Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:49 PM GMT

PDB ID	:	1VDE
Title	:	PI-SCEI, A HOMING ENDONUCLEASE WITH PROTEIN SPLICING ACTIVITY
Authors	:	Duan, X.; Quiocho, F.A.
Deposited on	:	1997-04-01
Resolution	:	2.40 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 ⓘ) were used in the production of this report:

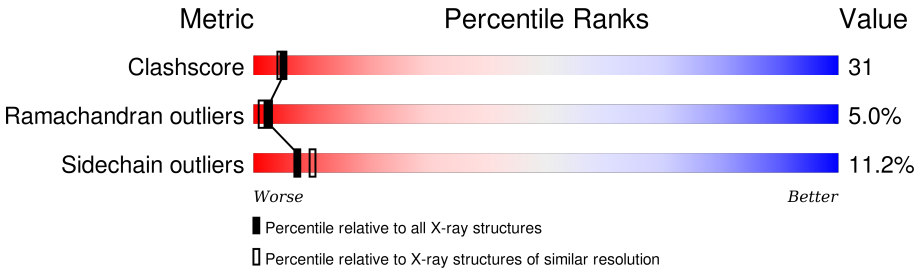
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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 2.40 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	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	454	55% 32% 6% • 6%
1	B	454	44% 40% 9% • 6%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 7116 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 PI-SCEI.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	429	Total	C	N	O	S	0	0	0
			3388	2141	587	647	13			
1	B	428	Total	C	N	O	S	0	0	0
			3381	2136	586	646	13			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	187	Total	O	0	0
			187	187		
2	B	160	Total	O	0	0
			160	160		

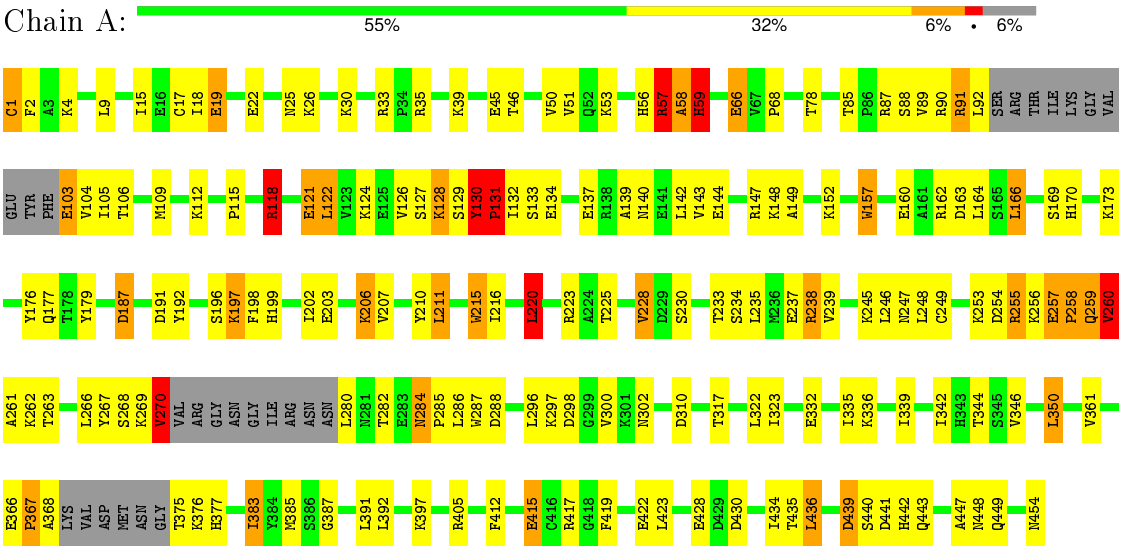
3 Residue-property plots (i)

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.

Note EDS was not executed.

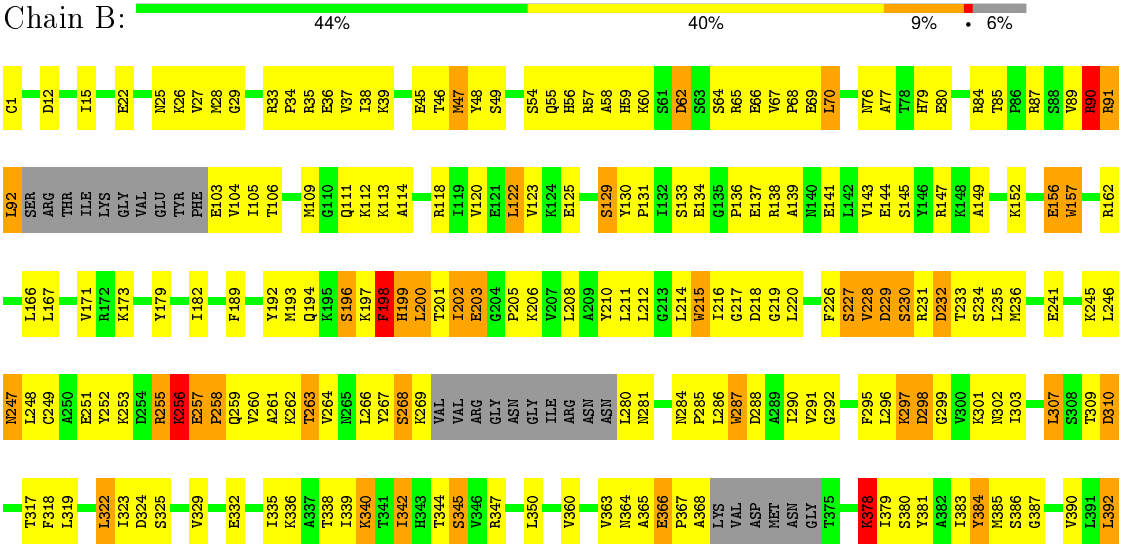
- Molecule 1: PI-SCEI

Chain A:



- Molecule 1: PI-SCEI

Chain B:




G400
S401
K402
K403
F404
R405
P406
A407
A411
R414
R417
L423
Q424
K427
E428
D429
I434
T435
L436
S437
D441
H442
N448
Q449
N454

