Full wwPDB X-ray Structure Validation Report (i)

Aug 27, 2023 – 01:25 AM EDT

PDB ID	:	3EYO
Title	:	Crystal structure of anti-human cytomegalovirus antibody 8F9
Authors	:	Thomson, C.A.; Bryson, S.; McLean, G.R.; Creagh, A.L.; Pai, E.F.; Schrader, J.W.
Deposited on	:	2008-10-21
Resolution	:	2.50 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 (i) 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 (1)) were used in the production of this report:

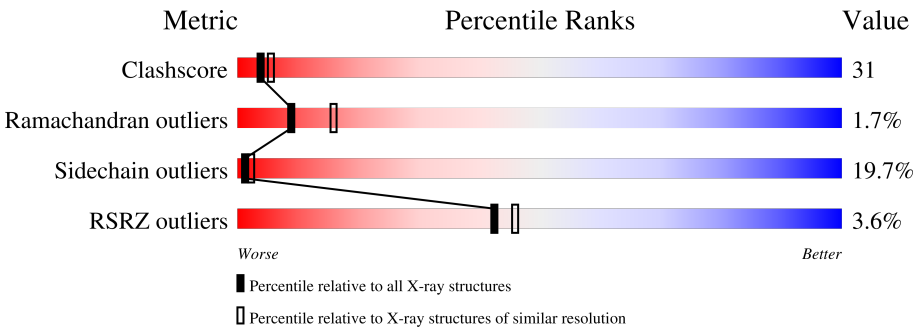
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 2.50 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))
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	216	4%, 56%, 30%, 10%, • •
1	C	216	2%, 55%, 37%, 7%, •
2	B	242	4%, 45%, 33%, 7%, •, 12%
2	D	242	3%, 46%, 32%, 12%, 10%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 6906 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 8f9 Fab.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	213	1643	1034	281	323	5	0	0	0
1	C	214	1652	1039	282	326	5	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	expression tag	PDB 3EYO
C	0	MET	-	expression tag	PDB 3EYO

- Molecule 2 is a protein called AD-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	212	1598	1003	274	313	8	0	0	0
2	D	218	1633	1021	283	319	10	0	0	0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	235	LEU	-	expression tag	PDB 3EYO
B	236	GLU	-	expression tag	PDB 3EYO
B	237	HIS	-	expression tag	PDB 3EYO
B	238	HIS	-	expression tag	PDB 3EYO
B	239	HIS	-	expression tag	PDB 3EYO
B	240	HIS	-	expression tag	PDB 3EYO
B	241	HIS	-	expression tag	PDB 3EYO
B	242	HIS	-	expression tag	PDB 3EYO
D	235	LEU	-	expression tag	PDB 3EYO
D	236	GLU	-	expression tag	PDB 3EYO

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Chain	Residue	Modelled	Actual	Comment	Reference
D	237	HIS	-	expression tag	PDB 3EYO
D	238	HIS	-	expression tag	PDB 3EYO
D	239	HIS	-	expression tag	PDB 3EYO
D	240	HIS	-	expression tag	PDB 3EYO
D	241	HIS	-	expression tag	PDB 3EYO
D	242	HIS	-	expression tag	PDB 3EYO

- Molecule 3 is water.

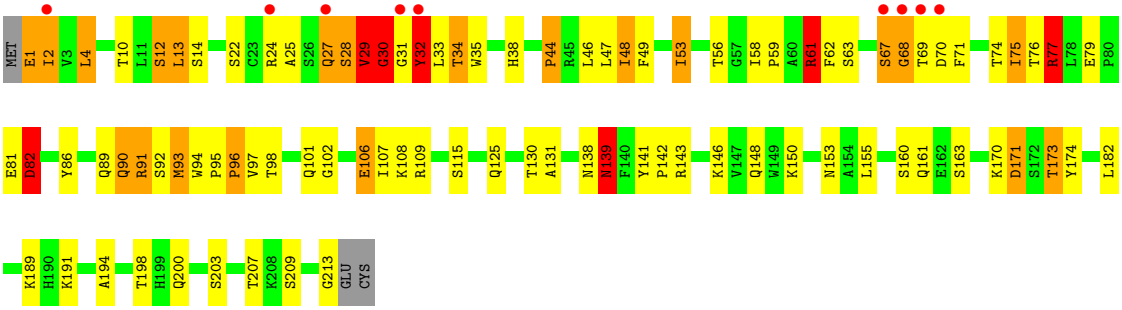
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	114	114	114	0	0
			Total	O		
3	B	96	96	96	0	0
			Total	O		
3	C	89	89	89	0	0
			Total	O		
3	D	81	81	81	0	0

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.

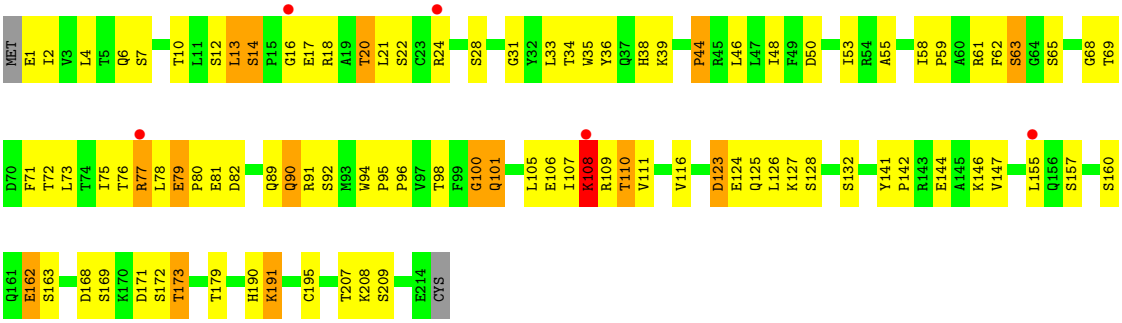
- Molecule 1: 8f9 Fab

Chain A:



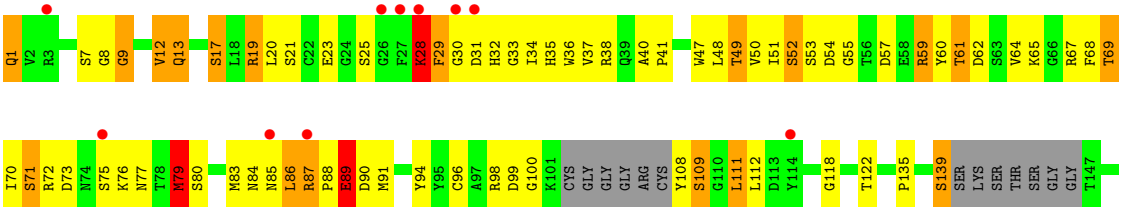
- Molecule 1: 8f9 Fab

Chain C:



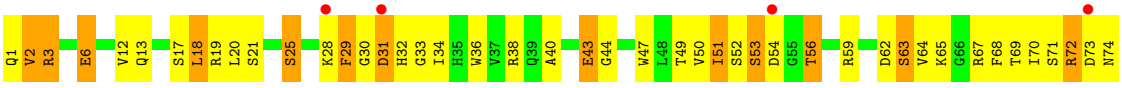
- Molecule 2: AD-2

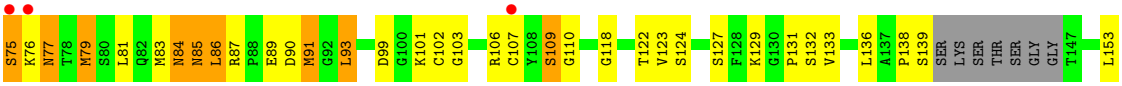
Chain B:



- Molecule 2: AD-2

Chain D:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	63.03Å 110.73Å 180.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.50 37.77 – 2.39	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-2.50) 94.1 (37.77-2.39)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.47 (at 2.39Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.241 , 0.268 0.238 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	39.7	Xtriage
Anisotropy	0.329	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 49.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	6906	wwPDB-VP
Average B, all atoms (Å^2)	40.0	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, 0.333 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	0.72	3/1681 (0.2%)	1.17	12/2285 (0.5%)
1	C	0.63	1/1690 (0.1%)	0.97	3/2297 (0.1%)
2	B	0.63	1/1634 (0.1%)	1.03	8/2217 (0.4%)
2	D	0.68	0/1670	1.15	11/2265 (0.5%)
All	All	0.67	5/6675 (0.1%)	1.08	34/9064 (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 (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	82	ASP	CA-C	-6.20	1.36	1.52
1	A	82	ASP	CB-CG	-6.13	1.38	1.51
1	C	124	GLU	CB-CG	-5.40	1.41	1.52
1	A	82	ASP	CA-CB	-5.18	1.42	1.53
2	B	29	PHE	CB-CG	-5.15	1.42	1.51

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	61	ARG	NE-CZ-NH2	-16.56	112.02	120.30
2	D	139	SER	N-CA-CB	-12.44	91.84	110.50
1	A	61	ARG	NE-CZ-NH1	9.81	125.20	120.30
2	D	138	PRO	CA-C-N	-9.10	97.19	117.20
1	A	77	ARG	NE-CZ-NH1	-8.03	116.28	120.30
2	D	139	SER	CB-CA-C	7.70	124.73	110.10
2	D	138	PRO	C-N-CA	7.64	140.81	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	190	LEU	CA-CB-CG	7.36	132.22	115.30
1	A	82	ASP	CB-CG-OD1	-7.05	111.96	118.30
2	D	86	LEU	CA-CB-CG	-6.97	99.27	115.30
1	C	108	LYS	CD-CE-NZ	-6.93	95.75	111.70
2	B	79	MET	N-CA-C	-6.92	92.33	111.00
1	A	32	TYR	N-CA-C	6.66	128.97	111.00
2	D	103	GLY	N-CA-C	6.59	129.59	113.10
2	B	29	PHE	N-CA-C	6.47	128.48	111.00
1	A	31	GLY	N-CA-C	-6.47	96.93	113.10
1	A	30	GLY	N-CA-C	6.43	129.17	113.10
1	A	29	VAL	N-CA-C	-6.40	93.72	111.00
2	D	138	PRO	N-CA-C	6.38	128.68	112.10
2	B	89	GLU	N-CA-C	-6.31	93.95	111.00
1	A	61	ARG	CG-CD-NE	-5.89	99.44	111.80
2	D	136	LEU	N-CA-C	-5.82	95.28	111.00
2	B	29	PHE	N-CA-CB	-5.74	100.27	110.60
2	D	200	SER	N-CA-C	-5.71	95.59	111.00
2	B	28	LYS	CA-C-N	-5.66	104.76	117.20
1	A	75	ILE	N-CA-C	-5.64	95.76	111.00
2	B	28	LYS	C-N-CA	5.60	135.70	121.70
1	C	13	LEU	CA-CB-CG	5.46	127.85	115.30
1	A	77	ARG	CB-CA-C	5.37	121.13	110.40
2	B	190	LEU	CB-CG-CD2	-5.35	101.90	111.00
1	C	100	GLY	N-CA-C	-5.26	99.95	113.10
2	D	110	GLY	N-CA-C	-5.11	100.33	113.10
1	A	115	SER	N-CA-C	-5.04	97.39	111.00
2	D	138	PRO	O-C-N	5.03	130.75	122.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	61	ARG	Sidechain

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	1643	0	1613	107	0
1	C	1652	0	1619	82	0
2	B	1598	0	1555	106	0
2	D	1633	0	1585	110	0
3	A	114	0	0	12	0
3	B	96	0	0	9	0
3	C	89	0	0	8	0
3	D	81	0	0	6	0
All	All	6906	0	6372	397	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 31.

