Full wwPDB X-ray Structure Validation Report (i)

May 14, 2020 – 06:28 am BST

PDB ID	:	1OLZ
Title	:	The ligand-binding face of the semaphorins revealed by the high resolution crystal structure of SEMA4D
Authors	:	Love, C.A.; Harlos, K.; Mavaddat, N.; Davis, S.J.; Stuart, D.I.; Jones, E.Y.; Esnouf, R.M.
Deposited on	:	2003-08-19
Resolution	:	2.00 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 following versions of software and data (see references (i)) were used in the production of this report:

|		
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
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)	:	2.11

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 2.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.
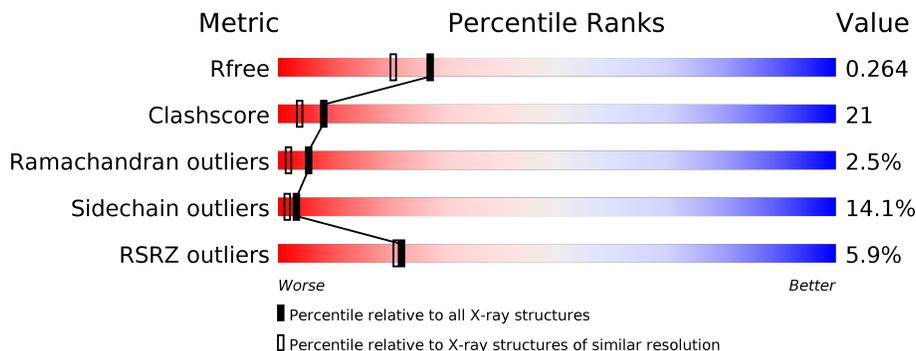
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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 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	663	5% 57% 28% 8% • 6%
1	B	663	6% 60% 26% 8% • 6%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 10669 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 SEMAPHORIN 4D.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	622	Total	C	N	O	S	0	0	1
			4914	3128	850	913	23			
1	B	622	Total	C	N	O	S	0	0	1
			4914	3128	850	913	23			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	398	Total	O	0	0
			398	398		
2	B	443	Total	O	0	0
			443	443		

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 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: SEMAPHORIN 4D
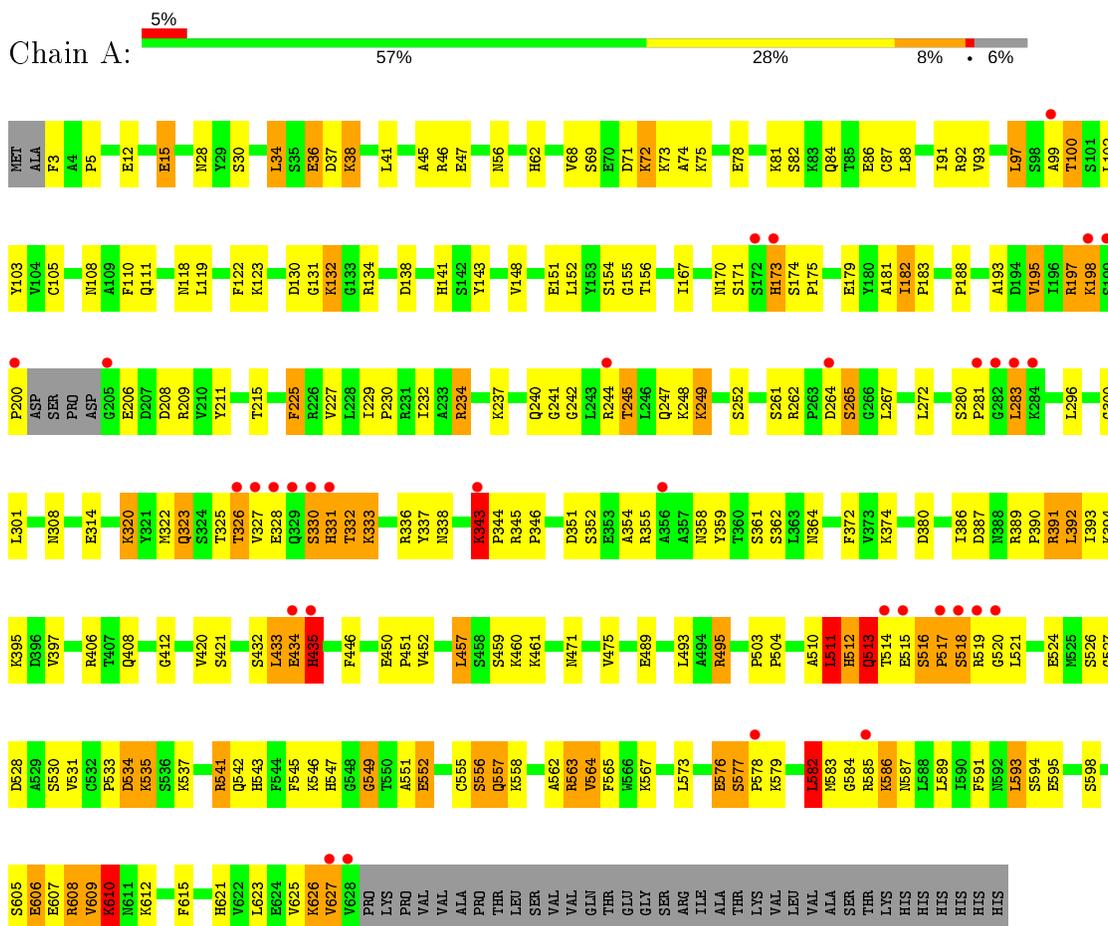
- Molecule 1: SEMAPHORIN 4D
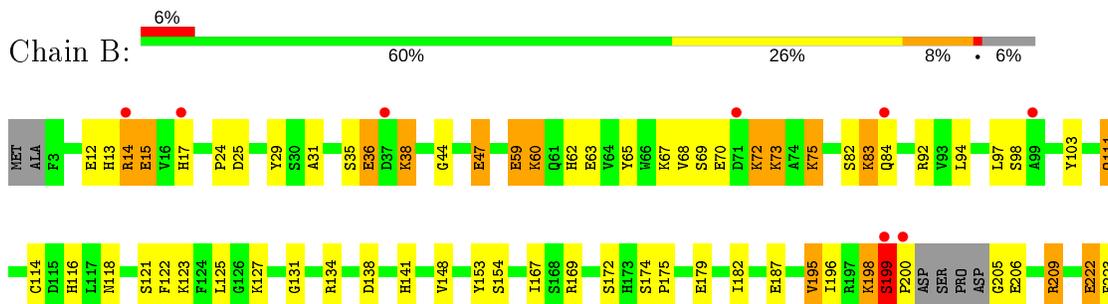
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	73.32Å　76.76Å　89.41Å 77.41°　73.35°　63.57°	Depositor
Resolution (Å)	20.00　–　2.00 19.51　–　2.00	Depositor EDS
% Data completeness (in resolution range)	96.7 (20.00-2.00) 96.7 (19.51-2.00)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	3.38 (at 2.01Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.206　,　0.270 0.204　,　0.264	Depositor DCC
R_{free} test set	5440 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	22.8	Xtriage
Anisotropy	0.192	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 72.5	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	0.95	EDS
Total number of atoms	10669	wwPDB-VP
Average B, all atoms (Å^2)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.47% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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	#$\vert Z\vert$ >5	RMSZ	#$\vert Z\vert$ >5
1	A	0.39	0/5034	0.64	1/6825 (0.0%)
1	B	0.39	0/5034	0.68	2/6825 (0.0%)
All	All	0.39	0/10068	0.66	3/13650 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	199	SER	C-N-CD	-7.49	104.11	120.60
1	B	199	SER	C-N-CA	6.12	147.71	122.00
1	A	457	LEU	CA-CB-CG	5.20	127.25	115.30

