:HE2	3:N:1509:HOH:O	1.99	0.61
2:F:55:GLU:HG2	2:F:56:ASP:H	1.65	0.61
2:F:58:SER:HB3	3:F:817:HOH:O	2.00	0.61
2:F:148:LYS:CD	2:F:149:ILE:C	2.70	0.61
2:B:149:ILE:CG2	3:B:1383:HOH:O	2.25	0.61
2:H:115:THR:O	2:H:116:LEU:CB	2.43	0.61
1:C:29:GLN:HE22	2:D:105:SER:H	1.49	0.61
1:E:84:GLY:O	1:E:85:ALA:CB	2.48	0.61
1:O:29:GLN:HE22	2:P:105:SER:H	1.48	0.61
2:D:42:GLN:OE1	2:D:148:LYS:HD2	2.00	0.60
1:C:129:PHE:HD1	3:D:1135:HOH:O	1.83	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:85:LYS:HZ3	2:L:88:VAL:HG21	1.66	0.60
2:H:18:ALA:N	2:H:46:TYR:HE1	1.99	0.60
2:J:61:ASP:HA	2:J:64:MET:HE2	1.83	0.60
3:A:2631:HOH:O	2:B:85:LYS:HD3	2.00	0.60
2:N:53:HIS:HE1	2:N:97:ALA:O	1.84	0.60
2:P:18:ALA:HB2	3:P:2170:HOH:O	2.00	0.60
1:C:23:LYS:O	3:C:1353:HOH:O	2.16	0.60
2:P:47:VAL:CG1	2:P:108:PHE:HE1	2.13	0.59
2:J:42:GLN:HG2	2:J:148:LYS:HD2	1.82	0.59
2:J:103:LYS:HE3	3:J:1545:HOH:O	2.02	0.59
1:K:81:PHE:O	1:K:83:GLY:N	2.35	0.59
1:M:174:CYS:C	3:M:477:HOH:O	2.44	0.59
2:B:66:GLN:HE21	2:B:93:ASN:HA	1.67	0.59
1:E:84:GLY:HA2	1:M:86:SER:HG	1.67	0.59
2:F:47:VAL:HG12	2:F:106:GLU:HB3	1.83	0.59
1:O:31:ILE:HD12	2:P:88:VAL:HG12	1.83	0.59
2:J:42:GLN:CG	2:J:148:LYS:HD2	2.33	0.59
2:P:148:LYS:CD	2:P:149:ILE:O	2.51	0.59
2:J:18:ALA:O	3:J:1682:HOH:O	2.16	0.59
1:I:110:ARG:HB3	3:I:437:HOH:O	2.02	0.59
2:F:64:MET:HE1	3:F:1420:HOH:O	2.03	0.59
1:I:29:GLN:NE2	2:J:105:SER:H	2.01	0.58
2:N:28:SER:CB	3:N:2112:HOH:O	1.75	0.58
2:N:47:VAL:HG12	2:N:108:PHE:HE1	1.68	0.58
2:H:122:GLU:HB3	2:H:149:ILE:HA	1.84	0.58
2:F:55:GLU:CG	2:F:56:ASP:N	2.66	0.58
2:H:18:ALA:CB	3:H:720:HOH:O	2.00	0.58
1:A:29:GLN:NE2	2:B:105:SER:H	2.01	0.58
2:D:47:VAL:CG1	2:D:108:PHE:CE1	2.85	0.58
1:G:86:SER:OG	1:G:87:SER:N	2.25	0.58
2:L:33:ARG:HG3	2:L:33:ARG:HH11	1.68	0.58
2:N:94:ARG:NH1	2:N:102:GLU:OE1	2.34	0.58
2:H:139:ARG:CB	3:H:1411:HOH:O	2.46	0.58
2:L:103:LYS:HE3	3:L:1726:HOH:O	2.03	0.58
2:J:18:ALA:HB3	2:J:45:ASP:HA	1.86	0.57
1:O:57:ASN:HB3	3:O:203:HOH:O	2.03	0.57
1:M:29:GLN:NE2	2:N:105:SER:H	2.00	0.57
2:L:115:THR:O	2:L:116:LEU:HG	2.03	0.57
2:N:82:PRO:HD3	2:N:129:ILE:HD11	1.85	0.57
1:E:39:MET:HB3	1:E:165:LEU:CD1	2.35	0.57
2:F:42:GLN:CD	2:F:148:LYS:HZ2	2.12	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:85:ALA:HB1	3:K:440:HOH:O	2.03	0.57
2:D:53:HIS:HE1	2:D:97:ALA:O	1.87	0.57
1:M:33:ASN:HB3	3:M:1776:HOH:O	2.03	0.57
1:O:1:GLU:HG2	3:O:2731:HOH:O	2.04	0.57
2:F:19:ASP:HB3	3:F:847:HOH:O	2.04	0.57
2:H:47:VAL:CG1	2:H:108:PHE:CE1	2.84	0.56
1:I:60:TYR:HE1	1:I:149:LYS:HE3	1.70	0.56
1:A:168:ARG:HD2	3:A:2282:HOH:O	2.04	0.56
1:K:80:SER:O	1:K:82:PRO:HD3	2.06	0.56
2:P:122:GLU:HB3	2:P:149:ILE:HA	1.86	0.56
2:J:115:THR:O	2:J:116:LEU:CG	2.53	0.56
2:L:33:ARG:NH1	3:L:2333:HOH:O	2.39	0.56
2:B:122:GLU:HB3	2:B:149:ILE:HG13	1.86	0.56