All (397) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34:THR:HG21	1:A:46:LEU:HD11	1.22	1.12
1:A:91:ARG:NH1	2:B:109:SER:O	1.83	1.11
2:B:62:ASP:HA	2:B:65:LYS:HE2	1.36	1.07
2:B:30:GLY:O	2:B:53:SER:HB2	1.57	1.04
1:C:28:SER:OG	1:C:68:GLY:HA2	1.56	1.03
1:C:171:ASP:HB3	1:C:173:THR:OG1	1.60	1.02
1:A:48:ILE:HD12	1:A:48:ILE:O	1.59	1.00
1:A:34:THR:HG21	1:A:46:LEU:CD1	1.93	0.98
1:A:61:ARG:HH22	1:A:82:ASP:CG	1.66	0.97
2:D:6:GLU:OE1	2:D:118:GLY:N	1.96	0.96
2:D:200:SER:O	2:D:201:LEU:HB2	1.64	0.96
2:B:29:PHE:O	2:B:72:ARG:NH2	2.01	0.94
1:A:34:THR:CG2	1:A:46:LEU:HD11	1.98	0.94
2:D:71:SER:O	2:D:72:ARG:HB2	1.70	0.91
1:A:30:GLY:HA2	1:A:68:GLY:HA2	1.52	0.91
2:B:17:SER:HB2	3:B:337:HOH:O	1.70	0.90
2:B:69:THR:HG22	3:B:334:HOH:O	1.71	0.90
3:C:229:HOH:O	2:D:155:LYS:HE3	1.70	0.90
1:A:77:ARG:O	1:A:77:ARG:HD3	1.71	0.90
1:A:48:ILE:HD12	1:A:48:ILE:C	1.92	0.88
2:D:63:SER:O	2:D:67:ARG:NH1	2.06	0.87
1:C:106:GLU:HG2	1:C:107:ILE:N	1.89	0.86
2:D:62:ASP:HA	2:D:65:LYS:HE2	1.56	0.86
2:D:32:HIS:O	2:D:72:ARG:NH2	2.08	0.86
2:D:91:MET:HE2	2:D:123:VAL:H	1.41	0.85
2:B:62:ASP:HA	2:B:65:LYS:CE	2.06	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2:ILE:O	1:A:98:THR:HG21	1.75	0.85
1:C:81:GLU:CD	1:C:81:GLU:H	1.80	0.84
2:D:52:SER:O	2:D:72:ARG:NH1	2.10	0.84
1:A:61:ARG:NH1	1:A:82:ASP:OD1	2.10	0.84
2:D:54:ASP:HB2	2:D:56:THR:HG23	1.57	0.84
1:A:28:SER:HA	1:A:68:GLY:O	1.78	0.83
2:D:91:MET:CE	2:D:123:VAL:H	1.93	0.82
1:C:123:ASP:HA	3:C:238:HOH:O	1.79	0.81
1:A:2:ILE:HD11	1:A:93:MET:CB	2.09	0.81
2:D:67:ARG:NH2	2:D:90:ASP:OD2	2.13	0.81
2:B:28:LYS:O	2:B:31:ASP:HB2	1.80	0.81
1:C:20:THR:C	1:C:21:LEU:HD23	2.02	0.80
1:A:34:THR:HG23	1:A:49:PHE:HA	1.64	0.79
2:D:12:VAL:HG11	2:D:86:LEU:HD13	1.65	0.79
2:D:129:LYS:HE2	3:D:268:HOH:O	1.84	0.78
1:C:171:ASP:CB	1:C:173:THR:OG1	2.32	0.78
1:A:161:GLN:HB3	2:B:181:VAL:HG11	1.66	0.78
2:D:17:SER:OG	2:D:84:ASN:HB3	1.83	0.77
1:C:95:PRO:CB	1:C:96:PRO:HA	2.15	0.77
1:A:61:ARG:NH2	1:A:82:ASP:CG	2.37	0.76
1:A:90:GLN:OE1	1:A:98:THR:OG1	2.04	0.76
1:A:150:LYS:HD3	3:A:219:HOH:O	1.86	0.75
1:C:79:GLU:HB3	1:C:81:GLU:OE1	1.86	0.75
1:A:34:THR:HG23	1:A:48:ILE:O	1.86	0.75
1:A:61:ARG:NH2	1:A:82:ASP:OD2	2.20	0.74
1:A:34:THR:CG2	1:A:48:ILE:O	2.35	0.74
1:A:106:GLU:HG2	1:A:107:ILE:N	2.03	0.74
1:A:89:GLN:HE21	1:A:97:VAL:HG12	1.52	0.74
1:C:106:GLU:OE2	1:C:141:TYR:OH	2.05	0.73
1:A:2:ILE:HD11	1:A:93:MET:HB2	1.69	0.73
1:A:35:TRP:HD1	1:A:48:ILE:HD11	1.54	0.73
1:A:77:ARG:O	1:A:77:ARG:CD	2.36	0.72
2:B:30:GLY:O	2:B:53:SER:O	2.07	0.72
1:C:14:SER:O	1:C:17:GLU:HG3	1.88	0.72
2:D:62:ASP:HA	2:D:65:LYS:CE	2.21	0.71
2:D:51:ILE:HG23	2:D:70:ILE:HD13	1.73	0.71
2:B:36:TRP:NE1	2:B:79:MET:CE	2.54	0.70
2:D:211:ASN:OD1	2:D:218:LYS:HE3	1.91	0.70
1:A:2:ILE:HD11	1:A:93:MET:HB3	1.72	0.70
1:A:4:LEU:HD12	1:A:25:ALA:HA	1.72	0.70
2:D:33:GLY:O	2:D:34:ILE:HG12	1.92	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:GLU:O	1:A:82:ASP:OD2	2.11	0.69
1:A:34:THR:HG22	1:A:35:TRP:H	1.55	0.69
1:C:81:GLU:CD	1:C:81:GLU:N	2.46	0.69
2:B:91:MET:CE	2:B:122:THR:HG23	2.23	0.69
2:D:54:ASP:CB	2:D:56:THR:HG23	2.22	0.69
2:D:200:SER:O	2:D:201:LEU:CB	2.41	0.69
2:D:71:SER:O	2:D:72:ARG:CB	2.40	0.69
1:A:30:GLY:HA2	1:A:68:GLY:CA	2.22	0.68
1:C:55:ALA:HB3	1:C:58:ILE:HD13	1.75	0.68
1:C:116:VAL:HG12	1:C:208:LYS:HG3	1.75	0.68
2:B:171:LEU:HD21	2:B:194:VAL:HG21	1.76	0.67
1:C:77:ARG:O	1:C:77:ARG:HG2	1.93	0.67
