Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 09:13 AM GMT

PDB ID	:	3HEI
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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

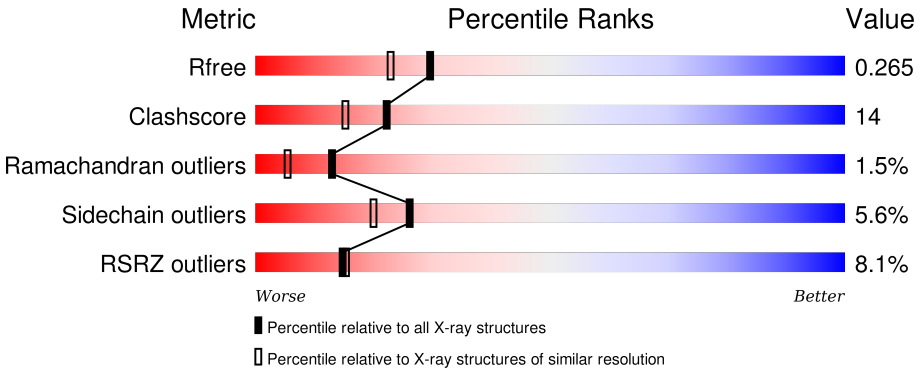
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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.



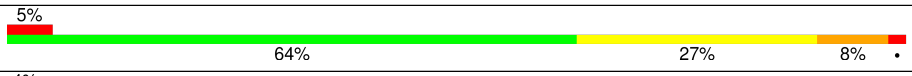
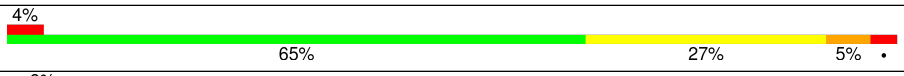
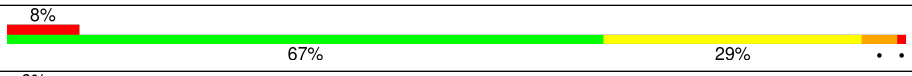
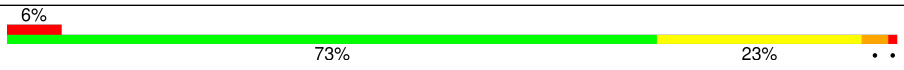
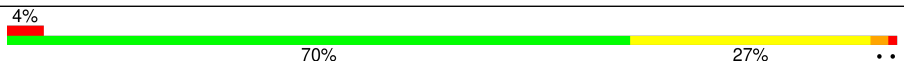
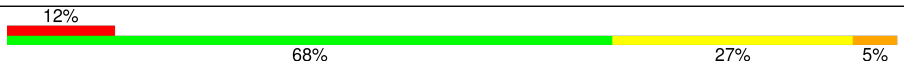
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	8% 79% 16% 5%
1	C	174	3% 78% 18% •
1	E	174	5% 79% 18% ••
1	G	174	77% 17% 5% •
1	I	174	21% 77% 21% ••

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...

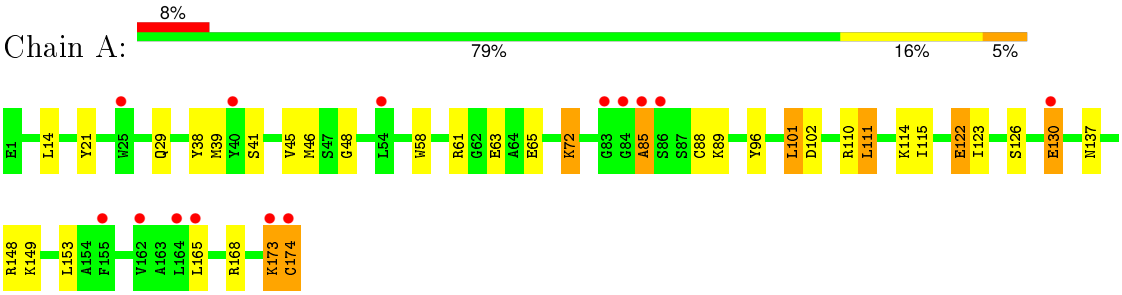
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	H	203	Total O 203 203	0	0
3	I	115	Total O 115 115	0	0
3	J	145	Total O 145 145	0	0
3	K	173	Total O 173 173	0	0
3	L	149	Total O 149 149	0	0
3	M	157	Total O 157 157	0	0
3	N	173	Total O 173 173	0	0
3	O	99	Total O 99 99	0	0
3	P	144	Total O 144 144	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

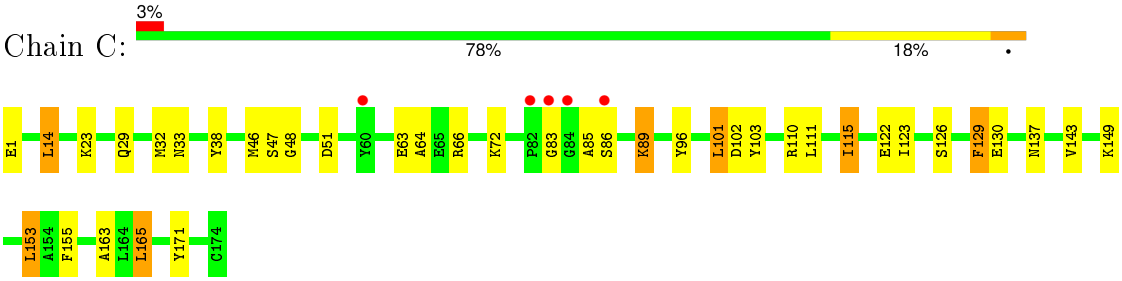
- Molecule 1: Ephrin type-A receptor 2

Chain A:



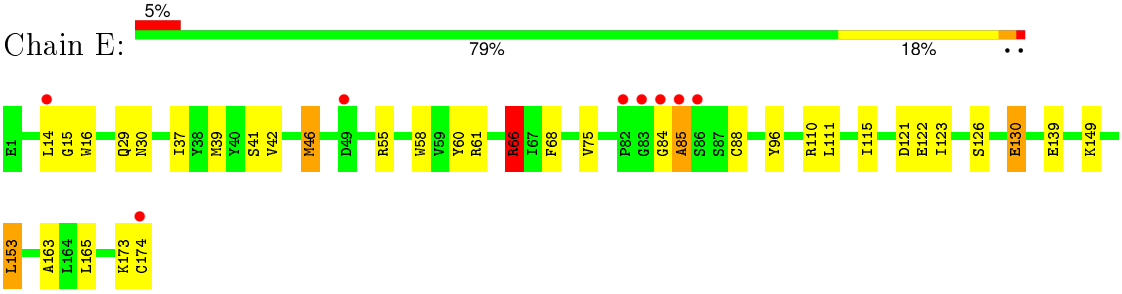
- Molecule 1: Ephrin type-A receptor 2

Chain C:



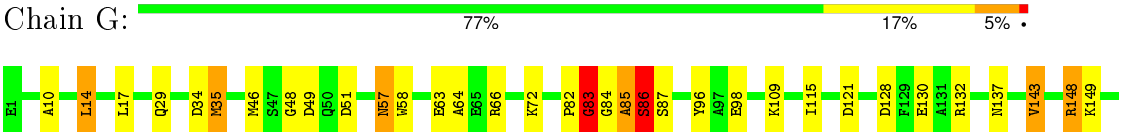
- Molecule 1: Ephrin type-A receptor 2

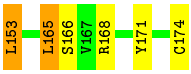
Chain E:



- Molecule 1: Ephrin type-A receptor 2

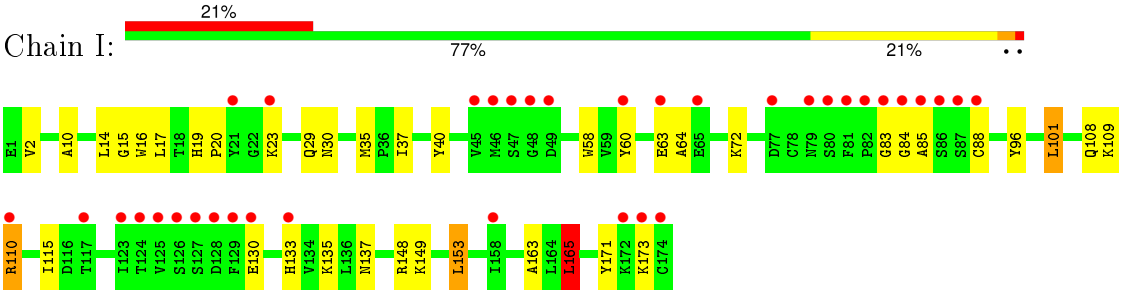
Chain G:





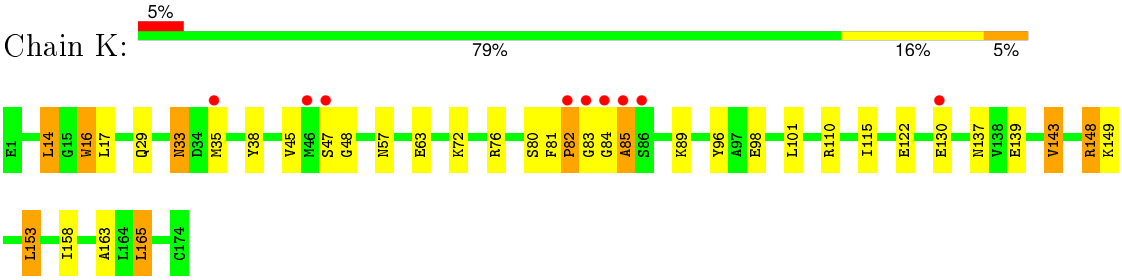
• Molecule 1: Ephrin type-A receptor 2

Chain I:



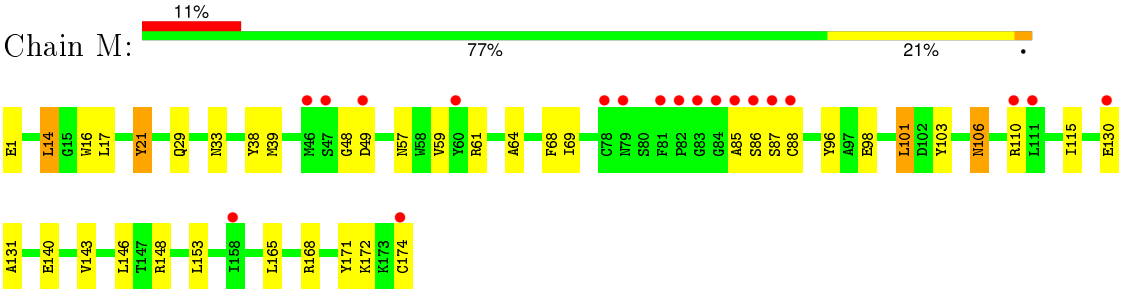
• Molecule 1: Ephrin type-A receptor 2

Chain K:



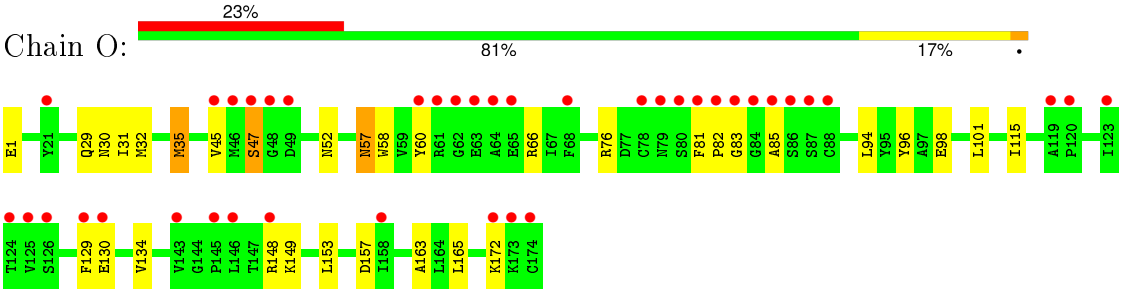
• Molecule 1: Ephrin type-A receptor 2

Chain M:



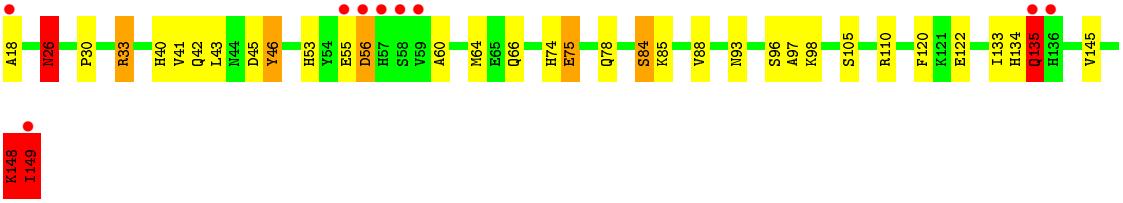
• Molecule 1: Ephrin type-A receptor 2

Chain O:

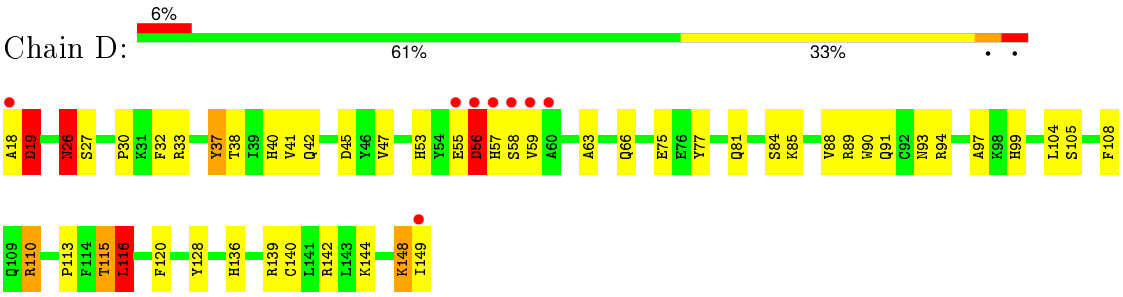


• Molecule 2: Ephrin-A1

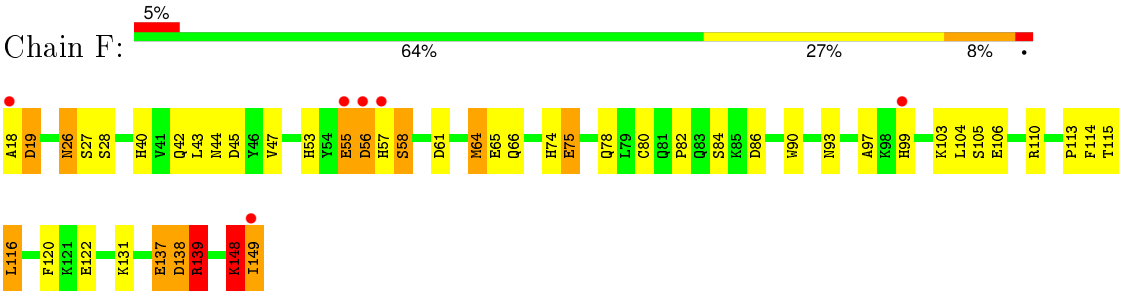
Chain B:



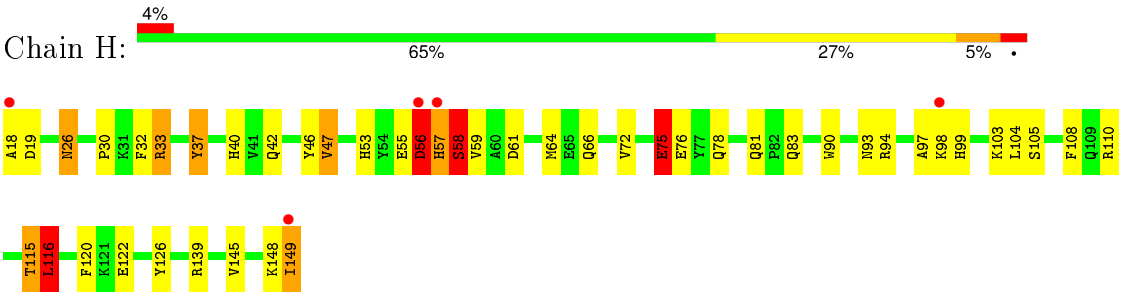
• Molecule 2: Ephrin-A1



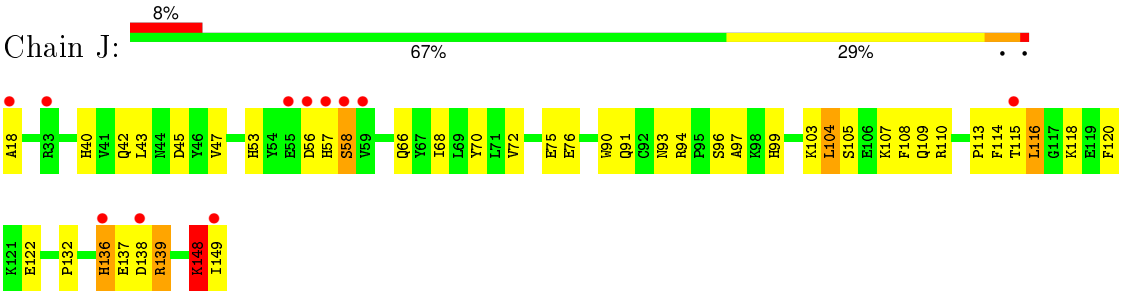
• Molecule 2: Ephrin-A1



• Molecule 2: Ephrin-A1

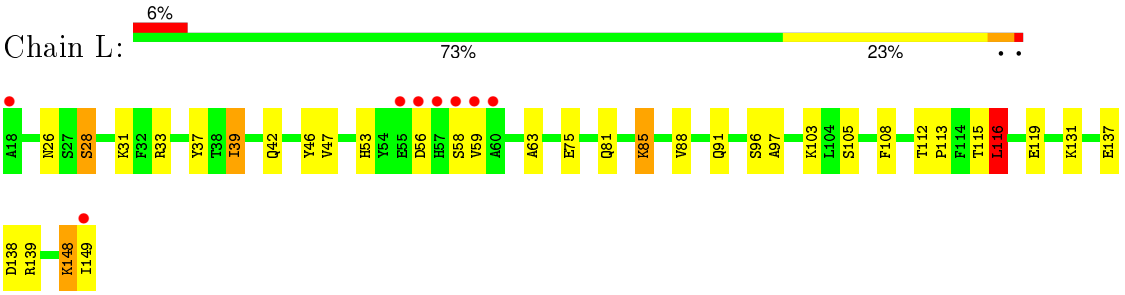


• Molecule 2: Ephrin-A1



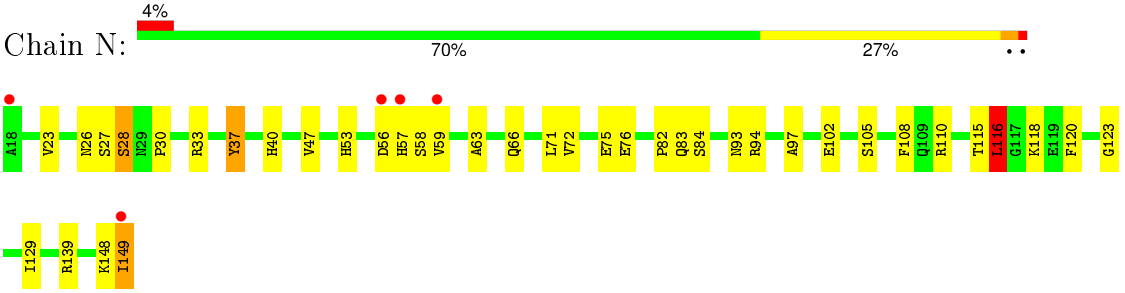
• Molecule 2: Ephrin-A1

Chain L:



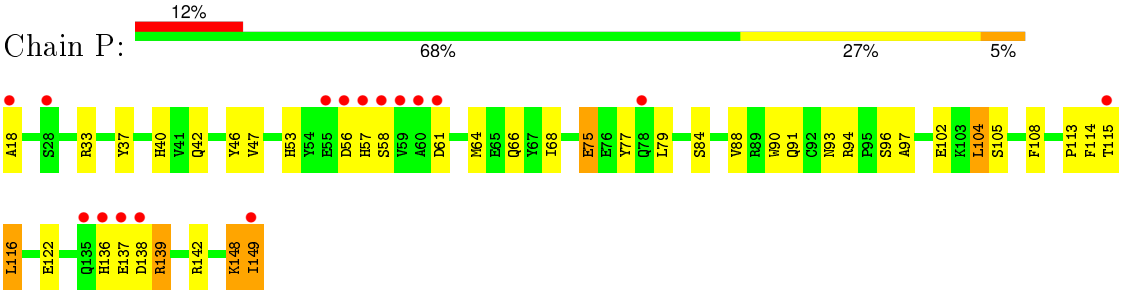
• Molecule 2: Ephrin-A1

Chain N:



• Molecule 2: Ephrin-A1

Chain P:



4 Data and refinement statistics (i)

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 43.60 – 2.00	Depositor EDS
% Data completeness (in resolution range)	96.0 (50.00-2.00) 94.4 (43.60-2.00)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.40 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.5.0093	Depositor
R, R_{free}	0.172 , 0.233 0.209 , 0.265	Depositor DCC
R_{free} test set	9696 reflections (5.32%)	DCC
Wilson B-factor (Å^2)	21.6	Xtriage
Anisotropy	0.193	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 44.6	EDS
Estimated twinning fraction	0.019 for h,h-k,h-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 192014 reflections	Xtriage
F_o,F_c correlation	0.94	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	1.32	4/1433 (0.3%)	1.15	8/1940 (0.4%)
1	C	1.27	2/1433 (0.1%)	1.26	14/1940 (0.7%)
1	E	1.17	2/1433 (0.1%)	1.03	6/1940 (0.3%)
1	G	1.29	9/1433 (0.6%)	1.06	5/1940 (0.3%)
1	I	0.92	1/1433 (0.1%)	0.90	2/1940 (0.1%)
1	K	1.19	2/1433 (0.1%)	1.04	5/1940 (0.3%)
1	M	1.00	1/1433 (0.1%)	0.93	0/1940
1	O	0.90	1/1433 (0.1%)	0.91	0/1940
2	B	1.36	7/1154 (0.6%)	1.09	3/1562 (0.2%)
2	D	1.34	9/1154 (0.8%)	1.07	8/1562 (0.5%)
2	F	1.29	5/1154 (0.4%)	1.11	3/1562 (0.2%)
2	H	1.45	12/1154 (1.0%)	1.15	8/1562 (0.5%)
2	J	1.14	4/1154 (0.3%)	0.99	2/1562 (0.1%)
2	L	1.23	2/1154 (0.2%)	0.97	3/1562 (0.2%)
2	N	1.24	5/1154 (0.4%)	1.00	3/1562 (0.2%)
2	P	1.15	4/1154 (0.3%)	0.97	1/1562 (0.1%)
All	All	1.21	70/20696 (0.3%)	1.04	71/28016 (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 (70) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	26	ASN	CG-ND2	9.52	1.56	1.32
2	N	37	TYR	CD2-CE2	9.47	1.53	1.39
2	H	26	ASN	CA-CB	9.43	1.77	1.53
2	B	26	ASN	CB-CG	9.11	1.72	1.51
2	D	26	ASN	CG-ND2	8.73	1.54	1.32
2	H	37	TYR	CD2-CE2	8.32	1.51	1.39
2	N	26	ASN	N-CA	8.11	1.62	1.46
2	B	75	GLU	CD-OE1	8.08	1.34	1.25
2	F	80	CYS	CB-SG	7.94	1.95	1.82
1	G	57	ASN	CB-CG	7.71	1.68	1.51
2	D	26	ASN	CB-CG	7.54	1.68	1.51
2	H	26	ASN	CG-OD1	7.50	1.40	1.24
2	N	26	ASN	CA-CB	7.32	1.72	1.53
1	I	40	TYR	CD1-CE1	6.90	1.49	1.39
2	D	116	LEU	N-CA	6.84	1.60	1.46
1	A	38	TYR	CD2-CE2	6.83	1.49	1.39
2	B	96	SER	CB-OG	-6.76	1.33	1.42
2	D	37	TYR	CD2-CE2	6.68	1.49	1.39
2	H	26	ASN	N-CA	6.65	1.59	1.46
2	L	137	GLU	CB-CG	6.59	1.64	1.52
2	F	75	GLU	CD-OE1	6.31	1.32	1.25
2	J	70	TYR	CD2-CE2	6.24	1.48	1.39
2	D	140	CYS	CB-SG	6.20	1.92	1.82
2	B	46	TYR	CG-CD1	6.14	1.47	1.39
1	O	57	ASN	CB-CG	6.09	1.65	1.51
1	K	16	TRP	CE3-CZ3	6.02	1.48	1.38
2	L	46	TYR	CD2-CE2	5.96	1.48	1.39
1	A	72	LYS	CD-CE	5.94	1.66	1.51
1	G	14	LEU	C-O	5.92	1.34	1.23
1	E	42	VAL	CB-CG2	5.88	1.65	1.52
2	D	41	VAL	CB-CG1	5.81	1.65	1.52
2	H	115	THR	C-O	-5.80	1.12	1.23
2	P	96	SER	CB-OG	-5.79	1.34	1.42
2	H	26	ASN	CB-CG	5.78	1.64	1.51
1	E	75	VAL	CB-CG2	5.75	1.65	1.52
1	G	86	SER	C-O	5.75	1.34	1.23
2	N	23	VAL	CB-CG1	5.70	1.64	1.52
2	H	126	TYR	CG-CD2	5.67	1.46	1.39
1	G	83	GLY	N-CA	5.66	1.54	1.46
2	H	47	VAL	CB-CG1	-5.65	1.41	1.52
1	C	129	PHE	CE1-CZ	5.63	1.48	1.37
1	A	89	LYS	CD-CE	5.63	1.65	1.51
2	B	145	VAL	CB-CG2	5.62	1.64	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	130	GLU	CG-CD	5.59	1.60	1.51
1	M	59	VAL	CB-CG1	5.58	1.64	1.52
1	G	143	VAL	CB-CG2	-5.58	1.41	1.52
2	H	145	VAL	CB-CG1	5.54	1.64	1.52
2	J	96	SER	CB-OG	-5.51	1.35	1.42
1	K	122	GLU	CG-CD	5.47	1.60	1.51
1	C	155	PHE	CD1-CE1	5.45	1.50	1.39
2	P	46	TYR	CG-CD2	5.41	1.46	1.39
2	F	55	GLU	CG-CD	5.35	1.59	1.51
2	N	75	GLU	CG-CD	5.35	1.59	1.51
2	H	90	TRP	CE3-CZ3	5.32	1.47	1.38
2	F	26	ASN	CA-CB	5.32	1.67	1.53
2	P	75	GLU	CD-OE1	5.32	1.31	1.25
2	H	32	PHE	CD2-CE2	5.31	1.49	1.39
2	J	75	GLU	CD-OE1	5.31	1.31	1.25
2	B	88	VAL	CB-CG1	5.30	1.64	1.52
2	D	128	TYR	CE1-CZ	5.26	1.45	1.38
2	H	75	GLU	CG-CD	5.22	1.59	1.51
2	D	90	TRP	CE3-CZ3	5.20	1.47	1.38
1	G	166	SER	CB-OG	5.16	1.49	1.42
2	J	107	LYS	CD-CE	5.14	1.64	1.51
1	A	122	GLU	CD-OE1	5.13	1.31	1.25
2	D	32	PHE	CD2-CE2	5.12	1.49	1.39
2	P	46	TYR	CE1-CZ	5.11	1.45	1.38
1	G	130	GLU	CB-CG	5.10	1.61	1.52
1	G	57	ASN	CG-ND2	5.08	1.45	1.32
2	F	116	LEU	N-CA	5.05	1.56	1.46