2:B:149:ILE:O	2:B:149:ILE:HG23	2.05	0.56
2:H:139:ARG:HG2	3:H:242:HOH:O	2.05	0.56
1:I:30:ASN:CB	3:I:370:HOH:O	2.41	0.56
1:E:96:TYR:HD2	1:E:115:ILE:HD11	1.69	0.55
3:E:571:HOH:O	1:K:14:LEU:HD23	2.06	0.55
2:H:56:ASP:O	3:H:879:HOH:O	2.18	0.55
3:L:980:HOH:O	2:P:40:HIS:CE1	2.59	0.55
2:L:75:GLU:H	2:L:75:GLU:CD	2.14	0.55
1:M:39:MET:HE2	1:M:165:LEU:HD11	1.89	0.55
1:M:33:ASN:CB	3:M:1776:HOH:O	2.54	0.55
2:P:122:GLU:CB	2:P:149:ILE:HG12	2.36	0.55
2:H:66:GLN:HE21	2:H:93:ASN:HA	1.71	0.55
1:K:29:GLN:HG2	1:K:38:TYR:CE2	2.41	0.55
1:E:30:ASN:HD22	1:E:39:MET:HE3	1.72	0.54
2:H:94:ARG:HH22	2:H:99:HIS:HE1	1.54	0.54
1:O:60:TYR:HB2	3:O:2250:HOH:O	2.08	0.54
2:F:137:GLU:CG	3:F:1077:HOH:O	2.55	0.54
2:H:55:GLU:O	2:H:57:HIS:O	2.26	0.54
2:D:55:GLU:HG2	2:D:56:ASP:N	2.22	0.54
2:F:122:GLU:OE2	2:F:149:ILE:HG23	2.06	0.54
2:N:47:VAL:CG1	2:N:108:PHE:CE1	2.90	0.54
2:D:40:HIS:CE1	2:D:148:LYS:CB	2.88	0.54
2:J:118:LYS:HE2	3:J:316:HOH:O	2.08	0.54
2:P:115:THR:O	2:P:116:LEU:HG	2.07	0.54
2:H:149:ILE:HG13	3:H:2104:HOH:O	2.06	0.54
2:D:75:GLU:CD	2:D:75:GLU:H	2.16	0.54
2:J:68:ILE:HG12	2:J:91:GLN:HE21	1.72	0.54
1:C:47:SER:HB2	3:C:2451:HOH:O	2.08	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:35:MET:HA	1:G:35:MET:HE2	1.90	0.54
2:H:75:GLU:CD	2:H:75:GLU:H	2.16	0.53
1:O:148:ARG:HD3	3:O:2285:HOH:O	2.07	0.53
1:C:46:MET:SD	1:C:85:ALA:HA	2.48	0.53
1:I:133:HIS:CD2	1:I:135:LYS:HG3	2.43	0.53
1:M:14:LEU:HD22	1:M:16:TRP:CD1	2.44	0.53
1:M:29:GLN:HG2	1:M:38:TYR:CE2	2.43	0.53
1:M:39:MET:HB3	1:M:165:LEU:HD13	1.89	0.53
2:F:115:THR:O	2:F:116:LEU:CB	2.56	0.53
1:I:20:PRO:HG2	1:I:23:LYS:HE2	1.89	0.53
1:C:86:SER:CB	3:C:1168:HOH:O	2.37	0.53
1:I:163:ALA:HB2	2:J:113:PRO:HG2	1.90	0.53
2:B:18:ALA:HB3	2:B:46:TYR:CD1	2.44	0.53
2:F:27:SER:CB	2:F:137:GLU:OE2	2.57	0.53
2:H:99:HIS:CD2	3:H:2644:HOH:O	2.62	0.53
2:N:40:HIS:NE2	2:N:148:LYS:HB3	2.23	0.53
2:F:66:GLN:HE21	2:F:93:ASN:HA	1.73	0.52
2:J:53:HIS:HE1	2:J:97:ALA:O	1.91	0.52
2:J:148:LYS:HD2	3:J:507:HOH:O	2.09	0.52
2:F:18:ALA:CB	3:F:819:HOH:O	2.49	0.52
1:K:72:LYS:HA	1:K:137:ASN:O	2.09	0.52
2:P:122:GLU:HB3	2:P:149:ILE:HG12	1.90	0.52
2:F:57:HIS:O	2:F:58:SER:CB	2.58	0.52
1:O:32:MET:HE3	1:O:134:VAL:HG21	1.90	0.52
1:A:45:VAL:O	1:A:85:ALA:HB1	2.09	0.52
1:O:45:VAL:O	1:O:85:ALA:HB1	2.09	0.52
1:K:139:GLU:OE2	3:K:363:HOH:O	2.19	0.52
3:I:1601:HOH:O	2:L:85:LYS:HE2	2.10	0.52
2:F:74:HIS:CE1	2:F:78:GLN:HG3	2.45	0.52
1:I:60:TYR:CE1	1:I:149:LYS:HE3	2.44	0.52
1:M:17:LEU:C	1:M:17:LEU:HD23	2.35	0.52
2:N:33:ARG:CG	3:N:1124:HOH:O	2.55	0.52
1:O:76:ARG:HD2	1:O:129:PHE:HZ	1.75	0.52
1:E:60:TYR:CD2	3:K:2016:HOH:O	2.54	0.51
1:O:30:ASN:OD1	3:O:604:HOH:O	2.19	0.51
1:O:96:TYR:HB3	1:O:115:ILE:HD11	1.92	0.51
2:P:68:ILE:HG12	2:P:91:GLN:HE21	1.75	0.51
1:K:89:LYS:HG3	1:K:158:ILE:HG13	1.92	0.51