2:B:67:ARG:NH2	2:B:90:ASP:OD2	2.28	0.67
2:B:174:GLY:O	2:B:194:VAL:HA	1.94	0.67
1:A:30:GLY:CA	1:A:68:GLY:HA2	2.24	0.67
1:A:163:SER:OG	2:B:179:PRO:HD2	1.95	0.67
2:D:36:TRP:NE1	2:D:79:MET:HE1	2.10	0.67
1:A:62:PHE:CD1	1:A:75:ILE:HG12	2.30	0.66
2:D:73:ASP:OD2	2:D:76:LYS:HB2	1.95	0.66
1:C:6:GLN:HG2	3:C:254:HOH:O	1.95	0.66
1:A:48:ILE:C	1:A:48:ILE:CD1	2.60	0.66
2:B:57:ASP:OD2	2:B:59:ARG:NE	2.29	0.66
1:A:27:GLN:HG2	1:A:27:GLN:O	1.94	0.66
1:A:171:ASP:HB3	1:A:173:THR:OG1	1.96	0.66
2:D:54:ASP:HB2	2:D:56:THR:CG2	2.25	0.65
2:B:36:TRP:NE1	2:B:79:MET:HE2	2.12	0.65
1:A:89:GLN:NE2	1:A:97:VAL:HG12	2.11	0.65
2:D:62:ASP:O	2:D:65:LYS:HG2	1.97	0.65
1:C:6:GLN:OE1	1:C:100:GLY:HA3	1.97	0.65
2:D:28:LYS:CB	2:D:31:ASP:OD2	2.45	0.65
2:D:174:GLY:O	2:D:194:VAL:HA	1.98	0.64
2:B:17:SER:HB3	2:B:83:MET:O	1.97	0.64
2:B:112:LEU:N	2:B:112:LEU:HD12	2.11	0.64
1:C:24:ARG:HA	1:C:69:THR:O	1.96	0.64
2:B:73:ASP:OD2	2:B:76:LYS:HG3	1.98	0.64
1:C:110:THR:HA	3:C:295:HOH:O	1.98	0.64
1:A:34:THR:HG23	1:A:49:PHE:CA	2.27	0.64
2:B:72:ARG:HA	2:B:79:MET:HA	1.79	0.64
2:D:6:GLU:OE1	2:D:118:GLY:CA	2.45	0.64
1:A:62:PHE:CE1	1:A:75:ILE:HG12	2.33	0.64
1:A:24:ARG:HD3	3:A:327:HOH:O	1.97	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:17:GLU:O	1:C:76:THR:O	2.15	0.63
1:C:106:GLU:CG	1:C:107:ILE:N	2.61	0.63
2:D:28:LYS:O	2:D:31:ASP:OD2	2.16	0.63
2:B:36:TRP:HE1	2:B:79:MET:HE2	1.62	0.63
1:A:2:ILE:HG13	1:A:90:GLN:OE1	1.99	0.62
2:B:224:GLU:HB2	2:B:225:PRO:HD2	1.80	0.62
2:B:62:ASP:CA	2:B:65:LYS:HE2	2.21	0.62
1:C:20:THR:O	1:C:21:LEU:HD23	1.99	0.62
1:C:13:LEU:HD23	1:C:78:LEU:HD11	1.82	0.62
2:D:51:ILE:HG21	2:D:70:ILE:HG12	1.79	0.62
1:A:48:ILE:O	1:A:48:ILE:CD1	2.43	0.62
1:C:77:ARG:O	1:C:77:ARG:CG	2.47	0.62
2:D:76:LYS:HD2	3:D:294:HOH:O	2.00	0.62
1:C:28:SER:HA	1:C:68:GLY:O	2.00	0.61
2:B:7:SER:OG	2:B:21:SER:HB3	2.01	0.61
1:C:1:GLU:HG2	1:C:2:ILE:H	1.65	0.61
2:B:41:PRO:HA	3:B:314:HOH:O	2.00	0.61
2:B:36:TRP:NE1	2:B:79:MET:HE1	2.16	0.61
2:B:87:ARG:O	2:B:90:ASP:HB2	2.01	0.60
1:C:162:GLU:HG2	3:C:222:HOH:O	2.00	0.60
2:B:1:GLN:OE1	2:B:1:GLN:N	2.31	0.60
1:A:94:TRP:HB2	1:A:95:PRO:HA	1.84	0.60
1:C:61:ARG:HH21	1:C:82:ASP:CG	2.04	0.60
2:D:52:SER:C	2:D:72:ARG:NH1	2.54	0.60
2:D:28:LYS:HB2	2:D:31:ASP:OD2	2.02	0.60
1:C:55:ALA:HB3	1:C:58:ILE:CD1	2.31	0.59
1:C:16:GLY:H	1:C:78:LEU:HB2	1.68	0.59
1:C:155:LEU:HD12	1:C:155:LEU:N	2.16	0.59
1:C:168:ASP:HB3	1:C:171:ASP:HB2	1.85	0.59
2:B:91:MET:HE3	2:B:122:THR:HG23	1.83	0.59
2:B:13:GLN:HB2	3:B:306:HOH:O	2.02	0.59
2:B:98:ARG:O	2:B:112:LEU:HA	2.03	0.58
2:D:59:ARG:HG2	2:D:59:ARG:HH11	1.69	0.58
1:A:1:GLU:N	3:A:277:HOH:O	2.37	0.58
2:B:34:ILE:O	2:B:50:VAL:HA	2.04	0.58
2:B:112:LEU:N	2:B:112:LEU:CD1	2.67	0.58
2:D:64:VAL:O	2:D:67:ARG:HB2	2.04	0.58
2:D:51:ILE:HG23	2:D:70:ILE:CD1	2.34	0.57
2:D:68:PHE:CZ	2:D:83:MET:HG2	2.39	0.57
2:B:52:SER:OG	2:B:54:ASP:OD1	2.21	0.57
2:D:91:MET:HE2	2:D:122:THR:HA	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:54:ASP:OD1	2:B:55:GLY:N	2.37	0.57
1:A:34:THR:HG22	1:A:35:TRP:N	2.20	0.57
2:D:32:HIS:HD2	2:D:99:ASP:O	1.87	0.57
2:D:36:TRP:CE2	2:D:79:MET:HE1	2.40	0.56
1:C:89:GLN:HG2	1:C:90:GLN:N	2.20	0.56
1:C:33:LEU:HD22	1:C:71:PHE:CG	2.40	0.56
1:A:141:TYR:CG	1:A:142:PRO:HA	2.41	0.56
1:A:47:LEU:HA	1:A:58:ILE:HG12	1.87	0.56
2:D:199:SER:C	2:D:200:SER:O	2.41	0.56
1:A:34:THR:HG22	1:A:48:ILE:O	2.05	0.56
2:D:40:ALA:HB3	2:D:43:GLU:HG3	1.88	0.56
2:D:51:ILE:CG2	2:D:70:ILE:CG2	2.84	0.56
