Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 07:10 PM GMT

PDB ID	:	1EEA
Title	:	Acetylcholinesterase
Authors	:	Raves, M.L.; Giles, K.; Schrag, J.D.; Schmid, M.F.; Phillips Jr., G.N.; Wah, C.; Howard, A.J.; Silman, I.; Sussman, J.L.
Deposited on	:	1999-01-26
Resolution	:	4.50 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

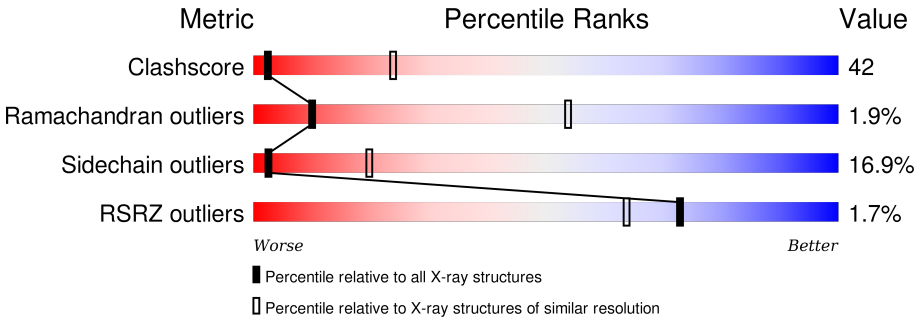
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 4.50 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	102246	1003 (5.30-3.62)
Ramachandran outliers	100387	1117 (5.40-3.60)
Sidechain outliers	100360	1099 (5.40-3.60)
RSRZ outliers	91569	1075 (5.40-3.60)

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	534	2% 35% 44% 16%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 4115 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 PROTEIN (ACETYLCHOLINESTERASE).

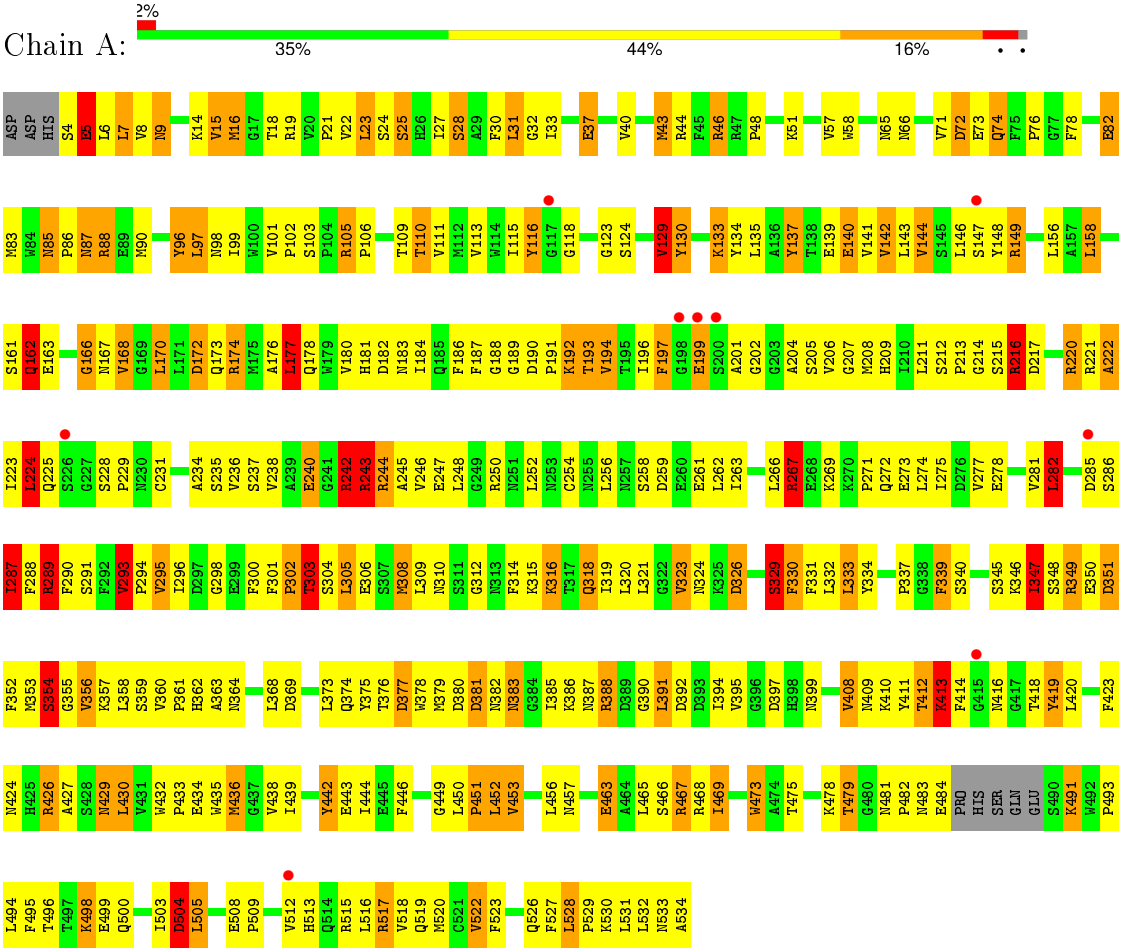
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	526	4115	2663	694	737	21	0	0	0

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: PROTEIN (ACETYLCHOLINESTERASE)

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	F 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	140.86Å 201.46Å 235.77Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 4.50 34.32 – 4.49	Depositor EDS
% Data completeness (in resolution range)	(Not available) ((Not available)-4.50) 81.9 (34.32-4.49)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.59 (at 4.43Å)	Xtriage
Refinement program	?	Depositor
R, R_{free}	(Not available) , (Not available) 0.378 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	107.7	Xtriage
Anisotropy	0.228	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.24 , 34.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	0 of 9717 reflections	Xtriage
F_o,F_c correlation	0.73	EDS
Total number of atoms	4115	wwPDB-VP
Average B, all atoms (Å^2)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.68% 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	1.19	0/4234	2.05	130/5751 (2.3%)

There are no bond length outliers.

