Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:19 AM GMT

PDB ID	:	2Q6W
Title	:	The structure of HLA-DRA, DRB3*0101 (DR52a) with bound platelet integrin peptide associated with fetal and neonatal alloimmune thrombocytopenia
Authors	:	Parry, C.S.
Deposited on	:	2007-06-05
Resolution	:	2.25 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 ⓘ symbol.

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

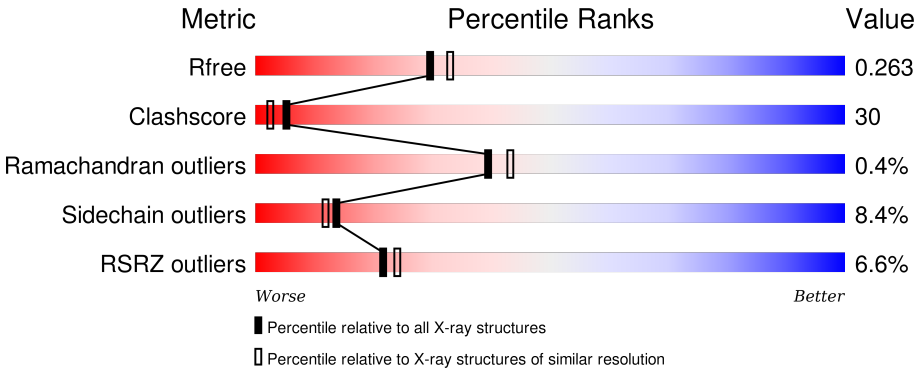
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.25 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	1640 (2.28-2.24)
Clashscore	102246	1095 (2.26-2.26)
Ramachandran outliers	100387	1063 (2.26-2.26)
Sidechain outliers	100360	1063 (2.26-2.26)
RSRZ outliers	91569	1647 (2.28-2.24)

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	182	4% 47% 46% 5%
1	D	182	4% 47% 43% 7%
2	B	190	5% 52% 40% 7%
2	E	190	11% 48% 44% 6%
3	C	12	17% 50% 42% 8%

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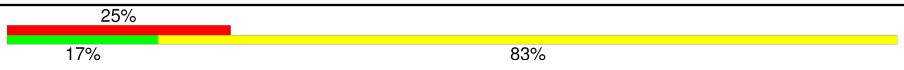
Mol	Chain	Length	Quality of chain
3	F	12	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6530 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 HLA class II histocompatibility antigen, DR alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	180	Total	C	N	O	S	0	0	1
			1442	939	235	263	5			
1	D	180	Total	C	N	O	S	3	0	0
			1462	949	236	272	5			

- Molecule 2 is a protein called HLA class II histocompatibility antigen, DRB3-1 beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	188	Total	C	N	O	S	0	0	0
			1485	943	267	270	5			
2	E	188	Total	C	N	O	S	0	0	0
			1477	934	271	267	5			

- Molecule 3 is a protein called Integrin beta-3.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	11	Total	C	N	O	0	0	0
			85	54	15	16			
3	F	12	Total	C	N	O	2	0	0
			92	57	16	19			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	26	ARG	CYS	ENGINEERED	UNP P05106
F	26	ARG	CYS	ENGINEERED	UNP P05106

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	131	Total	O	0	0
			131	131		

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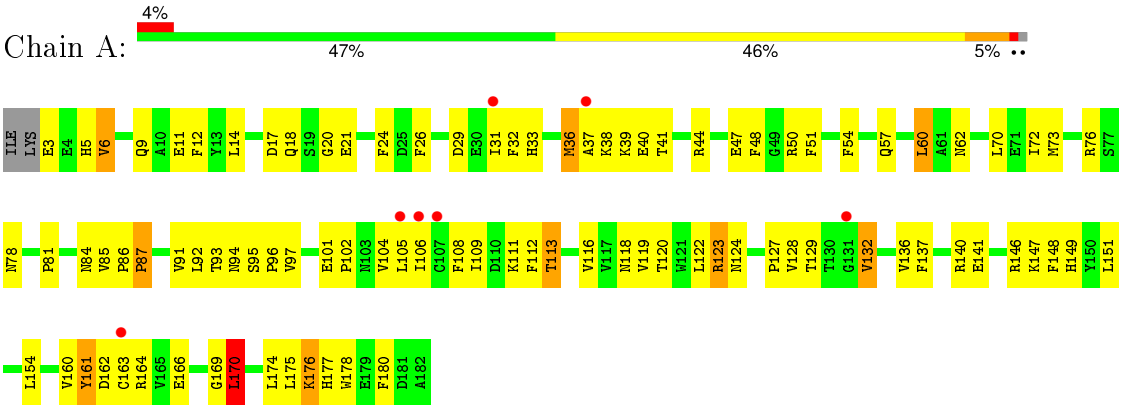
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	124	Total O 124 124	0	0
4	C	4	Total O 4 4	0	0
4	D	122	Total O 122 122	0	0
4	E	99	Total O 99 99	0	0
4	F	7	Total O 7 7	0	0

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.

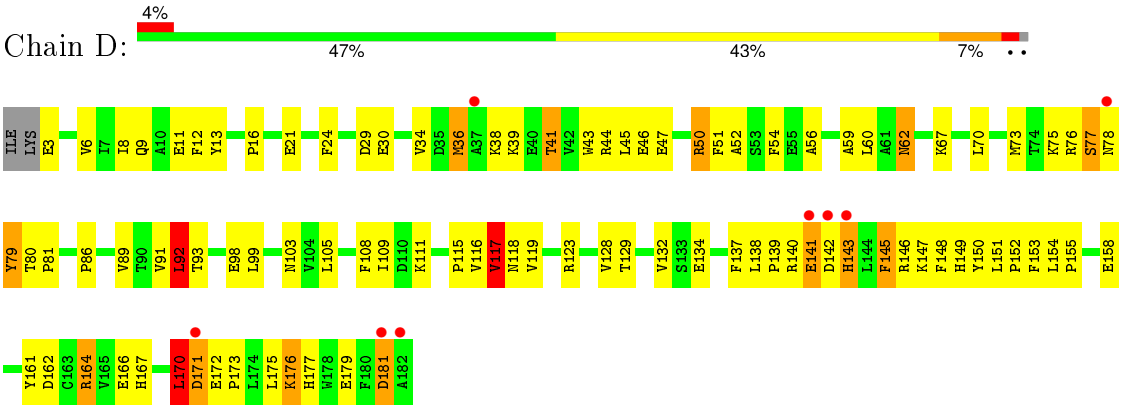
- Molecule 1: HLA class II histocompatibility antigen, DR alpha chain