1:C:21:LEU:HD23	1:C:21:LEU:N	2.21	0.55
1:A:94:TRP:HB2	1:A:97:VAL:HG22	1.87	0.55
1:C:90:GLN:HG2	1:C:92:SER:H	1.69	0.55
2:B:32:HIS:C	2:B:53:SER:HB3	2.27	0.55
2:B:99:ASP:OD2	2:B:109:SER:OG	2.13	0.55
1:C:61:ARG:NH2	1:C:82:ASP:OD1	2.39	0.55
1:A:34:THR:CG2	1:A:46:LEU:CD1	2.71	0.55
1:A:61:ARG:HH12	1:A:82:ASP:CG	2.09	0.55
2:B:60:TYR:OH	2:B:70:ILE:HG22	2.07	0.55
2:D:51:ILE:CG2	2:D:70:ILE:HG12	2.36	0.55
2:B:36:TRP:CE2	2:B:79:MET:HE1	2.43	0.54
1:C:79:GLU:CB	1:C:81:GLU:OE1	2.55	0.54
2:B:64:VAL:HB	2:B:68:PHE:CG	2.43	0.54
1:A:27:GLN:O	1:A:28:SER:C	2.46	0.54
1:A:91:ARG:HG3	1:A:91:ARG:HH11	1.73	0.54
2:D:74:ASN:O	2:D:77:ASN:N	2.40	0.54
2:D:12:VAL:HG11	2:D:86:LEU:CD1	2.34	0.54
1:C:20:THR:HG22	1:C:72:THR:CG2	2.38	0.53
1:C:125:GLN:HE22	1:C:132:SER:H	1.54	0.53
2:B:48:LEU:HA	2:B:61:THR:CG2	2.38	0.53
1:C:76:THR:O	1:C:78:LEU:N	2.41	0.53
2:D:28:LYS:HB3	2:D:31:ASP:OD2	2.09	0.53
2:D:73:ASP:OD2	2:D:76:LYS:N	2.41	0.53
1:A:90:GLN:HG2	1:A:91:ARG:N	2.24	0.53
2:B:48:LEU:HA	2:B:61:THR:HG22	1.91	0.53
1:A:29:VAL:O	1:A:32:TYR:HB2	2.09	0.53
1:C:171:ASP:O	1:C:172:SER:HB2	2.09	0.53
1:C:195:CYS:O	1:C:207:THR:HA	2.10	0.52
2:D:74:ASN:O	2:D:76:LYS:N	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:91:MET:HE2	2:D:123:VAL:N	2.18	0.52
1:C:146:LYS:HZ1	1:C:147:VAL:H	1.58	0.52
1:A:61:ARG:HH21	1:A:75:ILE:CG2	2.22	0.52
1:A:29:VAL:HG23	1:A:32:TYR:HB2	1.92	0.51
1:A:91:ARG:CG	1:A:91:ARG:O	2.58	0.51
1:C:125:GLN:O	1:C:128:SER:HB2	2.11	0.51
2:B:12:VAL:HG13	2:B:13:GLN:N	2.24	0.51
2:D:84:ASN:O	2:D:85:ASN:HB2	2.09	0.51
2:B:139:SER:CB	3:B:316:HOH:O	2.59	0.51
2:D:62:ASP:O	2:D:65:LYS:CG	2.58	0.51
1:A:94:TRP:HZ2	2:B:108:TYR:HB3	1.76	0.51
1:A:130:THR:HG22	1:A:131:ALA:N	2.26	0.51
1:A:12:SER:O	1:A:13:LEU:HD13	2.11	0.50
2:D:28:LYS:O	2:D:30:GLY:N	2.45	0.50
2:B:64:VAL:HG13	3:B:318:HOH:O	2.11	0.50
1:C:146:LYS:NZ	1:C:147:VAL:H	2.09	0.50
2:B:62:ASP:O	2:B:65:LYS:HB2	2.12	0.50
2:B:67:ARG:HH22	2:B:90:ASP:CG	2.15	0.50
2:B:139:SER:HB3	3:B:316:HOH:O	2.12	0.50
2:D:1:GLN:CB	3:D:274:HOH:O	2.59	0.50
1:A:153:ASN:HB3	3:A:298:HOH:O	2.12	0.50
2:B:36:TRP:HE1	2:B:79:MET:CE	2.21	0.50
2:D:74:ASN:C	2:D:76:LYS:N	2.62	0.50
1:A:91:ARG:NH1	1:A:91:ARG:HG3	2.27	0.49
1:C:95:PRO:HB2	1:C:96:PRO:HA	1.94	0.49
2:B:34:ILE:HG13	2:B:72:ARG:NH1	2.26	0.49
1:C:63:SER:HB3	3:C:224:HOH:O	2.11	0.49
2:D:76:LYS:O	2:D:77:ASN:HB2	2.11	0.49
2:D:131:PRO:HB3	2:D:157:TYR:HB3	1.94	0.49
1:A:146:LYS:HB3	1:A:198:THR:HB	1.94	0.49
2:B:51:ILE:HD12	2:B:71:SER:HA	1.94	0.49
2:D:199:SER:OG	2:D:200:SER:N	2.43	0.49
1:A:49:PHE:HB2	2:B:111:LEU:HD11	1.95	0.49
1:C:12:SER:HB3	1:C:108:LYS:HD2	1.95	0.49
2:B:12:VAL:HG13	2:B:13:GLN:O	2.13	0.49
2:D:33:GLY:C	2:D:34:ILE:CG1	2.81	0.49
2:B:37:VAL:HG22	2:B:47:TRP:HA	1.95	0.48
2:B:67:ARG:NH2	2:B:90:ASP:CG	2.67	0.48
2:D:12:VAL:O	2:D:123:VAL:HA	2.13	0.48
2:D:211:ASN:OD1	2:D:218:LYS:HD2	2.13	0.48
2:B:30:GLY:O	2:B:53:SER:CB	2.45	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:160:SER:HA	1:C:179:THR:O	2.13	0.48
2:D:68:PHE:HB3	2:D:81:LEU:HD11	1.95	0.48
1:C:94:TRP:HB2	1:C:95:PRO:HA	1.96	0.48
2:B:59:ARG:CD	2:B:59:ARG:N	2.76	0.48
2:B:76:LYS:O	2:B:77:ASN:HB2	2.14	0.48
2:B:17:SER:HA	2:B:86:LEU:HD12	1.95	0.48
2:D:87:ARG:O	2:D:90:ASP:HB2	2.14	0.48
2:B:84:ASN:O	2:B:85:ASN:C	2.52	0.48
2:D:18:LEU:HD23	2:D:18:LEU:HA	1.73	0.48
2:B:36:TRP:HB2	2:B:49:THR:HG23	1.96	0.48
1:C:155:LEU:N	1:C:155:LEU:CD1	2.77	0.48