All (130) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	216	ARG	NE-CZ-NH1	23.85	132.23	120.30
1	A	243	ARG	NE-CZ-NH1	-15.51	112.55	120.30
1	A	243	ARG	NE-CZ-NH2	15.04	127.82	120.30
1	A	244	ARG	NE-CZ-NH1	14.71	127.65	120.30
1	A	244	ARG	NE-CZ-NH2	-14.21	113.20	120.30
1	A	267	ARG	NE-CZ-NH1	13.37	126.98	120.30
1	A	216	ARG	CD-NE-CZ	12.89	141.65	123.60
1	A	289	ARG	NE-CZ-NH1	12.75	126.67	120.30
1	A	267	ARG	CD-NE-CZ	12.74	141.44	123.60
1	A	216	ARG	NE-CZ-NH2	-11.73	114.43	120.30
1	A	289	ARG	NE-CZ-NH2	-11.55	114.53	120.30
1	A	174	ARG	NE-CZ-NH1	-11.03	114.78	120.30
1	A	273	GLU	OE1-CD-OE2	10.76	136.21	123.30
1	A	434	GLU	CA-CB-CG	10.34	136.15	113.40
1	A	392	ASP	CB-CG-OD1	-10.27	109.06	118.30
1	A	166	GLY	C-N-CA	10.18	147.16	121.70
1	A	293	VAL	N-CA-CB	-9.91	89.70	111.50
1	A	388	ARG	NE-CZ-NH1	9.74	125.17	120.30
1	A	285	ASP	CB-CA-C	9.49	129.37	110.40
1	A	494	LEU	CA-CB-CG	9.40	136.92	115.30
1	A	326	ASP	CB-CG-OD1	-9.38	109.86	118.30
1	A	97	LEU	CA-CB-CG	9.22	136.50	115.30
1	A	426	ARG	CD-NE-CZ	8.82	135.94	123.60
1	A	16	MET	CA-CB-CG	8.68	128.06	113.30
1	A	391	LEU	CB-CA-C	8.64	126.62	110.20
1	A	172	ASP	CB-CG-OD1	8.55	126.00	118.30
1	A	468	ARG	NE-CZ-NH1	-8.36	116.12	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	168	VAL	CA-CB-CG1	8.30	123.36	110.90
1	A	46	ARG	NE-CZ-NH1	7.83	124.22	120.30
1	A	293	VAL	CB-CA-C	7.81	126.23	111.40
1	A	220	ARG	NE-CZ-NH1	7.80	124.20	120.30
1	A	242	ARG	CD-NE-CZ	-7.74	112.77	123.60
1	A	426	ARG	NE-CZ-NH1	-7.70	116.45	120.30
1	A	259	ASP	CB-CG-OD1	7.70	125.23	118.30
1	A	72	ASP	CB-CG-OD1	7.68	125.21	118.30
1	A	105	ARG	NE-CZ-NH1	7.57	124.09	120.30
1	A	242	ARG	NE-CZ-NH1	-7.48	116.56	120.30
1	A	522	VAL	CA-CB-CG1	7.43	122.05	110.90
1	A	220	ARG	NE-CZ-NH2	-7.34	116.63	120.30
1	A	170	LEU	CB-CA-C	7.34	124.15	110.20
1	A	504	ASP	N-CA-CB	7.33	123.80	110.60
1	A	436	MET	CA-CB-CG	7.32	125.74	113.30
1	A	289	ARG	CB-CA-C	7.30	124.99	110.40
1	A	484	GLU	CA-CB-CG	7.26	129.37	113.40
1	A	305	LEU	CA-CB-CG	7.23	131.93	115.30
1	A	442	TYR	CB-CA-C	7.22	124.85	110.40
1	A	217	ASP	CB-CG-OD1	7.14	124.73	118.30
1	A	168	VAL	CB-CA-C	7.02	124.74	111.40
1	A	228	SER	CB-CA-C	6.99	123.37	110.10
1	A	174	ARG	CD-NE-CZ	-6.98	113.82	123.60
1	A	220	ARG	CA-CB-CG	6.95	128.68	113.40
1	A	282	LEU	CA-CB-CG	6.93	131.23	115.30
1	A	351	ASP	CB-CG-OD1	-6.78	112.20	118.30
1	A	323	VAL	N-CA-CB	-6.75	96.65	111.50
1	A	194	VAL	O-C-N	6.66	133.35	122.70
1	A	368	LEU	CB-CA-C	6.52	122.59	110.20
1	A	201	ALA	CB-CA-C	6.48	119.83	110.10
1	A	137	TYR	CB-CG-CD1	6.39	124.83	121.00
1	A	308	MET	CG-SD-CE	6.38	110.40	100.20
1	A	85	ASN	CA-CB-CG	6.37	127.42	113.40
1	A	144	VAL	CA-CB-CG2	6.36	120.44	110.90
1	A	285	ASP	N-CA-C	-6.25	94.14	111.00
1	A	468	ARG	NE-CZ-NH2	6.24	123.42	120.30
1	A	326	ASP	CB-CG-OD2	6.23	123.91	118.30
1	A	436	MET	CB-CA-C	6.20	122.79	110.40
1	A	221	ARG	NE-CZ-NH2	-6.19	117.21	120.30
1	A	463	GLU	CG-CD-OE1	6.15	130.60	118.30
1	A	391	LEU	CA-CB-CG	6.11	129.35	115.30
1	A	170	LEU	CA-CB-CG	6.09	129.30	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	129	VAL	O-C-N	6.04	132.37	122.70
1	A	97	LEU	CB-CA-C	6.03	121.66	110.20
1	A	413	LYS	N-CA-CB	6.01	121.43	110.60
1	A	147	SER	N-CA-CB	6.01	119.51	110.50
1	A	290	PHE	CB-CA-C	6.00	122.41	110.40
1	A	149	ARG	CD-NE-CZ	5.94	131.91	123.60
1	A	148	TYR	CA-CB-CG	5.91	124.63	113.40
1	A	354	SER	N-CA-CB	5.91	119.36	110.50
1	A	303	THR	N-CA-CB	5.90	121.51	110.30
1	A	302	PRO	N-CD-CG	-5.89	94.36	103.20
1	A	16	MET	CB-CA-C	5.89	122.17	110.40
1	A	293	VAL	CG1-CB-CG2	5.83	120.23	110.90
1	A	254	CYS	O-C-N	5.82	132.01	122.70
1	A	65	ASN	O-C-N	5.82	132.01	122.70
1	A	380	ASP	CB-CG-OD2	5.81	123.53	118.30
1	A	467	ARG	CD-NE-CZ	5.79	131.71	123.60
1	A	222	ALA	N-CA-CB	-5.78	102.01	110.10
1	A	37	GLU	OE1-CD-OE2	5.77	130.23	123.30
1	A	339	PHE	O-C-N	5.77	131.94	122.70
1	A	442	TYR	CA-CB-CG	-5.76	102.45	113.40
1	A	505	LEU	CA-CB-CG	5.74	128.51	115.30
1	A	505	LEU	CB-CA-C	5.74	121.10	110.20
1	A	278	GLU	CB-CG-CD	5.71	129.62	114.20
1	A	177	LEU	CB-CA-C	5.71	121.04	110.20
1	A	88	ARG	CA-CB-CG	5.68	125.90	113.40
1	A	43	MET	CA-CB-CG	-5.67	103.66	113.30
1	A	347	ILE	CB-CG1-CD1	5.63	129.67	113.90
1	A	244	ARG	CD-NE-CZ	5.62	131.46	123.60
1	A	96	TYR	CA-CB-CG	-5.61	102.73	113.40
1	A	31	LEU	CA-C-O	5.61	131.88	120.10
1	A	426	ARG	CA-CB-CG	5.59	125.70	113.40
1	A	442	TYR	CB-CG-CD2	-5.58	117.66	121.00
1	A	273	GLU	CG-CD-OE2	-5.55	107.19	118.30
1	A	419	TYR	CB-CG-CD1	-5.54	117.68	121.00
1	A	217	ASP	OD1-CG-OD2	-5.53	112.79	123.30
1	A	216	ARG	NH1-CZ-NH2	-5.53	113.32	119.40
1	A	162	GLN	CB-CG-CD	5.52	125.94	111.60
1	A	224	LEU	O-C-N	5.49	131.48	122.70
1	A	174	ARG	NH1-CZ-NH2	5.47	125.42	119.40
1	A	162	GLN	N-CA-CB	5.46	120.42	110.60
1	A	158	LEU	CA-CB-CG	5.46	127.85	115.30
1	A	231	CYS	CA-CB-SG	-5.43	104.22	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	130	TYR	CB-CG-CD1	5.41	124.25	121.00
1	A	377	ASP	CB-CG-OD1	5.38	123.14	118.30
1	A	287	ILE	CB-CA-C	5.36	122.32	111.60
1	A	526	GLN	CA-CB-CG	5.34	125.14	113.40
1	A	339	PHE	CA-C-O	-5.33	108.92	120.10
1	A	137	TYR	CB-CG-CD2	-5.26	117.85	121.00
1	A	199	GLU	CB-CA-C	-5.25	99.91	110.40
1	A	350	GLU	N-CA-CB	5.21	119.98	110.60
1	A	382	ASN	O-C-N	5.17	130.98	122.70
1	A	522	VAL	CB-CA-C	5.16	121.20	111.40
1	A	517	ARG	CA-CB-CG	5.13	124.69	113.40
1	A	305	LEU	CB-CG-CD1	5.10	119.68	111.00
1	A	388	ARG	CG-CD-NE	5.10	122.52	111.80
1	A	130	TYR	CB-CG-CD2	-5.09	117.95	121.00
1	A	142	VAL	CB-CA-C	5.09	121.07	111.40
1	A	517	ARG	NE-CZ-NH1	-5.08	117.76	120.30
1	A	161	SER	N-CA-CB	-5.06	102.92	110.50
1	A	267	ARG	NE-CZ-NH2	-5.05	117.77	120.30
1	A	83	MET	CB-CG-SD	-5.00	97.40	112.40