Chain A:



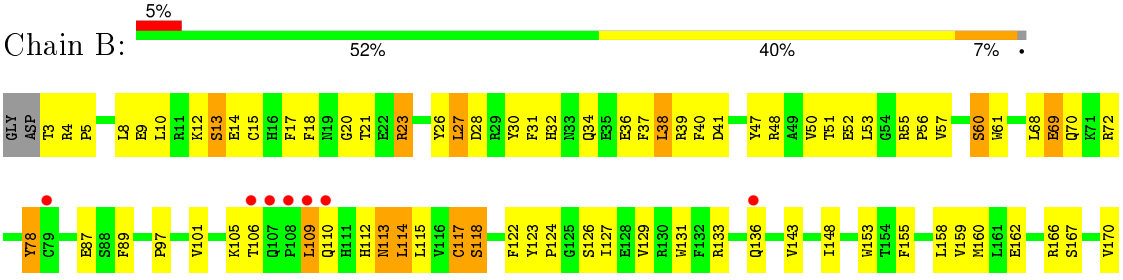
- Molecule 1: HLA class II histocompatibility antigen, DR alpha chain

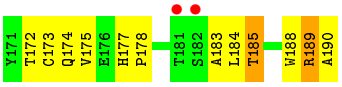
Chain D:



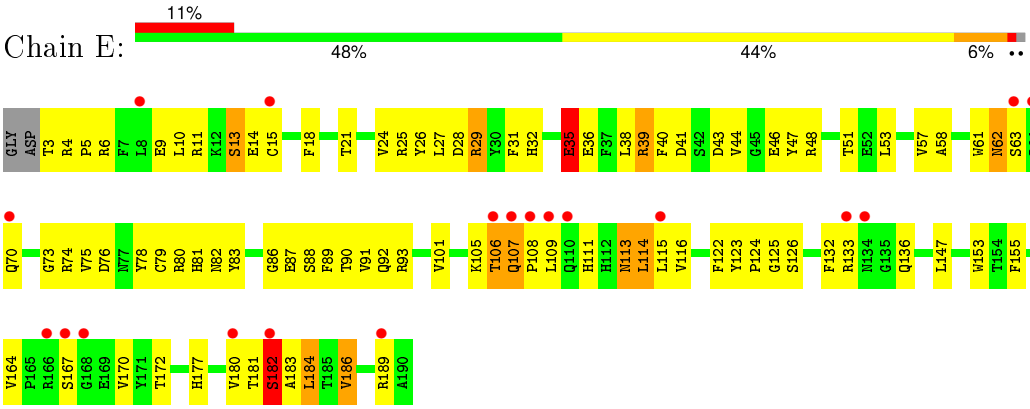
- Molecule 2: HLA class II histocompatibility antigen, DRB3-1 beta chain

Chain B:

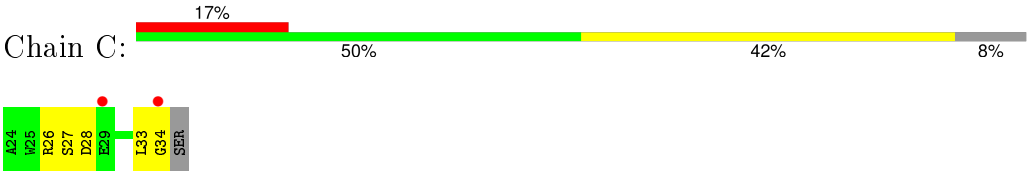




• Molecule 2: HLA class II histocompatibility antigen, DRB3-1 beta chain



• Molecule 3: Integrin beta-3



• Molecule 3: Integrin beta-3

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	92.17Å 92.17Å 248.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.05 – 2.25 20.05 – 2.20	Depositor EDS
% Data completeness (in resolution range)	93.3 (20.05-2.25) 89.7 (20.05-2.20)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.79 (at 2.19Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.210 , 0.265 0.206 , 0.263	Depositor DCC
R_{free} test set	3684 reflections (8.27%)	DCC
Wilson B-factor (Å^2)	44.0	Xtriage
Anisotropy	0.349	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 38.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Outliers	1 of 49533 reflections (0.002%)	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	6530	wwPDB-VP
Average B, all atoms (Å^2)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.09% 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	1.42	4/1485 (0.3%)	1.23	9/2027 (0.4%)
1	D	1.38	3/1506 (0.2%)	1.22	9/2052 (0.4%)
2	B	1.56	9/1523 (0.6%)	1.26	9/2068 (0.4%)
2	E	1.26	2/1517 (0.1%)	1.19	6/2059 (0.3%)
3	C	1.32	0/87	1.29	1/118 (0.8%)
3	F	1.73	1/94 (1.1%)	1.37	2/126 (1.6%)
All	All	1.41	19/6212 (0.3%)	1.23	36/8450 (0.4%)

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

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	35	SER	CA-CB	11.72	1.70	1.52
2	B	78	TYR	CE2-CZ	-7.16	1.29	1.38
1	D	150	TYR	CD2-CE2	-7.13	1.28	1.39
1	A	163	CYS	CB-SG	-7.06	1.70	1.82
2	B	52	GLU	CG-CD	7.01	1.62	1.51
2	B	13	SER	CB-OG	-6.74	1.33	1.42
2	B	87	GLU	CB-CG	-6.52	1.39	1.52
2	B	70	GLN	C-O	6.12	1.34	1.23
2	E	35	GLU	CD-OE1	5.83	1.32	1.25
2	B	143	VAL	CB-CG1	-5.80	1.40	1.52
2	B	69	GLU	CG-CD	5.69	1.60	1.51
1	A	6	VAL	CB-CG2	-5.68	1.41	1.52
1	D	145	PHE	CE2-CZ	5.67	1.48	1.37
2	B	117	CYS	CB-SG	-5.58	1.72	1.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	35	GLU	CB-CG	5.57	1.62	1.52
1	A	161	TYR	CE1-CZ	-5.48	1.31	1.38
1	D	117	VAL	CB-CG1	-5.34	1.41	1.52
1	A	112	PHE	CE2-CZ	5.28	1.47	1.37
2	B	173	CYS	CB-SG	-5.20	1.73	1.81