All (71) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	66	ARG	NE-CZ-NH2	-16.20	112.20	120.30
1	E	66	ARG	NE-CZ-NH1	11.75	126.18	120.30
1	C	66	ARG	NE-CZ-NH1	10.44	125.52	120.30
1	A	102	ASP	CB-CG-OD1	10.05	127.34	118.30
1	A	102	ASP	CB-CG-OD2	-9.33	109.91	118.30
1	C	102	ASP	CB-CG-OD1	8.91	126.32	118.30
2	H	26	ASN	N-CA-C	-8.08	89.19	111.00
1	G	153	LEU	CB-CG-CD1	7.72	124.12	111.00
2	D	19	ASP	N-CA-C	7.71	131.81	111.00
2	N	26	ASN	N-CA-C	-7.45	90.90	111.00
2	D	115	THR	O-C-N	-7.36	110.93	122.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	165	LEU	CB-CG-CD2	7.18	123.21	111.00
2	H	116	LEU	N-CA-CB	7.15	124.69	110.40
2	H	104	LEU	CA-CB-CG	-6.86	99.53	115.30
1	C	14	LEU	CB-CG-CD2	6.79	122.55	111.00
1	E	66	ARG	NE-CZ-NH2	-6.78	116.91	120.30
1	I	153	LEU	CB-CG-CD1	6.75	122.47	111.00
2	D	104	LEU	CA-CB-CG	-6.62	100.06	115.30
2	J	104	LEU	CA-CB-CG	-6.60	100.11	115.30
2	H	26	ASN	CB-CA-C	-6.59	97.22	110.40
2	P	104	LEU	CA-CB-CG	-6.56	100.21	115.30
1	A	111	LEU	CB-CG-CD2	6.55	122.13	111.00
2	D	116	LEU	CA-CB-CG	6.46	130.16	115.30
2	H	115	THR	O-C-N	-6.46	112.37	122.70
2	F	116	LEU	CA-CB-CG	6.44	130.11	115.30
2	H	26	ASN	N-CA-CB	6.39	122.11	110.60
1	E	121	ASP	CB-CG-OD2	6.36	124.03	118.30
1	G	165	LEU	CB-CG-CD1	6.29	121.69	111.00
2	D	110	ARG	NE-CZ-NH2	-6.27	117.17	120.30
1	C	143	VAL	CG1-CB-CG2	-6.24	100.92	110.90
2	L	28	SER	CB-CA-C	6.19	121.86	110.10
1	I	165	LEU	CB-CG-CD2	6.16	121.47	111.00
2	L	39	ILE	CG1-CB-CG2	-6.07	98.05	111.40
1	C	51	ASP	CB-CG-OD2	6.05	123.75	118.30
1	K	153	LEU	CB-CG-CD1	6.02	121.23	111.00
2	N	26	ASN	CB-CA-C	-6.00	98.41	110.40
1	E	111	LEU	CB-CG-CD2	5.96	121.14	111.00
2	J	94	ARG	NE-CZ-NH1	5.94	123.27	120.30
2	D	89	ARG	NE-CZ-NH1	-5.91	117.35	120.30
2	H	116	LEU	CA-CB-CG	5.88	128.83	115.30
2	L	116	LEU	CA-CB-CG	5.83	128.71	115.30
2	B	149	ILE	CG1-CB-CG2	-5.81	98.62	111.40
1	K	143	VAL	CB-CA-C	-5.80	100.38	111.40
2	D	115	THR	C-N-CA	-5.72	107.39	121.70
1	C	111	LEU	CB-CG-CD2	5.72	120.72	111.00
1	C	110	ARG	NE-CZ-NH1	5.68	123.14	120.30
2	B	43	LEU	CB-CG-CD2	-5.66	101.38	111.00
2	N	116	LEU	CA-CB-CG	5.61	128.19	115.30
1	C	153	LEU	CB-CG-CD1	5.59	120.50	111.00
2	F	149	ILE	N-CA-CB	5.58	123.63	110.80
1	A	41	SER	N-CA-CB	-5.57	102.14	110.50
1	E	153	LEU	CB-CG-CD1	5.53	120.40	111.00
1	A	114	LYS	CD-CE-NZ	-5.47	99.12	111.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	110	ARG	NE-CZ-NH2	-5.44	117.58	120.30
1	E	55	ARG	NE-CZ-NH2	-5.42	117.59	120.30
2	H	57	HIS	CB-CA-C	5.42	121.24	110.40
2	D	116	LEU	N-CA-CB	5.39	121.19	110.40
1	G	165	LEU	CB-CG-CD2	5.36	120.11	111.00
1	K	76	ARG	NE-CZ-NH2	-5.35	117.62	120.30
1	C	153	LEU	CB-CG-CD2	5.31	120.02	111.00
2	B	134	HIS	C-N-CA	5.28	134.90	121.70
1	K	101	LEU	CB-CG-CD1	-5.28	102.03	111.00
1	K	165	LEU	CA-CB-CG	5.26	127.39	115.30
1	C	32	MET	CG-SD-CE	-5.19	91.89	100.20
1	C	165	LEU	CB-CG-CD1	5.18	119.81	111.00
1	G	66	ARG	CG-CD-NE	-5.16	100.97	111.80
1	A	61	ARG	NE-CZ-NH1	5.13	122.87	120.30
1	A	38	TYR	CB-CG-CD1	-5.13	117.92	121.00
2	F	64	MET	CG-SD-CE	5.12	108.40	100.20
1	A	110	ARG	NE-CZ-NH2	-5.08	117.76	120.30
1	G	14	LEU	N-CA-C	-5.07	97.31	111.00