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	4115	0	3958	340	17
All	All	4115	0	3958	340	17

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 42.

All (340) 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:25:SER:HB2	1:A:137:TYR:HE2	1.15	1.11
1:A:433:PRO:HD2	1:A:436:MET:HE3	1.24	1.09
1:A:349:ARG:HH11	1:A:349:ARG:HG3	1.25	0.98
1:A:339:PHE:HZ	1:A:391:LEU:HD23	1.33	0.94
1:A:25:SER:HB2	1:A:137:TYR:CE2	2.05	0.92
1:A:240:GLU:OE1	1:A:243:ARG:HD3	1.70	0.92
1:A:453:VAL:CG2	1:A:456:LEU:HG	1.98	0.92
1:A:225:GLN:HE22	1:A:473:TRP:HE1	1.19	0.91
1:A:479:THR:HG22	1:A:481:ASN:H	1.35	0.90
1:A:243:ARG:HH12	1:A:244:ARG:HG2	1.34	0.90
1:A:87:ASN:HD22	1:A:87:ASN:H	1.22	0.87
1:A:27:ILE:HD12	1:A:137:TYR:HB2	1.54	0.86
1:A:410:LYS:O	1:A:413:LYS:HE2	1.75	0.86
1:A:449:GLY:HA2	1:A:466:SER:OG	1.77	0.85
1:A:190:ASP:OD1	1:A:192:LYS:HG2	1.77	0.84
1:A:27:ILE:CD1	1:A:137:TYR:HB2	2.07	0.84
1:A:349:ARG:HG3	1:A:349:ARG:NH1	1.85	0.84
1:A:303:THR:HG22	1:A:304:SER:H	1.40	0.84
1:A:508:GLU:HB3	1:A:509:PRO:HD2	1.59	0.84
1:A:208:MET:HG2	1:A:229:PRO:HB3	1.61	0.81
1:A:170:LEU:HD11	1:A:208:MET:HE3	1.59	0.81
1:A:433:PRO:HD2	1:A:436:MET:CE	2.09	0.80
1:A:73:GLU:O	1:A:76:PRO:HD3	1.83	0.79
1:A:433:PRO:CD	1:A:436:MET:HE3	2.11	0.78
1:A:339:PHE:CZ	1:A:391:LEU:HD23	2.19	0.78
1:A:296:ILE:HD12	1:A:305:LEU:HD13	1.64	0.78
1:A:408:VAL:O	1:A:412:THR:HG23	1.84	0.78
1:A:360:VAL:HG12	1:A:363:ALA:HB2	1.64	0.78
1:A:345:SER:O	1:A:347:ILE:HD13	1.83	0.77
1:A:176:ALA:O	1:A:180:VAL:HG23	1.85	0.77
1:A:413:LYS:HE3	1:A:414:PHE:CE1	2.21	0.76
1:A:243:ARG:NH1	1:A:244:ARG:HG2	1.99	0.76
1:A:48:PRO:HG3	1:A:172:ASP:OD1	1.85	0.76
1:A:178:GLN:O	1:A:181:HIS:HB3	1.86	0.76
1:A:306:GLU:O	1:A:310:ASN:HB2	1.86	0.75
1:A:432:TRP:CE3	1:A:436:MET:HE1	2.22	0.75
1:A:9:ASN:ND2	1:A:14:LYS:HZ3	1.85	0.75
1:A:289:ARG:NH2	1:A:399:ASN:OD1	2.19	0.74
1:A:452:LEU:HD12	1:A:463:GLU:HG2	1.69	0.74
1:A:496:THR:CG2	1:A:498:LYS:HB3	2.17	0.74
1:A:87:ASN:HD22	1:A:87:ASN:N	1.81	0.74
1:A:258:SER:OG	1:A:261:GLU:HG2	1.88	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:282:LEU:HD13	1:A:291:SER:OG	1.88	0.74
1:A:312:GLY:O	1:A:316:LYS:HE2	1.86	0.73
1:A:193:THR:HG23	1:A:220:ARG:NH1	2.03	0.73
1:A:87:ASN:H	1:A:87:ASN:ND2	1.87	0.73
1:A:321:LEU:O	1:A:420:LEU:HA	1.89	0.72
1:A:469:ILE:HD11	1:A:505:LEU:HG	1.72	0.72
1:A:211:LEU:HD11	1:A:309:LEU:HD12	1.73	0.71
1:A:134:TYR:CE2	1:A:453:VAL:HG12	2.25	0.71
1:A:427:ALA:HB1	1:A:429:ASN:ND2	2.06	0.70
1:A:453:VAL:HG22	1:A:456:LEU:HG	1.74	0.69
1:A:346:LYS:HD3	1:A:385:ILE:HD11	1.72	0.69
1:A:170:LEU:HD11	1:A:208:MET:CE	2.22	0.69
1:A:216:ARG:CG	1:A:315:LYS:HB2	2.23	0.69
1:A:40:VAL:O	1:A:43:MET:HB2	1.92	0.68
1:A:216:ARG:HG3	1:A:315:LYS:HB2	1.76	0.68
1:A:339:PHE:HA	1:A:345:SER:HB3	1.76	0.68
1:A:349:ARG:NE	1:A:381:ASP:O	2.27	0.67
1:A:146:LEU:C	1:A:146:LEU:HD12	2.15	0.67
1:A:452:LEU:HD12	1:A:463:GLU:CG	2.24	0.67
1:A:192:LYS:O	1:A:220:ARG:NH1	2.26	0.67
1:A:7:LEU:HB2	1:A:16:MET:HE2	1.74	0.67
1:A:261:GLU:OE1	1:A:261:GLU:HA	1.95	0.66
1:A:19:ARG:HG3	1:A:19:ARG:HH11	1.60	0.66
1:A:216:ARG:O	1:A:315:LYS:HD2	1.95	0.66
1:A:475:THR:O	1:A:479:THR:HB	1.96	0.66
1:A:19:ARG:HG3	1:A:19:ARG:NH1	2.11	0.66
1:A:46:ARG:HD2	1:A:162:GLN:NE2	2.11	0.66
1:A:320:LEU:C	1:A:320:LEU:HD23	2.17	0.65
1:A:110:THR:OG1	1:A:478:LYS:HB3	1.96	0.65
1:A:429:ASN:ND2	1:A:429:ASN:H	1.94	0.64
1:A:225:GLN:NE2	1:A:473:TRP:HE1	1.93	0.64
1:A:170:LEU:HD21	1:A:208:MET:HE1	1.78	0.64
1:A:347:ILE:HG23	1:A:351:ASP:HB3	1.79	0.64
1:A:349:ARG:CG	1:A:349:ARG:HH11	2.06	0.64
1:A:346:LYS:HD3	1:A:385:ILE:CD1	2.28	0.64
1:A:166:GLY:O	1:A:168:VAL:HG23	1.98	0.64
1:A:106:PRO:CG	1:A:109:THR:HG21	2.28	0.63
1:A:193:THR:HG22	1:A:220:ARG:HG2	1.78	0.63
1:A:347:ILE:HG23	1:A:351:ASP:CB	2.29	0.63