2:F:148:LYS:HZ3	2:F:149:ILE:C	2.18	0.51
1:K:96:TYR:CD2	1:K:115:ILE:CD1	2.82	0.51
2:L:115:THR:O	2:L:116:LEU:CG	2.59	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:101:LEU:HD12	3:C:1586:HOH:O	2.11	0.51
1:C:96:TYR:CD2	1:C:115:ILE:CD1	2.79	0.51
2:H:33:ARG:HG2	2:H:33:ARG:NH1	2.21	0.51
2:P:75:GLU:CD	2:P:75:GLU:H	2.19	0.51
2:D:42:GLN:HE22	2:D:148:LYS:HE3	1.76	0.51
1:C:115:ILE:N	1:C:115:ILE:CD1	2.70	0.50
2:F:57:HIS:O	2:F:58:SER:HB3	2.10	0.50
1:K:110:ARG:HA	3:K:2352:HOH:O	2.09	0.50
1:O:32:MET:O	1:O:35:MET:HG2	2.10	0.50
2:F:149:ILE:HG22	2:F:149:ILE:O	2.10	0.50
1:E:66:ARG:HD3	1:E:68:PHE:CZ	2.46	0.50
2:F:42:GLN:OE1	2:F:148:LYS:NZ	2.42	0.50
2:D:148:LYS:HD3	2:D:149:ILE:C	2.36	0.50
1:E:46:MET:HE1	1:E:84:GLY:N	2.19	0.50
1:A:39:MET:CB	1:A:165:LEU:HD13	2.34	0.50
1:E:58:TRP:CH2	1:E:149:LYS:HG2	2.46	0.50
2:J:40:HIS:CE1	3:J:475:HOH:O	2.64	0.50
1:M:69:ILE:O	1:M:140:GLU:HA	2.11	0.50
2:P:47:VAL:HG12	2:P:108:PHE:CE1	2.40	0.49
2:B:41:VAL:O	2:B:148:LYS:HG2	2.12	0.49
1:G:48:GLY:O	1:G:49:ASP:HB2	2.11	0.49
2:P:115:THR:O	2:P:116:LEU:CB	2.59	0.49
1:C:29:GLN:NE2	2:D:105:SER:H	2.08	0.49
2:F:53:HIS:HE1	2:F:97:ALA:O	1.94	0.49
1:I:17:LEU:C	1:I:17:LEU:HD23	2.37	0.49
2:L:31:LYS:NZ	2:P:149:ILE:HD12	2.21	0.49
1:M:21:TYR:C	1:M:21:TYR:CD2	2.89	0.49
2:N:72:VAL:HB	2:N:76:GLU:HB2	1.95	0.49
1:A:46:MET:SD	1:A:85:ALA:HB2	2.52	0.49
2:F:18:ALA:CB	3:F:2722:HOH:O	1.66	0.49
1:A:111:LEU:HB3	3:A:2074:HOH:O	2.13	0.49
1:M:48:GLY:O	1:M:49:ASP:HB2	2.13	0.49
2:J:136:HIS:C	2:J:138:ASP:H	2.20	0.48
2:L:115:THR:O	2:L:116:LEU:HB2	2.12	0.48
2:P:94:ARG:HD3	2:P:102:GLU:OE1	2.14	0.48
2:F:19:ASP:HA	2:F:45:ASP:OD1	2.13	0.48
2:B:53:HIS:HE1	2:B:97:ALA:O	1.96	0.48
1:C:64:ALA:HB2	1:C:171:TYR:CD2	2.49	0.48
2:H:40:HIS:NE2	2:H:148:LYS:HB3	2.27	0.48
2:H:57:HIS:HD2	3:H:1307:HOH:O	1.96	0.48
2:H:72:VAL:HB	2:H:76:GLU:HB2	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:163:ALA:HB2	2:F:113:PRO:HG2	1.96	0.48
2:H:115:THR:O	2:H:116:LEU:HB2	2.13	0.48
2:N:61:ASP:HA	2:N:64:MET:HE2	1.96	0.48
1:A:35:MET:HE1	2:N:82:PRO:HD2	1.95	0.48
2:F:115:THR:O	2:F:116:LEU:HB2	2.14	0.48
2:N:71:LEU:HD21	2:N:118:LYS:HG2	1.95	0.48
2:D:40:HIS:NE2	2:D:148:LYS:HB3	2.28	0.48
2:F:64:MET:HE3	3:F:786:HOH:O	2.14	0.48
2:J:109:GLN:NE2	3:J:1390:HOH:O	2.44	0.48
2:B:133:ILE:C	2:B:135:GLN:N	2.71	0.47
3:E:571:HOH:O	1:K:57:ASN:HB3	2.12	0.47
1:A:39:MET:HE2	1:A:165:LEU:CD1	2.31	0.47
1:C:163:ALA:HB2	2:D:113:PRO:HG2	1.96	0.47
1:G:84:GLY:O	1:G:85:ALA:HB3	2.14	0.47
2:F:43:LEU:HD22	2:F:122:GLU:HG3	1.96	0.47
1:G:17:LEU:C	1:G:17:LEU:HD23	2.39	0.47
1:G:64:ALA:HB2	1:G:171:TYR:CD2	2.49	0.47
1:O:163:ALA:HB2	2:P:113:PRO:HG2	1.96	0.47
1:A:85:ALA:CB	1:A:88:CYS:HB2	2.45	0.47
2:D:85:LYS:HE3	2:D:88:VAL:HG21	1.97	0.47
2:H:94:ARG:HH22	2:H:99:HIS:CE1	2.31	0.47