2:D:13:GLN:HA	2:D:124:SER:O	2.14	0.48
2:B:53:SER:HA	2:B:72:ARG:NH1	2.29	0.47
2:B:94:TYR:O	2:B:118:GLY:HA2	2.14	0.47
2:D:1:GLN:HB3	3:D:274:HOH:O	2.14	0.47
2:B:19:ARG:HH21	2:B:80:SER:HB2	1.80	0.47
2:B:48:LEU:O	2:B:61:THR:HG22	2.15	0.47
1:A:30:GLY:N	1:A:68:GLY:HA2	2.29	0.47
1:A:61:ARG:O	1:A:75:ILE:HA	2.14	0.47
1:C:146:LYS:HA	1:C:146:LYS:HZ2	1.80	0.47
2:D:91:MET:CE	2:D:123:VAL:N	2.72	0.47
2:D:159:PRO:O	2:D:212:HIS:NE2	2.40	0.47
2:D:190:LEU:C	2:D:190:LEU:HD12	2.35	0.47
1:A:58:ILE:HA	1:A:59:PRO:HD3	1.71	0.47
1:C:80:PRO:N	1:C:81:GLU:OE1	2.48	0.47
1:C:190:HIS:HE1	3:C:285:HOH:O	1.98	0.47
2:D:2:VAL:C	2:D:3:ARG:CG	2.83	0.47
2:D:52:SER:OG	2:D:54:ASP:OD1	2.27	0.47
2:B:135:PRO:HD3	2:B:221:LYS:HE2	1.96	0.46
2:B:197:PRO:O	2:B:200:SER:OG	2.30	0.46
1:A:30:GLY:H	1:A:68:GLY:HA2	1.80	0.46
2:B:158:PHE:HA	2:B:159:PRO:HA	1.67	0.46
2:D:70:ILE:HD11	2:D:79:MET:SD	2.55	0.46
1:A:61:ARG:CZ	1:A:82:ASP:CG	2.83	0.46
1:A:94:TRP:CE3	1:A:97:VAL:HG22	2.50	0.46
2:D:102:CYS:SG	2:D:107:CYS:C	2.94	0.46
2:B:51:ILE:O	2:B:52:SER:O	2.33	0.46
2:B:98:ARG:HG2	2:B:99:ASP:N	2.31	0.46
2:D:59:ARG:HG2	2:D:59:ARG:NH1	2.31	0.46
2:B:64:VAL:HB	2:B:68:PHE:CD1	2.51	0.46
1:C:6:GLN:N	1:C:101:GLN:OE1	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:211:ASN:HD21	2:D:213:LYS:HE3	1.80	0.46
1:A:69:THR:C	1:A:70:ASP:OD2	2.54	0.46
1:A:141:TYR:CD1	1:A:142:PRO:HA	2.50	0.46
1:A:189:LYS:HE2	1:A:189:LYS:HB3	1.37	0.46
2:B:41:PRO:HB3	3:B:314:HOH:O	2.16	0.46
2:D:38:ARG:HA	2:D:93:LEU:O	2.16	0.46
1:A:95:PRO:HA	1:A:96:PRO:HA	1.51	0.45
2:D:51:ILE:CG2	2:D:70:ILE:HG21	2.45	0.45
2:D:201:LEU:HD23	2:D:201:LEU:HA	1.67	0.45
2:B:73:ASP:CG	2:B:76:LYS:HG3	2.36	0.45
1:A:61:ARG:NH1	1:A:82:ASP:CG	2.69	0.45
2:B:79:MET:C	2:B:79:MET:SD	2.95	0.45
1:C:31:GLY:O	1:C:50:ASP:HA	2.16	0.45
1:C:94:TRP:HA	1:C:95:PRO:C	2.37	0.45
2:D:62:ASP:OD1	2:D:65:LYS:HE3	2.17	0.45
2:D:156:ASP:HB3	2:D:187:LEU:HD13	1.99	0.45
1:C:126:LEU:C	1:C:128:SER:N	2.68	0.45
2:D:2:VAL:C	2:D:3:ARG:HG3	2.36	0.45
1:A:130:THR:CG2	1:A:131:ALA:N	2.79	0.45
1:C:91:ARG:HD2	2:D:109:SER:O	2.17	0.45
1:C:144:GLU:CD	1:C:144:GLU:H	2.20	0.45
2:D:54:ASP:O	2:D:56:THR:CG2	2.65	0.45
1:C:168:ASP:OD1	1:C:169:SER:N	2.50	0.45
1:A:213:GLY:CA	3:A:319:HOH:O	2.65	0.44
2:B:35:HIS:NE2	2:B:99:ASP:OD1	2.49	0.44
2:B:83:MET:HB2	2:B:86:LEU:HD11	1.98	0.44
1:A:94:TRP:CZ2	2:B:108:TYR:HB3	2.52	0.44
1:A:148:GLN:OE1	1:A:155:LEU:HG	2.17	0.44
2:B:33:GLY:N	2:B:53:SER:HB3	2.32	0.44
2:D:28:LYS:C	2:D:30:GLY:H	2.20	0.44
1:C:36:TYR:HE2	1:C:89:GLN:OE1	2.01	0.44
1:A:2:ILE:H	1:A:2:ILE:HG12	1.34	0.44
2:B:70:ILE:HG12	2:B:71:SER:N	2.32	0.44
1:C:141:TYR:CD1	1:C:142:PRO:HA	2.52	0.44
2:D:43:GLU:HB2	2:D:44:GLY:H	1.46	0.44
2:D:52:SER:CB	2:D:54:ASP:OD1	2.65	0.44
1:C:50:ASP:HB2	1:C:53:ILE:HD12	1.98	0.44
2:D:31:ASP:OD2	2:D:31:ASP:N	2.50	0.44
2:D:84:ASN:HB3	3:D:272:HOH:O	2.18	0.44
2:B:17:SER:HB3	2:B:84:ASN:HA	2.00	0.44
2:B:17:SER:HB3	2:B:84:ASN:OD1	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:85:ASN:O	2:D:86:LEU:C	2.51	0.44
1:A:207:THR:HG21	3:A:303:HOH:O	2.18	0.43
1:C:1:GLU:HG2	1:C:2:ILE:N	2.31	0.43
1:A:139:ASN:HB3	1:A:173:THR:HG21	2.00	0.43
2:B:8:GLY:O	2:B:9:GLY:O	2.35	0.43
2:B:156:ASP:HB3	2:B:187:LEU:HD13	2.00	0.43
2:D:49:THR:OG1	2:D:50:VAL:N	2.51	0.43
1:A:61:ARG:CZ	1:A:82:ASP:OD2	2.66	0.43
1:A:106:GLU:HG3	1:A:174:TYR:OH	2.19	0.43
2:B:156:ASP:HA	2:B:187:LEU:HB3	2.01	0.43