1:A:7:LEU:HD23	1:A:16:MET:CE	2.29	0.63
1:A:246:VAL:HG23	1:A:256:LEU:HD13	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:355:GLY:HA3	1:A:391:LEU:HD11	1.81	0.62
1:A:413:LYS:HE3	1:A:414:PHE:HE1	1.65	0.62
1:A:72:ASP:OD2	1:A:334:TYR:HE2	1.83	0.62
1:A:236:VAL:O	1:A:295:VAL:HA	1.99	0.61
1:A:6:LEU:HD12	1:A:28:SER:OG	2.01	0.61
1:A:450:LEU:C	1:A:452:LEU:H	2.04	0.61
1:A:303:THR:CG2	1:A:304:SER:H	2.02	0.61
1:A:177:LEU:HD11	1:A:196:ILE:HG22	1.83	0.61
1:A:324:ASN:ND2	1:A:423:PHE:HB3	2.16	0.61
1:A:359:SER:C	1:A:361:PRO:HD3	2.21	0.61
1:A:212:SER:HB2	1:A:300:PHE:O	2.00	0.61
1:A:433:PRO:HB2	1:A:435:TRP:CD1	2.36	0.61
1:A:170:LEU:HD21	1:A:208:MET:CE	2.31	0.60
1:A:397:ASP:OD1	1:A:517:ARG:NH1	2.34	0.60
1:A:204:ALA:O	1:A:208:MET:HG3	2.02	0.60
1:A:345:SER:O	1:A:388:ARG:HG3	2.02	0.60
1:A:240:GLU:OE2	1:A:244:ARG:NE	2.34	0.59
1:A:86:PRO:HG2	1:A:90:MET:HE1	1.84	0.59
1:A:243:ARG:HH12	1:A:244:ARG:CG	2.13	0.59
1:A:85:ASN:HB3	1:A:86:PRO:HD2	1.83	0.59
1:A:353:MET:O	1:A:357:LYS:HE3	2.03	0.59
1:A:408:VAL:CG1	1:A:409:ASN:N	2.66	0.58
1:A:223:ILE:HA	1:A:320:LEU:O	2.02	0.58
1:A:316:LYS:HB3	1:A:414:PHE:O	2.03	0.58
1:A:339:PHE:HA	1:A:345:SER:CB	2.33	0.58
1:A:184:ILE:HA	1:A:187:PHE:HD2	1.67	0.58
1:A:354:SER:HA	1:A:357:LYS:HE3	1.85	0.58
1:A:504:ASP:OD2	1:A:513:HIS:HE1	1.86	0.58
1:A:395:VAL:O	1:A:399:ASN:HB2	2.03	0.58
1:A:106:PRO:HG2	1:A:109:THR:HG21	1.86	0.58
1:A:333:LEU:HD12	1:A:436:MET:HE1	1.86	0.57
1:A:9:ASN:ND2	1:A:14:LYS:NZ	2.52	0.57
1:A:208:MET:HE1	1:A:294:PRO:HG2	1.85	0.57
1:A:189:GLY:O	1:A:191:PRO:HD3	2.04	0.57
1:A:449:GLY:O	1:A:452:LEU:HB2	2.05	0.57
1:A:235:SER:HA	1:A:294:PRO:O	2.04	0.57
1:A:247:GLU:CD	1:A:250:ARG:HE	2.07	0.57
1:A:496:THR:HG22	1:A:498:LYS:HB3	1.87	0.56
1:A:46:ARG:CD	1:A:162:GLN:NE2	2.69	0.56
1:A:324:ASN:HD22	1:A:423:PHE:HB3	1.69	0.56
1:A:32:GLY:HA2	1:A:96:TYR:HB3	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:418:THR:HB	1:A:495:PHE:HB3	1.87	0.56
1:A:427:ALA:HB1	1:A:429:ASN:HD21	1.70	0.56
1:A:349:ARG:HH21	1:A:376:THR:HG23	1.71	0.56
1:A:450:LEU:N	1:A:451:PRO:CD	2.69	0.56
1:A:360:VAL:CG1	1:A:363:ALA:HB2	2.32	0.56
1:A:78:PHE:HE2	1:A:432:TRP:CZ3	2.23	0.56
1:A:27:ILE:HD11	1:A:137:TYR:HB2	1.87	0.55
1:A:498:LYS:HG3	1:A:499:GLU:CG	2.36	0.55
1:A:192:LYS:O	1:A:193:THR:HG23	2.07	0.55
1:A:258:SER:O	1:A:261:GLU:HB2	2.06	0.55
1:A:37:GLU:HG2	1:A:51:LYS:HA	1.86	0.55
1:A:98:ASN:O	1:A:144:VAL:HA	2.07	0.55
1:A:349:ARG:CD	1:A:381:ASP:O	2.55	0.55
1:A:528:LEU:HB3	1:A:529:PRO:HD3	1.89	0.55
1:A:432:TRP:CE3	1:A:436:MET:CE	2.89	0.55
1:A:302:PRO:HD2	1:A:308:MET:CE	2.36	0.55
1:A:7:LEU:HD13	1:A:7:LEU:C	2.27	0.55
1:A:520:MET:O	1:A:523:PHE:HB3	2.07	0.54
1:A:310:ASN:OD1	1:A:410:LYS:NZ	2.38	0.54
1:A:286:SER:HB3	1:A:361:PRO:HG3	1.89	0.54
1:A:208:MET:HB3	1:A:301:PHE:CZ	2.43	0.54
1:A:211:LEU:HD11	1:A:309:LEU:CD1	2.38	0.54
1:A:408:VAL:HG22	1:A:418:THR:HG21	1.89	0.54
1:A:72:ASP:OD2	1:A:334:TYR:CE2	2.61	0.53
1:A:479:THR:HG22	1:A:481:ASN:N	2.13	0.53
1:A:247:GLU:HB3	1:A:281:VAL:HG12	1.89	0.53
1:A:296:ILE:CD1	1:A:305:LEU:HD13	2.35	0.53
1:A:7:LEU:HD23	1:A:16:MET:HE2	1.90	0.53
1:A:7:LEU:HD23	1:A:16:MET:HE3	1.90	0.53
1:A:74:GLN:C	1:A:76:PRO:HD3	2.29	0.53
1:A:110:THR:OG1	1:A:478:LYS:CB	2.56	0.52
1:A:321:LEU:HD21	1:A:408:VAL:HG23	1.91	0.52
1:A:424:ASN:N	1:A:424:ASN:OD1	2.41	0.52
1:A:286:SER:CB	1:A:361:PRO:HG3	2.39	0.52
1:A:9:ASN:HD21	1:A:14:LYS:NZ	2.08	0.52
1:A:8:VAL:HG11	1:A:187:PHE:CE1	2.44	0.52
1:A:242:ARG:O	1:A:245:ALA:HB3	2.09	0.52
1:A:22:VAL:O	1:A:23:LEU:C	2.48	0.52
1:A:412:THR:HG21	1:A:495:PHE:HD2	1.75	0.52
1:A:446:PHE:CE2	1:A:465:LEU:HD23	2.45	0.52
1:A:15:VAL:HG22	1:A:58:TRP:HB3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:208:MET:CE	1:A:294:PRO:HG2	2.40	0.52
1:A:208:MET:HE1	1:A:294:PRO:CG	2.40	0.51
