Full wwPDB X-ray Structure Validation Report ⓘ

Aug 27, 2023 – 06:48 AM EDT

PDB ID	:	3H2V
Title	:	Human raver1 RRM1 domain in complex with human vinculin tail domain Vt
Authors	:	Lee, J.H.; Rangarajan, E.S.; Yogesha, S.D.; Izard, T.
Deposited on	:	2009-04-14
Resolution	:	2.90 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:

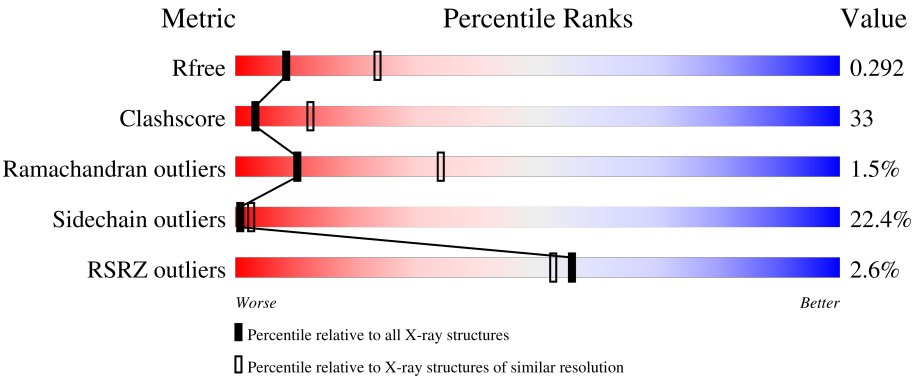
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 2.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	188	39% 37% 15% • 7%
1	B	188	3% 41% 35% 12% • 11%
1	C	188	3% 41% 35% 12% • 11%
1	D	188	3% 40% 38% 13% • 7%
2	E	74	54% 41% 5%

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Mol	Chain	Length	Quality of chain
2	F	74	4% 54% 41%
2	G	74	% 51% 45%
2	H	74	5% 53% 41% 5%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 7693 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 Vinculin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	174	Total	C	N	O	S	0	0	0
			1351	830	255	254	12			
1	B	167	Total	C	N	O	S	0	0	0
			1299	796	243	248	12			
1	C	167	Total	C	N	O	S	0	0	0
			1298	797	243	246	12			
1	D	175	Total	C	N	O	S	0	0	0
			1361	837	255	257	12			

- Molecule 2 is a protein called Raver-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	74	Total	C	N	O	S	0	0	0
			600	378	107	113	2			
2	F	73	Total	C	N	O	S	0	0	0
			590	372	104	112	2			
2	G	74	Total	C	N	O	S	0	0	0
			600	378	107	113	2			
2	H	73	Total	C	N	O	S	0	0	0
			590	372	104	112	2			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	57	HIS	-	cloning artifact	UNP Q8IY67
E	58	MET	-	cloning artifact	UNP Q8IY67
F	57	HIS	-	cloning artifact	UNP Q8IY67
F	58	MET	-	cloning artifact	UNP Q8IY67
G	57	HIS	-	cloning artifact	UNP Q8IY67
G	58	MET	-	cloning artifact	UNP Q8IY67
H	57	HIS	-	cloning artifact	UNP Q8IY67
H	58	MET	-	cloning artifact	UNP Q8IY67

- Molecule 3 is water.

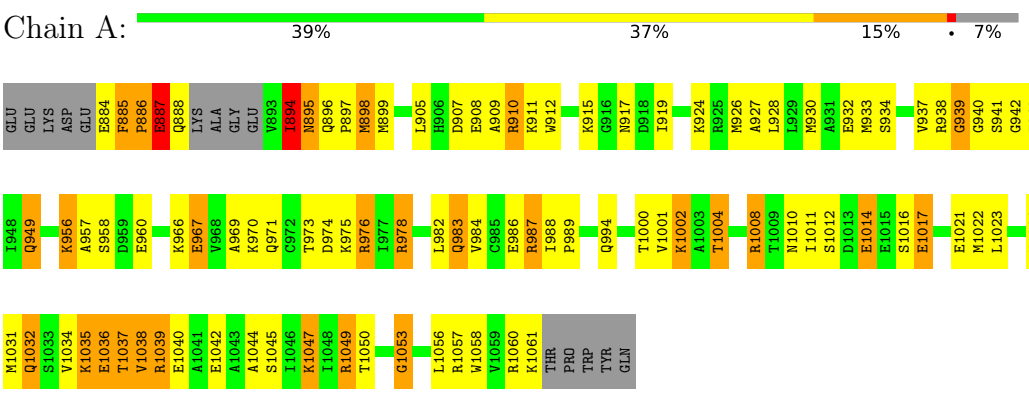
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O 1 1	0	0
3	B	1	Total O 1 1	0	0
3	F	1	Total O 1 1	0	0
3	G	1	Total O 1 1	0	0

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.

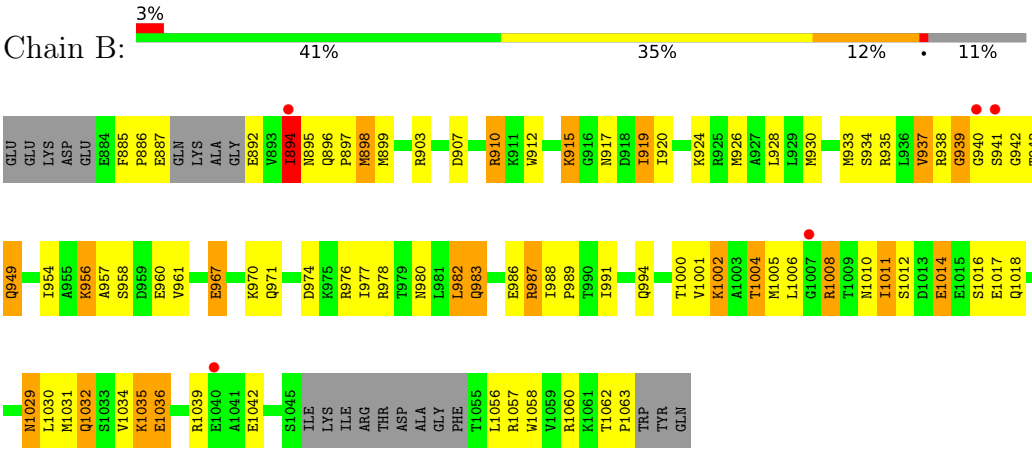
• Molecule 1: Vinculin

Chain A:



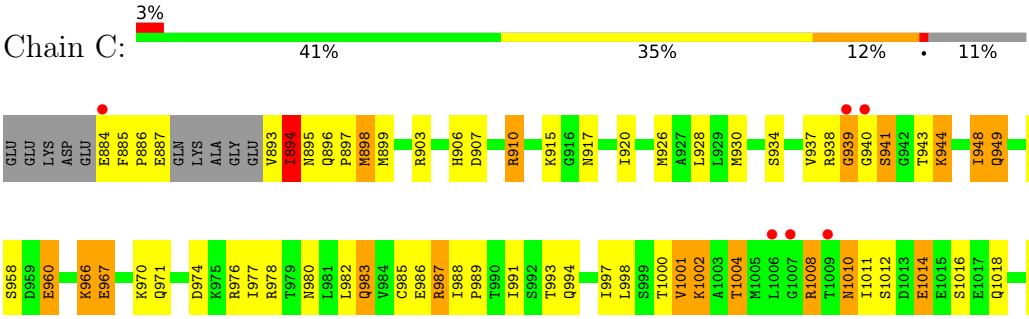
• Molecule 1: Vinculin

Chain B:

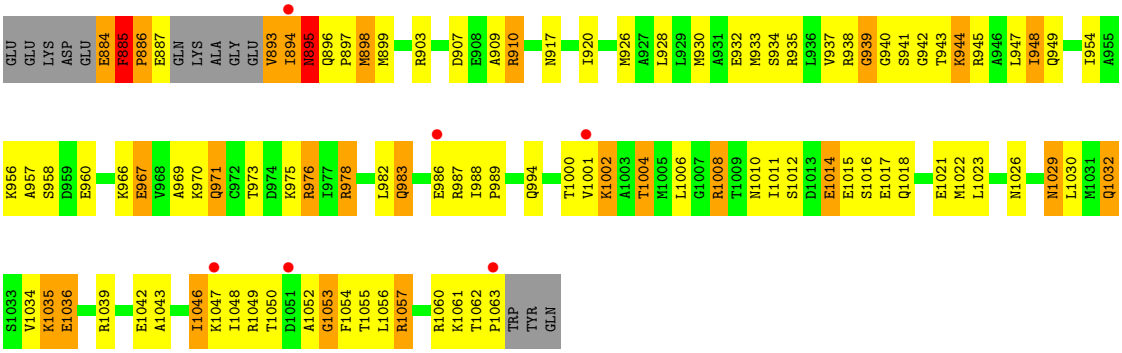


• Molecule 1: Vinculin

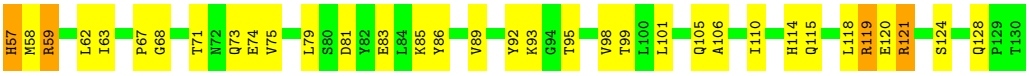
Chain C:



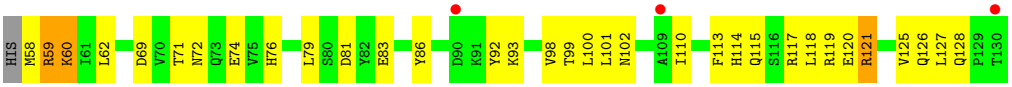
• Molecule 1: Vinculin



• Molecule 2: Raver-1

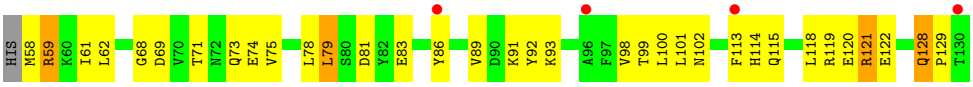


• Molecule 2: Raver-1



• Molecule 2: Raver-1

• Molecule 2: Raver-1



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	41.82Å 70.92Å 99.34Å 89.77° 90.04° 104.04°	Depositor
Resolution (Å)	20.00 – 2.90 40.57 – 2.89	Depositor EDS
% Data completeness (in resolution range)	94.0 (20.00-2.90) 93.2 (40.57-2.89)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.46 (at 2.90Å)	Xtriage
Refinement program	BUSTER-TNT 2.3.0	Depositor
R, R_{free}	0.210 , 0.277 0.221 , 0.292	Depositor DCC
R_{free} test set	1191 reflections (5.14%)	wwPDB-VP
Wilson B-factor (Å^2)	56.0	Xtriage
Anisotropy	0.310	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 23.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.429 for -h,-k,l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	7693	wwPDB-VP
Average B, all atoms (Å^2)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.26% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	1.41	26/1360 (1.9%)	0.92	5/1821 (0.3%)
1	B	0.76	1/1307 (0.1%)	0.79	1/1751 (0.1%)
1	C	0.75	1/1306 (0.1%)	0.81	1/1750 (0.1%)
1	D	0.73	0/1371	0.81	1/1838 (0.1%)
2	E	0.97	4/610 (0.7%)	0.75	1/821 (0.1%)
2	F	0.63	0/599	0.68	0/806
2	G	0.65	0/610	0.70	0/821
2	H	0.65	0/599	0.68	0/806
All	All	0.90	32/7762 (0.4%)	0.80	9/10414 (0.1%)

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1038	VAL	CB-CG1	-16.49	1.18	1.52
1	A	1038	VAL	CA-CB	-12.68	1.28	1.54
1	A	1038	VAL	C-O	-10.21	1.03	1.23
1	A	885	PHE	CE2-CZ	-10.01	1.18	1.37
1	A	1040	GLU	C-O	-9.99	1.04	1.23
1	A	1039	ARG	C-O	-9.41	1.05	1.23
1	A	885	PHE	CG-CD1	-8.57	1.25	1.38
1	A	1038	VAL	CB-CG2	-8.43	1.35	1.52
2	E	119	ARG	C-O	-8.21	1.07	1.23
1	A	1040	GLU	CD-OE2	-8.01	1.16	1.25
2	E	119	ARG	CZ-NH1	-7.99	1.22	1.33
1	A	885	PHE	CD2-CE2	-7.84	1.23	1.39
1	A	886	PRO	CG-CD	-7.30	1.26	1.50
1	A	1039	ARG	CB-CG	-7.20	1.33	1.52
2	E	119	ARG	CZ-NH2	-7.08	1.23	1.33
1	A	1038	VAL	CA-C	-6.70	1.35	1.52
1	A	1039	ARG	CA-C	-6.62	1.35	1.52
1	A	1039	ARG	CZ-NH2	-6.47	1.24	1.33
1	A	1040	GLU	N-CA	-6.32	1.33	1.46
1	A	885	PHE	C-O	-6.14	1.11	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1038	VAL	N-CA	-6.10	1.34	1.46
1	A	1040	GLU	CA-C	-5.87	1.37	1.52
1	B	1017	GLU	CB-CG	5.78	1.63	1.52
1	A	1037	THR	C-N	-5.77	1.20	1.34
1	A	1040	GLU	CB-CG	-5.76	1.41	1.52
2	E	119	ARG	CB-CG	-5.52	1.37	1.52
1	A	1039	ARG	CG-CD	-5.50	1.38	1.51
1	A	887	GLU	C-O	-5.38	1.13	1.23
1	A	1017	GLU	CG-CD	5.24	1.59	1.51
1	A	886	PRO	CB-CG	-5.24	1.23	1.50
1	A	885	PHE	CD1-CE1	-5.11	1.29	1.39
1	C	960	GLU	CG-CD	5.04	1.59	1.51

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	885	PHE	C-N-CD	-11.37	95.59	120.60
1	A	1040	GLU	OE1-CD-OE2	-8.34	113.29	123.30
1	A	1039	ARG	NE-CZ-NH1	8.31	124.45	120.30
2	E	119	ARG	NE-CZ-NH1	7.86	124.23	120.30
1	C	1062	THR	C-N-CD	-5.90	107.63	120.60
1	A	1039	ARG	NE-CZ-NH2	-5.65	117.48	120.30
1	A	885	PHE	N-CA-C	-5.50	96.15	111.00
1	B	982	LEU	CA-CB-CG	-5.45	102.77	115.30
1	A	942	GLY	N-CA-C	-5.22	100.05	113.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1351	0	1412	98	0
1	B	1299	0	1352	105	0
1	C	1298	0	1357	108	0
1	D	1361	0	1423	115	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	600	0	597	29	0
2	F	590	0	590	34	0
2	G	600	0	597	37	0
2	H	590	0	590	33	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
All	All	7693	0	7918	513	0

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 33.