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	123	ARG	NE-CZ-NH1	10.88	125.74	120.30
1	D	36	MET	CA-CB-CG	-10.40	95.62	113.30
1	D	146	ARG	NE-CZ-NH2	-9.72	115.44	120.30
2	E	93	ARG	NE-CZ-NH1	-8.81	115.89	120.30
3	F	35	SER	N-CA-CB	8.65	123.48	110.50
2	B	69	GLU	CA-C-N	-8.44	98.63	117.20
2	E	126	SER	N-CA-CB	-8.02	98.47	110.50
2	B	20	GLY	CA-C-N	-7.80	100.03	117.20
2	B	158	LEU	CB-CG-CD2	-7.30	98.59	111.00
1	A	44	ARG	NE-CZ-NH1	-7.25	116.67	120.30
2	E	29	ARG	NE-CZ-NH2	-7.24	116.68	120.30
1	A	176	LYS	CD-CE-NZ	-7.01	95.58	111.70
2	B	23	ARG	NE-CZ-NH1	6.70	123.65	120.30
2	E	29	ARG	NE-CZ-NH1	6.39	123.49	120.30
1	D	92	LEU	CA-CB-CG	6.09	129.32	115.30
2	B	173	CYS	CA-CB-SG	-6.08	103.06	114.00
1	A	146	ARG	N-CA-C	-5.91	95.05	111.00
2	E	161	LEU	CB-CG-CD2	-5.68	101.34	111.00
1	D	99	LEU	CB-CG-CD1	-5.62	101.45	111.00
1	A	146	ARG	NE-CZ-NH2	-5.61	117.50	120.30
1	D	50	ARG	CB-CG-CD	-5.44	97.45	111.60
1	A	174	LEU	CA-CB-CG	5.43	127.79	115.30
2	B	118	SER	N-CA-CB	-5.42	102.37	110.50
1	D	170	LEU	CB-CG-CD1	5.39	120.16	111.00
1	A	170	LEU	CA-CB-CG	5.38	127.67	115.30
1	D	154	LEU	CB-CG-CD2	-5.34	101.92	111.00
2	E	69	GLU	CA-C-O	5.20	131.01	120.10
1	A	123	ARG	CD-NE-CZ	5.13	130.78	123.60
1	D	164	ARG	NE-CZ-NH1	-5.11	117.74	120.30
3	F	26	ARG	NE-CZ-NH2	-5.08	117.76	120.30
3	C	26	ARG	NE-CZ-NH2	-5.07	117.76	120.30
2	B	4	ARG	NE-CZ-NH2	-5.06	117.77	120.30
1	A	154	LEU	CB-CG-CD2	-5.05	102.41	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	176	LYS	CB-CG-CD	-5.05	98.47	111.60
2	B	52	GLU	CB-CA-C	5.02	120.45	110.40
2	B	23	ARG	NE-CZ-NH2	-5.01	117.79	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	87	PRO	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	1442	0	1372	89	0
1	D	1462	0	1378	105	0
2	B	1485	0	1386	69	0
2	E	1477	0	1367	115	0
3	C	85	0	79	9	0
3	F	92	0	84	18	0
4	A	131	0	0	19	0
4	B	124	0	0	17	0
4	C	4	0	0	1	0
4	D	122	0	0	20	0
4	E	99	0	0	20	0
4	F	7	0	0	0	0
All	All	6530	0	5666	354	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 30.