1:A:503:ILE:HG22	1:A:512:VAL:HG22	1.91	0.51
1:A:66:ASN:ND2	1:A:88:ARG:H	2.09	0.51
1:A:312:GLY:HA2	1:A:314:PHE:CE2	2.45	0.51
1:A:208:MET:HB3	1:A:301:PHE:CE1	2.45	0.51
1:A:496:THR:HG22	1:A:499:GLU:H	1.76	0.51
1:A:109:THR:HG22	1:A:188:GLY:O	2.11	0.51
1:A:252:LEU:HD13	1:A:269:LYS:HG3	1.92	0.51
1:A:44:ARG:O	1:A:267:ARG:NH1	2.37	0.51
1:A:377:ASP:OD1	1:A:377:ASP:O	2.27	0.51
1:A:106:PRO:HG2	1:A:109:THR:CG2	2.41	0.50
1:A:216:ARG:HG2	1:A:315:LYS:HB2	1.92	0.50
1:A:319:ILE:HG13	1:A:319:ILE:O	2.11	0.50
1:A:177:LEU:HD11	1:A:196:ILE:CG2	2.40	0.50
1:A:173:GLN:OE1	1:A:209:HIS:HE1	1.95	0.50
1:A:22:VAL:HG23	1:A:133:LYS:HG3	1.93	0.50
1:A:135:LEU:HB3	1:A:143:LEU:CD1	2.42	0.50
1:A:129:VAL:HG12	1:A:450:LEU:HD22	1.94	0.49
1:A:450:LEU:O	1:A:452:LEU:N	2.46	0.49
1:A:204:ALA:O	1:A:208:MET:CG	2.60	0.49
1:A:238:VAL:HA	1:A:295:VAL:HG22	1.94	0.49
1:A:87:ASN:N	1:A:87:ASN:ND2	2.45	0.49
1:A:111:VAL:HG13	1:A:142:VAL:HG12	1.94	0.49
1:A:4:SER:O	1:A:6:LEU:N	2.46	0.49
1:A:314:PHE:CE1	1:A:411:TYR:CE1	3.01	0.49
1:A:456:LEU:O	1:A:457:ASN:HB2	2.14	0.48
1:A:527:PHE:CZ	1:A:531:LEU:HD12	2.48	0.48
1:A:5:GLU:HA	1:A:5:GLU:OE1	2.14	0.48
1:A:450:LEU:C	1:A:452:LEU:N	2.66	0.48
1:A:515:ARG:HB3	1:A:518:VAL:HB	1.96	0.48
1:A:333:LEU:HD12	1:A:436:MET:CE	2.44	0.48
1:A:243:ARG:NH1	1:A:244:ARG:CG	2.72	0.48
1:A:46:ARG:NE	1:A:162:GLN:NE2	2.60	0.48
1:A:207:GLY:HA3	1:A:229:PRO:HD3	1.95	0.48
1:A:234:ALA:O	1:A:294:PRO:HD2	2.14	0.48
1:A:349:ARG:HD3	1:A:381:ASP:O	2.12	0.48
1:A:376:THR:HG22	1:A:378:TRP:H	1.79	0.48
1:A:413:LYS:CE	1:A:414:PHE:CE1	2.94	0.48
1:A:346:LYS:CD	1:A:385:ILE:CD1	2.92	0.48
1:A:71:VAL:CG2	1:A:90:MET:HE1	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:46:ARG:NH2	1:A:162:GLN:OE1	2.47	0.47
1:A:330:PHE:HE2	1:A:442:TYR:HE1	1.61	0.47
1:A:432:TRP:HB3	1:A:436:MET:HE3	1.95	0.47
1:A:491:LYS:N	1:A:491:LYS:HE2	2.29	0.47
1:A:451:PRO:HG2	1:A:466:SER:HB2	1.97	0.47
1:A:7:LEU:CD1	1:A:7:LEU:C	2.82	0.47
1:A:158:LEU:HD12	1:A:263:ILE:HD11	1.97	0.47
1:A:170:LEU:HG	1:A:300:PHE:CZ	2.50	0.47
1:A:346:LYS:HG2	1:A:385:ILE:HD13	1.96	0.47
1:A:429:ASN:N	1:A:429:ASN:ND2	2.60	0.47
1:A:246:VAL:HG23	1:A:256:LEU:CD1	2.45	0.47
1:A:213:PRO:HA	1:A:216:ARG:HD3	1.96	0.47
1:A:503:ILE:CG2	1:A:512:VAL:HG22	2.45	0.47
1:A:287:ILE:HD11	1:A:331:PHE:C	2.36	0.46
1:A:7:LEU:HD21	1:A:57:VAL:HG22	1.98	0.46
1:A:263:ILE:O	1:A:267:ARG:HG3	2.16	0.46
1:A:452:LEU:CD1	1:A:463:GLU:HG2	2.43	0.46
1:A:339:PHE:CZ	1:A:391:LEU:CD2	2.96	0.46
1:A:46:ARG:CZ	1:A:162:GLN:OE1	2.64	0.46
1:A:130:TYR:HE1	1:A:444:ILE:HD13	1.80	0.46
1:A:433:PRO:HG2	1:A:436:MET:HE2	1.98	0.46
1:A:223:ILE:HG23	1:A:320:LEU:HD22	1.98	0.46
1:A:223:ILE:HD13	1:A:473:TRP:CD1	2.50	0.46
1:A:163:GLU:HB3	1:A:267:ARG:HH22	1.80	0.46
1:A:491:LYS:O	1:A:493:PRO:HD3	2.15	0.46
1:A:139:GLU:O	1:A:140:GLU:C	2.53	0.46
1:A:223:ILE:HG23	1:A:320:LEU:CD2	2.46	0.46
1:A:73:GLU:O	1:A:76:PRO:CD	2.58	0.46
1:A:364:ASN:N	1:A:364:ASN:OD1	2.47	0.46
1:A:348:SER:OG	1:A:351:ASP:HB2	2.15	0.45
1:A:413:LYS:CE	1:A:414:PHE:HE1	2.29	0.45
1:A:360:VAL:N	1:A:361:PRO:HD3	2.32	0.45
1:A:199:GLU:HA	1:A:225:GLN:O	2.15	0.45
1:A:321:LEU:HD21	1:A:408:VAL:CG2	2.46	0.45
1:A:82:GLU:HA	1:A:85:ASN:HD22	1.81	0.45
1:A:177:LEU:HD21	1:A:196:ILE:HG21	1.97	0.45
1:A:6:LEU:CD1	1:A:28:SER:OG	2.64	0.45
1:A:298:GLY:HA2	1:A:301:PHE:O	2.15	0.45
1:A:430:LEU:HA	1:A:430:LEU:HD23	1.79	0.45
1:A:236:VAL:HG13	1:A:293:VAL:HG12	1.98	0.45
1:A:116:TYR:CE1	1:A:123:GLY:HA3	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:22:VAL:HG13	1:A:137:TYR:CD2	2.51	0.45
1:A:72:ASP:N	1:A:85:ASN:OD1	2.48	0.45
1:A:33:ILE:HD12	1:A:99:ILE:HD12	1.98	0.45
1:A:333:LEU:C	1:A:333:LEU:CD2	2.84	0.45
1:A:149:ARG:NH2	1:A:168:VAL:HG13	2.32	0.45
1:A:375:TYR:CZ	1:A:520:MET:SD	3.10	0.45
1:A:135:LEU:HD23	1:A:143:LEU:HD11	1.98	0.45