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	4914	0	4841	223	0
1	B	4914	0	4841	198	0
2	A	398	0	0	24	0
2	B	443	0	0	39	0
All	All	10669	0	9682	414	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 21.

All (414) 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:495:ARG:HG3	1:A:495:ARG:HH11	1.06	1.12
1:A:608:ARG:HD2	1:A:608:ARG:H	1.13	1.12
1:B:200:PRO:HD3	1:B:205:GLY:HA2	1.35	1.08
1:B:343:LYS:HB3	1:B:344:PRO:HD3	1.33	1.07
1:B:199:SER:HB3	1:B:200:PRO:C	1.82	1.00
1:B:543:HIS:HB2	1:B:623:LEU:HB2	1.43	0.96
1:A:609:VAL:HG22	1:A:610:LYS:H	1.31	0.96
1:A:527:GLY:HA3	1:A:609:VAL:HG21	1.50	0.94
1:A:323:GLN:HE21	1:A:325:THR:HG22	1.32	0.93
1:A:200:PRO:HD2	1:A:206:GLU:HB2	1.51	0.92
1:A:557:GLN:HE22	1:A:562:ALA:HB3	1.35	0.91
1:A:608:ARG:CD	1:A:608:ARG:H	1.81	0.91
1:B:460:LYS:HA	1:B:464:ARG:HE	1.36	0.91
1:B:600:VAL:HG22	1:B:622:VAL:HG22	1.51	0.90
1:B:343:LYS:HB3	1:B:344:PRO:CD	2.01	0.89
1:A:495:ARG:HG3	1:A:495:ARG:NH1	1.84	0.89
1:B:410:LEU:HD13	1:B:511:LEU:HD11	1.56	0.88
1:A:608:ARG:HD2	1:A:608:ARG:N	1.88	0.87
1:A:197:ARG:HG3	1:A:198:LYS:H	1.39	0.86
1:B:94:LEU:HD22	2:B:2042:HOH:O	1.74	0.86
1:A:200:PRO:HD2	1:A:206:GLU:CB	2.07	0.82
1:A:36:GLU:OE2	1:A:99:ALA:HA	1.78	0.82
1:A:280:SER:OG	1:A:283:LEU:HB2	1.81	0.81
1:A:609:VAL:HG22	1:A:610:LYS:N	1.95	0.81
1:A:283:LEU:HG	1:A:406:ARG:HH12	1.47	0.79
1:A:330:SER:HB2	2:A:2254:HOH:O	1.83	0.77
1:A:557:GLN:NE2	1:A:562:ALA:HB3	1.99	0.77
1:B:545:PHE:O	1:B:625:VAL:HA	1.84	0.77
1:A:584:GLY:O	1:A:586:LYS:HG2	1.84	0.77
1:A:343:LYS:HB3	1:A:344:PRO:HD3	1.66	0.77
1:B:12:GLU:HB2	1:B:15:GLU:HG2	1.67	0.76
1:A:320:LYS:HE3	1:A:336:ARG:HD3	1.69	0.74
1:A:325:THR:O	1:A:326:THR:HG22	1.86	0.74
1:B:495:ARG:NH1	1:B:609:VAL:HG23	2.01	0.74
1:B:343:LYS:CB	1:B:344:PRO:HD3	2.14	0.73
1:B:543:HIS:HB2	1:B:623:LEU:CB	2.19	0.73
1:A:504:PRO:CG	1:A:517:PRO:HG3	2.18	0.73
1:B:199:SER:HB3	1:B:200:PRO:O	1.89	0.72
1:B:537:LYS:HD3	1:B:617:VAL:O	1.88	0.72
1:A:265:SER:HB3	1:A:267:LEU:HG	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:434:GLU:O	1:A:435:HIS:HB2	1.89	0.71
1:B:460:LYS:CA	1:B:464:ARG:HE	2.04	0.70
1:B:44:GLY:HA3	2:B:2042:HOH:O	1.90	0.70
1:A:552:GLU:O	1:A:552:GLU:HG3	1.92	0.70
1:A:549:GLY:O	1:A:593:LEU:HB2	1.93	0.69
1:B:543:HIS:CB	1:B:623:LEU:HB2	2.19	0.69
1:B:513:GLN:HG3	2:B:2398:HOH:O	1.93	0.69
1:A:608:ARG:HH11	1:A:608:ARG:HG3	1.56	0.68
1:B:408:GLN:HG3	1:B:414:VAL:HG22	1.76	0.68
1:A:134:ARG:NH2	1:A:170:ASN:HB3	2.08	0.68
1:B:527:GLY:HA3	1:B:609:VAL:HG21	1.75	0.68
1:B:537:LYS:NZ	1:B:617:VAL:H	1.91	0.68
1:B:557:GLN:HB2	2:B:2431:HOH:O	1.92	0.68
1:A:326:THR:O	1:A:332:THR:HA	1.94	0.68
1:A:541:ARG:HG2	1:A:543:HIS:NE2	2.08	0.68
1:B:610:LYS:HB2	2:B:2439:HOH:O	1.93	0.67
1:A:323:GLN:NE2	1:A:325:THR:HG22	2.08	0.67
1:A:283:LEU:HG	1:A:406:ARG:NH1	2.08	0.67
1:A:533:PRO:HG2	2:A:2363:HOH:O	1.95	0.66
1:B:585:ARG:O	1:B:586:LYS:HB2	1.93	0.66
1:A:330:SER:HB3	2:A:2256:HOH:O	1.94	0.66
1:B:545:PHE:HD2	1:B:623:LEU:HD12	1.61	0.66
1:A:504:PRO:HG3	1:A:517:PRO:HG3	1.77	0.66
1:A:594:SER:O	1:A:625:VAL:HG11	1.96	0.66
1:B:573:LEU:HD23	1:B:573:LEU:C	2.16	0.65
1:A:333:LYS:NZ	1:B:333:LYS:HB2	2.12	0.65
1:B:262:ARG:HG2	1:B:264:ASP:OD1	1.97	0.65
1:B:447:GLN:HG3	2:B:2012:HOH:O	1.97	0.65
1:A:545:PHE:CD2	1:A:623:LEU:HD11	2.31	0.65
1:B:35:SER:HB3	1:B:38:LYS:O	1.96	0.65
1:B:535:LYS:O	1:B:537:LYS:N	2.28	0.65
1:A:516:SER:HB3	1:A:517:PRO:HD2	1.79	0.64
1:B:200:PRO:HD3	1:B:205:GLY:CA	2.22	0.64
1:A:512:HIS:O	1:A:513:GLN:HB3	1.97	0.64
1:A:557:GLN:HG2	1:A:558:LYS:N	2.13	0.63
1:B:333:LYS:HE2	1:B:335:VAL:HG12	1.80	0.63
1:B:458:SER:O	1:B:464:ARG:NH2	2.31	0.63
1:A:576:GLU:CD	1:A:577:SER:H	2.01	0.63
1:A:12:GLU:HG2	1:A:15:GLU:OE1	1.98	0.63