All (354) 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:D:92:LEU:CD2	1:D:108:PHE:CE1	1.92	1.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:92:LEU:CD2	1:D:108:PHE:HE1	1.19	1.49
1:D:92:LEU:HD21	1:D:108:PHE:CE1	1.51	1.36
2:E:3:THR:HG21	4:E:279:HOH:O	1.05	1.24
2:B:53:LEU:CB	4:B:304:HOH:O	1.87	1.20
1:D:92:LEU:HD21	1:D:108:PHE:CZ	1.84	1.11
1:D:92:LEU:HD22	1:D:108:PHE:CE1	1.86	1.11
1:D:73:MET:HE3	2:E:53:LEU:HD13	1.14	1.07
1:A:37:ALA:O	1:A:38:LYS:HB3	1.53	1.06
1:D:36:MET:O	4:D:253:HOH:O	1.74	1.04
4:D:303:HOH:O	3:F:25:TRP:CE3	2.10	1.04
1:D:36:MET:C	4:D:253:HOH:O	1.95	1.03
1:D:73:MET:CE	2:E:53:LEU:HD13	1.89	1.03
4:E:280:HOH:O	3:F:25:TRP:CE2	2.17	0.97
4:E:280:HOH:O	3:F:25:TRP:CD2	2.15	0.97
1:D:92:LEU:HD23	1:D:108:PHE:HE1	1.26	0.96
1:D:81:PRO:HB3	2:E:5:PRO:HB2	1.48	0.95
2:E:53:LEU:HB2	4:E:281:HOH:O	1.67	0.92
1:D:86:PRO:HB2	1:D:170:LEU:HD13	1.52	0.92
2:B:68:LEU:O	2:B:72:ARG:HG3	1.68	0.92
2:B:48:ARG:HH11	2:B:48:ARG:HG2	1.35	0.91
1:D:73:MET:HE3	2:E:53:LEU:CD1	1.99	0.91
1:D:46:GLU:CA	1:D:47:GLU:N	2.34	0.90
4:D:303:HOH:O	3:F:25:TRP:HE3	1.46	0.89
2:E:81:HIS:HE1	3:F:24:ALA:O	1.56	0.87
1:A:37:ALA:HB1	4:A:303:HOH:O	1.73	0.87
1:A:166:GLU:CG	4:A:229:HOH:O	2.22	0.87
1:D:47:GLU:N	4:D:294:HOH:O	2.07	0.86
2:E:29:ARG:HD2	2:E:36:GLU:OE2	1.74	0.86
1:D:73:MET:O	1:D:77:SER:HB2	1.75	0.86
1:D:118:ASN:ND2	4:D:295:HOH:O	1.95	0.86
4:D:241:HOH:O	2:E:32:HIS:HE1	1.59	0.85
4:D:303:HOH:O	3:F:25:TRP:HB2	1.76	0.85
2:E:113:ASN:HD22	2:E:114:LEU:H	1.21	0.84
1:D:73:MET:HE1	2:E:53:LEU:HB3	1.60	0.83
1:A:149:HIS:HD2	4:A:262:HOH:O	1.60	0.83
4:A:301:HOH:O	2:B:32:HIS:HE1	1.62	0.83
1:A:37:ALA:O	1:A:38:LYS:CB	2.27	0.82
2:E:26:TYR:OH	3:F:28:ASP:OD2	1.96	0.81
4:D:287:HOH:O	2:E:155:PHE:CE1	2.34	0.78
1:A:149:HIS:CD2	4:A:262:HOH:O	2.35	0.77
2:E:164:VAL:HB	4:E:236:HOH:O	1.85	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:139:PRO:HB3	4:D:273:HOH:O	1.86	0.76
2:B:3:THR:N	4:B:295:HOH:O	2.20	0.74
1:D:98:GLU:O	1:D:155:PRO:HG2	1.88	0.74
2:E:167:SER:CA	4:E:259:HOH:O	2.37	0.73
2:E:101:VAL:HG23	2:E:186:VAL:HG22	1.72	0.71
1:A:92:LEU:HB2	1:A:108:PHE:HE1	1.54	0.71
2:E:73:GLY:HA3	4:E:282:HOH:O	1.89	0.70
2:B:36:GLU:O	2:B:50:VAL:HG22	1.91	0.70
1:D:46:GLU:CA	4:D:294:HOH:O	2.39	0.70
1:D:147:LYS:HE3	1:D:149:HIS:HE1	1.55	0.70
2:E:101:VAL:CG2	2:E:186:VAL:HG22	2.22	0.69
4:B:308:HOH:O	1:D:176:LYS:HG2	1.93	0.69
2:E:109:LEU:HD12	2:E:109:LEU:H	1.58	0.69
1:D:86:PRO:CB	1:D:170:LEU:HD13	2.23	0.69
1:A:3:GLU:OE2	1:A:6:VAL:CG2	2.41	0.69
2:E:47:TYR:H	2:E:62:ASN:HD21	1.42	0.68
2:E:43:ASP:OD2	4:E:267:HOH:O	2.11	0.68
2:E:9:GLU:OE1	2:E:32:HIS:HD2	1.77	0.68
2:B:10:LEU:HD21	2:B:12:LYS:HE3	1.76	0.68
2:E:107:GLN:HE21	2:E:107:GLN:N	1.90	0.68
1:D:147:LYS:HE3	1:D:149:HIS:CE1	2.29	0.68
1:A:141:GLU:CB	4:A:269:HOH:O	2.41	0.68
2:E:3:THR:HA	4:E:264:HOH:O	1.94	0.67
2:B:48:ARG:NH1	2:B:48:ARG:HG2	2.08	0.67
1:A:92:LEU:HB2	1:A:108:PHE:CE1	2.30	0.66
2:E:109:LEU:O	4:E:261:HOH:O	2.13	0.66
2:E:3:THR:CG2	2:E:6:ARG:HH12	2.09	0.65
1:D:76:ARG:HD3	4:E:277:HOH:O	1.96	0.65
2:B:113:ASN:HD22	2:B:114:LEU:H	1.44	0.65
1:D:81:PRO:HB3	2:E:5:PRO:CB	2.26	0.65
2:E:57:VAL:HG11	3:F:33:LEU:HD22	1.79	0.64
1:A:86:PRO:HB2	1:A:170:LEU:HD13	1.80	0.64
1:A:70:LEU:HB2	2:B:9:GLU:HB2	1.79	0.64
1:D:50:ARG:CG	1:D:50:ARG:HH11	2.09	0.63
1:A:96:PRO:HG3	2:B:118:SER:OG	1.99	0.62
2:E:3:THR:CG2	4:E:279:HOH:O	1.87	0.62
2:B:109:LEU:O	2:B:110:GLN:HB2	1.99	0.62
2:E:113:ASN:ND2	2:E:114:LEU:H	1.94	0.62
1:D:129:THR:O	1:D:132:VAL:HG22	2.00	0.62
1:A:21:GLU:OE1	4:A:283:HOH:O	2.16	0.62
2:E:18:PHE:HB3	4:E:248:HOH:O	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:111:HIS:HB2	4:E:289:HOH:O	2.01	0.61
1:A:36:MET:HE3	1:A:60:LEU:HD23	1.83	0.60
1:D:123:ARG:HG3	1:D:161:TYR:CE2	2.36	0.60
1:D:43:TRP:HH2	4:D:303:HOH:O	1.83	0.60
2:B:174:GLN:HG3	2:B:183:ALA:HB1	1.84	0.59
1:A:109:ILE:HD11	1:A:119:VAL:HG21	1.84	0.59