1:E:130:GLU:OE1	1:E:130:GLU:HA	2.09	0.47
1:G:57:ASN:HB3	3:G:176:HOH:O	2.15	0.47
2:N:66:GLN:HE21	2:N:93:ASN:HA	1.79	0.47
1:E:58:TRP:HH2	1:E:149:LYS:HG2	1.80	0.47
1:I:16:TRP:O	3:I:740:HOH:O	2.20	0.46
1:M:33:ASN:CG	3:M:1776:HOH:O	2.57	0.46
2:D:19:ASP:HB3	3:D:417:HOH:O	2.15	0.46
2:D:136:HIS:ND1	3:D:1881:HOH:O	2.35	0.46
1:I:58:TRP:CH2	1:I:149:LYS:HE2	2.47	0.46
2:J:47:VAL:CG1	2:J:108:PHE:HE1	2.27	0.46
2:H:40:HIS:CE1	2:H:148:LYS:HB3	2.50	0.46
1:I:85:ALA:HB1	1:I:88:CYS:HB2	1.97	0.46
2:B:61:ASP:HA	2:B:64:MET:HE2	1.97	0.46
2:F:61:ASP:HA	2:F:64:MET:HE2	1.97	0.46
1:M:57:ASN:HB3	3:M:509:HOH:O	2.15	0.46
1:G:82:PRO:O	1:G:83:GLY:C	2.58	0.46
1:K:80:SER:HB3	3:K:863:HOH:O	2.15	0.46
1:G:34:ASP:O	1:G:35:MET:HE3	2.16	0.46
2:B:18:ALA:HB1	2:B:45:ASP:HA	1.98	0.46
2:F:27:SER:HB3	2:F:137:GLU:OE2	2.16	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:30:ASN:HD22	1:I:39:MET:HE3	1.81	0.46
2:L:112:THR:HG22	2:L:119:GLU:HG2	1.96	0.46
2:B:60:ALA:HB1	3:B:2173:HOH:O	2.16	0.46
2:D:59:VAL:HG12	2:D:63:ALA:HB3	1.97	0.46
2:L:96:SER:HB2	3:L:2628:HOH:O	2.15	0.46
2:F:58:SER:CA	3:F:952:HOH:O	2.64	0.45
2:H:110:ARG:HA	2:H:120:PHE:O	2.16	0.45
2:J:149:ILE:O	2:J:149:ILE:HG22	2.16	0.45
2:J:40:HIS:CE1	2:J:148:LYS:CB	2.82	0.45
2:L:33:ARG:HG3	3:L:2333:HOH:O	2.17	0.45
2:P:77:TYR:CE1	2:P:142:ARG:HD2	2.51	0.45
2:J:132:PRO:HG3	2:J:137:GLU:HA	1.98	0.45
2:F:27:SER:OG	2:F:65:GLU:OE1	2.34	0.45
2:F:43:LEU:O	2:F:44:ASN:HB2	2.16	0.45
2:F:58:SER:HA	3:F:952:HOH:O	2.16	0.45
2:F:103:LYS:HE2	3:F:2499:HOH:O	2.16	0.45
1:C:72:LYS:HA	1:C:137:ASN:O	2.15	0.45
2:F:42:GLN:OE1	2:F:148:LYS:CE	2.65	0.45
2:F:82:PRO:HD2	2:F:131:LYS:HE2	1.98	0.45
1:M:39:MET:HE2	1:M:165:LEU:CD1	2.46	0.45
1:M:106:ASN:HD22	1:M:106:ASN:HA	1.50	0.45
2:D:42:GLN:OE1	2:D:148:LYS:CG	2.65	0.45
2:J:103:LYS:HD3	3:J:2091:HOH:O	2.17	0.45
2:L:47:VAL:HG12	2:L:108:PHE:CE1	2.41	0.45
1:A:85:ALA:HB1	1:A:88:CYS:HB2	1.99	0.45
1:C:89:LYS:HA	1:C:89:LYS:HD3	1.80	0.45
1:K:17:LEU:HD23	1:K:17:LEU:C	2.42	0.45
1:M:110:ARG:HA	3:M:1791:HOH:O	2.17	0.45
1:A:130:GLU:HB2	3:A:1137:HOH:O	2.16	0.45
2:H:94:ARG:NH1	3:H:929:HOH:O	2.50	0.45
1:I:96:TYR:CE2	1:I:115:ILE:HD11	2.53	0.44
2:B:149:ILE:HG22	2:B:149:ILE:O	2.15	0.44
1:G:132:ARG:HD3	3:G:1957:HOH:O	2.16	0.44
1:M:61:ARG:HD2	1:M:146:LEU:HB2	1.99	0.44
2:F:110:ARG:HA	2:F:120:PHE:O	2.17	0.44
1:M:64:ALA:HB2	1:M:171:TYR:CD2	2.52	0.44
1:G:96:TYR:CD2	1:G:115:ILE:CD1	2.94	0.44
2:B:84:SER:CB	3:B:2286:HOH:O	2.58	0.44
2:J:115:THR:O	2:J:115:THR:OG1	2.35	0.44
1:M:68:PHE:CZ	1:M:172:LYS:HD2	2.52	0.44
1:A:111:LEU:HD12	3:A:1660:HOH:O	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:42:GLN:HG3	2:J:148:LYS:CD	2.48	0.44
1:K:96:TYR:HD2	1:K:115:ILE:CD1	2.22	0.44
2:F:148:LYS:CE	2:F:149:ILE:C	2.90	0.44
1:G:58:TRP:HH2	1:G:149:LYS:HG2	1.83	0.44