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 (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	1399	0	1348	23	0
1	C	1399	0	1348	30	0
1	E	1399	0	1348	33	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	1399	0	1348	30	0
1	I	1399	0	1348	31	0
1	K	1399	0	1348	27	0
1	M	1399	0	1348	43	0
1	O	1399	0	1348	27	0
2	B	1120	0	1058	31	0
2	D	1120	0	1058	39	0
2	F	1120	0	1058	61	0
2	H	1120	0	1058	53	0
2	J	1120	0	1058	45	0
2	L	1120	0	1058	34	0
2	N	1120	0	1058	29	0
2	P	1120	0	1058	41	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	19	0
3	G	219	0	0	11	0
3	H	203	0	0	19	1
3	I	115	0	0	7	0
3	J	145	0	0	11	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	542	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 (542) 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:CB	2:H:26:ASN:CA	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:J:99:HIS:HE1	3:J:1893:HOH:O	1.30	1.11
1:G:86:SER:HB3	3:G:1220:HOH:O	1.50	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: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:G:174:CYS:C	3:G:1254:HOH:O	2.00	0.99
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
2:D:19:ASP:OD2	2:D:45:ASP:OD1	1.84	0.95
2:P:114:PHE:HB3	3:P:1231:HOH:O	1.66	0.95
1:G:46:MET:SD	3:G:2602:HOH:O	2.22	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: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
2:F:148:LYS:HD2	2:F:149:ILE:C	1.91	0.91
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:P:114:PHE:CD2	3:P:1231:HOH:O	2.28	0.85
1:E:84:GLY:HA2	1:M:86:SER:OG	1.76	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:HE1	1:A:165:LEU:HD11	1.56	0.85
2:L:31:LYS:HZ1	2:P:149:ILE:HD12	1.42	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
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
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
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
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
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
1:E:39:MET:HE2	1:E:165:LEU:HD11	1.63	0.79
2:H:57:HIS:O	2:H:58:SER:CB	2.27	0.79
1:M:101:LEU:HD23	1:M:101:LEU:N	1.96	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:H:26:ASN:CB	2:H:26:ASN:C	2.52	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:O:30:ASN:CB	3:O:604:HOH:O	2.20	0.77
1:E:84:GLY:O	1:E:85:ALA:HB3	1.85	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
1:M:174:CYS:C	3:M:910:HOH:O	2.23	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
1:C:115:ILE:HD13	1:C:115:ILE:N	2.01	0.74
2:D:19:ASP:CG	3:D:1471:HOH:O	2.25	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
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:HD23	1:I:101:LEU:N	2.05	0.71
1:I:29:GLN:HE22	2:J:105:SER:H	1.38	0.71
2:D:47:VAL:CG1	2:D:108:PHE:HE1	2.02	0.71
2:J:115:THR:O	2:J:116:LEU:HG	1.90	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:64:MET:CE	3:F:1420:HOH:O	2.39	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: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
2:B:133:ILE:C	2:B:135:GLN:H	1.96	0.69
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:N:115:THR:O	2:N:116:LEU:CB	2.37	0.69
2:B:84:SER:HB3	3:B:2286:HOH:O	1.92	0.69
2:J:66:GLN:HE21	2:J:93:ASN:HA	1.58	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
2:P:40:HIS:HE1	2:P:148:LYS:CB	2.00	0.67
1:E:139:GLU:OE2	3:E:271:HOH:O	2.13	0.67
2:B:26:ASN:OD1	3:B:1251:HOH:O	2.13	0.67
2:L:31:LYS:HZ1	2:P:149:ILE:CD1	2.07	0.67
1:E:29:GLN:NE2	2:F:105:SER:H	1.93	0.66
2:P:18:ALA:C	3:P:1057:HOH:O	2.18	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
2:P:138:ASP:OD1	2:P:139:ARG:N	2.28	0.66
2:H:115:THR:O	2:H:116:LEU:CB	2.43	0.65
1:K:29:GLN:NE2	2:L:105:SER:H	1.94	0.65
2:N:33:ARG:HG2	3:N:1124:HOH:O	1.95	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
1:A:39:MET:CE	1:A:165:LEU:HD11	2.25	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:CD2	1:M:101:LEU:N	2.59	0.65
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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:168:ARG:HD3	3:G:1511:HOH:O	1.94	0.63
1:G:121:ASP:OD2	3:G:314:HOH:O	2.15	0.63
2:N:59:VAL:HG12	2:N:63:ALA:HB3	1.78	0.63
2:N:47:VAL:CG1	2:N:108:PHE:HE1	2.12	0.63
1:E:174:CYS:SG	3:E:2217:HOH:O	1.99	0.63
2:P:53:HIS:HE1	2:P:97:ALA:O	1.82	0.63
1:M:14:LEU:HD22	1:M:16:TRP:NE1	2.14	0.63
1:I:58:TRP:HH2	1:I:149:LYS:HE2	1.64	0.63
1:G:86:SER:OG	1:G:87:SER:N	2.25	0.62
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
1:M:101:LEU:H	1:M:101:LEU:HD23	1.64	0.62
2:F:137:GLU:HG3	3:F:1077:HOH:O	1.98	0.62
1:E:30:ASN:CB	3:E:687:HOH:O	2.28	0.62
2:N:40:HIS:HE1	3:N:2682:HOH:O	1.82	0.62
2:F:55:GLU:CG	2:F:56:ASP:H	2.12	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:B:149:ILE:CG2	3:B:1383:HOH:O	2.25	0.61
1:E:84:GLY:O	1:E:85:ALA:CB	2.48	0.61
1:C:29:GLN:HE22	2:D:105:SER:H	1.49	0.61
1:O:29:GLN:HE22	2:P:105:SER:H	1.48	0.61
1:E:46:MET:HE1	1:E:84:GLY:H	1.66	0.60
2:D:42:GLN:OE1	2:D:148:LYS:HD2	2.00	0.60
2:L:85:LYS:HZ3	2:L:88:VAL:HG21	1.66	0.60
1:C:129:PHE:HD1	3:D:1135:HOH:O	1.83	0.60
2:H:18:ALA:N	2:H:46:TYR:HE1	1.99	0.60
2:P:18:ALA:HB2	3:P:2170:HOH:O	2.00	0.60
2:N:53:HIS:HE1	2:N:97:ALA:O	1.84	0.60
3:A:2631:HOH:O	2:B:85:LYS:HD3	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:81:PHE:O	1:K:83:GLY:N	2.35	0.59
2:J:103:LYS:HE3	3:J:1545:HOH:O	2.02	0.59
2:B:66:GLN:HE21	2:B:93:ASN:HA	1.67	0.59
2:F:47:VAL:HG12	2:F:106:GLU:HB3	1.83	0.59
1:E:84:GLY:HA2	1:M:86:SER:HG	1.67	0.59
1:O:31:ILE:HD12	2:P:88:VAL:HG12	1.83	0.59
2:P:148:LYS:CD	2:P:149:ILE:O	2.51	0.59
2:J:42:GLN:CG	2:J:148:LYS:HD2	2.33	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
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:H:18:ALA:CB	3:H:720:HOH:O	2.00	0.58
2:F:55:GLU:CG	2:F:56:ASP:N	2.66	0.58
2:D:47:VAL:CG1	2:D:108:PHE:CE1	2.85	0.58
1:A:29:GLN:NE2	2:B:105:SER:H	2.01	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
1:O:57:ASN:HB3	3:O:203:HOH:O	2.03	0.57
2:J:18:ALA:HB3	2:J:45:ASP:HA	1.86	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:B:64:MET:HE3	3:B:798:HOH:O	2.03	0.57
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
2:F:148:LYS:CD	2:F:149:ILE:C	2.70	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
2:P:122:GLU:HB3	2:P:149:ILE:HA	1.86	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:J:115:THR:O	2:J:116:LEU:CG	2.53	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:33:ARG:NH1	3:L:2333:HOH:O	2.39	0.56
2:H:139:ARG:HG2	3:H:242:HOH:O	2.05	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
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:L:980:HOH:O	2:P:40:HIS:CE1	2.59	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
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
1:M:174:CYS:C	3:M:477:HOH:O	2.44	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:O:60:TYR:HB2	3:O:2250:HOH:O	2.08	0.54
2:H:94:ARG:HH22	2:H:99:HIS:HE1	1.54	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:F:122:GLU:OE2	2:F:149:ILE:HG23	2.06	0.54
2:D:55:GLU:HG2	2:D:56:ASP:N	2.22	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:P:115:THR:O	2:P:116:LEU:HG	2.07	0.54
2:J:118:LYS:HE2	3:J:316:HOH:O	2.08	0.54
2:H:149:ILE:HG13	3:H:2104:HOH:O	2.06	0.54
1:G:34:ASP:O	1:G:35:MET:HE3	2.08	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
1:O:148:ARG:HD3	3:O:2285:HOH:O	2.07	0.53
1:M:14:LEU:HD22	1:M:16:TRP:CD1	2.44	0.53
1:I:133:HIS:CD2	1:I:135:LYS:HG3	2.43	0.53
1:C:46:MET:SD	1:C:85:ALA:HA	2.48	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:N:40:HIS:NE2	2:N:148:LYS:HB3	2.23	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:18:ALA:HB3	2:B:46:TYR:CD1	2.44	0.53
2:J:53:HIS:HE1	2:J:97:ALA:O	1.91	0.52
2:F:66:GLN:HE21	2:F:93:ASN:HA	1.73	0.52
2:J:148:LYS:HD2	3:J:507:HOH:O	2.09	0.52
2:F:42:GLN:OE1	2:F:148:LYS:NZ	2.42	0.52
2:P:122:GLU:HB3	2:P:149:ILE:HG12	1.90	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:F:57:HIS:O	2:F:58:SER:CB	2.58	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:N:33:ARG:CG	3:N:1124:HOH:O	2.55	0.52
1:I:60:TYR:CE1	1:I:149:LYS:HE3	2.44	0.52
2:F:74:HIS:CE1	2:F:78:GLN:HG3	2.45	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
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
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:D:42:GLN:HE22	2:D:148:LYS:HE3	1.76	0.51
1:C:115:ILE:CD1	1:C:115:ILE:N	2.70	0.50
1:O:32:MET:O	1:O:35:MET:HG2	2.10	0.50
1:K:110:ARG:HA	3:K:2352:HOH:O	2.09	0.50
2:F:57:HIS:O	2:F:58:SER:HB3	2.10	0.50
2:F:149:ILE:O	2:F:149:ILE:HG22	2.10	0.50