2:E:74:ARG:NH2	4:E:256:HOH:O	2.34	0.59
1:D:91:VAL:HG23	1:D:176:LYS:HB3	1.84	0.59
2:B:160:MET:HE2	4:B:258:HOH:O	2.03	0.59
1:A:51:PHE:CB	4:A:310:HOH:O	2.50	0.59
1:D:73:MET:CE	2:E:53:LEU:HB3	2.33	0.58
1:A:109:ILE:CD1	1:A:119:VAL:HG21	2.33	0.58
2:E:184:LEU:H	2:E:184:LEU:HD22	1.69	0.58
2:E:101:VAL:HA	2:E:116:VAL:O	2.04	0.58
2:B:57:VAL:HG11	3:C:33:LEU:HD23	1.85	0.58
2:B:68:LEU:O	2:B:72:ARG:CG	2.46	0.58
1:A:51:PHE:CB	4:A:313:HOH:O	2.52	0.58
2:B:133:ARG:NH2	4:B:267:HOH:O	2.36	0.57
1:D:54:PHE:CZ	3:F:27:SER:HB3	2.40	0.57
2:E:28:ASP:O	2:E:39:ARG:HA	2.04	0.57
1:D:141:GLU:OE1	2:E:29:ARG:NH2	2.36	0.57
1:A:37:ALA:CA	4:A:303:HOH:O	2.53	0.57
1:A:37:ALA:CB	4:A:308:HOH:O	2.53	0.57
1:D:176:LYS:HD3	4:D:296:HOH:O	2.05	0.56
2:E:123:TYR:O	2:E:177:HIS:HE1	1.89	0.56
2:E:3:THR:HG22	2:E:6:ARG:HH12	1.69	0.56
2:B:117:CYS:HB2	2:B:131:TRP:CZ2	2.41	0.56
1:A:37:ALA:HB3	4:A:308:HOH:O	2.05	0.56
1:D:176:LYS:CE	4:D:296:HOH:O	2.54	0.56
1:A:111:LYS:HG2	1:A:140:ARG:CZ	2.35	0.56
1:A:57:GLN:HA	1:A:60:LEU:HD12	1.87	0.55
2:B:188:TRP:CH2	2:B:190:ALA:HA	2.41	0.55
2:B:167:SER:HB3	4:B:270:HOH:O	2.06	0.55
2:E:133:ARG:O	2:E:170:VAL:O	2.24	0.55
1:D:128:VAL:HG11	1:D:151:LEU:HD11	1.88	0.55
1:D:13:TYR:CE2	1:D:67:LYS:HG3	2.42	0.55
2:B:101:VAL:HG11	2:B:188:TRP:HB2	1.88	0.54
1:D:118:ASN:HB3	4:D:298:HOH:O	2.07	0.54
1:D:115:PRO:HD3	1:D:145:PHE:CE2	2.43	0.54
1:A:93:THR:HG21	1:A:97:VAL:CG2	2.38	0.54
2:E:69:GLU:HA	4:E:225:HOH:O	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:81:HIS:CE1	3:F:24:ALA:O	2.48	0.54
2:E:47:TYR:N	2:E:62:ASN:HD21	2.04	0.54
2:E:31:PHE:HA	2:E:35:GLU:O	2.08	0.54
2:B:113:ASN:ND2	2:B:114:LEU:H	2.06	0.54
2:E:108:PRO:HD2	4:E:289:HOH:O	2.07	0.54
2:B:9:GLU:OE1	2:B:32:HIS:HD2	1.91	0.53
1:D:93:THR:HG22	1:D:105:LEU:HD23	1.90	0.53
1:D:3:GLU:HB3	2:E:18:PHE:CE2	2.43	0.53
1:D:16:PRO:HD2	2:E:6:ARG:NE	2.24	0.53
2:B:50:VAL:O	2:E:51:THR:HG22	2.09	0.53
2:E:122:PHE:HE2	2:E:125:GLY:O	1.91	0.53
1:A:128:VAL:HG12	1:A:151:LEU:HD11	1.90	0.53
1:D:77:SER:HB3	4:D:241:HOH:O	2.08	0.52
1:D:79:TYR:CD1	1:D:79:TYR:N	2.77	0.52
1:A:160:VAL:HB	1:A:177:HIS:CE1	2.45	0.52
2:B:185:THR:HG23	4:B:239:HOH:O	2.09	0.52
2:B:27:LEU:HD12	2:B:41:ASP:HA	1.89	0.52
1:D:111:LYS:HG2	1:D:140:ARG:CZ	2.39	0.52
2:B:30:TYR:HB2	2:B:38:LEU:HB3	1.92	0.52
2:B:38:LEU:HD11	2:B:61:TRP:CZ3	2.44	0.52
1:D:3:GLU:HA	2:E:18:PHE:CD2	2.45	0.52
2:E:123:TYR:CD1	2:E:124:PRO:HA	2.45	0.52
1:D:50:ARG:HG2	1:D:50:ARG:HH11	1.73	0.52
2:E:75:VAL:CG1	2:E:80:ARG:NH1	2.73	0.52
2:E:109:LEU:N	2:E:109:LEU:HD12	2.24	0.51
1:D:117:VAL:HG22	1:D:137:PHE:HE2	1.75	0.51
2:E:9:GLU:OE1	2:E:32:HIS:CD2	2.61	0.51
1:A:180:PHE:HE1	4:A:306:HOH:O	1.93	0.51
1:A:118:ASN:HB2	1:A:166:GLU:HB2	1.93	0.51
1:A:147:LYS:HE2	1:A:149:HIS:HE1	1.75	0.51
1:A:123:ARG:O	1:A:124:ASN:C	2.46	0.51
2:B:38:LEU:CD1	2:B:61:TRP:CZ3	2.94	0.50
2:E:41:ASP:HB3	2:E:44:VAL:HB	1.93	0.50
2:E:113:ASN:HD22	2:E:114:LEU:N	2.00	0.50
1:D:50:ARG:HD2	4:D:233:HOH:O	2.11	0.50
2:E:189:ARG:HG3	4:E:255:HOH:O	2.11	0.50
2:E:90:THR:OG1	2:E:91:VAL:N	2.43	0.50
1:A:122:LEU:HD23	1:A:127:PRO:HA	1.93	0.50
1:A:140:ARG:NH2	4:A:311:HOH:O	2.45	0.50
2:B:34:GLN:NE2	4:B:227:HOH:O	2.40	0.50
1:D:103:ASN:O	1:D:152:PRO:HA	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:34:GLY:HA3	4:C:315:HOH:O	2.12	0.50
2:B:57:VAL:HG11	3:C:33:LEU:CD2	2.42	0.50
2:B:28:ASP:O	2:B:39:ARG:HA	2.11	0.50
2:E:105:LYS:H	2:E:113:ASN:HD21	1.60	0.49
2:E:39:ARG:HD2	4:E:260:HOH:O	2.11	0.49
2:B:162:GLU:OE2	1:D:177:HIS:ND1	2.45	0.49
2:E:132:PHE:HA	2:E:136:GLN:O	2.13	0.49
1:A:94:ASN:CB	4:B:247:HOH:O	2.60	0.49
1:A:91:VAL:HG11	1:A:178:TRP:HB2	1.93	0.49
4:B:308:HOH:O	1:D:176:LYS:CG	2.55	0.49
2:B:166:ARG:HD3	4:B:293:HOH:O	2.13	0.49
1:D:12:PHE:HA	2:E:9:GLU:O	2.13	0.49
2:E:14:GLU:HB2	2:E:27:LEU:HB2	1.94	0.49
2:E:109:LEU:H	2:E:109:LEU:CD1	2.24	0.49
2:B:18:PHE:HB3	2:B:23:ARG:HH11	1.77	0.49