4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	59.75Å 102.40Å 87.10Å 90.00° 94.10° 90.00°	Depositor
Resolution (Å)	10.00 – 2.40	Depositor
% Data completeness (in resolution range)	95.6 (10.00-2.40)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.192 , 0.238	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7116	wwPDB-VP
Average B, all atoms (Å^2)	37.0	wwPDB-VP

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	0.72	2/3450 (0.1%)	0.94	8/4654 (0.2%)
1	B	0.67	2/3443 (0.1%)	0.89	7/4644 (0.2%)
All	All	0.70	4/6893 (0.1%)	0.92	15/9298 (0.2%)

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 (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1	CYS	CB-SG	9.00	1.97	1.82
1	B	157	TRP	CB-CG	-6.48	1.38	1.50
1	B	47	MET	SD-CE	-6.46	1.41	1.77
1	A	270	VAL	CB-CG2	5.69	1.64	1.52

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	220	LEU	CB-CG-CD1	-9.11	95.51	111.00
1	B	368	ALA	N-CA-C	-7.34	91.19	111.00
1	B	429	ASP	N-CA-C	6.92	129.70	111.00
1	B	92	LEU	CA-CB-CG	-6.41	100.55	115.30
1	B	122	LEU	CA-CB-CG	6.31	129.81	115.30
1	A	59	HIS	N-CA-C	6.12	127.52	111.00
1	B	28	MET	CG-SD-CE	-5.91	90.74	100.20
1	A	1	CYS	CB-CA-C	5.91	122.22	110.40
1	B	199	HIS	N-CA-C	5.70	126.38	111.00
1	A	440	SER	N-CA-C	-5.61	95.85	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	238	ARG	NE-CZ-NH2	-5.39	117.60	120.30
1	A	131	PRO	N-CA-C	5.36	126.03	112.10
1	A	118	ARG	NE-CZ-NH2	-5.31	117.64	120.30
1	A	58	ALA	N-CA-C	5.30	125.31	111.00
1	B	90	ARG	NE-CZ-NH1	5.23	122.92	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	220	LEU	Mainchain