1:O:32:MET:HE3	1:O:134:VAL:HG21	1.93	0.50
1:E:66:ARG:HD3	1:E:68:PHE:CZ	2.46	0.50
2:L:75:GLU:H	2:L:75:GLU:CD	2.14	0.50
2:J:40:HIS:CE1	3:J:475:HOH:O	2.64	0.50
1:A:39:MET:CB	1:A:165:LEU:HD13	2.34	0.50
1:M:69:ILE:O	1:M:140:GLU:HA	2.11	0.50
1:E:58:TRP:CH2	1:E:149:LYS:HG2	2.46	0.50
2:P:47:VAL:HG12	2:P:108:PHE:CE1	2.40	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:115:THR:O	2:P:116:LEU:CB	2.59	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
1:C:29:GLN:NE2	2:D:105:SER:H	2.08	0.49
2:H:61:ASP:HA	2:H:64:MET:CE	2.43	0.49
2:F:53:HIS:HE1	2:F:97:ALA:O	1.94	0.49
2:L:31:LYS:NZ	2:P:149:ILE:HD12	2.21	0.49
2:F:148:LYS:HZ3	2:F:149:ILE:C	2.16	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:H:75:GLU:H	2:H:75:GLU:CD	2.16	0.49
2:D:75:GLU:H	2:D:75:GLU:CD	2.16	0.49
2:F:18:ALA:CB	3:F:2722:HOH:O	1.66	0.49
1:M:48:GLY:O	1:M:49:ASP:HB2	2.13	0.49
1:A:111:LEU:HB3	3:A:2074:HOH:O	2.13	0.49
2:P:61:ASP:HA	2:P:64:MET:CE	2.43	0.49
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:H:57:HIS:HD2	3:H:1307:HOH:O	1.96	0.48
2:H:40:HIS:NE2	2:H:148:LYS:HB3	2.27	0.48
2:B:53:HIS:HE1	2:B:97:ALA:O	1.96	0.48
2:H:72:VAL:HB	2:H:76:GLU:HB2	1.95	0.48
1:C:64:ALA:HB2	1:C:171:TYR:CD2	2.49	0.48
2:H:115:THR:O	2:H:116:LEU:HB2	2.13	0.48
1:E:163:ALA:HB2	2:F:113:PRO:HG2	1.96	0.48
2:N:71:LEU:HD21	2:N:118:LYS:HG2	1.95	0.48
2:F:115:THR:O	2:F:116:LEU:HB2	2.14	0.48
2:D:40:HIS:NE2	2:D:148:LYS:HB3	2.28	0.48
2:J:109:GLN:NE2	3:J:1390:HOH:O	2.44	0.48
1:O:32:MET:HE3	1:O:134:VAL:HG11	1.96	0.47
3:E:571:HOH:O	1:K:57:ASN:HB3	2.12	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:O:163:ALA:HB2	2:P:113:PRO:HG2	1.96	0.47
1:G:64:ALA:HB2	1:G:171:TYR:CD2	2.49	0.47
2:H:94:ARG:HH22	2:H:99:HIS:CE1	2.31	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
1:G:57:ASN:HB3	3:G:176:HOH:O	2.15	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:130:GLU:HA	1:E:130:GLU:OE1	2.09	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:17:LEU:C	1:M:17:LEU:HD23	2.35	0.46
2:D:19:ASP:HB3	3:D:417:HOH:O	2.15	0.46
2:J:47:VAL:CG1	2:J:108:PHE:HE1	2.27	0.46
1:I:58:TRP:CH2	1:I:149:LYS:HE2	2.47	0.46
2:D:136:HIS:ND1	3:D:1881:HOH:O	2.35	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
1:M:57:ASN:HB3	3:M:509:HOH:O	2.15	0.46
1:K:80:SER:HB3	3:K:863:HOH:O	2.15	0.46
2:P:75:GLU:CD	2:P:75:GLU:H	2.19	0.46
2:F:27:SER:HB3	2:F:137:GLU:OE2	2.16	0.46
2:B:18:ALA:HB1	2:B:45:ASP:HA	1.98	0.46
2:L:112:THR:HG22	2:L:119:GLU:HG2	1.96	0.46
2:L:96:SER:HB2	3:L:2628:HOH:O	2.15	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:J:149:ILE:O	2:J:149:ILE:HG22	2.16	0.45
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: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: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
2:F:42:GLN:OE1	2:F:148:LYS:CE	2.65	0.45
2:D:148:LYS:HD3	2:D:149:ILE:C	2.36	0.45
1:C:72:LYS:HA	1:C:137:ASN:O	2.15	0.45
2:F:82:PRO:HD2	2:F:131:LYS:HE2	1.98	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:L:47:VAL:HG12	2:L:108:PHE:CE1	2.41	0.45
2:J:103:LYS:HD3	3:J:2091:HOH:O	2.17	0.45
1:C:89:LYS:HA	1:C:89:LYS:HD3	1.80	0.45
1:A:85:ALA:HB1	1:A:88:CYS:HB2	1.99	0.45
1:M:110:ARG:HA	3:M:1791:HOH:O	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:94:ARG:NH1	3:H:929:HOH:O	2.50	0.45
1:A:130:GLU:HB2	3:A:1137:HOH:O	2.16	0.45
1:I:96:TYR:CE2	1:I:115:ILE:HD11	2.53	0.44
1:M:21:TYR:C	1:M:21:TYR:CD2	2.89	0.44
1:I:17:LEU:C	1:I:17:LEU:HD23	2.37	0.44
2:B:149:ILE:O	2:B:149:ILE:HG22	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
1:M:64:ALA:HB2	1:M:171:TYR:CD2	2.52	0.44
2:F:110:ARG:HA	2:F:120:PHE:O	2.17	0.44
1:G:96:TYR:CD2	1:G:115:ILE:CD1	2.94	0.44
1:M:68:PHE:CZ	1:M:172:LYS:HD2	2.52	0.44
2:J:115:THR:O	2:J:115:THR:OG1	2.35	0.44
2:B:84:SER:CB	3:B:2286:HOH:O	2.58	0.44
1:K:96:TYR:HD2	1:K:115:ILE:CD1	2.22	0.44
2:J:42:GLN:HG3	2:J:148:LYS:CD	2.48	0.44
1:A:111:LEU:HD12	3:A:1660:HOH:O	2.17	0.44
2:J:136:HIS:C	2:J:138:ASP:H	2.20	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
2:P:122:GLU:HB2	2:P:149:ILE:HG12	2.00	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
1:C:130:GLU:OE1	1:C:130:GLU:HA	2.18	0.43
2:D:27:SER:O	2:D:139:ARG:NH1	2.51	0.43
1:M:96:TYR:CD2	1:M:115:ILE:CD1	2.96	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:115:ILE:HD13	1:M:115:ILE:N	2.32	0.43
2:F:103:LYS:CE	3:F:2499:HOH:O	2.66	0.43
2:D:66:GLN:HE21	2:D:93:ASN:HA	1.83	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:F:64:MET:HE1	3:F:1420:HOH:O	2.08	0.43
2:J:90:TRP:HB2	2:J:104:LEU:HD13	2.00	0.43
2:F:114:PHE:C	2:F:115:THR:O	2.56	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:172:LYS:HE3	3:M:1532:HOH:O	2.18	0.43
2:H:99:HIS:NE2	3:H:929:HOH:O	2.13	0.43
1:O:81:PHE:HA	1:O:82:PRO:HD2	1.77	0.43
1:E:66:ARG:HG3	1:E:66:ARG:NH1	2.21	0.43
1:K:14:LEU:HD22	1:K:16:TRP:CD1	2.53	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
2:F:64:MET:CE	3:F:786:HOH:O	2.67	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
2:H:57:HIS:HB3	3:H:1662:HOH:O	2.18	0.42
1:G:35:MET:HE2	1:G:35:MET:HA	2.00	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
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
1:K:45:VAL:O	1:K:85:ALA:HB1	2.19	0.42
1:G:17:LEU:C	1:G:17:LEU:HD23	2.39	0.42
2:L:33:ARG:HA	2:L:139:ARG:HH21	1.84	0.42
2:P:61:ASP:HA	2:P:64:MET:HE2	2.01	0.42
2:D:110:ARG:HA	2:D:120:PHE:O	2.20	0.42
1:A:173:LYS:HG2	1:A:174:CYS:SG	2.59	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
2:J:72:VAL:HB	2:J:76:GLU:HB2	2.02	0.42
1:I:64:ALA:HB2	1:I:171:TYR:CD2	2.55	0.42
1:C:38:TYR:CD1	1:C:38:TYR:N	2.86	0.42
1:M:33:ASN:CG	3:M:1776:HOH:O	2.57	0.42
1:O:98:GLU:CB	1:O:148:ARG:HG3	2.50	0.42
2:F:47:VAL:CG1	2:F:106:GLU:HB3	2.50	0.42
2:J:43:LEU:HD22	2:J:122:GLU:CG	2.50	0.42
1:I:37:ILE:HD12	1:I:165:LEU:HD13	2.02	0.42
1:K:163:ALA:HB2	2:L:113:PRO:HG2	2.02	0.42
1:I:173:LYS:HB2	1:I:173:LYS:HE3	1.72	0.42
2:B:110:ARG:HA	2:B:120:PHE:O	2.20	0.42
1:C:48:GLY:HA2	3:C:1343:HOH:O	2.20	0.41
2:H:149:ILE:CG2	2:H:149:ILE:O	2.67	0.41
1:I:2:VAL:HG22	2:P:79:LEU:CD2	2.50	0.41
2:F:42:GLN:HE22	2:F:148:LYS:HZ1	1.67	0.41
1:M:14:LEU:HD21	1:M:57:ASN:OD1	2.21	0.41
1:G:128:ASP:OD2	3:G:2232:HOH:O	2.22	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:84:SER:OG	2:F:86:ASP:HB2	2.20	0.41
1:G:86:SER:CB	3:G:1220:HOH:O	2.33	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
2:L:33:ARG:HG3	2:L:33:ARG:NH1	2.35	0.41
1:I:109:LYS:H	1:I:109:LYS:HG3	1.66	0.41
1:G:82:PRO:O	1:G:83:GLY:C	2.58	0.41
1:A:96:TYR:HD2	1:A:115:ILE:HD11	1.74	0.41
2:J:115:THR:O	2:J:116:LEU:CB	2.69	0.41
1:G:132:ARG:HB3	2:H:116:LEU:HD23	2.01	0.41
1:C:101:LEU:HD21	1:C:103:TYR:CE1	2.55	0.41
2:N:110:ARG:HA	2:N:120:PHE:O	2.20	0.41
1:E:37:ILE:HD12	1:E:165:LEU:HD12	2.02	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:A:72:LYS:HA	1:A:137:ASN:O	2.20	0.41
2:B:74:HIS:CE1	2:B:78:GLN:HG3	2.56	0.41
2:J:57:HIS:O	2:J:58:SER:HB3	2.21	0.41
2:F:27:SER:OG	2:F:65:GLU:OE1	2.34	0.41
1:I:19:HIS:ND1	1:I:20:PRO:HA	2.35	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
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
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:J:148:LYS:NZ	2:J:149:ILE:O	2.51	0.41
1:O:32:MET:CE	1:O:134:VAL:HG11	2.50	0.41
2:B:18:ALA:HB3	2:B:46:TYR:CE1	2.56	0.41
2:L:59:VAL:HG12	2:L:63:ALA:HB3	2.02	0.41
1:I:10:ALA:CB	1:I:14:LEU:HG	2.51	0.41
2:L:39:ILE:HG21	2:L:39:ILE:HD13	1.57	0.41
1:G:98:GLU:HB3	1:G:148:ARG:HG3	2.01	0.41
2:J:114:PHE:HA	3:J:1608:HOH:O	2.20	0.41
1:G:115:ILE:HD12	1:G:143:VAL:HG22	2.02	0.41
2:P:114:PHE:CE2	2:P:116:LEU:HB2	2.56	0.40
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
1:E:84:GLY:CA	1:M:86:SER:OG	2.60	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:61:ASP:HA	2:F:64:MET:HE2	2.02	0.40
2:N:30:PRO:O	2:N:33:ARG:HG2	2.22	0.40
2:F:137:GLU:HG3	2:F:137:GLU:O	2.21	0.40
1:O:58:TRP:HH2	1:O:149:LYS:HD3	1.86	0.40
1:K:17:LEU:C	1:K:17:LEU:HD23	2.42	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 (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	172/174 (99%)	166 (96%)	5 (3%)	1 (1%)	30 22
1	C	172/174 (99%)	165 (96%)	6 (4%)	1 (1%)	30 22
1	E	172/174 (99%)	163 (95%)	7 (4%)	2 (1%)	16 8
1	G	172/174 (99%)	164 (95%)	5 (3%)	3 (2%)	11 4
1	I	172/174 (99%)	165 (96%)	5 (3%)	2 (1%)	16 8
1	K	172/174 (99%)	164 (95%)	5 (3%)	3 (2%)	11 4
1	M	172/174 (99%)	161 (94%)	11 (6%)	0	100 100
1	O	172/174 (99%)	159 (92%)	12 (7%)	1 (1%)	30 22
2	B	130/132 (98%)	125 (96%)	3 (2%)	2 (2%)	13 5
2	D	130/132 (98%)	125 (96%)	1 (1%)	4 (3%)	5 1
2	F	130/132 (98%)	125 (96%)	2 (2%)	3 (2%)	8 3

