



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 06:41 PM UTC

PDB ID : 1OLZ / pdb_00001olz
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 ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

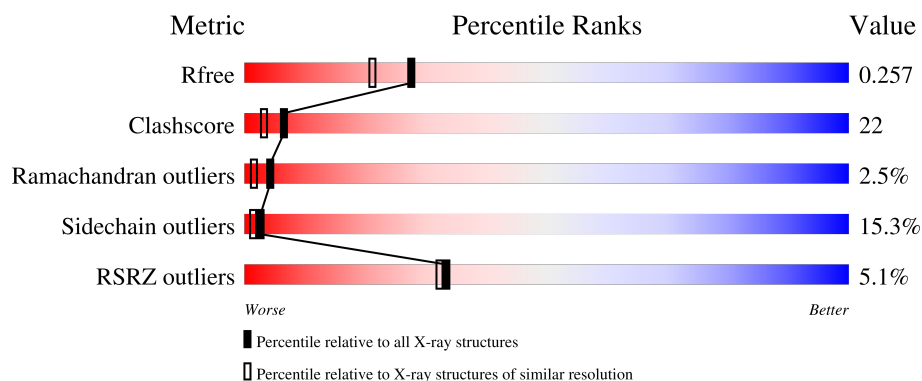
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	4% 55% 29% 9% 6%
1	B	663	5% 58% 26% 9% 6%

2 Entry composition

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			

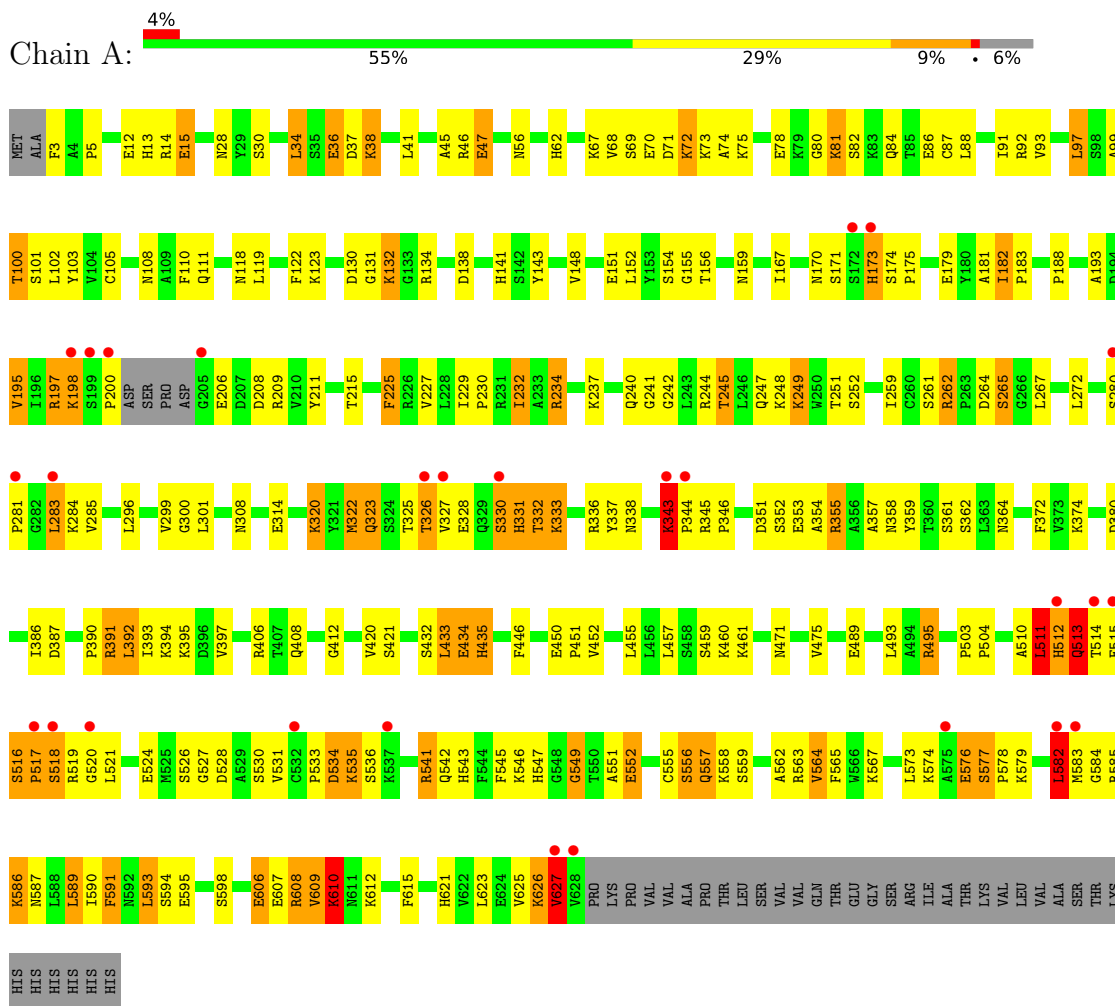
- Molecule 2 is water.