1:A:174:ARG:NH2	1:A:214:GLY:HA3	2.32	0.45
1:A:333:LEU:O	1:A:333:LEU:HD23	2.17	0.45
1:A:463:GLU:O	1:A:467:ARG:HG3	2.17	0.45
1:A:346:LYS:CD	1:A:385:ILE:HD13	2.46	0.45
1:A:360:VAL:N	1:A:361:PRO:CD	2.80	0.45
1:A:158:LEU:HD11	1:A:262:LEU:HD13	1.98	0.44
1:A:349:ARG:HA	1:A:349:ARG:HD2	1.81	0.44
1:A:432:TRP:HE3	1:A:436:MET:CE	2.30	0.44
1:A:453:VAL:HG22	1:A:456:LEU:CG	2.44	0.44
1:A:134:TYR:CE2	1:A:453:VAL:CG1	2.97	0.44
1:A:149:ARG:HH22	1:A:168:VAL:HG13	1.82	0.44
1:A:236:VAL:HG13	1:A:293:VAL:CG1	2.48	0.44
1:A:491:LYS:HE2	1:A:491:LYS:H	1.81	0.44
1:A:66:ASN:O	1:A:90:MET:HA	2.18	0.44
1:A:412:THR:HG22	1:A:418:THR:OG1	2.17	0.44
1:A:71:VAL:HG22	1:A:90:MET:HE1	2.00	0.44
1:A:287:ILE:HG22	1:A:358:LEU:C	2.38	0.44
1:A:450:LEU:N	1:A:451:PRO:HD2	2.33	0.44
1:A:453:VAL:CG2	1:A:456:LEU:CG	2.83	0.43
1:A:272:GLN:NE2	1:A:275:ILE:HB	2.33	0.43
1:A:326:ASP:HB2	1:A:438:VAL:O	2.19	0.43
1:A:197:PHE:HD1	1:A:197:PHE:H	1.65	0.43
1:A:504:ASP:OD2	1:A:513:HIS:CE1	2.68	0.43
1:A:330:PHE:CD2	1:A:439:ILE:CG2	3.01	0.43
1:A:113:VAL:HG13	1:A:144:VAL:HG22	2.01	0.43
1:A:101:VAL:HA	1:A:102:PRO:HD3	1.85	0.43
1:A:258:SER:OG	1:A:261:GLU:CG	2.62	0.43
1:A:44:ARG:NH1	1:A:266:LEU:O	2.52	0.43
1:A:224:LEU:HD12	1:A:224:LEU:N	2.34	0.43
1:A:318:GLN:HE22	1:A:416:ASN:HD22	1.67	0.43
1:A:196:ILE:O	1:A:196:ILE:HG13	2.19	0.42
1:A:115:ILE:O	1:A:202:GLY:HA3	2.19	0.42
1:A:332:LEU:O	1:A:333:LEU:C	2.56	0.42
1:A:240:GLU:O	1:A:244:ARG:HG3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:206:VAL:O	1:A:207:GLY:C	2.57	0.42
1:A:337:PRO:HG2	1:A:337:PRO:O	2.19	0.42
1:A:433:PRO:HG2	1:A:436:MET:CE	2.48	0.42
1:A:360:VAL:HG12	1:A:363:ALA:CB	2.43	0.42
1:A:383:ASN:OD1	1:A:386:LYS:HG3	2.19	0.42
1:A:352:PHE:O	1:A:356:VAL:HG13	2.19	0.42
1:A:314:PHE:CE1	1:A:411:TYR:CD1	3.08	0.42
1:A:209:HIS:HD2	1:A:215:SER:OG	2.03	0.42
1:A:182:ASP:C	1:A:183:ASN:ND2	2.73	0.42
1:A:139:GLU:O	1:A:140:GLU:O	2.37	0.42
1:A:78:PHE:HE2	1:A:432:TRP:CE3	2.38	0.42
1:A:349:ARG:HD3	1:A:387:ASN:HD21	1.84	0.42
1:A:21:PRO:O	1:A:133:LYS:HE2	2.20	0.42
1:A:178:GLN:O	1:A:181:HIS:CB	2.63	0.42
1:A:528:LEU:HD22	1:A:532:LEU:HG	2.01	0.42
1:A:22:VAL:CG1	1:A:137:TYR:CD2	3.03	0.41
1:A:129:VAL:HG12	1:A:450:LEU:CD2	2.50	0.41
1:A:298:GLY:CA	1:A:301:PHE:O	2.68	0.41
1:A:236:VAL:HG23	1:A:237:SER:O	2.20	0.41
1:A:498:LYS:HG3	1:A:499:GLU:N	2.34	0.41
1:A:430:LEU:HD21	1:A:442:TYR:CD2	2.55	0.41
1:A:355:GLY:O	1:A:358:LEU:HB2	2.20	0.41
1:A:481:ASN:OD1	1:A:483:ASN:HB2	2.19	0.41
1:A:378:TRP:CE3	1:A:378:TRP:HA	2.56	0.41
1:A:222:ALA:HB3	1:A:319:ILE:HG22	2.02	0.41
1:A:271:PRO:O	1:A:275:ILE:HG13	2.21	0.41
1:A:419:TYR:CE2	1:A:482:PRO:HD2	2.55	0.41
1:A:170:LEU:CD2	1:A:208:MET:HE1	2.47	0.41
1:A:250:ARG:HG3	1:A:256:LEU:HD11	2.02	0.41
1:A:242:ARG:HH11	1:A:242:ARG:HD2	1.54	0.41
1:A:408:VAL:HG12	1:A:409:ASN:N	2.36	0.41
1:A:96:TYR:CD1	1:A:96:TYR:N	2.89	0.41
1:A:318:GLN:NE2	1:A:416:ASN:HD22	2.18	0.41
1:A:533:ASN:O	1:A:534:ALA:C	2.59	0.41
1:A:433:PRO:CD	1:A:436:MET:CE	2.85	0.41
1:A:173:GLN:OE1	1:A:205:SER:HB3	2.20	0.41
1:A:443:GLU:HG2	1:A:444:ILE:N	2.35	0.41
1:A:27:ILE:CG2	1:A:28:SER:N	2.84	0.41
1:A:329:SER:HB3	1:A:436:MET:HB3	2.02	0.41
1:A:7:LEU:HD13	1:A:8:VAL:N	2.36	0.41
1:A:149:ARG:NH2	1:A:168:VAL:CG1	2.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:439:ILE:O	1:A:442:TYR:HB2	2.21	0.41
1:A:248:LEU:HD12	1:A:277:VAL:HG23	2.03	0.41
1:A:390:GLY:O	1:A:394:ILE:HG13	2.21	0.41
1:A:410:LYS:HD2	1:A:410:LYS:HA	1.84	0.41
1:A:182:ASP:OD1	1:A:182:ASP:N	2.53	0.41
1:A:453:VAL:HG23	1:A:456:LEU:HG	1.97	0.40
1:A:354:SER:HA	1:A:357:LYS:CE	2.51	0.40
1:A:135:LEU:HB3	1:A:143:LEU:HD12	2.03	0.40
1:A:443:GLU:O	1:A:444:ILE:C	2.59	0.40
1:A:30:PHE:HB3	1:A:33:ILE:HD11	2.02	0.40
1:A:246:VAL:CG2	1:A:256:LEU:HD13	2.51	0.40