All (513) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:939:GLY:HA3	1:B:943:THR:HG21	1.22	1.17
1:C:938:ARG:HH22	1:D:938:ARG:NH1	1.47	1.11
1:C:939:GLY:HA3	1:C:943:THR:HG21	1.22	1.10
1:C:896:GLN:NE2	1:D:896:GLN:HE22	1.51	1.09
1:D:939:GLY:HA3	1:D:943:THR:HG21	1.28	1.08
1:A:939:GLY:HA3	1:A:943:THR:HG21	1.37	1.05
1:A:973:THR:HG22	1:A:1049:ARG:HG3	1.43	1.00
1:B:894:ILE:HD12	1:B:899:MET:HG3	1.44	0.99
1:C:949:GLN:HG2	2:G:120:GLU:HB2	1.40	0.98
1:B:886:PRO:HG2	2:F:92:TYR:CE2	1.98	0.98
1:D:1047:LYS:H	1:D:1047:LYS:HD2	1.29	0.97
1:A:1047:LYS:H	1:A:1047:LYS:HZ2	1.11	0.96
1:B:949:GLN:HG2	2:F:120:GLU:HB2	1.47	0.95
1:A:949:GLN:HG2	2:E:120:GLU:HB2	1.50	0.93
1:D:1057:ARG:HG2	1:D:1057:ARG:HH11	1.32	0.92
1:C:896:GLN:HE22	1:D:896:GLN:HE22	1.04	0.92
1:A:898:MET:HB2	1:A:934:SER:HB3	1.52	0.91
1:B:917:ASN:HA	1:B:1056:LEU:HD22	1.53	0.91
1:C:894:ILE:HD12	1:C:899:MET:HG3	1.51	0.90
2:F:58:MET:HG3	2:F:59:ARG:H	1.38	0.89
1:C:917:ASN:HA	1:C:1056:LEU:HD22	1.52	0.89
1:A:1050:THR:HG23	1:A:1053:GLY:H	1.37	0.88
2:E:86:TYR:HB3	2:E:99:THR:HB	1.55	0.87
1:A:1038:VAL:HG12	1:A:1038:VAL:O	1.71	0.87
2:H:58:MET:HG3	2:H:59:ARG:H	1.41	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:92:TYR:CD2	2:G:93:LYS:HD3	2.11	0.84
2:G:92:TYR:CE2	2:G:93:LYS:HD3	2.12	0.84
1:C:917:ASN:HA	1:C:1056:LEU:CD2	2.07	0.84
1:C:938:ARG:HH22	1:D:938:ARG:HH12	1.22	0.84
1:C:938:ARG:NH2	1:D:938:ARG:NH1	2.26	0.84
1:C:896:GLN:NE2	1:D:896:GLN:NE2	2.25	0.83
1:D:949:GLN:HG2	2:H:120:GLU:HB2	1.58	0.83
1:A:1029:ASN:N	1:A:1029:ASN:HD22	1.75	0.83
1:C:949:GLN:HG2	2:G:120:GLU:CB	2.08	0.82
1:D:898:MET:HB2	1:D:934:SER:HB3	1.61	0.82
2:H:86:TYR:HB3	2:H:99:THR:HB	1.60	0.81
1:C:896:GLN:HE22	1:D:896:GLN:NE2	1.79	0.81
1:A:907:ASP:HA	1:A:910:ARG:HD3	1.61	0.80
1:B:907:ASP:HA	1:B:910:ARG:HD3	1.63	0.80
2:E:118:LEU:O	2:E:121:ARG:HG2	1.81	0.80
2:F:118:LEU:O	2:F:121:ARG:HG2	1.82	0.80
1:C:938:ARG:NH2	1:D:938:ARG:HH12	1.79	0.79
1:B:910:ARG:HB2	1:B:910:ARG:HH11	1.47	0.79
1:B:982:LEU:O	1:B:986:GLU:HG2	1.83	0.79
1:C:982:LEU:O	1:C:986:GLU:HG2	1.83	0.79
1:C:939:GLY:CA	1:C:943:THR:HG21	2.08	0.79
2:F:92:TYR:CE2	2:F:93:LYS:HD3	2.19	0.78
2:F:83:GLU:OE2	2:F:101:LEU:HD22	1.83	0.78
1:D:893:VAL:O	1:D:938:ARG:HG3	1.84	0.78
1:D:982:LEU:O	1:D:986:GLU:HG2	1.84	0.78
1:C:907:ASP:HA	1:C:910:ARG:HD3	1.64	0.77
1:C:926:MET:CE	1:C:1034:VAL:HG21	2.15	0.76
1:C:967:GLU:OE1	1:C:970:LYS:HD3	1.86	0.76
1:B:919:ILE:HG13	1:B:1056:LEU:HD11	1.67	0.76
2:G:86:TYR:HB3	2:G:99:THR:HB	1.68	0.76
1:B:949:GLN:HG2	2:F:120:GLU:CB	2.16	0.76
2:E:83:GLU:OE2	2:E:101:LEU:HD22	1.85	0.76
1:A:986:GLU:O	1:A:989:PRO:HD2	1.86	0.76
2:F:92:TYR:CD2	2:F:93:LYS:HD3	2.21	0.76
2:E:119:ARG:O	2:E:120:GLU:HB2	1.86	0.75
1:A:982:LEU:O	1:A:986:GLU:HG2	1.86	0.75
2:H:92:TYR:CE2	2:H:93:LYS:HD3	2.22	0.75
1:A:973:THR:CG2	1:A:1049:ARG:HG3	2.16	0.74
1:C:894:ILE:O	1:C:938:ARG:HD3	1.86	0.74
1:C:1029:ASN:N	1:C:1029:ASN:HD22	1.84	0.74
1:D:1029:ASN:HD22	1:D:1029:ASN:N	1.84	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:894:ILE:O	1:A:938:ARG:HD3	1.87	0.74
1:B:910:ARG:HH11	1:B:910:ARG:CB	2.00	0.74
2:F:86:TYR:HB3	2:F:99:THR:HB	1.69	0.74
2:H:83:GLU:OE2	2:H:101:LEU:HD22	1.87	0.74
1:C:939:GLY:HA3	1:C:943:THR:CG2	2.11	0.73
2:E:58:MET:HG3	2:E:59:ARG:H	1.54	0.73
1:C:1000:THR:O	1:C:1004:THR:HG23	1.88	0.73
1:D:986:GLU:O	1:D:989:PRO:HD2	1.88	0.73
1:D:1047:LYS:HD2	1:D:1047:LYS:N	2.03	0.73
1:B:939:GLY:CA	1:B:943:THR:HG21	2.10	0.72
1:D:939:GLY:HA3	1:D:943:THR:CG2	2.16	0.72
1:A:1008:ARG:HG2	1:A:1011:ILE:CD1	2.19	0.72
1:C:1057:ARG:HG2	1:C:1057:ARG:HH11	1.53	0.72
1:D:1052:ALA:HA	1:D:1053:GLY:O	1.90	0.71
1:A:1038:VAL:O	1:A:1038:VAL:CG1	2.27	0.71
2:H:119:ARG:O	2:H:120:GLU:HB2	1.91	0.71
1:B:1000:THR:O	1:B:1004:THR:HG23	1.90	0.71
1:B:967:GLU:OE1	1:B:970:LYS:HD3	1.91	0.71
1:D:1008:ARG:HG2	1:D:1011:ILE:CD1	2.21	0.70
2:H:92:TYR:CD2	2:H:93:LYS:HD3	2.25	0.70
1:B:894:ILE:O	1:B:938:ARG:HD3	1.90	0.70
1:B:895:ASN:ND2	1:B:898:MET:HG3	2.06	0.70
1:B:907:ASP:HA	1:B:910:ARG:CD	2.20	0.70
1:C:907:ASP:HA	1:C:910:ARG:CD	2.21	0.70
1:B:912:TRP:CH2	1:B:1060:ARG:HD3	2.27	0.70
1:A:949:GLN:HG2	2:E:120:GLU:CB	2.21	0.69
1:C:1008:ARG:HG2	1:C:1011:ILE:CD1	2.23	0.69
1:D:907:ASP:HA	1:D:910:ARG:HD3	1.75	0.69
1:C:1032:GLN:NE2	1:C:1036:GLU:OE2	2.23	0.69
1:B:1029:ASN:N	1:B:1029:ASN:HD22	1.90	0.69
1:C:887:GLU:OE2	1:C:887:GLU:N	2.25	0.69
1:D:1014:GLU:HA	1:D:1014:GLU:OE1	1.92	0.69
2:F:119:ARG:O	2:F:120:GLU:HB2	1.92	0.69
1:C:910:ARG:HB2	1:C:910:ARG:HH11	1.58	0.69
1:C:938:ARG:HH12	1:D:938:ARG:HH12	1.40	0.69
1:B:1008:ARG:HG2	1:B:1011:ILE:CD1	2.24	0.68
1:D:1057:ARG:HG2	1:D:1057:ARG:NH1	2.03	0.68
1:B:898:MET:HB2	1:B:934:SER:HB3	1.74	0.68
2:F:58:MET:HG3	2:F:59:ARG:N	2.08	0.68
1:C:938:ARG:NH1	1:D:938:ARG:HH12	1.91	0.68
2:G:83:GLU:OE2	2:G:101:LEU:HD22	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1030:LEU:O	1:D:1034:VAL:HG23	1.94	0.67
1:B:899:MET:HG2	1:B:934:SER:OG	1.95	0.67
1:C:895:ASN:HD22	1:C:898:MET:H	1.43	0.67
1:C:899:MET:HG2	1:C:934:SER:OG	1.94	0.67
2:F:69:ASP:OD1	2:F:119:ARG:NH2	2.26	0.67
1:A:1014:GLU:HA	1:A:1014:GLU:OE1	1.93	0.66
2:E:71:THR:OG1	2:E:74:GLU:HG3	1.95	0.66
1:D:939:GLY:CA	1:D:943:THR:HG21	2.17	0.66
2:G:119:ARG:O	2:G:120:GLU:HB2	1.95	0.66
1:B:1018:GLN:O	1:B:1022:MET:HG3	1.96	0.66
1:D:942:GLY:CA	1:D:944:LYS:HE3	2.26	0.66
2:H:71:THR:OG1	2:H:74:GLU:HG3	1.96	0.65
1:A:967:GLU:OE1	1:A:970:LYS:HD3	1.96	0.65
1:B:938:ARG:O	1:B:940:GLY:N	2.28	0.65
1:A:1049:ARG:HH11	1:A:1049:ARG:HB3	1.60	0.65
1:C:986:GLU:HA	1:C:986:GLU:OE2	1.96	0.65
1:C:1008:ARG:HG2	1:C:1008:ARG:NH1	2.11	0.65
2:H:58:MET:HG3	2:H:59:ARG:N	2.11	0.65
1:B:895:ASN:HD22	1:B:898:MET:H	1.44	0.64
1:C:910:ARG:HH11	1:C:910:ARG:CB	2.09	0.64