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	3388	0	3387	165	0
1	B	3381	0	3378	254	0
2	A	187	0	0	23	0
2	B	160	0	0	26	0
All	All	7116	0	6765	415	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 (415) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:257:GLU:HB2	1:B:261:ALA:HB3	1.41	1.03
1:A:130:TYR:HB3	1:A:131:PRO:CD	1.91	0.99
1:B:125:GLU:HB3	2:B:576:HOH:O	1.66	0.95
1:B:26:LYS:HD2	1:B:34:PRO:HB2	1.50	0.93
1:A:297:LYS:HG2	1:A:302:ASN:HB2	1.48	0.93
1:B:256:LYS:HD3	1:B:263:THR:HG23	1.49	0.93
2:A:525:HOH:O	1:B:386:SER:HB2	1.69	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:350:LEU:HD13	1:A:383:ILE:HG12	1.50	0.92
1:A:130:TYR:HB3	1:A:131:PRO:HD2	1.52	0.90
1:B:366:GLU:HB2	1:B:367:PRO:HD2	1.53	0.90
1:B:268:SER:H	1:B:280:LEU:HD13	1.37	0.89
1:B:92:LEU:HG	1:B:139:ALA:HB1	1.56	0.88
1:B:194:GLN:HA	1:B:198:PHE:HB2	1.58	0.86
1:B:46:THR:OG1	1:B:427:LYS:HG3	1.76	0.86
1:B:297:LYS:HE3	1:B:345:SER:HB3	1.57	0.85
1:B:114:ALA:HB3	2:B:541:HOH:O	1.76	0.85
1:A:442:HIS:HD2	1:A:454:ASN:HD21	1.24	0.85
1:A:187:ASP:HB2	2:A:551:HOH:O	1.75	0.85
1:B:46:THR:HG23	1:B:427:LYS:HA	1.59	0.85
1:B:91:ARG:HD3	2:B:494:HOH:O	1.76	0.84
1:A:233:THR:O	1:A:237:GLU:HG3	1.77	0.83
1:B:90:ARG:HH11	1:B:90:ARG:HG2	1.43	0.83
1:A:248:LEU:HD21	1:A:285:PRO:HD2	1.61	0.82
1:A:103:GLU:HA	1:A:129:SER:HB3	1.59	0.82
1:B:220:LEU:HD21	1:B:256:LYS:HE3	1.61	0.82
1:B:46:THR:HG23	1:B:427:LYS:CA	2.10	0.82
1:B:255:ARG:HD2	1:B:259:GLN:HA	1.61	0.81
1:B:125:GLU:HG3	1:B:171:VAL:HG23	1.62	0.81
1:B:217:GLY:HA3	1:B:325:SER:OG	1.81	0.80
1:B:247:ASN:ND2	1:B:269:LYS:HD3	1.95	0.80
1:B:319:LEU:O	1:B:323:ILE:HG12	1.81	0.80
1:B:428:GLU:HG3	1:B:429:ASP:N	1.99	0.78
1:B:227:SER:HA	1:B:262:LYS:O	1.84	0.77
1:A:269:LYS:HG2	1:A:270:VAL:N	1.99	0.77
1:B:227:SER:OG	1:B:261:ALA:HB1	1.84	0.76
1:B:232:ASP:HB3	1:B:402:LYS:NZ	2.00	0.76
1:B:85:THR:HG1	1:B:157:TRP:HH2	1.33	0.76
1:B:46:THR:HA	1:B:427:LYS:HA	1.67	0.76
1:B:323:ILE:HD13	1:B:339:ILE:HD11	1.66	0.76
1:A:199:HIS:NE2	1:A:246:LEU:HA	2.00	0.76
1:A:257:GLU:HB3	1:A:260:VAL:HG23	1.67	0.75
1:B:157:TRP:HZ2	2:B:588:HOH:O	1.68	0.75
1:A:197:LYS:HD3	1:A:288:ASP:HB2	1.68	0.74
1:B:229:ASP:HB2	1:B:261:ALA:C	2.06	0.74
1:B:65:ARG:HG2	1:B:379:ILE:HG21	1.69	0.73
1:A:199:HIS:HE2	1:A:246:LEU:HA	1.53	0.73
1:B:268:SER:N	1:B:280:LEU:HD13	2.04	0.73
1:B:229:ASP:H	1:B:262:LYS:HB2	1.54	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:58:ALA:HB1	2:A:578:HOH:O	1.87	0.72
1:A:53:LYS:HG2	1:A:422:GLU:HG3	1.71	0.72
1:B:291:VAL:HG12	1:B:296:LEU:HB3	1.71	0.72
1:B:215:TRP:HE1	1:B:295:PHE:HB3	1.55	0.71
1:B:45:GLU:O	1:B:47:MET:HE3	1.90	0.71
1:B:339:ILE:HD12	1:B:385:MET:HE3	1.72	0.71
1:B:194:GLN:HA	1:B:198:PHE:CB	2.21	0.71
1:B:194:GLN:NE2	1:B:198:PHE:HB3	2.06	0.70
1:A:220:LEU:HG	1:A:225:THR:OG1	1.91	0.70
1:A:147:ARG:HD3	1:B:411:ALA:N	2.06	0.70
1:B:267:TYR:HB3	1:B:280:LEU:HD12	1.73	0.70
1:B:92:LEU:HG	1:B:139:ALA:CB	2.22	0.70
1:A:256:LYS:HE2	2:A:608:HOH:O	1.90	0.70
1:B:339:ILE:HD12	1:B:385:MET:CE	2.21	0.70
1:A:255:ARG:HH11	1:A:259:GLN:HG2	1.57	0.70
1:B:280:LEU:HB3	1:B:284:ASN:OD1	1.92	0.69
1:B:47:MET:SD	2:B:611:HOH:O	2.50	0.69
1:A:144:GLU:O	1:A:148:LYS:HD2	1.93	0.69
1:A:33:ARG:HB3	1:A:33:ARG:CZ	2.23	0.69
1:B:29:GLY:HA3	1:B:35:ARG:HH11	1.58	0.69
1:B:255:ARG:HD2	1:B:259:GLN:H	1.58	0.69
1:A:442:HIS:CD2	1:A:454:ASN:HD21	2.10	0.68
1:A:130:TYR:HB3	1:A:131:PRO:HD3	1.76	0.68
1:B:255:ARG:HD2	1:B:259:GLN:CA	2.24	0.68
1:A:207:VAL:HG11	1:A:245:LYS:HD2	1.75	0.67
1:A:207:VAL:HG23	1:A:246:LEU:HG	1.77	0.67
1:B:350:LEU:HD23	1:B:383:ILE:HD12	1.76	0.67
1:A:45:GLU:HG3	1:A:46:THR:N	2.10	0.66
2:A:638:HOH:O	1:B:404:PHE:HE2	1.77	0.66
1:B:256:LYS:HD3	1:B:263:THR:CG2	2.25	0.66
1:B:231:ARG:HH21	1:B:235:LEU:HD23	1.61	0.65
1:B:442:HIS:N	2:B:493:HOH:O	2.29	0.65
1:A:17:CYS:HB3	1:A:19:GLU:OE2	1.97	0.65
1:B:367:PRO:HA	2:B:613:HOH:O	1.97	0.65
1:B:109:MET:HG2	2:B:575:HOH:O	1.96	0.64
1:A:104:VAL:CG1	1:A:128:LYS:HB2	2.27	0.64
1:B:255:ARG:HD2	1:B:259:GLN:N	2.12	0.64
1:B:427:LYS:O	1:B:428:GLU:HG2	1.98	0.64
1:B:247:ASN:HD21	1:B:269:LYS:HD3	1.62	0.64
1:B:203:GLU:CD	1:B:246:LEU:HD23	2.19	0.63
1:B:210:TYR:OH	1:B:235:LEU:HD11	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:48:TYR:HB3	1:B:423:LEU:HD22	1.80	0.63
1:A:230:SER:HB3	1:A:262:LYS:HG3	1.80	0.63
1:A:297:LYS:HG2	1:A:302:ASN:CB	2.27	0.63
1:B:90:ARG:NH1	1:B:90:ARG:HG2	2.12	0.63
1:A:33:ARG:NH1	1:A:33:ARG:HB3	2.14	0.63
1:A:87:ARG:NH2	1:A:149:ALA:HB3	2.14	0.62
1:B:258:PRO:O	1:B:260:VAL:HG22	1.98	0.62
1:B:257:GLU:HB3	1:B:260:VAL:HG23	1.82	0.62
1:B:303:ILE:HG23	1:B:307:LEU:HD23	1.81	0.62
1:A:122:LEU:HD11	1:A:124:LYS:HE3	1.80	0.62