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	H	130/132 (98%)	125 (96%)	1 (1%)	4 (3%)	5 1
2	J	130/132 (98%)	124 (95%)	3 (2%)	3 (2%)	8 3
2	L	130/132 (98%)	126 (97%)	2 (2%)	2 (2%)	13 5
2	N	130/132 (98%)	126 (97%)	2 (2%)	2 (2%)	13 5
2	P	130/132 (98%)	122 (94%)	4 (3%)	4 (3%)	5 1
All	All	2416/2448 (99%)	2305 (95%)	74 (3%)	37 (2%)	13 5

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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	150/150 (100%)	139 (93%)	11 (7%)	17	11
1	C	150/150 (100%)	142 (95%)	8 (5%)	28	22
1	E	150/150 (100%)	141 (94%)	9 (6%)	24	17
1	G	150/150 (100%)	145 (97%)	5 (3%)	45	43
1	I	150/150 (100%)	142 (95%)	8 (5%)	28	22
1	K	150/150 (100%)	140 (93%)	10 (7%)	20	14
1	M	150/150 (100%)	143 (95%)	7 (5%)	32	27
1	O	150/150 (100%)	142 (95%)	8 (5%)	28	22
2	B	124/124 (100%)	117 (94%)	7 (6%)	26	20
2	D	124/124 (100%)	118 (95%)	6 (5%)	31	26
2	F	124/124 (100%)	116 (94%)	8 (6%)	21	15
2	H	124/124 (100%)	115 (93%)	9 (7%)	17	11
2	J	124/124 (100%)	121 (98%)	3 (2%)	57	58
2	L	124/124 (100%)	116 (94%)	8 (6%)	21	15
2	N	124/124 (100%)	117 (94%)	7 (6%)	26	20
2	P	124/124 (100%)	116 (94%)	8 (6%)	21	15
All	All	2192/2192 (100%)	2070 (94%)	122 (6%)	26	20

All (122) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	LEU
1	A	21	TYR
1	A	65	GLU
1	A	101	LEU
1	A	123	ILE
1	A	126	SER
1	A	130	GLU
1	A	148	ARG
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	56	ASP
2	B	84	SER
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	37	TYR
2	D	56	ASP
2	D	84	SER
2	D	91	GLN
2	D	148	LYS
1	E	41	SER
1	E	46	MET
1	E	61	ARG
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	F	28	SER
2	F	75	GLU
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	148	ARG
1	G	153	LEU
1	G	165	LEU
2	H	33	ARG
2	H	37	TYR
2	H	56	ASP
2	H	58	SER
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	148	ARG
1	I	153	LEU
1	I	165	LEU
2	J	56	ASP
2	J	136	HIS
2	J	148	LYS
1	K	14	LEU
1	K	33	ASN
1	K	47	SER
1	K	63	GLU
1	K	130	GLU
1	K	143	VAL
1	K	148	ARG
1	K	149	LYS
1	K	153	LEU
1	K	165	LEU
2	L	26	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	L	28	SER
2	L	37	TYR
2	L	56	ASP
2	L	85	LYS
2	L	91	GLN
2	L	138	ASP
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	130	GLU
1	M	153	LEU
2	N	28	SER
2	N	37	TYR
2	N	56	ASP
2	N	57	HIS
2	N	83	GLN
2	N	84	SER
2	N	149	ILE
1	O	35	MET
1	O	47	SER
1	O	66	ARG
1	O	101	LEU
1	O	130	GLU
1	O	153	LEU
1	O	165	LEU
1	O	172	LYS
2	P	33	ARG
2	P	37	TYR
2	P	42	GLN
2	P	57	HIS
2	P	84	SER
2	P	136	HIS
2	P	148	LYS
2	P	149	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (86) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	29	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	44	ASN
1	A	106	ASN
1	A	108	GLN
2	B	34	ASN
2	B	40	HIS
2	B	53	HIS
2	B	66	GLN
2	B	91	GLN
1	C	19	HIS
1	C	29	GLN
1	C	30	ASN
1	C	44	ASN
1	C	79	ASN
1	C	106	ASN
1	C	108	GLN
2	D	40	HIS
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	44	ASN
1	E	106	ASN
1	E	108	GLN
2	F	40	HIS
2	F	53	HIS
2	F	66	GLN
2	F	91	GLN
2	F	99	HIS
1	G	29	GLN
1	G	30	ASN
1	G	44	ASN
1	G	106	ASN
1	G	108	GLN
2	H	26	ASN
2	H	53	HIS
2	H	57	HIS
2	H	66	GLN
2	H	99	HIS
1	I	29	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	I	44	ASN
1	I	108	GLN
1	I	133	HIS
2	J	40	HIS
2	J	53	HIS
2	J	66	GLN
2	J	81	GLN
2	J	83	GLN
2	J	91	GLN
2	J	99	HIS
1	K	29	GLN
1	K	44	ASN
1	K	79	ASN
1	K	106	ASN
2	L	26	ASN
2	L	53	HIS
2	L	66	GLN
2	L	83	GLN
2	L	91	GLN
2	L	124	HIS
1	M	29	GLN
1	M	44	ASN
1	M	106	ASN
1	M	108	GLN
2	N	26	ASN
2	N	40	HIS
2	N	53	HIS
2	N	66	GLN
2	N	78	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	44	ASN
1	O	106	ASN
1	O	108	GLN
2	P	40	HIS
2	P	42	GLN
2	P	53	HIS
2	P	66	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	P	91	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 carbohydrates 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