1:D:942:GLY:HA2	1:D:944:LYS:HE3	1.79	0.64
1:A:910:ARG:HH11	1:A:910:ARG:HB2	1.63	0.64
1:C:1008:ARG:HG2	1:C:1008:ARG:HH11	1.62	0.64
1:B:986:GLU:OE2	1:B:986:GLU:HA	1.98	0.64
1:C:1014:GLU:OE1	1:C:1014:GLU:HA	1.98	0.64
1:C:895:ASN:ND2	1:C:898:MET:HG3	2.13	0.64
1:A:1008:ARG:HG2	1:A:1008:ARG:NH1	2.13	0.64
2:G:72:ASN:O	2:G:76:HIS:HD2	1.80	0.64
1:C:898:MET:HB2	1:C:934:SER:HB3	1.79	0.63
1:C:926:MET:HE2	1:C:1034:VAL:HG21	1.79	0.63
2:G:58:MET:HG3	2:G:59:ARG:H	1.63	0.63
1:D:1008:ARG:HG2	1:D:1011:ILE:HD12	1.79	0.63
1:B:886:PRO:HG2	2:F:92:TYR:CZ	2.32	0.63
1:B:1032:GLN:NE2	1:B:1036:GLU:OE2	2.29	0.63
1:A:939:GLY:CA	1:A:943:THR:HG21	2.21	0.62
2:F:72:ASN:O	2:F:76:HIS:HD2	1.81	0.62
1:C:938:ARG:CZ	1:D:938:ARG:HH12	2.12	0.62
1:C:1008:ARG:HH11	1:C:1008:ARG:CG	2.12	0.62
1:B:926:MET:CE	1:B:1034:VAL:HG21	2.29	0.62
1:C:938:ARG:HH22	1:D:938:ARG:CZ	2.12	0.62
1:A:938:ARG:O	1:A:940:GLY:N	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:930:MET:HE2	1:D:954:ILE:CD1	2.30	0.62
1:A:1008:ARG:HH11	1:A:1008:ARG:CG	2.13	0.62
1:D:1000:THR:O	1:D:1004:THR:HG23	2.00	0.62
1:A:1008:ARG:HG2	1:A:1011:ILE:HD12	1.81	0.61
1:B:1008:ARG:HH11	1:B:1008:ARG:CG	2.13	0.61
1:A:1030:LEU:O	1:A:1034:VAL:HG23	2.00	0.61
1:B:939:GLY:HA3	1:B:943:THR:CG2	2.15	0.61
1:C:1008:ARG:HG2	1:C:1011:ILE:HD12	1.81	0.61
1:D:910:ARG:HH11	1:D:910:ARG:HB2	1.65	0.61
1:A:907:ASP:HA	1:A:910:ARG:CD	2.30	0.61
2:F:92:TYR:HE2	2:F:93:LYS:HZ2	1.47	0.61
1:A:939:GLY:HA3	1:A:943:THR:CG2	2.23	0.61
1:B:917:ASN:HA	1:B:1056:LEU:CD2	2.29	0.61
2:H:78:LEU:O	2:H:113:PHE:CZ	2.53	0.61
1:A:1000:THR:O	1:A:1004:THR:HG23	2.01	0.61
1:A:986:GLU:HA	1:A:986:GLU:OE2	2.00	0.61
1:D:930:MET:HE2	1:D:954:ILE:HD11	1.80	0.61
2:G:110:ILE:HD11	2:G:127:LEU:HD23	1.83	0.61
1:C:986:GLU:O	1:C:989:PRO:HD2	2.01	0.60
1:D:949:GLN:HG2	2:H:120:GLU:CB	2.30	0.60
1:C:938:ARG:NH1	1:D:938:ARG:HH22	1.99	0.60
1:A:1008:ARG:HG2	1:A:1008:ARG:HH11	1.66	0.60
1:D:986:GLU:OE2	1:D:986:GLU:HA	1.98	0.60
1:A:899:MET:HG2	1:A:934:SER:OG	2.01	0.60
1:A:917:ASN:HA	1:A:1056:LEU:HD22	1.83	0.60
2:E:74:GLU:OE1	2:E:119:ARG:NH1	2.35	0.60
2:H:74:GLU:OE1	2:H:119:ARG:NH1	2.33	0.60
1:A:1029:ASN:N	1:A:1029:ASN:ND2	2.44	0.59
1:C:949:GLN:HG3	2:G:121:ARG:HH11	1.67	0.59
1:B:1014:GLU:HA	1:B:1014:GLU:OE1	2.02	0.59
2:F:92:TYR:HE2	2:F:93:LYS:NZ	2.00	0.59
1:D:895:ASN:HD22	1:D:898:MET:H	1.49	0.59
1:D:1008:ARG:HH11	1:D:1008:ARG:CG	2.16	0.59
2:G:59:ARG:HD2	2:G:100:LEU:O	2.02	0.58
2:E:114:HIS:O	2:E:115:GLN:HB2	2.03	0.58
1:D:1029:ASN:N	1:D:1029:ASN:ND2	2.50	0.58
1:C:938:ARG:HH12	1:D:938:ARG:NH1	2.00	0.58
2:F:114:HIS:O	2:F:115:GLN:HB2	2.03	0.58
1:C:949:GLN:CG	2:G:120:GLU:HB2	2.23	0.58
1:C:896:GLN:HB3	1:C:897:PRO:HD3	1.86	0.57
1:A:895:ASN:HD22	1:A:898:MET:H	1.52	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1008:ARG:HG2	1:B:1008:ARG:NH1	2.19	0.57
2:G:69:ASP:OD1	2:G:119:ARG:NH2	2.26	0.57
1:B:949:GLN:CG	2:F:120:GLU:HB2	2.29	0.57
1:B:1030:LEU:O	1:B:1034:VAL:HG23	2.03	0.57
1:C:941:SER:C	1:C:943:THR:H	2.07	0.57
1:A:1044:ALA:HA	1:A:1047:LYS:NZ	2.19	0.57
1:B:1035:LYS:O	1:B:1039:ARG:HG3	2.04	0.57
2:F:71:THR:OG1	2:F:74:GLU:HG3	2.05	0.57
1:A:894:ILE:HD12	1:A:899:MET:HG3	1.86	0.57
1:C:938:ARG:CZ	1:D:938:ARG:HH22	2.18	0.57
1:D:886:PRO:HA	1:D:887:GLU:OE1	2.05	0.57
1:A:905:LEU:HD23	1:A:927:ALA:HB2	1.85	0.57
1:C:1010:ASN:O	2:H:129:PRO:HB3	2.04	0.56
1:D:895:ASN:CG	1:D:898:MET:HG3	2.25	0.56
1:D:896:GLN:HB3	1:D:897:PRO:HD3	1.87	0.56
1:A:1017:GLU:O	1:A:1021:GLU:HG3	2.06	0.56
1:C:1018:GLN:O	1:C:1022:MET:HG3	2.05	0.56
2:H:69:ASP:OD1	2:H:119:ARG:NH2	2.32	0.56
2:H:118:LEU:O	2:H:121:ARG:HG2	2.05	0.56
1:D:1008:ARG:HG2	1:D:1008:ARG:NH1	2.20	0.56
1:D:1035:LYS:O	1:D:1039:ARG:HG3	2.06	0.56
1:C:1057:ARG:HG2	1:C:1057:ARG:NH1	2.14	0.56
2:G:114:HIS:CD2	2:G:115:GLN:HG3	2.40	0.56
2:G:114:HIS:O	2:G:115:GLN:HB2	2.06	0.56
1:C:938:ARG:O	1:C:940:GLY:N	2.39	0.56
1:D:894:ILE:HG12	1:D:894:ILE:O	2.04	0.55
1:D:899:MET:HG2	1:D:934:SER:OG	2.06	0.55
2:G:118:LEU:O	2:G:121:ARG:HG2	2.07	0.55
1:B:941:SER:C	1:B:943:THR:H	2.10	0.55
1:B:896:GLN:HB3	1:B:897:PRO:HD3	1.88	0.55
1:A:988:ILE:HB	1:A:989:PRO:HD3	1.87	0.55
1:D:967:GLU:OE1	1:D:970:LYS:HD3	2.07	0.55
1:D:1032:GLN:NE2	1:D:1036:GLU:OE2	2.34	0.55
1:B:974:ASP:OD2	1:B:977:ILE:HG12	2.07	0.55
1:B:988:ILE:HB	1:B:989:PRO:HD3	1.87	0.55
1:C:895:ASN:CG	1:C:898:MET:HG3	2.27	0.55
2:G:86:TYR:HB3	2:G:99:THR:CB	2.36	0.54
1:B:930:MET:HE3	1:B:1031:MET:CE	2.38	0.54
1:A:915:LYS:O	1:A:1057:ARG:NH1	2.40	0.54
1:A:895:ASN:ND2	1:A:898:MET:HG3	2.22	0.54
1:B:894:ILE:CD1	1:B:899:MET:HG3	2.29	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:926:MET:CE	1:A:1034:VAL:HG21	2.38	0.54
1:B:1008:ARG:HG2	1:B:1008:ARG:HH11	1.71	0.54
1:A:895:ASN:ND2	1:A:897:PRO:HD2	2.22	0.53
1:A:910:ARG:HH11	1:A:910:ARG:CB	2.21	0.53
1:C:896:GLN:CB	1:C:897:PRO:HD3	2.38	0.53
2:E:58:MET:HG3	2:E:59:ARG:N	2.21	0.53
1:B:895:ASN:CG	1:B:898:MET:HG3	2.29	0.53
1:A:1001:VAL:HG22	1:A:1002:LYS:N	2.22	0.53
1:D:1008:ARG:CG	1:D:1011:ILE:HD12	2.38	0.53
1:A:941:SER:C	1:A:943:THR:H	2.12	0.52
1:B:894:ILE:HG22	1:B:935:ARG:HG2	1.90	0.52
1:D:1062:THR:CG2	1:D:1063:PRO:HD2	2.38	0.52
1:A:1032:GLN:NE2	1:A:1036:GLU:OE2	2.42	0.52
1:C:1008:ARG:CG	1:C:1011:ILE:HD12	2.38	0.52
1:D:976:ARG:C	1:D:976:ARG:HD2	2.27	0.52
1:D:894:ILE:HG13	1:D:899:MET:HG3	1.91	0.52
1:D:896:GLN:CB	1:D:897:PRO:HD3	2.39	0.52
1:B:920:ILE:HD11	1:B:1058:TRP:CZ3	2.45	0.52
1:B:910:ARG:HB2	1:B:910:ARG:NH1	2.22	0.52
1:C:988:ILE:HB	1:C:989:PRO:HD3	1.91	0.52
1:B:1001:VAL:HG22	1:B:1002:LYS:N	2.25	0.52
2:E:86:TYR:HB3	2:E:99:THR:CB	2.33	0.52
2:E:101:LEU:HD12	2:E:101:LEU:O	2.10	0.52
1:C:884:GLU:HG2	1:C:910:ARG:NH1	2.25	0.52