1:A:258:PRO:O	1:A:260:VAL:HG22	1.99	0.62
1:A:130:TYR:CB	1:A:131:PRO:CD	2.76	0.62
1:B:85:THR:OG1	1:B:157:TRP:HH2	1.82	0.62
1:B:130:TYR:OH	1:B:136:PRO:HA	1.99	0.62
1:B:266:LEU:HD12	1:B:286:LEU:HD22	1.82	0.61
1:B:287:TRP:CD1	1:B:290:ILE:HD12	2.35	0.61
1:A:430:ASP:HB3	2:A:574:HOH:O	2.00	0.61
1:B:38:ILE:HG13	1:B:39:LYS:HG3	1.81	0.61
1:A:109:MET:HG3	1:A:121:GLU:OE1	2.00	0.61
1:A:51:VAL:HG12	2:A:577:HOH:O	1.99	0.61
1:B:365:ALA:HB1	1:B:379:ILE:HD11	1.82	0.60
1:B:322:LEU:HD13	1:B:339:ILE:HD13	1.81	0.60
1:B:231:ARG:NH2	1:B:235:LEU:HD23	2.15	0.60
1:B:46:THR:CA	1:B:427:LYS:HA	2.31	0.60
1:B:57:ARG:NH2	1:B:67:VAL:O	2.34	0.60
1:A:215:TRP:CZ3	1:A:220:LEU:O	2.55	0.60
1:B:366:GLU:HB2	1:B:367:PRO:CD	2.30	0.60
1:B:206:LYS:N	1:B:206:LYS:HD2	2.16	0.60
1:B:297:LYS:O	1:B:299:GLY:N	2.35	0.59
1:B:125:GLU:CG	1:B:171:VAL:HG23	2.30	0.59
1:B:84:ARG:HD3	1:B:156:GLU:HG2	1.82	0.59
1:A:22:GLU:H	1:A:25:ASN:ND2	1.99	0.59
1:B:35:ARG:HB3	1:B:436:LEU:HD13	1.84	0.59
1:B:92:LEU:HD22	1:B:92:LEU:N	2.17	0.59
1:B:46:THR:CG2	1:B:427:LYS:HA	2.29	0.59
1:B:342:ILE:HG22	1:B:379:ILE:O	2.03	0.59
1:A:144:GLU:HB3	1:A:148:LYS:NZ	2.17	0.59
1:A:4:LYS:HG3	1:A:19:GLU:HG2	1.85	0.59
1:A:197:LYS:HD3	1:A:288:ASP:CB	2.31	0.58
1:B:232:ASP:HB2	1:B:400:GLY:HA2	1.86	0.58
1:A:215:TRP:HZ3	1:A:220:LEU:O	1.87	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:103:GLU:HG2	1:B:129:SER:HB3	1.85	0.58
1:B:230:SER:O	1:B:231:ARG:HB3	2.04	0.58
1:B:112:LYS:HD3	1:B:166:LEU:HD12	1.86	0.58
1:B:118:ARG:N	2:B:541:HOH:O	2.34	0.58
1:B:144:GLU:HB2	2:B:564:HOH:O	2.04	0.57
1:A:50:VAL:HG22	1:A:423:LEU:HD12	1.87	0.57
1:A:58:ALA:HB3	1:A:68:PRO:HB3	1.86	0.57
1:B:29:GLY:HA3	1:B:35:ARG:NH1	2.20	0.57
1:A:284:ASN:C	1:A:284:ASN:HD22	2.07	0.57
1:B:442:HIS:HB3	1:B:454:ASN:ND2	2.19	0.57
1:A:104:VAL:HG11	1:A:142:LEU:HD13	1.85	0.57
1:A:30:LYS:HE3	1:A:443:GLN:OE1	2.04	0.57
1:B:253:LYS:HB2	1:B:263:THR:OG1	2.04	0.57
1:B:267:TYR:HD1	1:B:280:LEU:HB2	1.69	0.57
1:B:249:CYS:O	1:B:266:LEU:HA	2.05	0.57
1:B:131:PRO:HB2	1:B:134:GLU:HG3	1.87	0.57
1:B:113:LYS:HD2	1:B:113:LYS:N	2.19	0.56
1:A:58:ALA:HB3	1:A:68:PRO:CA	2.34	0.56
2:A:640:HOH:O	1:B:173:LYS:HD2	2.04	0.56
1:A:436:LEU:HD23	2:A:572:HOH:O	2.05	0.56
1:A:442:HIS:HD2	1:A:454:ASN:ND2	1.98	0.56
1:B:65:ARG:NH2	1:B:378:LYS:HE3	2.20	0.56
1:B:232:ASP:HB2	1:B:401:SER:H	1.69	0.56
1:B:123:VAL:HG22	2:B:575:HOH:O	2.05	0.56
1:A:297:LYS:HZ2	1:A:300:VAL:CG1	2.17	0.56
1:B:92:LEU:CG	1:B:139:ALA:HB1	2.33	0.56
1:B:202:ILE:H	1:B:202:ILE:HD12	1.71	0.56
1:A:448:ASN:O	1:A:449:GLN:HB2	2.06	0.56
1:B:287:TRP:O	1:B:291:VAL:HG22	2.04	0.56
1:B:47:MET:HE1	1:B:76:ASN:HB3	1.88	0.56
1:B:231:ARG:HH21	1:B:235:LEU:CD2	2.19	0.55
1:B:56:HIS:HB3	2:B:599:HOH:O	2.05	0.55
1:A:15:ILE:HD13	1:A:447:ALA:HB1	1.89	0.55
1:A:249:CYS:SG	1:A:269:LYS:HA	2.47	0.55
1:A:269:LYS:HG2	1:A:270:VAL:H	1.66	0.55
1:A:211:LEU:HD23	1:A:246:LEU:HD12	1.88	0.55
1:A:58:ALA:HB3	1:A:68:PRO:HA	1.88	0.55
1:A:170:HIS:HB3	2:A:638:HOH:O	2.05	0.55
1:B:229:ASP:HB2	1:B:261:ALA:CA	2.36	0.55
1:B:196:SER:O	1:B:197:LYS:HB3	2.06	0.55
1:A:104:VAL:O	1:A:127:SER:HA	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:412:PHE:HD1	2:A:637:HOH:O	1.90	0.55
1:B:257:GLU:CB	1:B:261:ALA:HB3	2.26	0.55
1:B:33:ARG:HH11	1:B:33:ARG:HG3	1.72	0.55
1:A:361:VAL:HG13	1:A:383:ILE:CD1	2.37	0.55
1:A:104:VAL:HG13	1:A:128:LYS:HB2	1.89	0.54
1:A:441:ASP:O	1:A:443:GLN:HG3	2.07	0.54
1:B:338:THR:HG1	1:B:384:TYR:HD2	1.55	0.54
1:B:143:VAL:O	1:B:147:ARG:HG3	2.08	0.54
1:B:77:ALA:O	1:B:162:ARG:HG2	2.07	0.54
1:B:424:GLN:HB2	2:B:610:HOH:O	2.07	0.54
1:B:248:LEU:HD21	1:B:285:PRO:HG2	1.89	0.54
1:B:363:VAL:HG12	1:B:364:ASN:N	2.23	0.54
1:B:303:ILE:HD13	1:B:318:PHE:CE1	2.43	0.54
1:B:297:LYS:HE3	1:B:345:SER:CB	2.32	0.53
1:B:256:LYS:O	1:B:257:GLU:HB2	2.08	0.53
1:B:347:ARG:HD2	1:B:363:VAL:HG11	1.91	0.53
1:A:361:VAL:HG13	1:A:383:ILE:HD12	1.89	0.53
1:A:144:GLU:HB3	1:A:148:LYS:HZ3	1.73	0.53
1:B:130:TYR:CE2	1:B:138:ARG:HB2	2.43	0.53
1:B:340:LYS:HD2	1:B:340:LYS:H	1.71	0.53
1:B:427:LYS:HG2	1:B:428:GLU:H	1.72	0.53
1:B:57:ARG:HH22	1:B:69:GLU:H	1.56	0.53
1:A:336:LYS:HG3	1:A:385:MET:O	2.09	0.53
1:A:266:LEU:O	1:A:280:LEU:HD22	2.08	0.53
1:B:26:LYS:HE3	1:B:36:GLU:HB2	1.91	0.53
1:A:238:ARG:NH2	1:A:397:LYS:O	2.41	0.52
1:B:26:LYS:CE	1:B:36:GLU:HB2	2.40	0.52
1:A:88:SER:O	1:A:106:THR:HA	2.10	0.52
1:B:241:GLU:O	1:B:245:LYS:HG3	2.09	0.52
1:B:1:CYS:SG	2:B:546:HOH:O	2.29	0.52
1:B:442:HIS:CD2	1:B:454:ASN:HD21	2.28	0.52
1:A:169:SER:O	1:A:173:LYS:HE2	2.09	0.52
1:A:91:ARG:O	1:A:92:LEU:HB2	2.09	0.52
1:A:223:ARG:HG3	1:A:225:THR:HG23	1.92	0.52
1:A:50:VAL:HG11	1:A:177:GLN:HE22	1.74	0.52