1:A:200:PRO:CD	1:A:206:GLU:HB2	2.27	0.62
1:B:75:LYS:HE3	1:B:111:GLN:OE1	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:125:LEU:HD12	1:B:127:LYS:HE2	1.80	0.62
1:B:179:GLU:HB2	2:B:2159:HOH:O	1.99	0.62
1:B:537:LYS:HZ3	1:B:617:VAL:H	1.47	0.62
1:A:148:VAL:HG22	1:A:195:VAL:CG1	2.30	0.62
1:A:28:ASN:HD22	1:A:471:ASN:ND2	1.97	0.62
1:B:542:GLN:H	1:B:542:GLN:CD	2.03	0.61
1:A:586:LYS:HE3	2:A:2390:HOH:O	2.00	0.61
1:B:585:ARG:O	1:B:586:LYS:CB	2.47	0.61
1:A:541:ARG:HG2	1:A:543:HIS:CE1	2.34	0.61
1:B:326:THR:O	1:B:326:THR:HG23	2.00	0.61
1:B:527:GLY:HA3	1:B:609:VAL:CG2	2.31	0.61
1:A:582:LEU:HD23	1:A:585:ARG:HA	1.83	0.60
1:A:582:LEU:HA	1:A:587:ASN:O	2.01	0.60
1:B:566:TRP:HB2	1:B:573:LEU:HD22	1.83	0.60
1:B:12:GLU:HG2	1:B:15:GLU:OE2	2.01	0.60
1:A:528:ASP:OD1	1:A:612:LYS:HD3	2.01	0.60
1:B:464:ARG:HD3	2:B:2329:HOH:O	2.01	0.60
1:B:73:LYS:HG2	1:B:83:LYS:HD3	1.83	0.60
1:B:38:LYS:HE2	1:B:38:LYS:H	1.66	0.60
1:B:551:ALA:HB3	2:B:2424:HOH:O	2.01	0.60
1:B:351:ASP:HB2	2:B:2281:HOH:O	2.01	0.59
1:B:503:PRO:N	1:B:504:PRO:HD2	2.17	0.59
1:A:30:SER:HB3	2:A:2322:HOH:O	2.01	0.59
1:A:391:ARG:HH11	1:A:391:ARG:CG	2.16	0.59
1:B:535:LYS:O	1:B:537:LYS:HE3	2.01	0.59
1:A:148:VAL:HG22	1:A:195:VAL:HG11	1.84	0.59
1:A:545:PHE:HD2	1:A:623:LEU:HD11	1.67	0.59
1:A:541:ARG:HB2	1:A:541:ARG:CZ	2.32	0.59
1:A:460:LYS:HD2	2:A:2336:HOH:O	2.02	0.59
1:B:279:ARG:O	1:B:280:SER:O	2.21	0.59
1:B:495:ARG:HH11	1:B:609:VAL:HG23	1.65	0.59
1:B:343:LYS:CB	1:B:344:PRO:CD	2.78	0.59
1:A:197:ARG:HG3	1:A:198:LYS:N	2.15	0.58
1:B:590:ILE:HB	2:B:2424:HOH:O	2.02	0.58
1:A:343:LYS:HZ2	1:A:343:LYS:HA	1.68	0.58
1:A:327:VAL:HG13	1:A:327:VAL:O	2.02	0.58
1:A:386:ILE:O	1:A:387:ASP:HB2	2.02	0.58
1:A:516:SER:HB3	1:A:521:LEU:HD21	1.86	0.57
1:A:333:LYS:HZ2	1:B:333:LYS:HB2	1.69	0.57
1:B:36:GLU:HA	2:B:2034:HOH:O	2.05	0.57
1:B:573:LEU:HA	1:B:574:LYS:HE3	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:60:LYS:HE2	1:B:63:GLU:OE2	2.04	0.57
1:A:495:ARG:HH11	1:A:495:ARG:CG	1.96	0.57
1:A:281:PRO:HD2	2:A:2234:HOH:O	2.05	0.57
1:A:56:ASN:ND2	2:A:2072:HOH:O	2.37	0.57
1:B:240:GLN:HG2	2:B:2152:HOH:O	2.05	0.57
1:B:460:LYS:HA	1:B:464:ARG:NE	2.16	0.57
1:B:574:LYS:O	1:B:576:GLU:N	2.38	0.57
1:A:330:SER:O	1:A:331:HIS:HB2	2.06	0.56
1:A:434:GLU:O	1:A:435:HIS:CB	2.53	0.56
1:A:179:GLU:OE1	1:A:374:LYS:HE3	2.05	0.56
1:B:418:MET:HE2	2:B:2343:HOH:O	2.04	0.56
1:B:489:GLU:OE1	1:B:537:LYS:HE2	2.05	0.56
1:A:211:TYR:CE1	1:A:234:ARG:HG2	2.40	0.56
1:A:343:LYS:HB3	1:A:344:PRO:CD	2.34	0.56
1:A:394:LYS:HG2	1:A:397:VAL:HG11	1.88	0.56
1:A:71:ASP:O	1:A:74:ALA:HB3	2.06	0.56
1:A:563:ARG:HB3	1:A:606:GLU:OE2	2.06	0.55
1:B:131:GLY:HA2	1:B:134:ARG:HD2	1.88	0.55
1:B:31:ALA:HB3	2:B:2042:HOH:O	2.06	0.55
1:B:344:PRO:HD2	1:B:369:THR:OG1	2.06	0.55
1:A:3:PHE:CD1	1:A:395:LYS:HG3	2.41	0.55
1:B:229:ILE:HG12	1:B:257:ARG:HG2	1.88	0.55
1:B:200:PRO:CD	1:B:205:GLY:HA2	2.24	0.55
1:B:595:GLU:OE1	1:B:625:VAL:HG13	2.06	0.55
1:A:78:GLU:HA	2:A:2109:HOH:O	2.06	0.55
1:A:97:LEU:HG	1:A:103:TYR:HB2	1.89	0.55
1:B:463:ASN:ND2	1:B:513:GLN:NE2	2.54	0.55
1:A:545:PHE:O	1:A:626:LYS:HG3	2.07	0.55
1:B:327:VAL:HG22	1:B:328:GLU:OE2	2.05	0.55
1:A:81:LYS:HD2	1:A:110:PHE:CZ	2.42	0.55
1:B:121:SER:OG	1:B:123:LYS:HB2	2.07	0.55
1:B:392:LEU:C	1:B:392:LEU:HD23	2.27	0.55
1:A:151:GLU:CD	1:A:171:SER:HB3	2.28	0.54
1:A:326:THR:HG23	1:A:331:HIS:O	2.07	0.54
1:A:510:ALA:O	1:A:514:THR:HB	2.07	0.54
1:B:453:GLN:HE22	1:B:471:ASN:ND2	2.06	0.54
1:B:545:PHE:HB3	1:B:593:LEU:HD12	1.89	0.54
1:A:359:TYR:HA	1:A:364:ASN:OD1	2.07	0.54
1:B:594:SER:OG	1:B:595:GLU:N	2.40	0.54
1:A:151:GLU:HG3	2:A:2177:HOH:O	2.08	0.54
1:B:550:THR:HG23	2:B:2423:HOH:O	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:336:ARG:HD2	1:A:338:ASN:HD21	1.71	0.54