2:E:132:PHE:HB2	2:E:172:THR:HB	1.95	0.48
1:D:62:ASN:HD21	3:F:29:GLU:HA	1.77	0.48
2:E:76:ASP:HA	2:E:80:ARG:HB2	1.95	0.48
1:D:11:GLU:HA	1:D:21:GLU:O	2.13	0.48
1:D:8:ILE:O	1:D:24:PHE:HA	2.13	0.48
1:D:143:HIS:N	1:D:143:HIS:CD2	2.80	0.48
2:E:107:GLN:CA	2:E:107:GLN:HE21	2.27	0.48
1:D:132:VAL:HG12	1:D:151:LEU:HD13	1.95	0.48
1:A:78:ASN:ND2	4:A:304:HOH:O	2.39	0.48
1:A:24:PHE:HB3	1:A:31:ILE:HD12	1.95	0.48
1:A:40:GLU:HG2	1:A:41:THR:O	2.14	0.48
2:E:147:LEU:HG	2:E:155:PHE:CD2	2.49	0.48
2:E:83:TYR:O	2:E:87:GLU:HB2	2.14	0.47
2:E:115:LEU:O	2:E:160:MET:HA	2.14	0.47
2:E:74:ARG:O	2:E:75:VAL:C	2.51	0.47
2:B:148:ILE:O	2:B:155:PHE:HA	2.14	0.47
1:A:38:LYS:NZ	1:A:40:GLU:CD	2.67	0.47
2:B:172:THR:HG21	4:B:225:HOH:O	2.14	0.47
2:E:3:THR:HG22	2:E:4:ARG:N	2.29	0.47
2:E:62:ASN:HD22	2:E:68:LEU:HD21	1.79	0.47
1:D:62:ASN:ND2	3:F:30:ALA:H	2.12	0.47
1:A:93:THR:HA	1:A:104:VAL:O	2.15	0.47
1:D:50:ARG:CG	1:D:50:ARG:NH1	2.74	0.47
1:A:24:PHE:CD1	1:A:32:PHE:CZ	3.02	0.47
1:A:48:PHE:CD1	2:B:89:PHE:CD1	3.02	0.47
2:E:78:TYR:CZ	3:F:28:ASP:HB2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:26:TYR:O	2:E:27:LEU:HD12	2.16	0.46
1:A:106:ILE:HB	1:A:108:PHE:CE1	2.51	0.46
2:E:88:SER:HA	2:E:92:GLN:NE2	2.30	0.46
1:A:37:ALA:C	4:A:303:HOH:O	2.52	0.46
1:D:108:PHE:N	1:D:108:PHE:CD1	2.84	0.46
1:D:105:LEU:HD23	1:D:105:LEU:HA	1.73	0.46
1:D:11:GLU:HG3	2:E:11:ARG:HB3	1.98	0.46
1:D:138:LEU:HD12	1:D:148:PHE:HE1	1.80	0.46
1:A:11:GLU:HA	1:A:21:GLU:O	2.16	0.46
2:B:57:VAL:HG13	3:C:34:GLY:H	1.81	0.46
2:B:56:PRO:O	2:B:60:SER:OG	2.32	0.46
2:E:10:LEU:HB3	2:E:31:PHE:HB2	1.96	0.46
2:E:29:ARG:CD	2:E:36:GLU:OE2	2.57	0.46
1:A:6:VAL:HA	2:B:15:CYS:O	2.16	0.46
1:D:21:GLU:OE2	1:D:137:PHE:O	2.34	0.46
1:A:37:ALA:CB	4:A:303:HOH:O	2.44	0.46
2:B:48:ARG:NH1	2:B:48:ARG:CG	2.71	0.46
2:E:107:GLN:CA	2:E:107:GLN:NE2	2.79	0.46
2:E:31:PHE:CE2	2:E:36:GLU:HB2	2.51	0.45
1:D:41:THR:HG22	1:D:56:ALA:HB2	1.98	0.45
1:D:9:GLN:NE2	1:D:11:GLU:OE2	2.42	0.45
2:E:61:TRP:CH2	3:F:33:LEU:HD23	2.52	0.45
2:B:109:LEU:O	2:B:110:GLN:CB	2.65	0.45
1:D:92:LEU:HD22	1:D:108:PHE:CD1	2.45	0.45
1:A:140:ARG:O	2:B:12:LYS:NZ	2.50	0.45
1:A:5:HIS:HD2	4:B:191:HOH:O	2.00	0.45
1:D:38:LYS:N	4:D:253:HOH:O	2.50	0.45
1:D:103:ASN:HB3	1:D:153:PHE:CE1	2.51	0.45
2:B:31:PHE:CE2	2:B:36:GLU:HB2	2.52	0.45
2:E:24:VAL:HG11	2:E:79:CYS:HB3	1.98	0.45
2:E:44:VAL:HG12	2:E:46:GLU:H	1.82	0.45
2:B:112:HIS:HB2	4:B:311:HOH:O	2.16	0.45
2:E:13:SER:HA	2:E:27:LEU:O	2.17	0.45
1:A:26:PHE:HB2	1:A:31:ILE:HD11	1.99	0.45
1:A:14:LEU:CD2	1:A:116:VAL:CG2	2.94	0.45
1:A:162:ASP:HB3	1:A:175:LEU:HD22	1.99	0.45
1:A:12:PHE:CE2	1:A:21:GLU:HB3	2.52	0.44
1:D:41:THR:HG21	1:D:54:PHE:HB3	1.99	0.44
1:D:105:LEU:HG	1:D:153:PHE:CE1	2.52	0.44
1:A:33:HIS:CG	1:A:136:VAL:HG11	2.52	0.44
1:A:12:PHE:HB2	2:B:8:LEU:HD11	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:76:ARG:HH22	3:C:34:GLY:C	2.20	0.44
1:A:81:PRO:HB3	2:B:5:PRO:CB	2.47	0.44
1:D:123:ARG:HB2	1:D:128:VAL:HG21	2.00	0.44
2:E:123:TYR:CG	2:E:124:PRO:HA	2.52	0.44
2:E:46:GLU:OE2	2:E:48:ARG:NE	2.33	0.44
1:D:134:GLU:HA	1:D:148:PHE:O	2.18	0.44
1:A:47:GLU:HA	1:A:50:ARG:HD2	1.99	0.44
2:E:86:GLY:HA2	2:E:89:PHE:CE2	2.52	0.44
1:D:77:SER:O	1:D:78:ASN:HB2	2.18	0.44
2:E:115:LEU:HD22	2:E:163:THR:HG21	2.00	0.44
2:E:116:VAL:HG22	2:E:160:MET:HG2	2.00	0.44
1:A:164:ARG:HB2	1:A:175:LEU:CD2	2.47	0.44
1:D:70:LEU:HB2	2:E:9:GLU:HB2	1.98	0.44
1:D:167:HIS:HB3	1:D:170:LEU:HD22	1.99	0.44
2:B:55:ARG:O	2:B:56:PRO:C	2.55	0.44
1:D:172:GLU:HB2	1:D:173:PRO:HD2	2.00	0.44
1:D:171:ASP:OD1	1:D:171:ASP:N	2.39	0.44
2:B:36:GLU:O	2:B:51:THR:HG23	2.18	0.44
1:D:30:GLU:O	1:D:44:ARG:CB	2.66	0.44
1:D:118:ASN:HB2	1:D:166:GLU:HB2	2.00	0.44
2:B:136:GLN:CG	4:B:267:HOH:O	2.66	0.44
1:D:54:PHE:HZ	3:F:27:SER:HB3	1.80	0.44
1:A:129:THR:O	1:A:132:VAL:HB	2.18	0.43
1:D:91:VAL:H	1:D:176:LYS:NZ	2.16	0.43
1:D:54:PHE:CE1	3:F:27:SER:HB3	2.54	0.43
2:B:101:VAL:CG1	2:B:188:TRP:HB2	2.48	0.43