1:B:109:MET:SD	2:B:575:HOH:O	2.59	0.52
1:A:366:GLU:HB3	1:A:367:PRO:HD2	1.92	0.51
1:B:229:ASP:HA	1:B:262:LYS:HD3	1.92	0.51
1:A:46:THR:HA	1:A:428:GLU:HA	1.92	0.51
1:B:192:TYR:OH	1:B:292:GLY:HA3	2.10	0.51
1:A:234:SER:HB2	2:A:613:HOH:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:267:TYR:HB3	1:B:280:LEU:CD1	2.40	0.51
1:A:256:LYS:HB2	1:A:263:THR:CA	2.40	0.51
1:A:85:THR:OG1	1:A:157:TRP:CH2	2.60	0.51
1:A:368:ALA:HA	1:A:377:HIS:O	2.10	0.51
1:B:428:GLU:CG	1:B:429:ASP:N	2.68	0.51
1:B:215:TRP:CH2	1:B:301:LYS:HG2	2.46	0.51
1:B:137:GLU:HG3	1:B:138:ARG:HG3	1.93	0.51
1:B:251:GLU:O	1:B:264:VAL:HA	2.11	0.51
1:B:295:PHE:HA	1:B:302:ASN:O	2.11	0.50
1:A:143:VAL:O	1:A:147:ARG:HG3	2.11	0.50
1:B:69:GLU:HA	2:B:545:HOH:O	2.10	0.50
1:B:57:ARG:NH2	1:B:69:GLU:H	2.09	0.50
1:A:164:LEU:HD22	1:A:423:LEU:HD22	1.93	0.50
1:B:303:ILE:CG2	1:B:307:LEU:HD23	2.41	0.50
1:B:339:ILE:HD12	1:B:385:MET:HE1	1.94	0.50
1:A:228:VAL:HG21	1:A:239:VAL:HG21	1.92	0.50
1:B:54:SER:OG	1:B:57:ARG:HB2	2.11	0.50
1:A:50:VAL:HG22	1:A:423:LEU:CD1	2.42	0.49
1:A:179:TYR:CZ	1:A:417:ARG:HB2	2.47	0.49
1:B:59:HIS:HA	1:B:66:GLU:HB3	1.94	0.49
1:B:157:TRP:NE1	2:B:587:HOH:O	2.27	0.49
1:A:257:GLU:HB3	1:A:260:VAL:CG2	2.38	0.49
1:A:147:ARG:HH11	1:B:411:ALA:HB2	1.77	0.49
1:B:428:GLU:HG3	1:B:429:ASP:HB2	1.95	0.49
1:B:87:ARG:NH2	1:B:149:ALA:HB3	2.28	0.49
1:A:163:ASP:O	1:A:166:LEU:HB2	2.11	0.49
1:B:54:SER:HB2	2:B:602:HOH:O	2.13	0.49
1:A:256:LYS:HB2	1:A:263:THR:N	2.27	0.49
1:B:206:LYS:H	1:B:206:LYS:HD2	1.77	0.49
1:B:197:LYS:HD3	1:B:197:LYS:C	2.33	0.49
1:B:229:ASP:HA	1:B:262:LYS:CD	2.42	0.49
1:A:297:LYS:HZ2	1:A:300:VAL:HB	1.78	0.49
1:A:58:ALA:HB3	1:A:68:PRO:CB	2.43	0.49
1:A:176:TYR:HB2	1:A:419:PHE:O	2.13	0.49
1:B:297:LYS:HG3	1:B:298:ASP:N	2.27	0.48
1:A:105:ILE:HA	1:A:126:VAL:O	2.12	0.48
1:A:284:ASN:ND2	1:A:287:TRP:H	2.11	0.48
1:B:189:PHE:CD1	1:B:205:PRO:HB3	2.47	0.48
1:A:210:TYR:HB2	1:A:317:THR:HG22	1.95	0.48
1:B:268:SER:OG	1:B:280:LEU:HD22	2.14	0.48
1:A:104:VAL:CG1	1:A:142:LEU:HD13	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:48:TYR:HB3	1:B:423:LEU:CD2	2.42	0.48
1:B:211:LEU:HA	1:B:214:LEU:HD12	1.95	0.48
1:A:66:GLU:CD	1:A:66:GLU:H	2.17	0.48
1:B:194:GLN:CD	1:B:198:PHE:HD2	2.17	0.48
1:A:415:GLU:H	1:A:415:GLU:HG3	1.49	0.48
1:A:405:ARG:NH2	2:A:531:HOH:O	2.45	0.48
1:B:141:GLU:O	1:B:145:SER:HB2	2.13	0.48
1:B:232:ASP:HB3	1:B:402:LYS:HZ1	1.79	0.48
1:A:256:LYS:HD3	1:A:263:THR:OG1	2.12	0.48
2:A:525:HOH:O	1:B:360:VAL:HB	2.13	0.48
1:B:137:GLU:HG3	1:B:138:ARG:N	2.29	0.48
1:B:211:LEU:HD12	1:B:246:LEU:HD12	1.94	0.48
1:B:67:VAL:HG12	1:B:347:ARG:NH1	2.29	0.48
1:A:35:ARG:HB3	1:A:436:LEU:HG	1.95	0.47
1:A:215:TRP:CZ3	1:A:287:TRP:HZ3	2.31	0.47
1:B:85:THR:OG1	1:B:157:TRP:CH2	2.57	0.47
1:B:286:LEU:O	1:B:290:ILE:HG13	2.15	0.47
1:B:57:ARG:HH22	1:B:69:GLU:HB2	1.80	0.47
1:A:88:SER:HB2	1:B:407:ALA:O	2.14	0.47
1:B:235:LEU:HA	1:B:235:LEU:HD12	1.72	0.47
1:B:57:ARG:HA	1:B:57:ARG:HD2	1.63	0.47
1:B:302:ASN:CB	1:B:345:SER:HB2	2.44	0.47
1:B:65:ARG:HH21	1:B:378:LYS:HE3	1.79	0.47
1:B:111:GLN:HA	1:B:120:VAL:O	2.15	0.47
1:B:257:GLU:O	1:B:259:GLN:N	2.48	0.47
1:A:284:ASN:HA	1:A:285:PRO:HD3	1.70	0.47
1:B:130:TYR:HH	1:B:136:PRO:HA	1.80	0.47
1:B:26:LYS:NZ	1:B:36:GLU:HB2	2.30	0.46
1:A:268:SER:OG	1:A:284:ASN:HB3	2.16	0.46
1:B:212:LEU:HD21	1:B:290:ILE:HG12	1.98	0.46
1:A:147:ARG:NH1	1:B:411:ALA:HB2	2.29	0.46
1:B:384:TYR:CD1	1:B:384:TYR:N	2.83	0.46
1:A:191:ASP:HA	2:A:601:HOH:O	2.15	0.46
1:B:79:HIS:CE1	2:B:535:HOH:O	2.69	0.46
1:A:267:TYR:CD1	1:A:280:LEU:HD21	2.51	0.46
1:A:78:THR:HG22	1:A:162:ARG:CZ	2.45	0.46
1:B:210:TYR:HB2	1:B:317:THR:HG22	1.98	0.46
1:A:256:LYS:HD3	1:A:263:THR:HG23	1.97	0.46
1:B:89:VAL:HG23	1:B:106:THR:HG22	1.97	0.46
1:B:329:VAL:HG12	1:B:405:ARG:NH1	2.31	0.46
1:A:199:HIS:HE2	1:A:246:LEU:CA	2.27	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:197:LYS:HD2	1:A:285:PRO:HA	1.98	0.46
1:B:130:TYR:CD1	1:B:130:TYR:C	2.89	0.46
1:B:37:VAL:HG13	1:B:434:ILE:HB	1.98	0.46
1:A:50:VAL:HG11	1:A:177:GLN:NE2	2.31	0.46
1:A:129:SER:O	1:A:130:TYR:CB	2.64	0.46
1:B:57:ARG:NH2	1:B:69:GLU:HB2	2.30	0.46
1:A:207:VAL:HG11	1:A:245:LYS:CD	2.44	0.45
1:A:206:LYS:HB3	2:A:502:HOH:O	2.15	0.45
1:B:441:ASP:C	2:B:493:HOH:O	2.53	0.45
1:B:1:CYS:CB	1:B:79:HIS:CD2	2.99	0.45
1:B:288:ASP:O	1:B:292:GLY:N	2.48	0.45
1:A:160:GLU:OE1	1:A:162:ARG:NE	2.46	0.45
1:B:232:ASP:HB2	1:B:400:GLY:CA	2.46	0.45
1:A:256:LYS:HB2	1:A:263:THR:OG1	2.17	0.45
1:A:255:ARG:HG3	1:A:259:GLN:NE2	2.31	0.45
1:B:200:LEU:O	1:B:200:LEU:HG	2.17	0.45
1:A:192:TYR:HE2	1:A:197:LYS:NZ	2.14	0.45
1:A:246:LEU:O	1:A:247:ASN:HB2	2.17	0.45