1:B:386:ILE:O	1:B:387:ASP:HB2	2.08	0.54
1:A:516:SER:CB	1:A:521:LEU:HD21	2.38	0.53
1:B:222:GLU:HA	1:B:222:GLU:OE1	2.07	0.53
1:B:545:PHE:O	1:B:625:VAL:CA	2.54	0.53
1:B:568:PHE:O	1:B:569:GLN:C	2.47	0.53
1:B:97:LEU:HG	1:B:103:TYR:HB2	1.89	0.53
1:B:418:MET:CE	2:B:2343:HOH:O	2.56	0.53
1:B:544:PHE:HB3	1:B:626:LYS:NZ	2.24	0.53
1:A:242:GLY:HA3	1:A:245:THR:O	2.08	0.53
1:A:556:SER:HB2	1:A:586:LYS:HD2	1.91	0.53
1:A:606:GLU:HB3	1:A:615:PHE:CE1	2.44	0.53
1:B:604:LEU:HD23	1:B:604:LEU:N	2.24	0.53
1:B:59:GLU:HG3	2:B:2046:HOH:O	2.08	0.53
1:A:512:HIS:O	1:A:513:GLN:CB	2.56	0.53
1:A:93:VAL:HB	1:A:105:CYS:HB2	1.91	0.52
1:A:511:LEU:O	1:A:512:HIS:C	2.47	0.52
1:A:577:SER:OG	1:A:578:PRO:HA	2.09	0.52
1:B:118:ASN:O	1:B:122:PHE:N	2.42	0.52
1:A:69:SER:OG	1:A:72:LYS:HB2	2.09	0.52
1:B:460:LYS:N	1:B:464:ARG:HH21	2.07	0.52
1:A:130:ASP:OD2	1:A:132:LYS:HB2	2.10	0.52
1:A:5:PRO:HG2	2:A:2005:HOH:O	2.08	0.52
1:A:208:ASP:HB2	1:A:237:LYS:HE2	1.92	0.52
1:A:586:LYS:HG3	1:A:587:ASN:N	2.25	0.52
1:A:547:HIS:HB2	1:A:626:LYS:O	2.10	0.52
1:B:495:ARG:HG2	1:B:525:MET:O	2.09	0.52
1:A:173:HIS:O	1:A:175:PRO:HD3	2.10	0.52
1:A:234:ARG:NH2	1:A:252:SER:O	2.42	0.52
1:A:232:ILE:HG23	1:A:232:ILE:O	2.10	0.51
1:A:555:CYS:O	1:A:586:LYS:HB2	2.10	0.51
1:B:114:CYS:SG	1:B:134:ARG:HD3	2.50	0.51
1:A:75:LYS:HD3	2:A:2106:HOH:O	2.10	0.51
1:B:118:ASN:O	1:B:122:PHE:HA	2.09	0.51
1:B:308:ASN:HD22	1:B:309:LEU:N	2.08	0.51
1:A:323:GLN:HB3	1:A:337:TYR:HB2	1.91	0.51
1:A:517:PRO:HB2	1:A:520:GLY:HA3	1.93	0.51
1:A:320:LYS:HD3	2:A:2279:HOH:O	2.11	0.51
1:A:301:LEU:HD21	1:A:395:LYS:HG2	1.93	0.51
1:B:320:LYS:HE3	2:B:2039:HOH:O	2.10	0.51
1:A:103:TYR:HE2	1:A:152:LEU:HD22	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:118:ASN:O	1:A:122:PHE:N	2.44	0.50
1:A:433:LEU:O	1:A:434:GLU:C	2.50	0.50
1:B:333:LYS:HE2	1:B:335:VAL:CG1	2.40	0.50
1:B:435:HIS:ND1	1:B:435:HIS:N	2.57	0.50
1:B:601:TYR:N	1:B:621:HIS:O	2.33	0.50
1:B:63:GLU:HG3	1:B:65:TYR:HE2	1.76	0.50
1:A:343:LYS:C	1:A:343:LYS:HD3	2.32	0.50
1:B:584:GLY:O	1:B:585:ARG:O	2.29	0.50
1:A:45:ALA:O	1:A:91:ILE:HG12	2.12	0.50
1:A:503:PRO:N	1:A:504:PRO:HD2	2.26	0.50
1:A:608:ARG:CD	1:A:608:ARG:N	2.54	0.50
1:B:545:PHE:HB3	1:B:593:LEU:CD1	2.41	0.50
1:B:512:HIS:HD2	2:B:2156:HOH:O	1.94	0.50
1:A:134:ARG:HH21	1:A:170:ASN:HB3	1.76	0.50
1:A:193:ALA:HA	1:A:211:TYR:O	2.12	0.50
1:A:583:MET:O	1:A:587:ASN:HB2	2.12	0.50
1:A:543:HIS:HB2	1:A:623:LEU:HD13	1.93	0.49
1:B:537:LYS:HG2	2:B:2442:HOH:O	2.12	0.49
1:B:535:LYS:O	1:B:537:LYS:CE	2.60	0.49
1:B:322:MET:HE3	2:B:2304:HOH:O	2.12	0.49
1:B:279:ARG:HD2	2:B:2240:HOH:O	2.13	0.49
1:B:209:ARG:NE	2:B:2193:HOH:O	2.44	0.49
1:A:103:TYR:CE2	1:A:152:LEU:HD22	2.48	0.49
1:B:196:ILE:HG22	1:B:198:LYS:CE	2.43	0.49
1:B:199:SER:HB3	1:B:200:PRO:CA	2.40	0.49
1:B:582:LEU:HA	1:B:587:ASN:O	2.13	0.48
1:B:72:LYS:HA	1:B:75:LYS:HB3	1.93	0.48
1:A:322:MET:HG3	1:A:380:ASP:HA	1.94	0.48
1:A:390:PRO:HG2	1:A:393:ILE:HD11	1.94	0.48
1:A:391:ARG:NH1	1:A:391:ARG:CG	2.75	0.48
1:A:38:LYS:HG2	1:A:459:SER:OG	2.12	0.48
1:B:118:ASN:O	1:B:122:PHE:CA	2.62	0.48
1:B:357:ALA:O	1:B:358:ASN:HB2	2.14	0.48
1:B:403:VAL:HG23	1:B:419:PHE:HB2	1.96	0.48
1:A:577:SER:CB	1:A:578:PRO:HA	2.44	0.48
1:B:14:ARG:HG3	2:B:2008:HOH:O	2.13	0.48
1:A:34:LEU:HD13	1:A:41:LEU:CD1	2.44	0.48
1:A:151:GLU:HA	1:A:151:GLU:OE1	2.14	0.48
1:A:351:ASP:O	1:A:355:ARG:HB2	2.14	0.48
1:B:398:ASN:ND2	2:B:2325:HOH:O	2.37	0.48
1:B:544:PHE:HB3	1:B:626:LYS:HZ2	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:69:SER:O	1:B:73:LYS:HB2	2.13	0.48
1:A:267:LEU:HD23	1:B:297:ASN:HA	1.94	0.48
1:A:591:PHE:HD1	1:B:550:THR:HG21	1.79	0.48