2:B:30:PRO:O	2:B:33:ARG:HG2	2.18	0.44
1:E:14:LEU:O	1:E:16:TRP:N	2.50	0.44
1:C:130:GLU:OE1	1:C:130:GLU:HA	2.18	0.43
1:O:29:GLN:NE2	2:P:105:SER:H	2.14	0.43
2:P:90:TRP:HB2	2:P:104:LEU:HD13	2.00	0.43
2:P:122:GLU:HB2	2:P:149:ILE:HG12	2.00	0.43
2:B:64:MET:HE1	3:B:2182:HOH:O	2.18	0.43
2:D:27:SER:O	2:D:139:ARG:NH1	2.51	0.43
1:C:17:LEU:C	1:C:17:LEU:HD23	2.44	0.43
1:I:101:LEU:N	1:I:101:LEU:CD2	2.78	0.43
2:J:110:ARG:HA	2:J:120:PHE:O	2.18	0.43
1:M:96:TYR:CD2	1:M:115:ILE:CD1	2.96	0.43
2:D:66:GLN:HE21	2:D:93:ASN:HA	1.83	0.43
2:F:103:LYS:CE	3:F:2499:HOH:O	2.66	0.43
1:M:115:ILE:N	1:M:115:ILE:HD13	2.32	0.43
2:H:98:LYS:HG3	3:H:1113:HOH:O	2.18	0.43
1:I:35:MET:HG2	2:L:131:LYS:HD2	2.01	0.43
2:J:90:TRP:HB2	2:J:104:LEU:HD13	2.00	0.43
2:D:38:THR:HA	2:D:144:LYS:O	2.18	0.43
1:M:131:ALA:HB2	3:M:2699:HOH:O	2.18	0.43
1:O:83:GLY:HA3	3:O:2614:HOH:O	2.18	0.43
2:D:56:ASP:HB3	2:D:57:HIS:H	1.55	0.43
2:H:99:HIS:NE2	3:H:929:HOH:O	2.13	0.43
1:M:172:LYS:HE3	3:M:1532:HOH:O	2.18	0.43
1:O:81:PHE:HA	1:O:82:PRO:HD2	1.77	0.43
1:C:30:ASN:HD22	1:C:39:MET:HE3	1.84	0.43
1:E:66:ARG:HG3	1:E:66:ARG:NH1	2.21	0.43
1:E:173:LYS:HG3	3:E:1582:HOH:O	2.18	0.43
1:I:72:LYS:HA	1:I:137:ASN:O	2.19	0.43
1:K:14:LEU:HD22	1:K:16:TRP:CD1	2.53	0.43
2:F:64:MET:CE	3:F:786:HOH:O	2.67	0.43
2:H:64:MET:HE3	3:H:2280:HOH:O	2.18	0.43
1:O:157:ASP:HA	3:O:406:HOH:O	2.19	0.43
2:J:148:LYS:H	2:J:148:LYS:HG3	1.66	0.42
1:K:85:ALA:O	1:K:86:SER:C	2.62	0.42
1:A:101:LEU:HD12	3:A:2514:HOH:O	2.18	0.42
1:G:72:LYS:HA	1:G:137:ASN:O	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:85:ALA:O	1:G:86:SER:C	2.60	0.42
2:H:57:HIS:HB3	3:H:1662:HOH:O	2.18	0.42
1:K:45:VAL:O	1:K:85:ALA:HB1	2.19	0.42
1:M:96:TYR:CZ	1:M:143:VAL:HG11	2.54	0.42
2:N:33:ARG:HD3	3:N:1840:HOH:O	2.18	0.42
2:L:33:ARG:HA	2:L:139:ARG:HH21	1.84	0.42
1:A:173:LYS:HG2	1:A:174:CYS:SG	2.59	0.42
2:D:110:ARG:HA	2:D:120:PHE:O	2.20	0.42
2:D:42:GLN:OE1	2:D:148:LYS:CD	2.66	0.42
2:D:77:TYR:CE1	2:D:142:ARG:HD2	2.55	0.42
1:C:38:TYR:N	1:C:38:TYR:CD1	2.86	0.42
1:I:64:ALA:HB2	1:I:171:TYR:CD2	2.55	0.42
2:J:72:VAL:HB	2:J:76:GLU:HB2	2.02	0.42
2:F:114:PHE:C	2:F:115:THR:O	2.56	0.42
1:O:98:GLU:CB	1:O:148:ARG:HG3	2.50	0.42
2:B:75:GLU:H	2:B:75:GLU:CD	2.27	0.42
2:B:110:ARG:HA	2:B:120:PHE:O	2.20	0.42
2:F:47:VAL:CG1	2:F:106:GLU:HB3	2.50	0.42
1:I:35:MET:HE1	2:L:82:PRO:HG2	2.02	0.42
1:I:37:ILE:HD12	1:I:165:LEU:HD13	2.02	0.42
1:I:173:LYS:HE3	1:I:173:LYS:HB2	1.72	0.42
2:J:43:LEU:HD22	2:J:122:GLU:CG	2.50	0.42
2:J:148:LYS:NZ	2:J:149:ILE:O	2.51	0.42
1:K:163:ALA:HB2	2:L:113:PRO:HG2	2.02	0.42
1:C:48:GLY:HA2	3:C:1343:HOH:O	2.20	0.41
2:H:149:ILE:O	2:H:149:ILE:CG2	2.67	0.41
1:I:2:VAL:HG22	2:P:79:LEU:CD2	2.50	0.41
2:F:84:SER:OG	2:F:86:ASP:HB2	2.20	0.41
1:G:128:ASP:OD2	3:G:2232:HOH:O	2.22	0.41