1:A:9:GLN:O	2:B:12:LYS:HA	2.18	0.43
1:A:72:ILE:HG22	1:A:76:ARG:HD2	2.01	0.43
2:B:78:TYR:CZ	3:C:28:ASP:HB2	2.53	0.43
2:E:39:ARG:HG3	2:E:39:ARG:O	2.18	0.43
1:D:176:LYS:NZ	4:D:296:HOH:O	2.51	0.43
1:D:117:VAL:HG22	1:D:137:PHE:CE2	2.52	0.43
1:A:175:LEU:O	4:A:263:HOH:O	2.22	0.43
1:D:142:ASP:CG	4:D:224:HOH:O	2.56	0.43
2:B:27:LEU:HA	2:B:40:PHE:O	2.18	0.43
2:E:147:LEU:HD12	2:E:147:LEU:HA	1.86	0.43
2:B:26:TYR:OH	3:C:28:ASP:OD2	2.23	0.43
2:E:182:SER:HB2	2:E:183:ALA:H	1.60	0.43
1:D:75:LYS:HG2	1:D:79:TYR:OH	2.18	0.43
1:D:6:VAL:HA	2:E:15:CYS:O	2.19	0.43
1:D:34:VAL:HG21	1:D:59:ALA:HB2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:48:ARG:HH11	2:E:48:ARG:HG3	1.83	0.42
1:A:101:GLU:HA	1:A:102:PRO:HD3	1.92	0.42
2:B:127:ILE:HD11	2:B:175:VAL:HG13	2.01	0.42
1:A:21:GLU:OE2	1:A:137:PHE:O	2.36	0.42
1:A:17:ASP:O	1:A:18:GLN:HB2	2.20	0.42
1:A:12:PHE:O	1:A:20:GLY:HA2	2.20	0.42
1:A:76:ARG:HD3	1:A:76:ARG:HH11	1.65	0.42
1:A:92:LEU:HA	1:A:92:LEU:HD23	1.84	0.42
1:D:76:ARG:HB3	2:E:53:LEU:CD2	2.49	0.42
1:D:162:ASP:HA	1:D:176:LYS:O	2.19	0.42
1:A:86:PRO:HB3	1:A:169:GLY:C	2.39	0.42
2:B:123:TYR:CD1	2:B:124:PRO:HA	2.55	0.42
1:A:38:LYS:O	1:A:39:LYS:C	2.58	0.42
1:A:3:GLU:OE2	1:A:6:VAL:HG21	2.15	0.42
2:B:40:PHE:HB2	2:B:47:TYR:CE2	2.54	0.42
1:A:176:LYS:HA	1:A:176:LYS:HD2	1.76	0.42
1:A:3:GLU:OE2	1:A:6:VAL:HG23	2.18	0.42
2:E:57:VAL:HG11	3:F:33:LEU:CD2	2.46	0.42
1:D:116:VAL:O	1:D:167:HIS:HD2	2.03	0.42
1:A:85:VAL:HB	1:A:113:THR:HG22	2.02	0.42
1:A:29:ASP:HB3	2:B:153:TRP:CE2	2.54	0.42
2:E:24:VAL:HG21	2:E:80:ARG:HG3	2.02	0.42
1:A:105:LEU:HB2	1:A:151:LEU:HB3	2.02	0.42
1:D:67:LYS:O	1:D:70:LEU:HB3	2.19	0.42
1:A:38:LYS:HZ1	1:A:40:GLU:CD	2.22	0.42
1:A:122:LEU:O	1:A:161:TYR:HA	2.20	0.42
1:D:29:ASP:HB3	2:E:153:TRP:CE2	2.55	0.42
1:D:109:ILE:CD1	1:D:119:VAL:HG21	2.50	0.42
2:E:68:LEU:C	2:E:70:GLN:N	2.73	0.41
2:E:115:LEU:HD12	2:E:115:LEU:HA	1.82	0.41
2:E:61:TRP:CZ2	3:F:31:LEU:HB2	2.55	0.41
1:A:73:MET:SD	3:C:33:LEU:HD13	2.60	0.41
2:E:106:THR:C	2:E:107:GLN:HE21	2.23	0.41
2:B:37:PHE:CD1	2:B:38:LEU:HB2	2.55	0.41
2:E:83:TYR:CZ	2:E:91:VAL:HG21	2.55	0.41
2:B:177:HIS:CD2	2:B:178:PRO:HD2	2.55	0.41
1:A:38:LYS:N	4:A:303:HOH:O	2.54	0.41
2:B:15:CYS:HB3	2:B:17:PHE:CZ	2.56	0.41
1:A:128:VAL:CG1	1:A:151:LEU:HD11	2.50	0.41
2:E:86:GLY:HA2	2:E:89:PHE:CZ	2.55	0.41
2:B:170:VAL:HG22	2:B:189:ARG:HG2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:97:PRO:HA	2:B:122:PHE:HB3	2.03	0.41
2:B:106:THR:HA	4:B:286:HOH:O	2.19	0.41
1:A:94:ASN:HB2	4:B:247:HOH:O	2.21	0.41
1:D:164:ARG:HB2	1:D:175:LEU:CD2	2.50	0.41
2:E:27:LEU:HA	2:E:40:PHE:O	2.21	0.41
1:A:108:PHE:CD2	1:A:148:PHE:HE2	2.39	0.41
2:E:24:VAL:HB	2:E:75:VAL:HG13	2.03	0.41
1:D:45:LEU:HD11	2:E:153:TRP:HB2	2.02	0.41
1:D:51:PHE:O	1:D:52:ALA:HB2	2.21	0.41
2:B:129:VAL:HB	2:B:159:VAL:HG21	2.03	0.41
1:A:177:HIS:CD2	2:E:114:LEU:HD21	2.56	0.41
1:A:87:PRO:HB3	1:A:109:ILE:HG22	2.03	0.41
1:A:84:ASN:HB3	1:A:169:GLY:CA	2.51	0.40
2:E:24:VAL:HG11	2:E:79:CYS:CB	2.51	0.40
1:A:54:PHE:CE1	3:C:27:SER:HB2	2.57	0.40
2:E:3:THR:HG22	2:E:6:ARG:NH1	2.35	0.40
2:E:82:ASN:HA	4:E:280:HOH:O	2.21	0.40
1:D:147:LYS:CE	1:D:149:HIS:HE1	2.29	0.40
2:B:115:LEU:O	2:B:160:MET:HA	2.21	0.40
2:B:14:GLU:HB2	2:B:27:LEU:HB2	2.04	0.40
1:D:89:VAL:HA	1:D:108:PHE:O	2.21	0.40
1:A:91:VAL:CG1	1:A:178:TRP:HB2	2.51	0.40
2:E:68:LEU:C	2:E:70:GLN:H	2.24	0.40
1:D:164:ARG:HD2	1:D:175:LEU:HD21	2.03	0.40
1:D:179:GLU:OE2	1:D:181:ASP:OD1	2.40	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	177/182 (97%)	170 (96%)	7 (4%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	D	176/182 (97%)	169 (96%)	7 (4%)	0	100 100
2	B	186/190 (98%)	175 (94%)	11 (6%)	0	100 100
2	E	186/190 (98%)	169 (91%)	14 (8%)	3 (2%)	12 7
3	C	9/12 (75%)	9 (100%)	0	0	100 100
3	F	10/12 (83%)	10 (100%)	0	0	100 100
All	All	744/768 (97%)	702 (94%)	39 (5%)	3 (0%)	39 43