1:A:308:ASN:ND2	2:A:2242:HOH:O	2.43	0.48
1:A:392:LEU:C	1:A:392:LEU:HD23	2.34	0.48
1:A:517:PRO:O	1:A:520:GLY:N	2.47	0.48
1:A:626:LYS:O	1:A:627:VAL:HB	2.14	0.48
1:A:336:ARG:HD2	1:A:338:ASN:ND2	2.28	0.47
1:B:460:LYS:H	1:B:464:ARG:HH21	1.60	0.47
1:A:198:LYS:HB2	2:A:2127:HOH:O	2.14	0.47
1:A:301:LEU:HD23	1:A:395:LYS:HA	1.95	0.47
1:B:62:HIS:HB3	1:B:122:PHE:CD2	2.50	0.47
1:B:169:ARG:O	1:B:175:PRO:HA	2.14	0.47
1:B:572:VAL:O	1:B:572:VAL:HG23	2.15	0.47
1:B:196:ILE:HG22	1:B:198:LYS:HE2	1.96	0.47
1:B:138:ASP:HB3	1:B:141:HIS:CG	2.49	0.47
1:B:600:VAL:HA	1:B:621:HIS:O	2.15	0.47
1:B:556:SER:O	1:B:618:VAL:HG13	2.15	0.47
1:A:391:ARG:NH1	1:A:391:ARG:HG2	2.29	0.47
1:A:230:PRO:HB3	1:A:272:LEU:HB2	1.97	0.47
1:A:343:LYS:O	1:A:345:ARG:N	2.47	0.47
1:A:609:VAL:HG12	1:A:612:LYS:O	2.14	0.47
1:B:391:ARG:HD3	1:B:391:ARG:HA	1.76	0.47
1:B:460:LYS:O	1:B:461:LYS:HG2	2.15	0.47
1:A:261:SER:HB2	1:A:267:LEU:O	2.15	0.46
1:A:515:GLU:O	1:A:516:SER:O	2.33	0.46
1:A:84:GLN:OE1	1:A:84:GLN:HA	2.15	0.46
1:B:59:GLU:OE1	1:B:59:GLU:HA	2.15	0.46
1:A:86:GLU:HB3	1:A:110:PHE:HE2	1.79	0.46
1:A:100:THR:HG23	1:A:100:THR:O	2.14	0.46
1:B:47:GLU:OE2	1:B:67:LYS:HB3	2.15	0.46
1:A:346:PRO:HG2	1:A:372:PHE:CD2	2.50	0.46
1:A:517:PRO:O	1:A:518:SER:C	2.54	0.46
1:B:118:ASN:ND2	2:B:2100:HOH:O	2.49	0.46
1:A:495:ARG:CG	1:A:495:ARG:NH1	2.63	0.46
1:B:555:CYS:HB2	1:B:566:TRP:CZ2	2.50	0.46
1:A:608:ARG:NH1	1:A:608:ARG:HG3	2.29	0.46
1:A:108:ASN:HB3	1:A:111:GLN:O	2.15	0.46
1:B:495:ARG:HD2	2:B:2386:HOH:O	2.16	0.46
1:B:446:PHE:CE1	1:B:475:VAL:HG23	2.50	0.46
1:B:281:PRO:HB3	2:B:2247:HOH:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:188:PRO:HA	1:A:215:THR:O	2.16	0.45
1:A:234:ARG:NH1	2:A:2212:HOH:O	2.49	0.45
1:A:320:LYS:HE3	1:A:336:ARG:HH11	1.82	0.45
1:B:598:SER:OG	1:B:624:GLU:HA	2.16	0.45
1:A:181:ALA:HB1	1:A:183:PRO:HD2	1.98	0.45
1:A:151:GLU:OE1	1:A:171:SER:HB3	2.17	0.45
1:A:92:ARG:HD2	1:A:143:TYR:CE2	2.52	0.45
1:A:503:PRO:CD	1:A:504:PRO:HD2	2.47	0.45
1:B:536:SER:O	1:B:537:LYS:O	2.34	0.45
1:B:196:ILE:O	1:B:198:LYS:HE3	2.17	0.45
1:B:581:GLY:O	1:B:589:LEU:HD12	2.16	0.45
1:A:524:GLU:CG	1:A:531:VAL:HG21	2.47	0.44
1:A:37:ASP:O	1:A:38:LYS:HB2	2.17	0.44
1:A:528:ASP:O	1:A:531:VAL:HG22	2.17	0.44
1:A:262:ARG:HA	2:A:2220:HOH:O	2.17	0.44
1:A:343:LYS:O	1:A:344:PRO:C	2.51	0.44
1:B:370:LEU:HD11	2:B:2289:HOH:O	2.18	0.44
1:B:47:GLU:CD	1:B:67:LYS:HA	2.38	0.44
1:B:608:ARG:NH1	2:B:2435:HOH:O	2.35	0.44
1:A:100:THR:HG23	2:A:2134:HOH:O	2.18	0.44
1:A:247:GLN:O	1:A:248:LYS:HB2	2.17	0.44
1:A:420:VAL:O	1:A:420:VAL:HG23	2.18	0.44
1:A:489:GLU:O	1:A:493:LEU:HD12	2.18	0.44
1:B:63:GLU:HG3	1:B:65:TYR:CE2	2.52	0.44
1:A:446:PHE:CE1	1:A:475:VAL:HG23	2.53	0.44
1:A:504:PRO:CD	1:A:517:PRO:HG3	2.48	0.44
1:B:328:GLU:HB3	2:B:2266:HOH:O	2.18	0.44
1:A:576:GLU:OE1	1:A:577:SER:O	2.36	0.44
1:B:324:SER:HB2	1:B:334:TRP:CZ2	2.53	0.44
1:A:516:SER:O	1:A:518:SER:N	2.50	0.44
1:A:593:LEU:HA	1:A:593:LEU:HD12	1.84	0.44
1:A:543:HIS:HB2	1:A:623:LEU:CD1	2.47	0.44
1:B:153:TYR:CZ	1:B:169:ARG:HD3	2.53	0.44
1:A:526:SER:O	1:A:610:LYS:HB2	2.18	0.43
1:A:609:VAL:CG2	1:A:610:LYS:N	2.67	0.43
1:B:573:LEU:HD23	1:B:573:LEU:O	2.17	0.43
1:A:123:LYS:HD3	2:A:2137:HOH:O	2.18	0.43
1:B:154:SER:O	1:B:167:ILE:HA	2.18	0.43
1:A:595:GLU:HA	1:A:625:VAL:CG1	2.48	0.43
1:A:28:ASN:HA	1:A:471:ASN:HA	1.99	0.43
1:B:395:LYS:HZ2	1:B:395:LYS:HB3	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:598:SER:OG	1:A:625:VAL:HG12	2.18	0.43
1:B:336:ARG:NE	1:B:380:ASP:OD2	2.48	0.43
1:B:262:ARG:HD2	1:B:389:ARG:NH1	2.33	0.43
1:B:13:HIS:HB3	2:B:2008:HOH:O	2.19	0.43
1:B:301:LEU:HD11	1:B:395:LYS:HG3	2.00	0.43
1:A:102:LEU:HG	1:A:119:LEU:HD21	2.00	0.43
1:A:503:PRO:HD2	1:A:504:PRO:HD2	2.01	0.43