1:M:14:LEU:HD21	1:M:57:ASN:OD1	2.21	0.41
1:E:29:GLN:HB3	2:F:90:TRP:CZ3	2.55	0.41
2:F:90:TRP:HB2	2:F:104:LEU:HD13	2.02	0.41
1:G:86:SER:CB	3:G:1220:HOH:O	2.33	0.41
1:I:109:LYS:H	1:I:109:LYS:HG3	1.66	0.41
2:L:33:ARG:HG3	2:L:33:ARG:NH1	2.35	0.41
1:A:96:TYR:HD2	1:A:115:ILE:HD11	1.74	0.41
1:C:101:LEU:HD21	1:C:103:TYR:CE1	2.55	0.41
1:G:132:ARG:HB3	2:H:116:LEU:HD23	2.01	0.41
2:J:115:THR:O	2:J:116:LEU:CB	2.69	0.41
2:N:110:ARG:HA	2:N:120:PHE:O	2.20	0.41
1:A:72:LYS:HA	1:A:137:ASN:O	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:74:HIS:CE1	2:B:78:GLN:HG3	2.56	0.41
1:E:37:ILE:HD12	1:E:165:LEU:HD12	2.02	0.41
2:J:57:HIS:O	2:J:58:SER:HB3	2.21	0.41
2:N:59:VAL:CG1	2:N:63:ALA:HB3	2.49	0.41
1:O:52:ASN:HB2	1:O:157:ASP:HB3	2.02	0.41
2:P:137:GLU:O	2:P:137:GLU:HG3	2.21	0.41
1:G:10:ALA:CB	1:G:14:LEU:HG	2.50	0.41
1:G:51:ASP:OD1	1:G:109:LYS:NZ	2.54	0.41
1:I:19:HIS:ND1	1:I:20:PRO:HA	2.35	0.41
1:A:58:TRP:CH2	1:A:149:LYS:HG2	2.56	0.41
1:A:63:GLU:HG2	3:A:1877:HOH:O	2.19	0.41
2:B:42:GLN:HB2	2:B:148:LYS:HD3	2.02	0.41
2:D:94:ARG:HH12	2:D:99:HIS:CE1	2.39	0.41
1:M:85:ALA:HB1	1:M:88:CYS:HB2	2.02	0.41
2:B:18:ALA:HB3	2:B:46:TYR:CE1	2.56	0.41
1:G:98:GLU:HB3	1:G:148:ARG:HG3	2.01	0.41
1:I:10:ALA:CB	1:I:14:LEU:HG	2.51	0.41
2:J:114:PHE:HA	3:J:1608:HOH:O	2.20	0.41
2:L:39:ILE:HD13	2:L:39:ILE:HG21	1.57	0.41
2:L:59:VAL:HG12	2:L:63:ALA:HB3	2.02	0.41
1:G:115:ILE:HD12	1:G:143:VAL:HG22	2.02	0.41
2:H:30:PRO:O	2:H:33:ARG:HG2	2.21	0.40
1:O:94:LEU:HG	1:O:115:ILE:HD12	2.02	0.40
2:P:114:PHE:CE2	2:P:116:LEU:HB2	2.56	0.40
2:J:78:GLN:CD	3:J:2526:HOH:O	2.64	0.40
1:E:84:GLY:CA	1:M:86:SER:OG	2.60	0.40
2:F:137:GLU:HG3	2:F:137:GLU:O	2.21	0.40
2:N:30:PRO:O	2:N:33:ARG:HG2	2.22	0.40
1:O:58:TRP:HH2	1:O:149:LYS:HD3	1.86	0.40

All (2) 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)
3:K:438:HOH:O	3:M:1257:HOH:O[1_565]	1.97	0.23
3:B:2558:HOH:O	3:H:661:HOH:O[1_544]	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	172/174 (99%)	166 (96%)	5 (3%)	1 (1%)	21	17
1	C	172/174 (99%)	165 (96%)	6 (4%)	1 (1%)	21	17
1	E	172/174 (99%)	163 (95%)	7 (4%)	2 (1%)	10	6
1	G	172/174 (99%)	164 (95%)	5 (3%)	3 (2%)	7	3
1	I	172/174 (99%)	165 (96%)	5 (3%)	2 (1%)	10	6
1	K	172/174 (99%)	164 (95%)	5 (3%)	3 (2%)	7	3
1	M	172/174 (99%)	161 (94%)	11 (6%)	0	100	100
1	O	172/174 (99%)	159 (92%)	12 (7%)	1 (1%)	21	17
2	B	130/132 (98%)	125 (96%)	3 (2%)	2 (2%)	8	4
2	D	130/132 (98%)	125 (96%)	1 (1%)	4 (3%)	3	1
2	F	130/132 (98%)	125 (96%)	2 (2%)	3 (2%)	5	2
2	H	130/132 (98%)	125 (96%)	1 (1%)	4 (3%)	3	1
2	J	130/132 (98%)	124 (95%)	3 (2%)	3 (2%)	5	2
2	L	130/132 (98%)	126 (97%)	2 (2%)	2 (2%)	8	4
2	N	130/132 (98%)	126 (97%)	2 (2%)	2 (2%)	8	4
2	P	130/132 (98%)	122 (94%)	4 (3%)	4 (3%)	3	1
All	All	2416/2448 (99%)	2305 (95%)	74 (3%)	37 (2%)	8	4