All (17) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:379:MET:SD	1:A:515:ARG:CG[2_555]	0.62	1.58
1:A:379:MET:SD	1:A:515:ARG:CD[2_555]	1.08	1.12
1:A:14:LYS:CE	1:A:186:PHE:CE1[14_555]	1.17	1.03
1:A:379:MET:CG	1:A:515:ARG:CD[2_555]	1.51	0.69
1:A:14:LYS:CE	1:A:186:PHE:CZ[14_555]	1.53	0.67
1:A:369:ASP:OD2	1:A:530:LYS:NZ[2_555]	1.62	0.58
1:A:14:LYS:NZ	1:A:186:PHE:CE1[14_555]	1.63	0.57
1:A:379:MET:CB	1:A:515:ARG:NE[2_555]	1.76	0.44
1:A:379:MET:CB	1:A:515:ARG:CD[2_555]	1.87	0.33
1:A:373:LEU:CD2	1:A:527:PHE:CB[2_555]	1.91	0.29
1:A:19:ARG:NE	1:A:19:ARG:NE[8_555]	1.93	0.27
1:A:379:MET:SD	1:A:515:ARG:CB[2_555]	1.94	0.26
1:A:379:MET:CE	1:A:500:GLN:NE2[2_555]	2.00	0.20
1:A:379:MET:SD	1:A:515:ARG:NE[2_555]	2.06	0.14
1:A:14:LYS:NZ	1:A:186:PHE:CD1[14_555]	2.11	0.09
1:A:379:MET:CE	1:A:515:ARG:CG[2_555]	2.17	0.03
1:A:379:MET:CE	1:A:500:GLN:CD[2_555]	2.17	0.03