1:A:564:VAL:HG21	2:A:2389:HOH:O	2.18	0.43
1:B:12:GLU:HB2	1:B:14:ARG:HD3	2.00	0.43
1:B:562:ALA:HB2	1:B:607:GLU:HG3	2.01	0.43
1:A:333:LYS:HG3	1:B:333:LYS:NZ	2.34	0.42
1:B:394:LYS:HG2	1:B:397:VAL:HG11	2.00	0.42
1:A:408:GLN:HG2	1:A:412:GLY:O	2.19	0.42
1:A:516:SER:CB	1:A:517:PRO:HD2	2.44	0.42
1:A:517:PRO:O	1:A:521:LEU:HG	2.20	0.42
1:B:14:ARG:H	1:B:14:ARG:HG3	1.62	0.42
1:A:354:ALA:O	1:A:359:TYR:HB2	2.19	0.42
1:A:421:SER:HB2	1:A:452:VAL:HB	2.01	0.42
1:B:446:PHE:HB3	1:B:448:ASP:OD1	2.19	0.42
1:B:567:LYS:HG2	1:B:572:VAL:HA	2.01	0.42
1:A:563:ARG:HA	2:A:2383:HOH:O	2.19	0.42
1:A:241:GLY:HA2	1:A:249:LYS:O	2.20	0.42
1:B:463:ASN:HA	1:B:463:ASN:HD22	1.61	0.42
1:A:450:GLU:OE2	1:A:451:PRO:HD2	2.19	0.42
1:A:62:HIS:NE2	2:A:2088:HOH:O	2.36	0.42
1:B:327:VAL:O	1:B:328:GLU:HB2	2.19	0.42
1:B:345:ARG:HA	1:B:346:PRO:HD3	1.96	0.42
1:B:464:ARG:NH1	1:B:479:LEU:HD11	2.35	0.42
1:A:118:ASN:ND2	2:A:2135:HOH:O	2.52	0.42
1:A:46:ARG:O	1:A:47:GLU:HB2	2.19	0.42
1:A:92:ARG:HD2	1:A:143:TYR:CZ	2.55	0.42
1:B:13:HIS:ND1	1:B:447:GLN:HG2	2.34	0.42
1:B:285:VAL:O	1:B:285:VAL:HG13	2.20	0.42
1:A:534:ASP:CG	1:A:535:LYS:N	2.73	0.42
1:A:582:LEU:CD2	1:A:585:ARG:HA	2.49	0.42
1:A:225:PHE:HE2	1:A:296:LEU:CD2	2.33	0.41
1:A:34:LEU:HD13	1:A:41:LEU:HD13	2.02	0.41
1:B:116:HIS:CE1	1:B:127:LYS:HE3	2.55	0.41
1:B:532:CYS:HB2	1:B:535:LYS:HE2	2.01	0.41
1:A:513:GLN:HG3	1:A:514:THR:N	2.36	0.41
1:A:68:VAL:HG21	1:A:87:CYS:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:240:GLN:HB2	1:A:362:SER:OG	2.19	0.41
1:A:524:GLU:C	1:A:526:SER:H	2.23	0.41
1:B:552:GLU:HG3	1:B:552:GLU:H	1.78	0.41
1:A:408:GLN:NE2	1:A:412:GLY:O	2.51	0.41
1:B:148:VAL:HG22	1:B:195:VAL:HG22	2.02	0.41
1:B:182:ILE:HD11	2:B:2172:HOH:O	2.19	0.41
1:B:329:GLN:O	1:B:330:SER:CB	2.68	0.41
1:B:503:PRO:CD	1:B:504:PRO:HD2	2.51	0.41
1:A:565:PHE:CD1	1:A:565:PHE:N	2.88	0.41
1:B:563:ARG:HG2	2:B:2189:HOH:O	2.21	0.41
1:A:154:SER:O	1:A:167:ILE:HA	2.20	0.41
1:B:280:SER:HA	1:B:281:PRO:HD3	1.96	0.41
1:A:138:ASP:HB3	1:A:141:HIS:CG	2.55	0.41
1:A:12:GLU:H	1:A:15:GLU:CG	2.34	0.41
1:A:551:ALA:O	1:A:589:LEU:HA	2.20	0.41
1:A:333:LYS:CD	1:B:333:LYS:HD3	2.51	0.41
1:A:511:LEU:HA	1:A:511:LEU:HD12	1.75	0.41
1:B:353:GLU:H	1:B:353:GLU:HG2	1.65	0.41
1:B:532:CYS:HA	1:B:533:PRO:HD3	1.94	0.41
1:B:604:LEU:HD22	1:B:617:VAL:HG22	2.02	0.41
1:A:182:ILE:HA	1:A:182:ILE:HD12	1.86	0.41
1:B:187:GLU:HA	2:B:2142:HOH:O	2.20	0.41
1:B:395:LYS:NZ	1:B:395:LYS:HB3	2.36	0.41
1:B:625:VAL:O	1:B:625:VAL:HG22	2.21	0.41
1:A:608:ARG:NH1	1:A:608:ARG:CG	2.84	0.41
1:B:24:PRO:O	1:B:25:ASP:HB2	2.21	0.41
1:B:346:PRO:HG2	1:B:372:PHE:CD2	2.56	0.41
1:B:98:SER:HB2	2:B:2085:HOH:O	2.21	0.41
1:A:131:GLY:O	1:A:134:ARG:HG3	2.21	0.40
1:B:281:PRO:HA	2:B:2244:HOH:O	2.20	0.40
1:A:229:ILE:HA	1:A:230:PRO:HD3	1.91	0.40
1:A:610:LYS:HG3	2:A:2359:HOH:O	2.20	0.40
1:B:583:MET:HB3	1:B:587:ASN:HB2	2.03	0.40
1:A:543:HIS:NE2	1:A:621:HIS:ND1	2.55	0.40
1:B:231:ARG:NH1	1:B:257:ARG:HG3	2.36	0.40
1:A:333:LYS:HZ3	1:B:333:LYS:HB2	1.84	0.40
1:B:434:GLU:OE2	1:B:610:LYS:HE3	2.22	0.40
1:B:484:LYS:HD2	2:B:2009:HOH:O	2.20	0.40
1:A:609:VAL:HG13	1:A:610:LYS:N	2.36	0.40
1:B:291:LEU:HD11	1:B:399:TYR:HB2	2.03	0.40
1:B:29:TYR:CD2	1:B:473:GLY:HA2	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:70:GLU:OE1	1:B:83:LYS:NZ	2.48	0.40
1:A:155:GLY:O	1:A:156:THR:HB	2.22	0.40
1:A:73:LYS:HB2	1:A:73:LYS:HE3	1.82	0.40
1:A:97:LEU:HD23	1:A:97:LEU:HA	1.77	0.40
1:B:577:SER:CB	1:B:578:PRO:HA	2.51	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	618/663 (93%)	565 (91%)	35 (6%)	18 (3%)	4 1
1	B	618/663 (93%)	567 (92%)	38 (6%)	13 (2%)	7 2
All	All	1236/1326 (93%)	1132 (92%)	73 (6%)	31 (2%)	5 2