2:D:47:TRP:HZ2	2:D:50:VAL:HG12	1.83	0.43
2:B:165:SER:HB2	2:B:209:ASN:HB2	1.99	0.43
1:C:59:PRO:HG2	1:C:62:PHE:CE2	2.54	0.43
2:D:53:SER:HA	2:D:72:ARG:NH1	2.34	0.43
1:A:53:ILE:O	1:A:53:ILE:HG13	2.09	0.43
2:B:89:GLU:HG3	2:B:90:ASP:N	2.33	0.43
2:D:198:SER:C	2:D:200:SER:O	2.57	0.43
1:A:89:GLN:HG2	1:A:98:THR:O	2.19	0.43
1:A:153:ASN:CB	3:A:298:HOH:O	2.66	0.43
1:C:61:ARG:O	1:C:75:ILE:HA	2.19	0.43
1:A:95:PRO:HD3	3:A:279:HOH:O	2.18	0.43
2:B:73:ASP:OD1	2:B:75:SER:OG	2.34	0.43
1:A:86:TYR:O	1:A:102:GLY:HA2	2.19	0.42
2:B:29:PHE:O	2:B:29:PHE:CD2	2.72	0.42
1:C:125:GLN:NE2	1:C:132:SER:H	2.17	0.42
1:A:30:GLY:HA2	1:A:68:GLY:N	2.34	0.42
2:B:28:LYS:H	2:B:28:LYS:HZ2	1.65	0.42
2:D:74:ASN:C	2:D:76:LYS:H	2.22	0.42
1:A:1:GLU:OE1	1:A:96:PRO:HG2	2.18	0.42
2:D:54:ASP:OD1	2:D:54:ASP:N	2.47	0.42
2:B:91:MET:HE3	2:B:122:THR:CG2	2.49	0.42
2:D:52:SER:HB2	2:D:54:ASP:OD1	2.19	0.42
2:D:211:ASN:ND2	2:D:213:LYS:HE3	2.34	0.42
1:A:67:SER:HB2	3:A:324:HOH:O	2.19	0.42
2:B:38:ARG:HB3	2:B:48:LEU:HD11	2.02	0.42
2:D:29:PHE:O	2:D:29:PHE:CD2	2.72	0.42
2:D:51:ILE:HG22	2:D:70:ILE:HG21	2.01	0.42
1:A:1:GLU:O	1:A:1:GLU:HG3	2.18	0.42
1:C:38:HIS:CD2	1:C:44:PRO:HG3	2.55	0.42
1:A:213:GLY:HA2	3:A:319:HOH:O	2.20	0.42
2:D:51:ILE:HG22	2:D:70:ILE:CG2	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:71:PHE:CD2	1:A:71:PHE:N	2.87	0.42
2:D:84:ASN:O	2:D:85:ASN:CB	2.68	0.42
2:B:70:ILE:CG1	2:B:71:SER:N	2.83	0.42
2:B:178:PHE:O	2:B:190:LEU:HD22	2.20	0.42
1:C:90:GLN:OE1	1:C:98:THR:OG1	2.37	0.42
1:C:146:LYS:HA	1:C:146:LYS:HD2	1.80	0.42
1:C:191:LYS:HE3	1:C:191:LYS:HB3	1.76	0.42
2:B:86:LEU:HD23	2:B:90:ASP:CB	2.49	0.41
1:C:77:ARG:HG3	1:C:79:GLU:OE2	2.20	0.41
2:D:68:PHE:CE1	2:D:83:MET:HG2	2.54	0.41
2:D:133:VAL:O	2:D:221:LYS:HE3	2.20	0.41
1:A:125:GLN:NE2	3:A:225:HOH:O	2.53	0.41
1:C:28:SER:OG	1:C:68:GLY:CA	2.47	0.41
1:C:123:ASP:CA	3:C:238:HOH:O	2.55	0.41
2:B:77:ASN:HD22	2:B:77:ASN:HA	1.65	0.41
1:C:35:TRP:CE2	1:C:73:LEU:HB2	2.56	0.41
2:B:64:VAL:CG1	3:B:318:HOH:O	2.68	0.41
2:D:211:ASN:OD1	2:D:218:LYS:CE	2.66	0.41
2:B:100:GLY:O	2:B:109:SER:OG	2.38	0.41
2:D:65:LYS:HG2	2:D:65:LYS:H	1.51	0.41
1:C:34:THR:HG23	1:C:46:LEU:HD11	2.03	0.41
1:A:2:ILE:HG13	1:A:90:GLN:CD	2.41	0.41
1:A:38:HIS:CD2	1:A:44:PRO:HG3	2.56	0.41
2:B:40:ALA:HA	2:B:41:PRO:HD3	1.80	0.41
2:B:51:ILE:C	2:B:52:SER:O	2.57	0.41
2:D:1:GLN:HB2	3:D:274:HOH:O	2.19	0.41
2:D:166:TRP:CH2	2:D:208:CYS:HB3	2.55	0.41
2:D:36:TRP:NE1	2:D:79:MET:CE	2.80	0.41
1:A:34:THR:HG23	1:A:48:ILE:C	2.41	0.40
1:A:161:GLN:OE1	2:B:181:VAL:HG12	2.21	0.40
2:B:35:HIS:O	2:B:96:CYS:HA	2.21	0.40
1:C:36:TYR:CE2	1:C:89:GLN:OE1	2.74	0.40
1:A:194:ALA:HB2	1:A:209:SER:HB3	2.04	0.40
2:B:87:ARG:HA	2:B:88:PRO:HD3	1.79	0.40
2:D:51:ILE:CG2	2:D:70:ILE:CG1	2.98	0.40
1:A:207:THR:CG2	3:A:303:HOH:O	2.70	0.40
2:B:51:ILE:O	2:B:51:ILE:HG23	2.21	0.40
1:C:126:LEU:HA	1:C:126:LEU:HD23	1.84	0.40
1:A:30:GLY:HA2	1:A:68:GLY:H	1.86	0.40
1:A:33:LEU:HD22	1:A:71:PHE:CD1	2.57	0.40
1:C:13:LEU:HD23	1:C:78:LEU:CD1	2.49	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:141:TYR:CG	1:C:142:PRO:HA	2.56	0.40
1:A:67:SER:O	1:A:69:THR:N	2.53	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	211/216 (98%)	197 (93%)	9 (4%)	5 (2%)	6 9
1	C	212/216 (98%)	199 (94%)	12 (6%)	1 (0%)	29 48
2	B	206/242 (85%)	187 (91%)	17 (8%)	2 (1%)	15 28
2	D	214/242 (88%)	191 (89%)	17 (8%)	6 (3%)	5 7
All	All	843/916 (92%)	774 (92%)	55 (6%)	14 (2%)	9 16