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

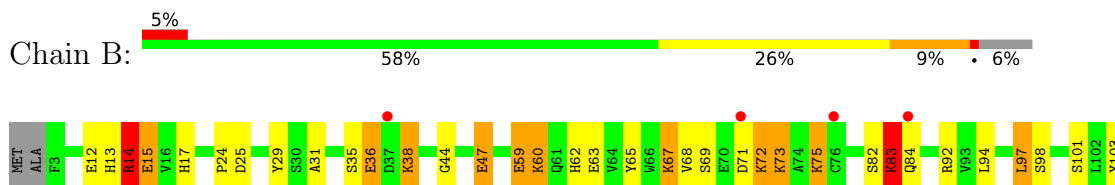
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: SEMAPHORIN 4D



• Molecule 1: SEMAPHORIN 4D



L623	E624	V625	K626	V627	V628	PRO	LYS	PRO	VAL	VAL	ALA	PRO	THR	THR	LEU	SER	VAL	VAL	GLN	THR	GLU	GLY	SER	SER	ILE	ALA	ALA	THR	LYS	VAL	LEU	VAL	ALA	SER	THR	LYS	HIS	HIS	HIS	HIS															
Q557	K558	A562	R563	V564	F565	W566	K567	F568	Q569	N570	G571	V572	L573	K574	A575	E576	S577	P578	Y579	Y580	G581	L582	M583	G584	R585	K586	N587	L588	L589	I590	F591	N592	L593	S594	E595	G596	D597	S598	G599	V600	Y601	L604	E607	R608	V609	K610	N611	K612	T613	V617	V618	A619	K620	H621	V622
Q453	S458	S459	K460	K461	G462	N463	R464	F465	V466	N471	S472	G473	A474	V475	L479	K484	E489	R495	P503	P504	L511	H512	Q513	T514	E515	M525	S526	G527	C532	P533	D534	K535	S536	K537	G538	R541	Q542	H543	F544	F545	T550	A551	E552	C555	S556										
V335	R336	V341	P342	K343	P344	R345	P346	D351	S352	E353	A354	R355	A356	A357	N358	T369	L370	Q371	F372	D380	V383	T386	D387	N388	R389	P390	R391	L392	I393	K394	K395	D396	V397	N398	Y399	V403	Q408	A409	L410	V414	M418	F419	E434	H435	F446	Q447	D448								
R209	E222	R226	V227	L228	I229	P230	R231	I232	Q240	R257	L258	I259	R262	P263	D264	S265	L272	L278	R279	S280	P281	G282	L283	K284	V285	L291	Q295	L296	N297	L301	N308	L309	K320	Q323	S324	T325	T326	V327	E328	Q329	S330	H331	T332	K333	W334										
Q111	P112	A113	C114	D115	H116	L117	N118	S121	F122	K123	F124	L125	K127	G131	R134	D138	H141	V148	Y153	S154	N159	I167	S168	R169	S172	H173	S174	P175	E179	I182	E187	V195	I196	R197	K198	S199	P200	ASP	SER	PRO	ASP	G205	E206												

4 Data and refinement statistics

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 20.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	96.7 (20.00-2.00) 96.6 (20.00-2.00)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.38 (at 2.01Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.206 , 0.270 (Not available) , 0.257	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)	0.33 , 71.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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	0.46	1/5034 (0.0%)	0.93	16/6825 (0.2%)
1	B	0.48	2/5034 (0.0%)	0.97	23/6825 (0.3%)
All	All	0.47	3/10068 (0.0%)	0.95	39/13650 (0.3%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	418	MET	SD-CE	-7.03	1.61	1.79
1	A	627	VAL	C-N	-5.58	1.25	1.33
1	B	627	VAL	C-N	-5.53	1.25	1.33