All (31) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	434	GLU
1	A	511	LEU
1	A	516	SER
1	A	610	LYS
1	B	199	SER
1	B	280	SER
1	B	343	LYS
1	B	537	LYS
1	B	585	ARG
1	B	586	LYS
1	B	610	LYS
1	A	326	THR
1	A	435	HIS

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Mol	Chain	Res	Type
1	A	512	HIS
1	A	513	GLN
1	A	517	PRO
1	A	582	LEU
1	A	586	LYS
1	A	609	VAL
1	A	627	VAL
1	B	593	LEU
1	A	549	GLY
1	B	594	SER
1	A	328	GLU
1	B	538	GLY
1	B	569	GLN
1	B	575	ALA
1	A	331	HIS
1	A	343	LYS
1	B	342	PRO
1	A	300	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	545/582 (94%)	471 (86%)	74 (14%)	3	2
1	B	545/582 (94%)	465 (85%)	80 (15%)	3	1
All	All	1090/1164 (94%)	936 (86%)	154 (14%)	3	1

All (154) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	GLU
1	A	34	LEU
1	A	36	GLU
1	A	38	LYS
1	A	72	LYS

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Mol	Chain	Res	Type
1	A	82	SER
1	A	88	LEU
1	A	97	LEU
1	A	100	THR
1	A	132	LYS
1	A	173	HIS
1	A	174	SER
1	A	182	ILE
1	A	195	VAL
1	A	197	ARG
1	A	198	LYS
1	A	209	ARG
1	A	225	PHE
1	A	227	VAL
1	A	234	ARG
1	A	244	ARG
1	A	245	THR
1	A	249	LYS
1	A	264	ASP
1	A	265	SER
1	A	283	LEU
1	A	314	GLU
1	A	320	LYS
1	A	323	GLN
1	A	330	SER
1	A	332	THR
1	A	333	LYS
1	A	343	LYS
1	A	352	SER
1	A	358	ASN
1	A	361	SER
1	A	389	ARG
1	A	391	ARG
1	A	392	LEU
1	A	432	SER
1	A	433	LEU
1	A	435	HIS
1	A	457	LEU
1	A	461	LYS
1	A	495	ARG
1	A	511	LEU
1	A	513	GLN