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	32	TYR
2	B	52	SER
2	D	2	VAL
2	D	72	ARG
1	A	30	GLY
1	A	68	GLY
1	A	139	ASN
2	B	9	GLY
2	D	29	PHE
2	D	75	SER
2	D	201	LEU
1	A	28	SER
1	C	77	ARG

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Mol	Chain	Res	Type
2	D	25	SER

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	184/187 (98%)	141 (77%)	43 (23%)	1 1
1	C	185/187 (99%)	157 (85%)	28 (15%)	3 5
2	B	180/204 (88%)	148 (82%)	32 (18%)	2 3
2	D	183/204 (90%)	142 (78%)	41 (22%)	1 1
All	All	732/782 (94%)	588 (80%)	144 (20%)	1 2

All (144) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	GLU
1	A	2	ILE
1	A	4	LEU
1	A	10	THR
1	A	12	SER
1	A	13	LEU
1	A	14	SER
1	A	22	SER
1	A	27	GLN
1	A	29	VAL
1	A	34	THR
1	A	44	PRO
1	A	48	ILE
1	A	53	ILE
1	A	56	THR
1	A	61	ARG
1	A	63	SER
1	A	67	SER
1	A	74	THR
1	A	76	THR

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Mol	Chain	Res	Type
1	A	77	ARG
1	A	81	GLU
1	A	82	ASP
1	A	90	GLN
1	A	91	ARG
1	A	92	SER
1	A	93	MET
1	A	96	PRO
1	A	101	GLN
1	A	106	GLU
1	A	108	LYS
1	A	109	ARG
1	A	138	ASN
1	A	139	ASN
1	A	143	ARG
1	A	160	SER
1	A	170	LYS
1	A	171	ASP
1	A	173	THR
1	A	182	LEU
1	A	191	LYS
1	A	200	GLN
1	A	203	SER
2	B	1	GLN
2	B	12	VAL
2	B	13	GLN
2	B	17	SER
2	B	19	ARG
2	B	20	LEU
2	B	23	GLU
2	B	25	SER
2	B	28	LYS
2	B	49	THR
2	B	59	ARG
2	B	61	THR
2	B	69	THR
2	B	71	SER
2	B	79	MET
2	B	86	LEU
2	B	87	ARG
2	B	89	GLU
2	B	109	SER

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Mol	Chain	Res	Type
2	B	111	LEU
2	B	139	SER
2	B	153	LEU
2	B	161	PRO
2	B	172	THR
2	B	173	SER
2	B	190	LEU
2	B	191	SER
2	B	195	THR
2	B	198	SER
2	B	211	ASN
2	B	216	ASN
2	B	222	LYS
1	C	4	LEU
1	C	7	SER
1	C	10	THR
1	C	14	SER
1	C	18	ARG
1	C	20	THR
1	C	22	SER
1	C	39	LYS
1	C	44	PRO
1	C	48	ILE
1	C	63	SER
1	C	65	SER
1	C	79	GLU
1	C	90	GLN
1	C	101	GLN
1	C	105	LEU
1	C	108	LYS
1	C	109	ARG
1	C	110	THR
1	C	111	VAL
1	C	123	ASP
1	C	127	LYS
1	C	157	SER
1	C	162	GLU
1	C	163	SER
1	C	173	THR
1	C	191	LYS
1	C	209	SER
2	D	3	ARG

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Mol	Chain	Res	Type
2	D	6	GLU
2	D	18	LEU
2	D	19	ARG
2	D	20	LEU
2	D	21	SER
2	D	25	SER
2	D	31	ASP
2	D	43	GLU
2	D	51	ILE
2	D	53	SER
2	D	56	THR
2	D	63	SER
2	D	69	THR
2	D	75	SER
2	D	77	ASN
2	D	79	MET
2	D	84	ASN
2	D	85	ASN
2	D	89	GLU
2	D	91	MET
2	D	93	LEU
2	D	101	LYS
2	D	106	ARG
2	D	109	SER
2	D	127	SER
2	D	132	SER
2	D	153	LEU
2	D	161	PRO
2	D	165	SER
2	D	172	THR
2	D	184	SER
2	D	189	SER
2	D	190	LEU
2	D	195	THR
2	D	198	SER
2	D	199	SER
2	D	201	LEU
2	D	203	THR
2	D	213	LYS
2	D	218	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	GLN
1	A	89	GLN
1	A	125	GLN
1	A	138	ASN
1	A	200	GLN
2	B	77	ASN
2	B	117	GLN
2	B	176	HIS
2	B	204	GLN
2	B	211	ASN
2	B	216	ASN
1	C	125	GLN
1	C	211	ASN
2	D	32	HIS
2	D	216	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	213/216 (98%)	0.07	9 (4%)	36	39	14, 36, 60, 75	0
1	C	214/216 (99%)	0.08	5 (2%)	60	63	23, 42, 56, 69	0
2	B	212/242 (87%)	0.19	10 (4%)	31	33	14, 41, 72, 82	0
2	D	218/242 (90%)	0.13	7 (3%)	47	51	17, 39, 65, 73	0
All	All	857/916 (93%)	0.12	31 (3%)	42	46	14, 39, 66, 82	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	68	GLY	3.6
1	C	77	ARG	3.6
1	A	24	ARG	3.5
2	D	75	SER	3.5
2	B	28	LYS	3.4
2	B	75	SER	3.3
2	B	31	ASP	3.3
2	D	107	CYS	3.3
2	B	30	GLY	2.8
1	A	32	TYR	2.7
1	A	70	ASP	2.6
1	A	31	GLY	2.6
2	B	27	PHE	2.6
2	B	85	ASN	2.5
2	D	76	LYS	2.5
1	C	108	LYS	2.5
2	B	26	GLY	2.4
2	D	28	LYS	2.4
2	D	31	ASP	2.4
1	A	2	ILE	2.4
1	C	24	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
2	B	114	TYR	2.3
1	A	67	SER	2.3
2	B	3	ARG	2.2
2	D	73	ASP	2.2
1	A	27	GLN	2.2
1	A	69	THR	2.1
1	C	16	GLY	2.1
1	C	155	LEU	2.1
2	D	54	ASP	2.1
2	B	87	ARG	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.