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	611	ASN	N-CA-C	-9.71	100.63	114.12
1	A	330	SER	N-CA-C	-8.78	102.47	113.01
1	A	591	PHE	N-CA-C	7.99	121.55	111.24
1	B	232	ILE	N-CA-C	-7.40	97.75	108.11
1	A	101	SER	N-CA-C	6.86	119.28	108.79
1	A	343	LYS	CA-C-N	-6.80	111.34	119.84
1	A	343	LYS	C-N-CA	-6.80	111.34	119.84
1	A	259	ILE	N-CA-C	6.62	118.11	108.58
1	A	232	ILE	N-CA-C	-6.40	99.21	108.17
1	A	262	ARG	CA-C-N	6.37	125.86	119.24
1	A	262	ARG	C-N-CA	6.37	125.86	119.24
1	B	596	GLY	N-CA-C	-6.37	105.61	115.73
1	A	251	THR	N-CA-C	-6.34	104.10	113.61
1	B	83	LYS	N-CA-C	6.28	118.93	111.71
1	B	543	HIS	N-CA-C	6.10	118.34	108.34
1	B	343	LYS	CA-C-N	-6.05	113.45	119.99
1	B	343	LYS	C-N-CA	-6.05	113.45	119.99
1	B	182	ILE	CB-CA-C	-5.88	108.11	113.70
1	B	101	SER	N-CA-C	5.76	118.04	108.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	532	CYS	N-CA-C	5.63	116.49	109.57
1	B	259	ILE	N-CA-C	5.62	116.39	108.36
1	B	159	ASN	N-CA-C	5.46	117.70	109.41
1	A	14	ARG	N-CA-C	5.39	116.85	110.97
1	B	344	PRO	N-CA-C	-5.39	102.10	111.32
1	B	341	VAL	CA-C-N	5.35	126.53	119.84
1	B	341	VAL	C-N-CA	5.35	126.53	119.84
1	B	14	ARG	N-CA-C	5.25	119.74	113.23
1	A	285	VAL	N-CA-C	5.24	113.84	107.61
1	B	295	GLN	N-CA-C	-5.24	105.17	112.45
1	A	322	MET	N-CA-C	-5.20	102.36	110.42
1	A	159	ASN	N-CA-C	5.18	116.54	109.18
1	A	559	SER	N-CA-C	5.12	117.73	110.10
1	B	199	SER	C-N-CD	-5.09	104.11	125.00
1	B	345	ARG	N-CA-C	5.09	116.94	109.71
1	B	383	VAL	N-CA-C	-5.09	100.45	108.23
1	A	284	LYS	N-CA-C	5.04	118.69	112.54
1	B	199	SER	CA-C-N	5.02	147.71	122.60
1	B	199	SER	C-N-CA	5.02	147.71	122.60
1	B	352	SER	N-CA-C	5.01	116.43	111.07

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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	227	0
1	B	4914	0	4841	204	0
2	A	398	0	0	24	0
2	B	443	0	0	39	0
All	All	10669	0	9682	425	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 22.