1:C:987:ARG:O	1:C:991:ILE:HD12	2.10	0.52
1:C:1029:ASN:N	1:C:1029:ASN:ND2	2.54	0.52
1:D:1054:PHE:CD1	1:D:1055:THR:N	2.78	0.52
1:D:926:MET:CE	1:D:1034:VAL:HG21	2.39	0.52
1:D:1001:VAL:HG22	1:D:1002:LYS:N	2.25	0.51
1:C:993:THR:O	1:C:997:ILE:HG13	2.11	0.51
1:A:994:GLN:CB	1:A:1026:ASN:HD21	2.23	0.51
1:D:884:GLU:O	1:D:885:PHE:HB2	2.08	0.51
1:D:1062:THR:CG2	1:D:1063:PRO:CD	2.88	0.51
2:E:92:TYR:HE2	2:E:93:LYS:HZ2	1.56	0.51
2:G:86:TYR:CB	2:G:99:THR:HB	2.39	0.51
1:A:930:MET:HE2	1:A:930:MET:HA	1.92	0.51
1:D:886:PRO:O	1:D:903:ARG:NH1	2.43	0.51
1:A:1027:ALA:O	1:A:1031:MET:HG2	2.10	0.51
1:A:1037:THR:O	1:A:1039:ARG:N	2.43	0.51
1:C:1035:LYS:O	1:C:1039:ARG:HG3	2.11	0.51
2:H:86:TYR:CB	2:H:99:THR:HB	2.36	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:933:MET:CE	1:B:947:LEU:HD12	2.41	0.51
1:C:886:PRO:O	1:C:903:ARG:NH1	2.43	0.51
2:G:101:LEU:HD12	2:G:101:LEU:O	2.10	0.51
1:A:886:PRO:O	1:A:887:GLU:O	2.28	0.51
1:C:886:PRO:HG2	2:G:92:TYR:CE2	2.45	0.51
1:D:932:GLU:OE2	2:H:68:GLY:N	2.44	0.51
1:D:938:ARG:O	1:D:940:GLY:N	2.44	0.51
1:D:944:LYS:HZ2	1:D:945:ARG:H	1.59	0.51
1:B:1008:ARG:HG2	1:B:1011:ILE:HD12	1.90	0.50
1:B:1008:ARG:CG	1:B:1008:ARG:NH1	2.74	0.50
2:E:75:VAL:HG21	2:E:89:VAL:CG2	2.40	0.50
1:A:1008:ARG:CG	1:A:1011:ILE:HD12	2.41	0.50
2:F:59:ARG:HD2	2:F:100:LEU:O	2.11	0.50
1:A:910:ARG:HB2	1:A:910:ARG:NH1	2.25	0.50
1:B:976:ARG:C	1:B:976:ARG:HD2	2.29	0.50
1:C:910:ARG:HH11	1:C:910:ARG:CG	2.25	0.50
1:B:910:ARG:HH11	1:B:910:ARG:CG	2.24	0.50
1:B:930:MET:HE3	1:B:1031:MET:HE1	1.94	0.50
1:B:949:GLN:HE21	2:F:120:GLU:HG3	1.76	0.50
2:F:86:TYR:HB3	2:F:99:THR:CB	2.38	0.50
1:D:907:ASP:HA	1:D:910:ARG:CD	2.40	0.50
2:F:114:HIS:CD2	2:F:115:GLN:HG3	2.47	0.50
2:H:58:MET:CG	2:H:59:ARG:H	2.20	0.50
2:H:59:ARG:HD2	2:H:100:LEU:O	2.12	0.50
1:D:969:ALA:O	1:D:978:ARG:HG3	2.12	0.50
1:B:942:GLY:HA2	1:B:944:LYS:HE3	1.94	0.49
2:H:92:TYR:HE2	2:H:93:LYS:HZ2	1.57	0.49
1:C:1030:LEU:O	1:C:1034:VAL:HG23	2.13	0.49
2:H:86:TYR:HB3	2:H:99:THR:CB	2.37	0.49
1:A:944:LYS:HZ2	1:A:945:ARG:H	1.60	0.49
1:D:1057:ARG:HH11	1:D:1057:ARG:CG	2.15	0.49
2:H:59:ARG:HB3	2:H:102:ASN:O	2.12	0.49
1:C:974:ASP:OD2	1:C:977:ILE:HG12	2.12	0.49
1:A:896:GLN:HB3	1:A:897:PRO:HD3	1.95	0.49
1:C:920:ILE:HD11	1:C:1058:TRP:CZ3	2.48	0.49
1:B:1002:LYS:HE3	1:B:1006:LEU:HD21	1.95	0.49
2:F:113:PHE:O	2:F:125:VAL:HG23	2.13	0.49
1:A:969:ALA:O	1:A:978:ARG:HG3	2.13	0.49
1:C:944:LYS:HZ1	2:G:117:ARG:HH22	1.61	0.49
1:C:949:GLN:HG2	2:G:120:GLU:CG	2.43	0.49
1:D:895:ASN:ND2	1:D:897:PRO:HD2	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:59:ARG:HB3	2:G:102:ASN:C	2.34	0.48
2:E:101:LEU:HB3	2:E:105:GLN:OE1	2.13	0.48
1:C:1062:THR:HG22	1:C:1063:PRO:N	2.29	0.48
1:D:942:GLY:HA3	1:D:944:LYS:HE3	1.96	0.48
1:D:917:ASN:HA	1:D:1056:LEU:HD22	1.96	0.48
1:A:994:GLN:HB3	1:A:1026:ASN:HD21	1.77	0.48
1:B:980:ASN:N	1:B:980:ASN:HD22	2.11	0.48
1:D:1043:ALA:O	1:D:1046:ILE:HG13	2.14	0.48
1:B:988:ILE:N	1:B:989:PRO:HD2	2.29	0.48
1:D:940:GLY:O	1:D:1006:LEU:HB3	2.14	0.48
1:D:1008:ARG:HG2	1:D:1008:ARG:HH11	1.76	0.48
2:E:92:TYR:CE2	2:E:93:LYS:HD3	2.49	0.48
2:E:106:ALA:O	2:E:110:ILE:HG13	2.14	0.48
1:B:1029:ASN:N	1:B:1029:ASN:ND2	2.61	0.47
1:D:1001:VAL:CG2	1:D:1002:LYS:N	2.76	0.47
2:F:86:TYR:CB	2:F:99:THR:HB	2.40	0.47
1:A:895:ASN:CG	1:A:898:MET:HG3	2.33	0.47
1:C:949:GLN:HE21	2:G:120:GLU:HG3	1.79	0.47
1:D:983:GLN:HE21	1:D:983:GLN:HB3	1.56	0.47
2:E:86:TYR:CB	2:E:99:THR:HB	2.34	0.47
2:F:110:ILE:HD11	2:F:127:LEU:HD23	1.95	0.47
1:B:1062:THR:HA	1:B:1063:PRO:HD3	1.68	0.47
1:A:926:MET:HG3	1:A:957:ALA:HB1	1.96	0.47
1:B:886:PRO:HG2	2:F:92:TYR:CD2	2.47	0.47
1:B:896:GLN:CB	1:B:897:PRO:HD3	2.45	0.47
1:C:930:MET:HE3	1:C:1031:MET:HE1	1.97	0.47
1:C:988:ILE:N	1:C:989:PRO:CD	2.77	0.47
1:C:1001:VAL:CG2	1:C:1002:LYS:N	2.77	0.47
2:H:115:GLN:HG2	2:H:122:GLU:OE1	2.15	0.47
1:C:894:ILE:HG13	1:C:895:ASN:N	2.29	0.47
1:D:933:MET:CE	1:D:947:LEU:HD12	2.45	0.47
1:A:1037:THR:C	1:A:1039:ARG:H	2.18	0.47
1:B:980:ASN:N	1:B:980:ASN:ND2	2.61	0.47
1:B:1008:ARG:CG	1:B:1011:ILE:HD12	2.45	0.47
1:D:1017:GLU:O	1:D:1021:GLU:HG3	2.15	0.47
1:A:898:MET:CB	1:A:934:SER:HB3	2.37	0.47
1:B:944:LYS:HZ1	2:F:117:ARG:HH22	1.62	0.47
1:B:949:GLN:HG2	2:F:120:GLU:CG	2.44	0.47
1:C:953:ASP:OD2	2:G:121:ARG:NH1	2.33	0.47
1:D:1062:THR:HG23	1:D:1063:PRO:HD2	1.97	0.47
2:G:64:ARG:HB2	2:G:124:SER:OG	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:92:TYR:HE2	2:H:93:LYS:NZ	2.14	0.46
2:F:117:ARG:HA	2:F:121:ARG:O	2.15	0.46
1:A:930:MET:HA	1:A:930:MET:CE	2.46	0.46
1:B:920:ILE:HG22	1:B:924:LYS:HE3	1.96	0.46
1:C:926:MET:HE1	1:C:1034:VAL:HG21	1.92	0.46
1:A:932:GLU:OE2	2:E:68:GLY:N	2.47	0.46
1:A:956:LYS:HB2	1:A:956:LYS:HE2	1.79	0.46
1:C:917:ASN:CA	1:C:1056:LEU:HD22	2.37	0.46
1:C:938:ARG:NH2	1:D:938:ARG:CZ	2.76	0.46
1:D:926:MET:HG3	1:D:957:ALA:HB1	1.96	0.46
1:C:1062:THR:HG23	1:C:1063:PRO:HD2	1.98	0.46
1:A:949:GLN:HE21	2:E:120:GLU:HG3	1.81	0.46
2:E:114:HIS:CD2	2:E:115:GLN:HG3	2.51	0.46
1:A:988:ILE:N	1:A:989:PRO:CD	2.79	0.46
1:B:944:LYS:H	1:B:944:LYS:HG3	1.52	0.46
2:H:101:LEU:HD12	2:H:101:LEU:O	2.16	0.46
1:B:910:ARG:NH1	1:B:910:ARG:CG	2.78	0.45
1:B:920:ILE:CG2	1:B:924:LYS:HE3	2.46	0.45
1:C:977:ILE:HG23	1:C:1040:GLU:OE2	2.17	0.45
1:C:1001:VAL:HG22	1:C:1002:LYS:N	2.31	0.45
1:D:1018:GLN:O	1:D:1022:MET:HG3	2.15	0.45
1:D:910:ARG:HH11	1:D:910:ARG:CB	2.29	0.45
1:B:988:ILE:N	1:B:989:PRO:CD	2.79	0.45
1:A:915:LYS:HB3	1:A:1057:ARG:NH1	2.32	0.45
1:B:933:MET:HE2	1:B:947:LEU:HD12	1.98	0.45
1:D:941:SER:HA	1:D:943:THR:H	1.82	0.45
1:B:956:LYS:HB2	1:B:956:LYS:HE2	1.79	0.45
1:C:1057:ARG:HH11	1:C:1057:ARG:CG	2.27	0.45
1:C:948:ILE:HG22	1:C:949:GLN:N	2.31	0.45
1:C:980:ASN:N	1:C:980:ASN:HD22	2.15	0.45