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	522/534 (98%)	455 (87%)	57 (11%)	10 (2%)	10 54

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	167	ASN
1	A	5	GLU
1	A	25	SER
1	A	381	ASP
1	A	216	ARG
1	A	329	SER
1	A	451	PRO
1	A	140	GLU
1	A	498	LYS
1	A	118	GLY

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	432/467 (92%)	359 (83%)	73 (17%)	2 20

All (73) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	GLU
1	A	7	LEU
1	A	9	ASN
1	A	15	VAL
1	A	18	THR
1	A	23	LEU
1	A	24	SER

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Mol	Chain	Res	Type
1	A	28	SER
1	A	31	LEU
1	A	74	GLN
1	A	82	GLU
1	A	87	ASN
1	A	97	LEU
1	A	103	SER
1	A	105	ARG
1	A	110	THR
1	A	116	TYR
1	A	124	SER
1	A	129	VAL
1	A	133	LYS
1	A	141	VAL
1	A	156	LEU
1	A	162	GLN
1	A	177	LEU
1	A	192	LYS
1	A	193	THR
1	A	194	VAL
1	A	197	PHE
1	A	216	ARG
1	A	224	LEU
1	A	240	GLU
1	A	242	ARG
1	A	243	ARG
1	A	267	ARG
1	A	274	LEU
1	A	282	LEU
1	A	287	ILE
1	A	288	PHE
1	A	289	ARG
1	A	293	VAL
1	A	295	VAL
1	A	303	THR
1	A	316	LYS
1	A	318	GLN
1	A	323	VAL
1	A	329	SER
1	A	330	PHE
1	A	333	LEU
1	A	340	SER

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Mol	Chain	Res	Type
1	A	347	ILE
1	A	349	ARG
1	A	354	SER
1	A	356	VAL
1	A	362	HIS
1	A	374	GLN
1	A	383	ASN
1	A	408	VAL
1	A	412	THR
1	A	413	LYS
1	A	426	ARG
1	A	429	ASN
1	A	430	LEU
1	A	452	LEU
1	A	453	VAL
1	A	469	ILE
1	A	473	TRP
1	A	479	THR
1	A	491	LYS
1	A	504	ASP
1	A	516	LEU
1	A	519	GLN
1	A	522	VAL
1	A	528	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	ASN
1	A	59	ASN
1	A	66	ASN
1	A	87	ASN
1	A	209	HIS
1	A	225	GLN
1	A	272	GLN
1	A	324	ASN
1	A	416	ASN
1	A	429	ASN
1	A	513	HIS

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	526/534 (98%)	-0.02	9 (1%)	73	64	20, 20, 20, 20	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	200	SER	2.9
1	A	199	GLU	2.5
1	A	226	SER	2.3
1	A	117	GLY	2.3
1	A	512	VAL	2.2
1	A	415	GLY	2.2
1	A	285	ASP	2.1
1	A	147	SER	2.1
1	A	198	GLY	2.1

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.