All (425) 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:H	1:A:608:ARG:HD2	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	1.04
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:H	1:A:608:ARG:CD	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
1:A:434:GLU:O	1:A:435:HIS:HB2	1.89	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:460:LYS:CA	1:B:464:ARG:HE	2.04	0.70
1:A:333:LYS:HZ2	1:B:333:LYS:HB2	1.55	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:B:573:LEU:HD23	1:B:573:LEU:C	2.16	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:576:GLU:CD	1:A:577:SER:H	2.01	0.69
1:B:418:MET:HE2	2:B:2343:HOH:O	1.92	0.68
1:A:608:ARG:HG3	1:A:608:ARG:HH11	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:542:GLN:H	1:B:542:GLN:CD	2.03	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: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:A:333:LYS:NZ	1:B:333:LYS:HB2	2.12	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:12:GLU:HG2	1:A:15:GLU:OE1	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:28:ASN:HD22	1:A:471:ASN:ND2	1.97	0.62
1:A:148:VAL:HG22	1:A:195:VAL:CG1	2.30	0.62
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: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:B:326:THR:HG23	1:B:326:THR:O	2.00	0.60
1:A:528:ASP:OD1	1:A:612:LYS:HD3	2.01	0.60
1:B:73:LYS:HG2	1:B:83:LYS:HD3	1.83	0.60
1:B:464:ARG:HD3	2:B:2329:HOH:O	2.01	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:151:GLU:CD	1:A:171:SER:HB3	2.28	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:B:392:LEU:C	1:B:392:LEU:HD23	2.27	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:327:VAL:O	1:A:327:VAL:HG13	2.02	0.58
1:A:386:ILE:O	1:A:387:ASP:HB2	2.02	0.58
1:B:568:PHE:O	1:B:569:GLN:C	2.47	0.58
1:A:516:SER:HB3	1:A:521:LEU:HD21	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:511:LEU:O	1:A:512:HIS:C	2.47	0.57
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:56:ASN:ND2	2:A:2072:HOH:O	2.37	0.57
1:A:281:PRO:HD2	2:A:2234:HOH:O	2.05	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:343:LYS:HZ2	1:A:343:LYS:HA	1.70	0.56
1:A:179:GLU:OE1	1:A:374:LYS:HE3	2.05	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:31:ALA:HB3	2:B:2042:HOH:O	2.06	0.55
1:B:131:GLY:HA2	1:B:134:ARG:HD2	1.88	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:A:433:LEU:O	1:A:434:GLU:C	2.50	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:336:ARG:HD2	1:A:338:ASN:HD21	1.71	0.54
1:A:343:LYS:HD3	1:A:343:LYS:C	2.32	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:OE1	1:B:222:GLU:HA	2.07	0.53
1:B:545:PHE:O	1:B:625:VAL:CA	2.54	0.53
1:B:97:LEU:HG	1:B:103:TYR:HB2	1.89	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:392:LEU:C	1:A:392:LEU:HD23	2.34	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:5:PRO:HG2	2:A:2005:HOH:O	2.08	0.52
1:A:130:ASP:OD2	1:A:132:LYS:HB2	2.10	0.52
1:A:208:ASP:HB2	1:A:237:LYS:HE2	1.92	0.52
1:A:547:HIS:HB2	1:A:626:LYS:O	2.10	0.52
1:A:586:LYS:HG3	1:A:587:ASN:N	2.25	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:301:LEU:HD21	1:A:395:LYS:HG2	1.93	0.51
1:A:320:LYS:HD3	2:A:2279:HOH:O	2.11	0.51
1:A:517:PRO:O	1:A:518:SER:C	2.54	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:118:ASN:O	1:A:122:PHE:N	2.44	0.50
1:B:63:GLU:HG3	1:B:65:TYR:HE2	1.76	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: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: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:47:GLU:CD	1:B:67:LYS:HA	2.38	0.49
1:B:196:ILE:HG22	1:B:198:LYS:CE	2.43	0.49
1:B:72:LYS:HA	1:B:75:LYS:HB3	1.93	0.48
1:B:582:LEU:HA	1:B:587:ASN:O	2.13	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:38:LYS:HG2	1:A:459:SER:OG	2.12	0.48
1:A:391:ARG:CG	1:A:391:ARG:NH1	2.75	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:343:LYS:O	1:A:344:PRO:C	2.51	0.48
1:B:418:MET:CE	2:B:2343:HOH:O	2.56	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:69:SER:O	1:B:73:LYS:HB2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:398:ASN:ND2	2:B:2325:HOH:O	2.37	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:517:PRO:O	1:A:520:GLY:N	2.47	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: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:391:ARG:NH1	1:A:391:ARG:HG2	2.29	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:84:GLN:HA	1:A:84:GLN:OE1	2.15	0.46
1:A:515:GLU:O	1:A:516:SER:O	2.33	0.46
1:A:534:ASP:CG	1:A:535:LYS:N	2.73	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:524:GLU:C	1:A:526:SER:H	2.23	0.46