1:B:894:ILE:CG1	1:B:895:ASN:N	2.78	0.45
1:C:930:MET:HE2	1:C:954:ILE:CD1	2.47	0.45
1:D:1062:THR:HG23	1:D:1063:PRO:CD	2.47	0.45
1:B:1001:VAL:CG2	1:B:1002:LYS:N	2.76	0.45
2:F:72:ASN:O	2:F:76:HIS:CD2	2.67	0.45
1:D:930:MET:CE	1:D:954:ILE:HD13	2.48	0.45
2:G:118:LEU:O	2:G:121:ARG:CG	2.64	0.45
2:H:78:LEU:O	2:H:113:PHE:HZ	1.96	0.45
1:A:974:ASP:HB2	1:A:1047:LYS:HG3	1.99	0.44
1:A:1044:ALA:HA	1:A:1047:LYS:HZ3	1.82	0.44
1:B:930:MET:HE3	1:B:930:MET:HB2	1.66	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:930:MET:HE2	1:D:930:MET:HA	1.99	0.44
2:E:85:LYS:HE3	2:E:101:LEU:HD13	1.99	0.44
1:C:886:PRO:HG2	2:G:92:TYR:CD2	2.52	0.44
1:C:980:ASN:N	1:C:980:ASN:ND2	2.65	0.44
1:D:949:GLN:HE21	2:H:120:GLU:HG3	1.82	0.44
1:A:930:MET:CE	1:A:930:MET:CA	2.95	0.44
1:A:930:MET:HE3	1:A:930:MET:HB2	1.79	0.44
1:B:948:ILE:HG22	1:B:949:GLN:N	2.30	0.44
1:C:953:ASP:CG	2:G:121:ARG:HH12	2.18	0.44
2:H:114:HIS:O	2:H:115:GLN:C	2.56	0.44
1:A:975:LYS:HA	1:A:978:ARG:NH2	2.33	0.44
1:B:983:GLN:HE21	1:B:983:GLN:HB3	1.64	0.44
2:G:113:PHE:O	2:G:125:VAL:HG23	2.18	0.44
1:C:910:ARG:NH1	1:C:910:ARG:CG	2.80	0.44
1:B:895:ASN:H	1:B:934:SER:HB2	1.83	0.44
1:A:1001:VAL:CG2	1:A:1002:LYS:N	2.78	0.43
1:A:1034:VAL:O	1:A:1038:VAL:HG23	2.17	0.43
1:B:894:ILE:HG13	1:B:895:ASN:N	2.33	0.43
1:C:886:PRO:HD2	2:G:92:TYR:CG	2.52	0.43
1:D:973:THR:HG21	1:D:1049:ARG:HA	1.99	0.43
1:D:930:MET:HB2	1:D:930:MET:HE3	1.65	0.43
2:E:92:TYR:CD2	2:E:93:LYS:HD3	2.54	0.43
1:A:894:ILE:CG1	1:A:895:ASN:N	2.79	0.43
1:A:895:ASN:H	1:A:934:SER:HB2	1.81	0.43
1:A:930:MET:HE2	1:A:930:MET:CA	2.48	0.43
1:A:983:GLN:HE21	1:A:983:GLN:HB3	1.57	0.43
1:B:930:MET:HE2	1:B:954:ILE:HD11	2.01	0.43
1:D:895:ASN:ND2	1:D:898:MET:HG3	2.33	0.43
2:G:93:LYS:O	2:G:95:THR:HG23	2.19	0.43
1:B:895:ASN:ND2	1:B:895:ASN:O	2.50	0.43
1:C:895:ASN:H	1:C:934:SER:HB2	1.82	0.43
1:C:1062:THR:CG2	1:C:1063:PRO:N	2.82	0.43
1:A:944:LYS:H	1:A:944:LYS:HG3	1.43	0.43
1:B:917:ASN:ND2	1:B:920:ILE:HG12	2.33	0.43
1:D:910:ARG:HB2	1:D:910:ARG:NH1	2.32	0.43
1:D:976:ARG:HD2	1:D:976:ARG:O	2.18	0.43
1:A:984:VAL:HG12	1:A:987:ARG:NH2	2.34	0.43
1:B:926:MET:HE1	1:B:1034:VAL:HG21	1.99	0.43
1:D:1055:THR:CG2	1:D:1056:LEU:N	2.79	0.43
2:E:93:LYS:O	2:E:95:THR:HG23	2.19	0.43
1:A:1037:THR:C	1:A:1039:ARG:N	2.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1005:MET:O	1:B:1008:ARG:HB2	2.19	0.43
1:C:994:GLN:CB	1:C:1026:ASN:HD21	2.31	0.43
1:A:976:ARG:HA	1:A:976:ARG:HD2	1.48	0.43
1:D:994:GLN:CB	1:D:1026:ASN:HD21	2.32	0.43
1:A:917:ASN:OD1	1:A:1056:LEU:HD13	2.18	0.43
1:B:930:MET:HE2	1:B:954:ILE:CD1	2.49	0.43
1:B:895:ASN:ND2	1:B:898:MET:CG	2.79	0.42
1:C:894:ILE:CG1	1:C:895:ASN:N	2.79	0.42
1:C:895:ASN:ND2	1:C:897:PRO:HD2	2.33	0.42
1:D:930:MET:CE	1:D:930:MET:CA	2.96	0.42
2:G:58:MET:HG3	2:G:59:ARG:N	2.33	0.42
1:B:982:LEU:HD23	1:B:982:LEU:HA	1.51	0.42
1:D:944:LYS:O	1:D:948:ILE:HD12	2.18	0.42
1:D:971:GLN:O	1:D:1049:ARG:HB2	2.19	0.42
1:D:926:MET:HE1	1:D:1034:VAL:HG21	2.01	0.42
1:D:1056:LEU:HA	1:D:1056:LEU:HD23	1.78	0.42
1:B:886:PRO:O	1:B:903:ARG:NH1	2.53	0.42
2:E:73:GLN:NE2	2:E:73:GLN:HA	2.35	0.42
1:A:1035:LYS:O	1:A:1039:ARG:HG3	2.20	0.42
1:A:1044:ALA:HA	1:A:1047:LYS:HZ1	1.84	0.42
1:B:976:ARG:HD2	1:B:976:ARG:O	2.20	0.42
1:D:930:MET:CE	1:D:930:MET:HA	2.50	0.42
1:A:944:LYS:NZ	1:A:945:ARG:H	2.16	0.42
1:B:939:GLY:O	1:B:941:SER:N	2.53	0.42
1:B:957:ALA:O	1:B:961:VAL:HG23	2.19	0.42
1:C:930:MET:HE3	1:C:1031:MET:CE	2.48	0.42
2:H:75:VAL:HG21	2:H:89:VAL:CG2	2.49	0.42
1:A:926:MET:HG3	1:A:957:ALA:CB	2.50	0.41
1:D:988:ILE:N	1:D:989:PRO:CD	2.82	0.41
1:D:1062:THR:HG22	1:D:1063:PRO:HD2	2.02	0.41
2:F:60:LYS:HZ2	2:F:60:LYS:HG2	1.69	0.41
2:H:59:ARG:HB3	2:H:102:ASN:C	2.40	0.41
1:D:944:LYS:H	1:D:944:LYS:HG3	1.48	0.41
1:B:892:GLU:HB3	1:B:894:ILE:HD13	2.02	0.41
1:B:895:ASN:ND2	1:B:897:PRO:HD2	2.35	0.41
1:B:926:MET:HE2	1:B:1034:VAL:HG21	1.99	0.41
1:A:909:ALA:O	1:A:924:LYS:HE3	2.21	0.41
1:B:926:MET:HG3	1:B:957:ALA:HB1	2.02	0.41
1:B:987:ARG:O	1:B:991:ILE:HD12	2.19	0.41
1:C:998:LEU:HD13	1:C:1022:MET:O	2.20	0.41
1:D:932:GLU:HA	1:D:935:ARG:CZ	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:988:ILE:HB	1:D:989:PRO:HD3	2.02	0.41
1:A:896:GLN:CB	1:A:897:PRO:HD3	2.50	0.41
1:C:884:GLU:HG3	1:C:906:HIS:HE1	1.85	0.41
1:B:930:MET:CE	1:B:1031:MET:HE3	2.50	0.41
1:B:994:GLN:OE1	1:B:1026:ASN:ND2	2.53	0.41
1:D:994:GLN:OE1	1:D:1026:ASN:ND2	2.54	0.41
2:E:63:ILE:O	2:E:95:THR:HA	2.21	0.41
1:D:1062:THR:HA	1:D:1063:PRO:HD3	1.90	0.41
1:A:1045:SER:OG	1:A:1058:TRP:NE1	2.53	0.41
1:B:930:MET:CE	1:B:1031:MET:CE	2.99	0.41
1:C:983:GLN:HE21	1:C:983:GLN:HB3	1.59	0.41
1:C:985:CYS:HA	1:C:988:ILE:HG13	2.03	0.41
1:D:982:LEU:HD23	1:D:982:LEU:HA	1.79	0.41
2:E:67:PRO:HG3	2:E:121:ARG:HG3	2.03	0.41
2:F:59:ARG:HB3	2:F:102:ASN:C	2.41	0.41
2:F:113:PHE:O	2:F:125:VAL:CG2	2.68	0.41
2:G:92:TYR:HE2	2:G:93:LYS:HZ2	1.64	0.41
2:G:71:THR:OG1	2:G:74:GLU:HG3	2.21	0.41
1:A:912:TRP:CH2	1:A:1060:ARG:HD3	2.56	0.40
1:A:1037:THR:O	1:A:1038:VAL:C	2.57	0.40
1:D:948:ILE:HG22	1:D:949:GLN:N	2.37	0.40
1:D:1047:LYS:H	1:D:1047:LYS:CD	2.14	0.40
1:A:908:GLU:O	1:A:911:LYS:HB2	2.21	0.40
1:B:986:GLU:O	1:B:989:PRO:HD2	2.21	0.40
1:A:894:ILE:HG13	1:A:895:ASN:N	2.36	0.40
1:C:966:LYS:HZ3	1:C:966:LYS:HG3	1.50	0.40
1:C:982:LEU:HA	1:C:982:LEU:HD23	1.60	0.40
1:D:909:ALA:HB1	1:D:920:ILE:HG23	2.03	0.40
2:E:57:HIS:HB3	2:E:58:MET:H	1.48	0.40
1:A:933:MET:HE3	1:A:947:LEU:HD12	2.04	0.40
1:A:966:LYS:HZ3	1:A:966:LYS:HG3	1.69	0.40
1:B:915:LYS:O	1:B:1057:ARG:HD3	2.22	0.40
2:G:60:LYS:HZ2	2:G:60:LYS:HG2	1.58	0.40
2:H:79:LEU:HD23	2:H:113:PHE:CE2	2.56	0.40
1:B:937:VAL:HG12	1:B:938:ARG:HD2	2.03	0.40
2:H:61:ILE:O	2:H:128:GLN:OE1	2.40	0.40
2:H:73:GLN:NE2	2:H:73:GLN:HA	2.35	0.40