1:B:189:PHE:HB2	1:B:310:ASP:OD2	2.16	0.45
1:A:297:LYS:NZ	1:A:300:VAL:HB	2.32	0.45
1:A:434:ILE:O	1:A:454:ASN:HB2	2.17	0.45
1:B:231:ARG:HD2	2:B:590:HOH:O	2.17	0.45
1:B:1:CYS:SG	1:B:454:ASN:O	2.74	0.45
1:A:56:HIS:O	1:A:57:ARG:NE	2.49	0.45
1:B:252:TYR:HB3	1:B:262:LYS:NZ	2.31	0.45
1:A:257:GLU:HB2	1:A:261:ALA:HB3	1.98	0.45
1:A:335:ILE:HG23	1:A:391:LEU:HD23	1.99	0.45
1:B:247:ASN:HD22	1:B:269:LYS:HD3	1.77	0.45
1:B:448:ASN:O	1:B:449:GLN:HB2	2.17	0.45
1:A:87:ARG:HD3	1:A:152:LYS:O	2.17	0.45
1:B:336:LYS:HE3	1:B:336:LYS:HB2	1.61	0.45
1:A:33:ARG:NH1	1:A:35:ARG:HH21	2.15	0.44
1:B:167:LEU:HD11	2:B:588:HOH:O	2.17	0.44
1:B:27:VAL:HG23	1:B:35:ARG:HB2	1.99	0.44
1:B:228:VAL:HG11	1:B:236:MET:CG	2.47	0.44
1:A:235:LEU:O	1:A:239:VAL:HG23	2.18	0.44
1:B:219:GLY:HA2	1:B:226:PHE:HA	1.99	0.44
1:B:257:GLU:HB2	1:B:261:ALA:CB	2.30	0.44
1:B:232:ASP:HB2	1:B:401:SER:N	2.31	0.44
1:B:79:HIS:HE1	2:B:535:HOH:O	2.01	0.44
1:A:118:ARG:HH22	1:A:163:ASP:CG	2.21	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:281:ASN:N	1:B:284:ASN:ND2	2.65	0.44
1:B:39:LYS:HB2	1:B:435:THR:HG23	1.98	0.44
1:A:255:ARG:NH1	2:A:619:HOH:O	2.48	0.44
1:B:62:ASP:C	1:B:64:SER:H	2.22	0.44
1:A:39:LYS:HB2	1:A:435:THR:HB	1.98	0.44
1:A:428:GLU:HG2	2:A:632:HOH:O	2.18	0.43
1:B:1:CYS:HB3	1:B:79:HIS:CD2	2.53	0.43
1:B:215:TRP:CZ2	1:B:301:LYS:HG2	2.54	0.43
1:A:103:GLU:CA	1:A:129:SER:HB3	2.37	0.43
1:A:297:LYS:NZ	1:A:300:VAL:CG1	2.81	0.43
1:B:379:ILE:HD13	1:B:381:TYR:OH	2.18	0.43
1:B:347:ARG:HA	1:B:383:ILE:HD11	2.01	0.43
1:A:342:ILE:HG12	2:A:473:HOH:O	2.19	0.43
1:B:90:ARG:NH2	2:B:485:HOH:O	2.52	0.43
1:B:201:THR:HG23	1:B:202:ILE:HD12	2.00	0.43
1:B:256:LYS:O	1:B:256:LYS:CG	2.67	0.43
1:A:89:VAL:HG21	1:A:143:VAL:HG22	2.00	0.43
1:B:392:LEU:HA	1:B:392:LEU:HD12	1.82	0.43
1:A:22:GLU:HG2	2:A:567:HOH:O	2.17	0.43
1:B:210:TYR:CE2	1:B:214:LEU:HD11	2.53	0.43
1:B:232:ASP:O	1:B:234:SER:N	2.52	0.43
1:A:59:HIS:CG	2:A:578:HOH:O	2.72	0.43
1:A:199:HIS:CE1	1:A:246:LEU:HD23	2.54	0.42
1:A:203:GLU:O	1:A:207:VAL:HG13	2.19	0.42
1:B:193:MET:HE2	1:B:208:LEU:HD22	2.01	0.42
1:B:229:ASP:N	1:B:262:LYS:HB2	2.29	0.42
1:B:367:PRO:O	1:B:380:SER:HB3	2.19	0.42
1:B:46:THR:HG23	1:B:427:LYS:CB	2.49	0.42
1:A:253:LYS:HB3	1:A:263:THR:HB	2.01	0.42
1:B:89:VAL:HA	1:B:105:ILE:O	2.19	0.42
1:A:132:ILE:HG22	1:A:133:SER:N	2.35	0.42
1:A:215:TRP:CD1	1:A:216:ILE:N	2.88	0.42
1:B:211:LEU:HD23	1:B:214:LEU:HD12	1.99	0.42
1:B:68:PRO:HD2	1:B:347:ARG:NH2	2.34	0.42
1:A:85:THR:OG1	1:A:157:TRP:CZ3	2.66	0.42
1:B:324:ASP:HA	1:B:403:LYS:HD3	2.01	0.42
1:B:202:ILE:O	1:B:203:GLU:O	2.38	0.42
1:B:378:LYS:HZ2	1:B:379:ILE:HB	1.83	0.42
1:B:45:GLU:O	1:B:47:MET:CE	2.62	0.42
1:A:2:PHE:HD1	1:A:18:ILE:HD13	1.83	0.42
1:A:248:LEU:CD2	1:A:285:PRO:HD2	2.40	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:46:THR:HG23	1:B:427:LYS:N	2.35	0.42
1:A:361:VAL:CG1	1:A:383:ILE:CD1	2.98	0.41
1:B:303:ILE:HD13	1:B:318:PHE:HE1	1.82	0.41
1:B:87:ARG:HD3	1:B:152:LYS:O	2.20	0.41
1:A:322:LEU:HB3	1:A:339:ILE:HD13	2.01	0.41
1:B:57:ARG:HD3	2:B:602:HOH:O	2.18	0.41
1:B:80:GLU:HG2	2:B:593:HOH:O	2.19	0.41
1:A:297:LYS:HZ2	1:A:300:VAL:CB	2.34	0.41
1:A:256:LYS:NZ	1:A:263:THR:HG23	2.36	0.41
1:A:1:CYS:SG	1:A:454:ASN:OXT	2.78	0.41
1:B:266:LEU:HD12	1:B:286:LEU:CD2	2.48	0.41
1:A:173:LYS:NZ	2:A:509:HOH:O	2.53	0.41
1:A:39:LYS:HD3	1:A:435:THR:HG21	2.03	0.41
1:B:179:TYR:CE2	1:B:417:ARG:HB2	2.56	0.41
1:B:229:ASP:HA	1:B:262:LYS:HG3	2.03	0.41
1:B:22:GLU:O	1:B:25:ASN:HB2	2.20	0.41
1:B:84:ARG:CD	1:B:156:GLU:HG2	2.50	0.41
1:A:346:VAL:O	1:A:350:LEU:HB2	2.21	0.41
1:B:92:LEU:HA	1:B:92:LEU:HD13	1.39	0.41
1:B:230:SER:O	1:B:232:ASP:N	2.54	0.41
1:B:65:ARG:NH2	1:B:378:LYS:HG3	2.36	0.41
1:A:2:PHE:N	1:A:2:PHE:CD1	2.89	0.41
1:B:256:LYS:HB3	1:B:262:LYS:O	2.21	0.41
1:B:229:ASP:HA	1:B:262:LYS:CG	2.50	0.41
1:B:87:ARG:HH22	1:B:149:ALA:HB3	1.86	0.41
1:B:390:VAL:HG13	1:B:414:ARG:NH1	2.36	0.41
1:B:125:GLU:CD	1:B:171:VAL:HG23	2.41	0.40
1:A:383:ILE:O	1:A:383:ILE:HG13	2.21	0.40
1:A:220:LEU:HG	2:A:537:HOH:O	2.20	0.40
1:B:216:ILE:HA	1:B:301:LYS:HD2	2.04	0.40
1:B:319:LEU:HA	1:B:319:LEU:HD23	1.96	0.40
1:B:46:THR:CB	1:B:427:LYS:HA	2.52	0.40
1:A:267:TYR:CD1	1:A:280:LEU:CD2	3.04	0.40
1:B:182:ILE:HG21	1:B:309:THR:HG22	2.02	0.40
1:B:228:VAL:H	1:B:262:LYS:H	1.69	0.40
1:A:196:SER:HB3	1:A:197:LYS:H	1.75	0.40
1:A:436:LEU:H	1:A:454:ASN:HD22	1.70	0.40
1:A:230:SER:CB	1:A:262:LYS:HG3	2.50	0.40
1:A:323:ILE:HG13	1:A:339:ILE:HD11	2.03	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	421/454 (93%)	378 (90%)	25 (6%)	18 (4%)	3	2
1	B	420/454 (92%)	361 (86%)	35 (8%)	24 (6%)	2	1
All	All	841/908 (93%)	739 (88%)	60 (7%)	42 (5%)	3	1