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	182	SER
2	E	58	ALA
2	E	62	ASN

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	154/166 (93%)	146 (95%)	8 (5%)	29 31
1	D	158/166 (95%)	143 (90%)	15 (10%)	11 8
2	B	152/170 (89%)	138 (91%)	14 (9%)	11 9
2	E	151/170 (89%)	135 (89%)	16 (11%)	8 6
3	C	8/9 (89%)	8 (100%)	0	100 100
3	F	9/9 (100%)	9 (100%)	0	100 100
All	All	632/690 (92%)	579 (92%)	53 (8%)	14 12

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	MET
1	A	60	LEU
1	A	62	ASN

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Mol	Chain	Res	Type
1	A	95	SER
1	A	113	THR
1	A	120	THR
1	A	132	VAL
1	A	170	LEU
2	B	13	SER
2	B	21	THR
2	B	27	LEU
2	B	38	LEU
2	B	60	SER
2	B	69	GLU
2	B	105	LYS
2	B	109	LEU
2	B	113	ASN
2	B	114	LEU
2	B	126	SER
2	B	184	LEU
2	B	185	THR
2	B	189	ARG
1	D	39	LYS
1	D	41	THR
1	D	60	LEU
1	D	62	ASN
1	D	77	SER
1	D	79	TYR
1	D	80	THR
1	D	92	LEU
1	D	117	VAL
1	D	141	GLU
1	D	143	HIS
1	D	158	GLU
1	D	170	LEU
1	D	171	ASP
1	D	181	ASP
2	E	13	SER
2	E	21	THR
2	E	25	ARG
2	E	35	GLU
2	E	38	LEU
2	E	39	ARG
2	E	63	SER
2	E	106	THR

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Mol	Chain	Res	Type
2	E	107	GLN
2	E	113	ASN
2	E	114	LEU
2	E	180	VAL
2	E	181	THR
2	E	182	SER
2	E	184	LEU
2	E	186	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	62	ASN
1	A	149	HIS
2	B	32	HIS
2	B	64	GLN
2	B	70	GLN
2	B	113	ASN
2	B	156	GLN
1	D	15	ASN
1	D	62	ASN
1	D	149	HIS
2	E	32	HIS
2	E	62	ASN
2	E	81	HIS
2	E	92	GLN
2	E	107	GLN
2	E	113	ASN
2	E	150	ASN
2	E	156	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	180/182 (98%)	0.07	7 (3%) 43 47	25, 39, 54, 63	0
1	D	180/182 (98%)	0.23	8 (4%) 38 41	25, 42, 62, 71	1 (0%)
2	B	188/190 (98%)	0.17	9 (4%) 34 38	23, 37, 59, 69	0
2	E	188/190 (98%)	0.42	21 (11%) 7 7	28, 47, 75, 81	0
3	C	11/12 (91%)	0.10	2 (18%) 2 1	39, 40, 60, 69	0
3	F	12/12 (100%)	1.40	3 (25%) 1 1	45, 54, 81, 86	1 (8%)
All	All	759/768 (98%)	0.24	50 (6%) 22 24	23, 41, 66, 86	2 (0%)

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	F	35	SER	7.6
1	D	37	ALA	7.1
2	E	110	GLN	5.5
3	F	34	GLY	4.8
2	E	109	LEU	4.6
2	B	109	LEU	4.0
2	B	106	THR	3.9
1	A	37	ALA	3.8
1	D	182	ALA	3.5
2	E	189	ARG	3.4
2	B	108	PRO	3.4
2	E	182	SER	3.0
1	D	171	ASP	3.0
2	E	64	GLN	2.9
1	A	131	GLY	2.9
1	D	142	ASP	2.9
2	E	70	GLN	2.9
2	B	181	THR	2.8
2	E	69	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
3	C	34	GLY	2.8
1	A	107	CYS	2.7
2	B	110	GLN	2.7
2	E	166	ARG	2.6
1	A	105	LEU	2.6
2	E	133	ARG	2.5
2	E	180	VAL	2.5
2	E	106	THR	2.5
1	A	31	ILE	2.5
2	E	168	GLY	2.4
1	D	78	ASN	2.3
1	D	181	ASP	2.3
2	E	8	LEU	2.3
2	E	134	ASN	2.3
2	E	167	SER	2.3
2	E	108	PRO	2.3
2	E	107	GLN	2.2
1	A	163	CYS	2.2
2	E	15	CYS	2.2
1	D	143	HIS	2.2
3	C	29	GLU	2.2
2	B	79	CYS	2.2
1	D	141	GLU	2.1
2	B	182	SER	2.1
2	E	115	LEU	2.1
2	B	136	GLN	2.1
1	A	106	ILE	2.1
2	E	67	LEU	2.1
3	F	29	GLU	2.1
2	E	63	SER	2.1
2	B	107	GLN	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

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.