There are no symmetry-related clashes.

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	170/188 (90%)	157 (92%)	9 (5%)	4 (2%)	6 22
1	B	161/188 (86%)	148 (92%)	10 (6%)	3 (2%)	8 28
1	C	161/188 (86%)	149 (92%)	10 (6%)	2 (1%)	13 40
1	D	171/188 (91%)	156 (91%)	10 (6%)	5 (3%)	4 18
2	E	72/74 (97%)	66 (92%)	6 (8%)	0	100 100
2	F	71/74 (96%)	67 (94%)	4 (6%)	0	100 100
2	G	72/74 (97%)	67 (93%)	5 (7%)	0	100 100
2	H	71/74 (96%)	67 (94%)	4 (6%)	0	100 100
All	All	949/1048 (91%)	877 (92%)	58 (6%)	14 (2%)	10 34

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	887	GLU
1	A	939	GLY
1	B	939	GLY
1	C	939	GLY
1	D	939	GLY
1	D	885	PHE
1	D	1053	GLY
1	D	895	ASN
1	B	915	LYS
1	D	886	PRO
1	A	1053	GLY
1	A	894	ILE
1	B	894	ILE
1	C	894	ILE

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	146/159 (92%)	108 (74%)	38 (26%)	0 1
1	B	142/159 (89%)	109 (77%)	33 (23%)	1 2
1	C	142/159 (89%)	103 (72%)	39 (28%)	0 1
1	D	148/159 (93%)	106 (72%)	42 (28%)	0 1
2	E	65/65 (100%)	56 (86%)	9 (14%)	3 10
2	F	64/65 (98%)	55 (86%)	9 (14%)	3 10
2	G	65/65 (100%)	56 (86%)	9 (14%)	3 10
2	H	64/65 (98%)	56 (88%)	8 (12%)	4 14
All	All	836/896 (93%)	649 (78%)	187 (22%)	1 2