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Mol	Chain	Res	Type
1	A	518	SER
1	A	519	ARG
1	A	530	SER
1	A	534	ASP
1	A	535	LYS
1	A	537	LYS
1	A	541	ARG
1	A	542	GLN
1	A	546	LYS
1	A	552	GLU
1	A	556	SER
1	A	557	GLN
1	A	563	ARG
1	A	564	VAL
1	A	567	LYS
1	A	573	LEU
1	A	576	GLU
1	A	577	SER
1	A	579	LYS
1	A	582	LEU
1	A	593	LEU
1	A	605	SER
1	A	606	GLU
1	A	607	GLU
1	A	608	ARG
1	A	610	LYS
1	A	626	LYS
1	B	14	ARG
1	B	15	GLU
1	B	17	HIS
1	B	36	GLU
1	B	38	LYS
1	B	47	GLU
1	B	59	GLU
1	B	60	LYS
1	B	68	VAL
1	B	72	LYS
1	B	73	LYS
1	B	75	LYS
1	B	82	SER
1	B	83	LYS
1	B	84	GLN

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Mol	Chain	Res	Type
1	B	92	ARG
1	B	111	GLN
1	B	172	SER
1	B	174	SER
1	B	195	VAL
1	B	198	LYS
1	B	206	GLU
1	B	209	ARG
1	B	222	GLU
1	B	223	PHE
1	B	225	PHE
1	B	226	ARG
1	B	234	ARG
1	B	264	ASP
1	B	265	SER
1	B	272	LEU
1	B	278	LEU
1	B	283	LEU
1	B	301	LEU
1	B	308	ASN
1	B	323	GLN
1	B	328	GLU
1	B	329	GLN
1	B	330	SER
1	B	332	THR
1	B	333	LYS
1	B	343	LYS
1	B	353	GLU
1	B	355	ARG
1	B	392	LEU
1	B	395	LYS
1	B	435	HIS
1	B	447	GLN
1	B	459	SER
1	B	460	LYS
1	B	464	ARG
1	B	495	ARG
1	B	537	LYS
1	B	541	ARG
1	B	542	GLN
1	B	550	THR
1	B	552	GLU

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Mol	Chain	Res	Type
1	B	557	GLN
1	B	563	ARG
1	B	564	VAL
1	B	569	GLN
1	B	570	ASN
1	B	573	LEU
1	B	574	LYS
1	B	577	SER
1	B	579	LYS
1	B	582	LEU
1	B	585	ARG
1	B	592	ASN
1	B	595	GLU
1	B	598	SER
1	B	604	LEU
1	B	610	LYS
1	B	612	LYS
1	B	613	THR
1	B	620	LYS
1	B	623	LEU
1	B	625	VAL
1	B	626	LYS
1	B	627	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	HIS
1	A	323	GLN
1	A	338	ASN
1	A	471	ASN
1	A	513	GLN
1	A	557	GLN
1	A	592	ASN
1	B	13	HIS
1	B	308	ASN
1	B	331	HIS
1	B	338	ASN
1	B	364	ASN
1	B	401	GLN
1	B	408	GLN
1	B	447	GLN

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Mol	Chain	Res	Type
1	B	463	ASN
1	B	471	ASN
1	B	513	GLN
1	B	547	HIS

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 carbohydrates 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(Å²)	Q<0.9
1	A	622/663 (93%)	-0.01	33 (5%)	26	25	13, 36, 81, 100	0
1	B	622/663 (93%)	-0.07	41 (6%)	18	17	8, 29, 85, 100	0
All	All	1244/1326 (93%)	-0.04	74 (5%)	22	21	8, 33, 84, 100	0

All (74) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	200	PRO	8.5
1	A	327	VAL	8.0
1	B	577	SER	7.7
1	A	628	VAL	7.5
1	A	199	SER	7.0
1	B	584	GLY	6.3
1	B	200	PRO	6.2
1	A	519	ARG	5.9
1	A	283	LEU	5.9
1	A	515	GLU	5.9
1	A	326	THR	5.2
1	B	626	LYS	5.2
1	A	328	GLU	4.9
1	A	514	THR	4.9
1	B	327	VAL	4.6
1	B	537	LYS	4.5
1	A	518	SER	4.5
1	B	627	VAL	4.5
1	A	585	ARG	4.1
1	B	199	SER	4.0
1	B	585	ARG	4.0
1	A	435	HIS	3.9
1	B	435	HIS	3.9
1	A	627	VAL	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	329	GLN	3.8
1	B	624	GLU	3.7
1	B	282	GLY	3.7
1	A	173	HIS	3.6
1	B	544	PHE	3.6
1	B	84	GLN	3.5
1	A	198	LYS	3.3
1	B	578	PRO	3.3
1	B	328	GLU	3.3
1	B	37	ASP	3.3
1	A	331	HIS	3.1
1	B	570	ASN	2.9
1	B	71	ASP	2.9
1	A	343	LYS	2.8
1	B	283	LEU	2.8
1	B	592	ASN	2.7
1	A	281	PRO	2.7
1	B	611	ASN	2.7
1	B	460	LYS	2.6
1	A	520	GLY	2.6
1	B	326	THR	2.6
1	B	281	PRO	2.5
1	B	576	GLU	2.5
1	B	459	SER	2.5
1	B	590	ILE	2.5
1	B	572	VAL	2.4
1	A	330	SER	2.4
1	B	628	VAL	2.4
1	A	205	GLY	2.4
1	B	625	VAL	2.4
1	A	172	SER	2.3
1	B	551	ALA	2.3
1	A	434	GLU	2.3
1	A	244	ARG	2.3
1	B	17	HIS	2.3
1	A	578	PRO	2.3
1	A	99	ALA	2.2
1	B	538	GLY	2.2
1	B	588	LEU	2.2
1	A	282	GLY	2.2
1	A	517	PRO	2.2
1	A	284	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	610	LYS	2.1
1	B	264	ASP	2.1
1	B	461	LYS	2.1
1	B	596	GLY	2.1
1	B	99	ALA	2.0
1	A	356	ALA	2.0
1	A	264	ASP	2.0
1	B	14	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 carbohydrates 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.