All (37) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	135	GLN
2	D	58	SER
2	F	58	SER
2	F	139	ARG
2	H	56	ASP
1	K	82	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	P	56	ASP
1	A	85	ALA
2	B	56	ASP
2	D	19	ASP
1	E	15	GLY
1	E	85	ALA
2	H	19	ASP
2	H	58	SER
2	H	116	LEU
2	J	58	SER
2	J	116	LEU
1	K	48	GLY
2	L	58	SER
2	L	116	LEU
2	N	58	SER
2	N	116	LEU
1	O	47	SER
2	P	116	LEU
2	D	56	ASP
2	D	116	LEU
2	F	56	ASP
2	P	58	SER
1	G	83	GLY
1	G	86	SER
1	G	85	ALA
2	J	139	ARG
1	K	85	ALA
2	P	139	ARG
1	C	83	GLY
1	I	83	GLY
1	I	84	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.

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	150/150 (100%)	141 (94%)	9 (6%)	17	14
1	C	150/150 (100%)	142 (95%)	8 (5%)	20	18
1	E	150/150 (100%)	142 (95%)	8 (5%)	20	18
1	G	150/150 (100%)	146 (97%)	4 (3%)	39	42
1	I	150/150 (100%)	143 (95%)	7 (5%)	23	22
1	K	150/150 (100%)	140 (93%)	10 (7%)	15	11
1	M	150/150 (100%)	142 (95%)	8 (5%)	20	18
1	O	150/150 (100%)	140 (93%)	10 (7%)	15	11
2	B	124/124 (100%)	117 (94%)	7 (6%)	19	16
2	D	124/124 (100%)	115 (93%)	9 (7%)	13	9
2	F	124/124 (100%)	115 (93%)	9 (7%)	13	9
2	H	124/124 (100%)	115 (93%)	9 (7%)	13	9
2	J	124/124 (100%)	118 (95%)	6 (5%)	23	21
2	L	124/124 (100%)	120 (97%)	4 (3%)	34	35
2	N	124/124 (100%)	116 (94%)	8 (6%)	15	12
2	P	124/124 (100%)	117 (94%)	7 (6%)	19	16
All	All	2192/2192 (100%)	2069 (94%)	123 (6%)	19	16

All (123) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	LEU
1	A	65	GLU
1	A	101	LEU
1	A	123	ILE
1	A	126	SER
1	A	130	GLU
1	A	153	LEU
1	A	173	LYS
1	A	174	CYS
2	B	26	ASN
2	B	33	ARG
2	B	55	GLU
2	B	75	GLU
2	B	84	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	148	LYS
2	B	149	ILE
1	C	14	LEU
1	C	89	LYS
1	C	101	LEU
1	C	115	ILE
1	C	123	ILE
1	C	126	SER
1	C	153	LEU
1	C	165	LEU
2	D	26	ASN
2	D	39	ILE
2	D	56	ASP
2	D	75	GLU
2	D	76	GLU
2	D	84	SER
2	D	116	LEU
2	D	148	LYS
2	D	149	ILE
1	E	41	SER
1	E	46	MET
1	E	66	ARG
1	E	110	ARG
1	E	123	ILE
1	E	126	SER
1	E	130	GLU
1	E	153	LEU
2	F	19	ASP
2	F	26	ASN
2	F	28	SER
2	F	75	GLU
2	F	116	LEU
2	F	137	GLU
2	F	138	ASP
2	F	139	ARG
2	F	148	LYS
1	G	35	MET
1	G	63	GLU
1	G	153	LEU
1	G	165	LEU
2	H	33	ARG
2	H	47	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	H	55	GLU
2	H	56	ASP
2	H	59	VAL
2	H	75	GLU
2	H	81	GLN
2	H	83	GLN
2	H	149	ILE
1	I	63	GLU
1	I	101	LEU
1	I	108	GLN
1	I	110	ARG
1	I	130	GLU
1	I	153	LEU
1	I	165	LEU
2	J	42	GLN
2	J	56	ASP
2	J	59	VAL
2	J	75	GLU
2	J	83	GLN
2	J	148	LYS
1	K	14	LEU
1	K	31	ILE
1	K	33	ASN
1	K	47	SER
1	K	63	GLU
1	K	130	GLU
1	K	143	VAL
1	K	149	LYS
1	K	153	LEU
1	K	165	LEU
2	L	26	ASN
2	L	28	SER
2	L	85	LYS
2	L	148	LYS
1	M	14	LEU
1	M	21	TYR
1	M	87	SER
1	M	101	LEU
1	M	106	ASN
1	M	115	ILE
1	M	130	GLU
1	M	153	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	N	28	SER
2	N	47	VAL
2	N	57	HIS
2	N	75	GLU
2	N	83	GLN
2	N	84	SER
2	N	116	LEU
2	N	149	ILE
1	O	35	MET
1	O	47	SER
1	O	101	LEU
1	O	110	ARG
1	O	130	GLU
1	O	148	ARG
1	O	153	LEU
1	O	165	LEU
1	O	172	LYS
1	O	173	LYS
2	P	33	ARG
2	P	42	GLN
2	P	57	HIS
2	P	75	GLU
2	P	84	SER
2	P	148	LYS
2	P	149	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (103) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	29	GLN
1	A	44	ASN
1	A	52	ASN
1	A	79	ASN
1	A	93	ASN
1	A	106	ASN
1	A	108	GLN
2	B	40	HIS
2	B	53	HIS
2	B	66	GLN
2	B	91	GLN
2	B	99	HIS
1	C	29	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	30	ASN
1	C	44	ASN
1	C	52	ASN
1	C	79	ASN
1	C	93	ASN
1	C	106	ASN
1	C	108	GLN
2	D	40	HIS
2	D	44	ASN
2	D	53	HIS
2	D	57	HIS
2	D	66	GLN
2	D	83	GLN
2	D	124	HIS
1	E	29	GLN
1	E	30	ASN
1	E	57	ASN
1	E	106	ASN
1	E	108	GLN
2	F	40	HIS
2	F	53	HIS
2	F	66	GLN