All (187) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	884	GLU
1	A	885	PHE
1	A	888	GLN
1	A	894	ILE
1	A	895	ASN
1	A	898	MET
1	A	910	ARG
1	A	919	ILE
1	A	928	LEU
1	A	937	VAL
1	A	944	LYS
1	A	949	GLN
1	A	956	LYS
1	A	958	SER
1	A	960	GLU
1	A	967	GLU
1	A	971	GLN
1	A	976	ARG
1	A	978	ARG

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Mol	Chain	Res	Type
1	A	983	GLN
1	A	987	ARG
1	A	1002	LYS
1	A	1004	THR
1	A	1008	ARG
1	A	1010	ASN
1	A	1012	SER
1	A	1014	GLU
1	A	1016	SER
1	A	1022	MET
1	A	1023	LEU
1	A	1029	ASN
1	A	1032	GLN
1	A	1035	LYS
1	A	1036	GLU
1	A	1042	GLU
1	A	1047	LYS
1	A	1049	ARG
1	A	1061	LYS
1	B	885	PHE
1	B	887	GLU
1	B	894	ILE
1	B	898	MET
1	B	910	ARG
1	B	919	ILE
1	B	928	LEU
1	B	937	VAL
1	B	944	LYS
1	B	948	ILE
1	B	949	GLN
1	B	956	LYS
1	B	958	SER
1	B	960	GLU
1	B	967	GLU
1	B	971	GLN
1	B	978	ARG
1	B	983	GLN
1	B	987	ARG
1	B	1002	LYS
1	B	1004	THR
1	B	1008	ARG
1	B	1010	ASN

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Mol	Chain	Res	Type
1	B	1011	ILE
1	B	1012	SER
1	B	1014	GLU
1	B	1016	SER
1	B	1023	LEU
1	B	1029	ASN
1	B	1032	GLN
1	B	1035	LYS
1	B	1036	GLU
1	B	1042	GLU
1	C	885	PHE
1	C	893	VAL
1	C	894	ILE
1	C	898	MET
1	C	910	ARG
1	C	915	LYS
1	C	928	LEU
1	C	937	VAL
1	C	941	SER
1	C	944	LYS
1	C	948	ILE
1	C	949	GLN
1	C	956	LYS
1	C	958	SER
1	C	960	GLU
1	C	966	LYS
1	C	967	GLU
1	C	971	GLN
1	C	976	ARG
1	C	978	ARG
1	C	983	GLN
1	C	987	ARG
1	C	1001	VAL
1	C	1002	LYS
1	C	1004	THR
1	C	1008	ARG
1	C	1010	ASN
1	C	1012	SER
1	C	1014	GLU
1	C	1016	SER
1	C	1023	LEU
1	C	1029	ASN

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Mol	Chain	Res	Type
1	C	1032	GLN
1	C	1035	LYS
1	C	1036	GLU
1	C	1042	GLU
1	C	1046	ILE
1	C	1060	ARG
1	C	1061	LYS
1	D	884	GLU
1	D	885	PHE
1	D	893	VAL
1	D	894	ILE
1	D	895	ASN
1	D	898	MET
1	D	910	ARG
1	D	928	LEU
1	D	937	VAL
1	D	944	LYS
1	D	948	ILE
1	D	956	LYS
1	D	958	SER
1	D	960	GLU
1	D	966	LYS
1	D	967	GLU
1	D	971	GLN
1	D	975	LYS
1	D	976	ARG
1	D	978	ARG
1	D	983	GLN
1	D	987	ARG
1	D	1002	LYS
1	D	1004	THR
1	D	1008	ARG
1	D	1010	ASN
1	D	1012	SER
1	D	1014	GLU
1	D	1015	GLU
1	D	1016	SER
1	D	1023	LEU
1	D	1029	ASN
1	D	1032	GLN
1	D	1035	LYS
1	D	1036	GLU

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Mol	Chain	Res	Type
1	D	1042	GLU
1	D	1046	ILE
1	D	1048	ILE
1	D	1050	THR
1	D	1057	ARG
1	D	1060	ARG
1	D	1061	LYS
2	E	57	HIS
2	E	59	ARG
2	E	62	LEU
2	E	79	LEU
2	E	81	ASP
2	E	98	VAL
2	E	121	ARG
2	E	124	SER
2	E	128	GLN
2	F	59	ARG
2	F	60	LYS
2	F	62	LEU
2	F	79	LEU
2	F	81	ASP
2	F	98	VAL
2	F	121	ARG
2	F	126	GLN
2	F	128	GLN
2	G	59	ARG
2	G	60	LYS
2	G	62	LEU
2	G	79	LEU
2	G	81	ASP
2	G	98	VAL
2	G	121	ARG
2	G	126	GLN
2	G	128	GLN
2	H	59	ARG
2	H	62	LEU
2	H	79	LEU
2	H	81	ASP
2	H	91	LYS
2	H	98	VAL
2	H	121	ARG
2	H	128	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	888	GLN
1	A	895	ASN
1	A	949	GLN
1	A	980	ASN
1	A	983	GLN
1	A	994	GLN
1	A	1018	GLN
1	A	1026	ASN
1	A	1029	ASN
1	B	895	ASN
1	B	949	GLN
1	B	980	ASN
1	B	983	GLN
1	B	994	GLN
1	B	1018	GLN
1	B	1026	ASN
1	B	1029	ASN
1	C	895	ASN
1	C	896	GLN
1	C	906	HIS
1	C	949	GLN
1	C	980	ASN
1	C	983	GLN
1	C	1026	ASN
1	C	1029	ASN
1	D	895	ASN
1	D	949	GLN
1	D	980	ASN
1	D	983	GLN
1	D	994	GLN
1	D	1018	GLN
1	D	1026	ASN
1	D	1029	ASN
2	E	76	HIS
2	E	128	GLN
2	F	76	HIS
2	F	128	GLN
2	G	72	ASN
2	G	76	HIS
2	G	128	GLN
2	H	73	GLN

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Mol	Chain	Res	Type
2	H	76	HIS
2	H	128	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 monosaccharides 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	174/188 (92%)	-0.12	0 100 100	31, 51, 81, 95	0
1	B	167/188 (88%)	0.06	5 (2%) 50 45	34, 54, 86, 104	0
1	C	167/188 (88%)	0.11	6 (3%) 42 37	34, 54, 86, 102	0
1	D	175/188 (93%)	0.04	6 (3%) 45 40	30, 51, 82, 95	0
2	E	74/74 (100%)	-0.03	0 100 100	42, 54, 73, 95	0
2	F	73/74 (98%)	0.09	3 (4%) 37 32	44, 55, 71, 90	0
2	G	74/74 (100%)	0.09	1 (1%) 75 75	43, 55, 74, 95	0
2	H	73/74 (98%)	0.03	4 (5%) 25 21	42, 54, 69, 87	0
All	All	977/1048 (93%)	0.03	25 (2%) 56 52	30, 54, 83, 104	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	1009	THR	4.5
2	F	130	THR	4.3
2	H	130	THR	4.1
2	G	130	THR	3.7
1	C	940	GLY	3.5
1	C	1007	GLY	3.3
1	B	1007	GLY	3.3
1	D	1063	PRO	3.2
1	B	1040	GLU	2.9
1	D	986	GLU	2.8
1	C	939	GLY	2.8
1	B	894	ILE	2.6
1	D	894	ILE	2.5
2	H	86	TYR	2.5
2	H	96	ALA	2.4
1	C	1006	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	1051	ASP	2.3
1	D	1001	VAL	2.2
1	B	940	GLY	2.2
1	B	941	SER	2.1
2	F	109	ALA	2.1
2	H	113	PHE	2.0
1	C	884	GLU	2.0
1	D	1047	LYS	2.0
2	F	90	ASP	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 monosaccharides 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.