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, 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	174/174 (100%)	0.64	14 (8%) 15 16	2, 5, 24, 42	0
1	C	174/174 (100%)	0.15	5 (2%) 55 56	2, 5, 20, 28	0
1	E	174/174 (100%)	0.27	8 (4%) 36 38	2, 8, 22, 36	0
1	G	174/174 (100%)	-0.03	0 100 100	2, 6, 20, 30	0
1	I	174/174 (100%)	1.00	36 (20%) 1 1	4, 11, 25, 35	0
1	K	174/174 (100%)	0.26	9 (5%) 31 33	2, 7, 23, 32	0
1	M	174/174 (100%)	0.51	19 (10%) 7 8	3, 8, 22, 27	0
1	O	174/174 (100%)	1.13	40 (22%) 1 1	4, 11, 24, 35	0
2	B	132/132 (100%)	0.28	9 (6%) 20 22	2, 6, 30, 41	0
2	D	132/132 (100%)	0.26	8 (6%) 25 26	2, 5, 24, 38	0
2	F	132/132 (100%)	0.10	6 (4%) 37 38	2, 6, 24, 37	0
2	H	132/132 (100%)	0.33	5 (3%) 44 45	2, 5, 22, 29	0
2	J	132/132 (100%)	0.19	11 (8%) 14 15	2, 6, 32, 39	0
2	L	132/132 (100%)	0.06	8 (6%) 25 26	2, 6, 21, 41	0
2	N	132/132 (100%)	0.07	5 (3%) 44 45	2, 6, 24, 39	0
2	P	132/132 (100%)	0.44	16 (12%) 6 6	2, 6, 29, 38	0
All	All	2448/2448 (100%)	0.37	199 (8%) 15 15	2, 7, 24, 42	0

All (199) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	18	ALA	11.6
1	O	174	CYS	11.1
1	I	174	CYS	10.4
1	K	82	PRO	10.0
2	N	18	ALA	10.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	174	CYS	9.7
2	H	18	ALA	9.7
2	P	18	ALA	8.5
1	K	85	ALA	8.4
1	M	85	ALA	8.1
2	B	18	ALA	7.8
2	J	18	ALA	7.7
2	F	56	ASP	7.4
2	D	57	HIS	7.1
2	P	136	HIS	6.9
2	F	18	ALA	6.9
1	K	83	GLY	6.8
1	M	83	GLY	6.8
2	L	57	HIS	6.8
1	I	85	ALA	6.6
2	B	136	HIS	6.5
1	O	82	PRO	6.3
1	I	86	SER	6.3
1	I	82	PRO	6.1
2	P	57	HIS	5.9
2	L	18	ALA	5.8
1	I	83	GLY	5.8
1	O	83	GLY	5.7
1	M	84	GLY	5.6
2	L	56	ASP	5.6
1	E	82	PRO	5.5
1	K	84	GLY	5.5
2	N	149	ILE	5.5
1	O	84	GLY	5.4
2	D	56	ASP	5.3
1	I	125	VAL	5.2
2	J	57	HIS	5.2
1	I	87	SER	5.2
2	J	56	ASP	5.2
2	P	56	ASP	5.1
1	O	60	TYR	5.0
1	M	86	SER	5.0
1	I	84	GLY	5.0
2	J	136	HIS	4.9
1	M	82	PRO	4.9
1	E	174	CYS	4.9
1	I	126	SER	4.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	K	86	SER	4.8
1	O	173	LYS	4.8
1	I	173	LYS	4.8
1	O	85	ALA	4.8
1	M	46	MET	4.7
1	E	85	ALA	4.7
1	A	86	SER	4.5
2	H	56	ASP	4.5
2	L	149	ILE	4.4
1	O	126	SER	4.4
1	I	130	GLU	4.4
1	O	47	SER	4.2
1	A	83	GLY	4.2
1	I	124	THR	4.2
2	P	135	GLN	4.1
2	D	59	VAL	4.1
1	I	46	MET	4.1
2	N	56	ASP	4.1
1	M	47	SER	4.0
2	F	57	HIS	4.0
1	I	47	SER	4.0
1	I	80	SER	4.0
1	I	158	ILE	3.9
2	N	57	HIS	3.9
1	O	48	GLY	3.9
2	B	56	ASP	3.9
2	P	138	ASP	3.9
1	I	127	SER	3.9
1	O	46	MET	3.8
2	P	59	VAL	3.8
2	P	55	GLU	3.7
1	O	86	SER	3.7
2	B	57	HIS	3.6
1	E	84	GLY	3.6
2	P	58	SER	3.5
2	P	149	ILE	3.4
2	J	149	ILE	3.4
1	C	86	SER	3.4
1	I	45	VAL	3.4
2	J	138	ASP	3.4
2	P	60	ALA	3.3
1	O	145	PRO	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	135	GLN	3.3
1	I	129	PHE	3.2
1	E	83	GLY	3.2
1	O	81	PHE	3.2
1	O	129	PHE	3.2
2	D	149	ILE	3.2
1	A	84	GLY	3.2
1	M	79	ASN	3.1
1	C	60	TYR	3.1
2	J	58	SER	3.1
1	M	110	ARG	3.1
1	O	172	LYS	3.1
2	D	60	ALA	3.1
1	C	84	GLY	3.1
1	I	49	ASP	3.1
1	O	62	GLY	3.1
1	M	60	TYR	3.0
2	F	55	GLU	3.0
1	E	49	ASP	3.0
1	O	125	VAL	3.0
1	K	46	MET	3.0
1	E	14	LEU	3.0
1	O	49	ASP	3.0
1	O	64	ALA	3.0
1	O	79	ASN	3.0
1	O	65	GLU	3.0
1	I	21	TYR	3.0
1	I	48	GLY	2.9
1	I	123	ILE	2.9
1	O	45	VAL	2.9
1	I	133	HIS	2.9
1	M	111	LEU	2.9
1	K	130	GLU	2.9
1	M	81	PHE	2.9
1	O	130	GLU	2.9
2	L	58	SER	2.9
2	H	149	ILE	2.8
2	D	55	GLU	2.8
1	O	87	SER	2.8
1	O	124	THR	2.8
2	J	115	THR	2.8
1	M	87	SER	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	O	119	ALA	2.7
1	O	146	LEU	2.7
1	O	143	VAL	2.7
1	M	49	ASP	2.7
2	B	55	GLU	2.7
1	A	165	LEU	2.7
2	J	33	ARG	2.7
1	I	172	LYS	2.7
1	O	63	GLU	2.7
2	D	58	SER	2.7
1	M	130	GLU	2.6
1	I	77	ASP	2.6
1	A	25	TRP	2.6
2	N	59	VAL	2.6
1	I	110	ARG	2.6
1	I	81	PHE	2.6
1	A	162	VAL	2.6
1	O	21	TYR	2.5
2	P	137	GLU	2.5
1	M	88	CYS	2.5
1	O	78	CYS	2.5
1	A	173	LYS	2.5
2	B	58	SER	2.5
1	I	60	TYR	2.4
1	O	68	PHE	2.4
2	L	55	GLU	2.4
1	O	88	CYS	2.4
1	C	82	PRO	2.4
1	I	128	ASP	2.4
1	O	80	SER	2.4
1	A	85	ALA	2.4
1	I	79	ASN	2.4
1	A	54	LEU	2.4
1	I	63	GLU	2.4
1	O	120	PRO	2.3
2	F	149	ILE	2.3
1	A	164	LEU	2.3
1	A	40	TYR	2.3
1	O	158	ILE	2.3
1	I	65	GLU	2.3
1	O	148	ARG	2.3
1	I	23	LYS	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	130	GLU	2.2
2	J	55	GLU	2.2
2	L	60	ALA	2.2
1	I	117	THR	2.2
2	P	61	ASP	2.2
1	O	61	ARG	2.1
2	L	59	VAL	2.1
1	O	123	ILE	2.1
2	H	98	LYS	2.1
2	F	99	HIS	2.1
2	J	59	VAL	2.1
1	K	47	SER	2.1
1	A	155	PHE	2.1
2	B	59	VAL	2.1
2	P	115	THR	2.0
2	H	57	HIS	2.0
1	E	86	SER	2.0
1	I	88	CYS	2.0
1	M	78	CYS	2.0
1	M	158	ILE	2.0
2	B	149	ILE	2.0
1	K	35	MET	2.0
2	P	78	GLN	2.0
1	C	83	GLY	2.0
1	M	174	CYS	2.0
2	P	28	SER	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.