2	F	81	GLN
2	F	99	HIS
1	G	29	GLN
1	G	44	ASN
1	G	93	ASN
1	G	106	ASN
1	G	108	GLN
2	H	53	HIS
2	H	57	HIS
2	H	66	GLN
2	H	91	GLN
2	H	99	HIS
1	I	29	GLN
1	I	30	ASN
1	I	44	ASN
1	I	106	ASN
1	I	108	GLN
2	J	34	ASN
2	J	40	HIS
2	J	53	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	J	66	GLN
2	J	81	GLN
2	J	91	GLN
2	J	99	HIS
2	J	109	GLN
1	K	29	GLN
1	K	33	ASN
1	K	44	ASN
1	K	52	ASN
1	K	79	ASN
1	K	93	ASN
1	K	106	ASN
1	K	108	GLN
2	L	53	HIS
2	L	66	GLN
2	L	83	GLN
2	L	91	GLN
2	L	109	GLN
2	L	124	HIS
1	M	29	GLN
1	M	44	ASN
1	M	52	ASN
1	M	93	ASN
1	M	106	ASN
1	M	108	GLN
1	M	156	GLN
2	N	26	ASN
2	N	40	HIS
2	N	53	HIS
2	N	66	GLN
2	N	83	GLN
2	N	109	GLN
2	N	124	HIS
1	O	19	HIS
1	O	29	GLN
1	O	30	ASN
1	O	50	GLN
1	O	52	ASN
1	O	106	ASN
1	O	108	GLN
2	P	40	HIS
2	P	42	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	P	53	HIS
2	P	66	GLN
2	P	78	GLN
2	P	83	GLN
2	P	91	GLN
2	P	135	GLN

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	174/174 (100%)	-0.36	5 (2%) 53 52	2, 5, 24, 42	0
1	C	174/174 (100%)	-0.49	4 (2%) 61 60	2, 5, 20, 28	0
1	E	174/174 (100%)	-0.31	4 (2%) 61 60	2, 8, 22, 36	0
1	G	174/174 (100%)	-0.29	2 (1%) 78 77	2, 6, 20, 30	0
1	I	174/174 (100%)	0.43	10 (5%) 29 28	4, 11, 25, 35	0
1	K	174/174 (100%)	-0.16	7 (4%) 42 41	2, 7, 23, 32	0
1	M	174/174 (100%)	0.52	12 (6%) 23 21	3, 8, 22, 27	0
1	O	174/174 (100%)	0.23	4 (2%) 61 60	4, 11, 24, 35	0
2	B	132/132 (100%)	-0.15	7 (5%) 32 31	2, 6, 30, 41	0
2	D	132/132 (100%)	-0.28	5 (3%) 44 43	2, 5, 24, 38	0
2	F	132/132 (100%)	-0.17	8 (6%) 27 26	2, 6, 24, 37	0
2	H	132/132 (100%)	-0.32	5 (3%) 44 43	2, 5, 22, 29	0
2	J	132/132 (100%)	0.01	7 (5%) 32 31	2, 6, 32, 39	0
2	L	132/132 (100%)	-0.26	2 (1%) 72 71	2, 6, 21, 41	0
2	N	132/132 (100%)	-0.31	3 (2%) 61 60	2, 6, 24, 39	0
2	P	132/132 (100%)	0.04	9 (6%) 23 22	2, 6, 29, 38	0
All	All	2448/2448 (100%)	-0.11	94 (3%) 44 43	2, 7, 24, 42	0

All (94) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	18	ALA	9.2
2	H	18	ALA	8.9
2	B	18	ALA	8.8
2	P	18	ALA	8.0
1	K	85	ALA	6.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	F	18	ALA	6.6
2	J	18	ALA	6.4
1	K	82	PRO	6.3
2	N	18	ALA	5.8
2	L	18	ALA	5.4
1	A	174	CYS	5.3
1	K	83	GLY	4.5
2	B	136	HIS	4.3
2	P	136	HIS	4.3
1	K	84	GLY	4.0
2	P	149	ILE	3.9
1	M	111	LEU	3.8
1	O	174	CYS	3.7
1	K	86	SER	3.7
1	M	83	GLY	3.6
1	M	85	ALA	3.5
1	C	84	GLY	3.5
2	J	136	HIS	3.4
2	P	55	GLU	3.4
1	C	60	TYR	3.3
2	P	56	ASP	3.3
1	E	174	CYS	3.2
2	J	56	ASP	3.2
2	L	57	HIS	3.2
1	G	83	GLY	3.2
2	J	115	THR	3.2
2	D	57	HIS	3.1
2	F	56	ASP	3.1
2	B	135	GLN	3.1
2	J	138	ASP	3.1
2	J	149	ILE	3.1
2	H	56	ASP	3.0
1	M	60	TYR	3.0
1	E	82	PRO	2.9
1	M	86	SER	2.9
1	I	174	CYS	2.8
1	I	173	LYS	2.7
2	J	57	HIS	2.7
1	I	21	TYR	2.7
2	P	57	HIS	2.6
1	M	38	TYR	2.6
1	C	47	SER	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	D	149	ILE	2.5
1	A	86	SER	2.5
1	M	33	ASN	2.5
2	H	57	HIS	2.5
1	I	130	GLU	2.4
1	M	110	ARG	2.4
2	N	57	HIS	2.4
1	I	84	GLY	2.4
1	I	38	TYR	2.4
2	D	56	ASP	2.4
1	K	47	SER	2.4
2	F	99	HIS	2.4
2	P	137	GLU	2.4
1	I	30	ASN	2.4
2	P	78	GLN	2.4
1	G	86	SER	2.4
2	N	149	ILE	2.3
2	B	55	GLU	2.3
1	A	21	TYR	2.3
1	O	60	TYR	2.3
2	H	99	HIS	2.3
2	H	149	ILE	2.3
2	F	55	GLU	2.3
1	A	85	ALA	2.3
1	I	83	GLY	2.3
2	B	138	ASP	2.3
1	E	21	TYR	2.3
2	F	19	ASP	2.2
1	M	32	MET	2.2
2	P	138	ASP	2.2
2	F	57	HIS	2.2
1	I	9	ALA	2.2
2	B	57	HIS	2.2
1	E	84	GLY	2.1
2	F	149	ILE	2.1
1	C	86	SER	2.1
2	B	56	ASP	2.1
2	F	138	ASP	2.1
1	O	21	TYR	2.1
1	M	125	VAL	2.1
1	I	110	ARG	2.0
1	A	173	LYS	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	M	12	GLY	2.0
1	M	46	MET	2.0
2	D	19	ASP	2.0
1	O	173	LYS	2.0
1	K	21	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.