All (42) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	118	ARG
1	A	130	TYR
1	A	131	PRO
1	A	137	GLU
1	A	197	LYS
1	A	257	GLU
1	B	60	LYS
1	B	196	SER
1	B	199	HIS
1	B	202	ILE
1	B	203	GLU
1	B	229	ASP
1	B	233	THR
1	B	256	LYS
1	B	298	ASP
1	B	378	LYS
1	B	442	HIS
1	A	57	ARG
1	A	260	VAL
1	A	332	GLU
1	A	367	PRO
1	A	439	ASP
1	A	139	ALA
1	A	259	GLN
1	B	58	ALA

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Mol	Chain	Res	Type
1	B	257	GLU
1	B	258	PRO
1	B	429	ASP
1	A	91	ARG
1	B	70	LEU
1	B	230	SER
1	B	255	ARG
1	A	255	ARG
1	B	91	ARG
1	B	228	VAL
1	B	332	GLU
1	A	202	ILE
1	B	198	PHE
1	B	218	ASP
1	A	258	PRO
1	A	387	GLY
1	B	387	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	371/392 (95%)	328 (88%)	43 (12%)	7 9
1	B	370/392 (94%)	330 (89%)	40 (11%)	8 11
All	All	741/784 (94%)	658 (89%)	83 (11%)	7 10

All (83) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	LEU
1	A	19	GLU
1	A	26	LYS
1	A	57	ARG
1	A	59	HIS
1	A	66	GLU

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Mol	Chain	Res	Type
1	A	90	ARG
1	A	103	GLU
1	A	112	LYS
1	A	115	PRO
1	A	121	GLU
1	A	122	LEU
1	A	128	LYS
1	A	130	TYR
1	A	134	GLU
1	A	140	ASN
1	A	157	TRP
1	A	166	LEU
1	A	187	ASP
1	A	198	PHE
1	A	206	LYS
1	A	211	LEU
1	A	215	TRP
1	A	220	LEU
1	A	228	VAL
1	A	254	ASP
1	A	260	VAL
1	A	270	VAL
1	A	282	THR
1	A	284	ASN
1	A	286	LEU
1	A	296	LEU
1	A	298	ASP
1	A	310	ASP
1	A	344	THR
1	A	350	LEU
1	A	375	THR
1	A	376	LYS
1	A	383	ILE
1	A	392	LEU
1	A	415	GLU
1	A	436	LEU
1	A	439	ASP
1	B	12	ASP
1	B	15	ILE
1	B	49	SER
1	B	55	GLN
1	B	62	ASP

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Mol	Chain	Res	Type
1	B	70	LEU
1	B	90	ARG
1	B	104	VAL
1	B	122	LEU
1	B	129	SER
1	B	133	SER
1	B	156	GLU
1	B	198	PHE
1	B	200	LEU
1	B	215	TRP
1	B	227	SER
1	B	232	ASP
1	B	247	ASN
1	B	256	LYS
1	B	263	THR
1	B	268	SER
1	B	287	TRP
1	B	297	LYS
1	B	307	LEU
1	B	310	ASP
1	B	322	LEU
1	B	335	ILE
1	B	340	LYS
1	B	342	ILE
1	B	344	THR
1	B	345	SER
1	B	366	GLU
1	B	378	LYS
1	B	384	TYR
1	B	392	LEU
1	B	423	LEU
1	B	429	ASP
1	B	435	THR
1	B	437	SER
1	B	441	ASP

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

Mol	Chain	Res	Type
1	A	20	ASN
1	A	25	ASN
1	A	56	HIS

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Mol	Chain	Res	Type
1	A	79	HIS
1	A	186	ASN
1	A	284	ASN
1	A	442	HIS
1	A	454	ASN
1	B	56	HIS
1	B	79	HIS
1	B	194	GLN
1	B	247	ASN
1	B	284	ASN
1	B	377	HIS
1	B	454	ASN

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

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.