1:A:626:LYS:O	1:A:627:VAL:HB	2.14	0.46
1:B:118:ASN:ND2	2:B:2100:HOH:O	2.49	0.46
1:A:495:ARG:NH1	1:A:495:ARG:CG	2.63	0.46
1:B:555:CYS:HB2	1:B:566:TRP:CZ2	2.50	0.46
1:A:608:ARG:HG3	1:A:608:ARG:NH1	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:92:ARG:HD2	1:A:143:TYR:CE2	2.52	0.45
1:A:151:GLU:OE1	1:A:171:SER:HB3	2.17	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:B:71:ASP:OD1	1:B:71:ASP:C	2.60	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:B:179:GLU:CD	2:B:2159:HOH:O	2.59	0.44
1:A:262:ARG:HA	2:A:2220:HOH:O	2.17	0.44
1:B:370:LEU:HD11	2:B:2289:HOH:O	2.18	0.44
1:B:570:ASN:CG	1:B:571:GLY:N	2.75	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:HG23	1:A:420:VAL:O	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:B:535:LYS:C	1:B:537:LYS:N	2.74	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:A:584:GLY:O	1:A:585:ARG:C	2.60	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:543:HIS:HB2	1:A:623:LEU:CD1	2.47	0.44
1:A:593:LEU:HD12	1:A:593:LEU:HA	1.84	0.44
1:B:153:TYR:CZ	1:B:169:ARG:HD3	2.53	0.44
1:B:542:GLN:CD	1:B:542:GLN:N	2.74	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:544:PHE:HB3	1:B:626:LYS:HZ3	1.82	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:HB3	1:B:395:LYS:HZ2	1.84	0.43
1:A:598:SER:OG	1:A:625:VAL:HG12	2.18	0.43
1:B:262:ARG:HD2	1:B:389:ARG:NH1	2.33	0.43
1:B:336:ARG:NE	1:B:380:ASP:OD2	2.48	0.43
1:B:13:HIS:HB3	2:B:2008:HOH:O	2.19	0.43
1:B:262:ARG:HG2	1:B:264:ASP:CG	2.43	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:HG3	1:B:14:ARG:H	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:B:111:GLN:O	1:B:112:PRO:C	2.62	0.42
1:A:241:GLY:HA2	1:A:249:LYS:O	2.20	0.42
1:B:463:ASN:HD22	1:B:463:ASN:HA	1.61	0.42
1:B:573:LEU:HD23	1:B:573:LEU:O	2.17	0.42
1:A:62:HIS:NE2	2:A:2088:HOH:O	2.36	0.42
1:A:450:GLU:OE2	1:A:451:PRO:HD2	2.19	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: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:A:118:ASN:ND2	2:A:2135:HOH:O	2.52	0.42
1:B:13:HIS:ND1	1:B:447:GLN:HG2	2.34	0.42
1:B:285:VAL:HG13	1:B:285:VAL:O	2.20	0.42
1:A:78:GLU:C	1:A:80:GLY:H	2.27	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:582:LEU:CD2	1:A:585:ARG:HA	2.49	0.42
1:B:308:ASN:HD22	1:B:308:ASN:C	2.28	0.42
1:A:34:LEU:HD13	1:A:41:LEU:HD13	2.02	0.41
1:A:225:PHE:HE2	1:A:296:LEU:CD2	2.33	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:68:VAL:HG21	1:A:87:CYS:O	2.20	0.41
1:A:240:GLN:HB2	1:A:362:SER:OG	2.19	0.41
1:A:535:LYS:O	1:A:536:SER:C	2.61	0.41
1:B:552:GLU:H	1:B:552:GLU:HG3	1.78	0.41
1:B:595:GLU:C	1:B:597:ASP:H	2.26	0.41
1:A:408:GLN:NE2	1:A:412:GLY:O	2.51	0.41
1:A:513:GLN:HG3	1:A:514:THR:N	2.36	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:12:GLU:H	1:A:15:GLU:CG	2.34	0.41
1:A:138:ASP:HB3	1:A:141:HIS:CG	2.55	0.41
1:A:551:ALA:O	1:A:589:LEU:HA	2.20	0.41
1:A:182:ILE:HD12	1:A:182:ILE:HA	1.86	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:187:GLU:HA	2:B:2142:HOH:O	2.20	0.41
1:B:353:GLU:H	1:B:353:GLU:HG2	1.65	0.41
1:B:395:LYS:HB3	1:B:395:LYS:NZ	2.36	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:B:625:VAL:O	1:B:625:VAL:HG22	2.21	0.41
1:A:12:GLU:O	1:A:13:HIS:C	2.64	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:98:SER:HB2	2:B:2085:HOH:O	2.21	0.41
1:B:346:PRO:HG2	1:B:372:PHE:CD2	2.56	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:610:LYS:HG3	2:A:2359:HOH:O	2.20	0.40
1:B:463:ASN:HD22	1:B:513:GLN:CD	2.30	0.40
1:B:583:MET:HB3	1:B:587:ASN:HB2	2.03	0.40
1:A:355:ARG:C	1:A:357:ALA:H	2.30	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: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:29:TYR:CD2	1:B:473:GLY:HA2	2.57	0.40
1:B:291:LEU:HD11	1:B:399:TYR:HB2	2.03	0.40
1:A:73:LYS:HE3	1:A:73:LYS:HB2	1.82	0.40
1:A:97:LEU:HA	1:A:97:LEU:HD23	1.77	0.40
1:A:155:GLY:O	1:A:156:THR:HB	2.22	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

5.3.1 Protein backbone

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%)	 
1	B	618/663 (93%)	567 (92%)	38 (6%)	13 (2%)	 
All	All	1236/1326 (93%)	1132 (92%)	73 (6%)	31 (2%)	 

All (31) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	434	GLU
1	A	511	LEU
1	A	516	SER

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Mol	Chain	Res	Type
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
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 ⓘ

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%)	466 (86%)	79 (14%)	3	2
1	B	545/582 (94%)	457 (84%)	88 (16%)	2	1
All	All	1090/1164 (94%)	923 (85%)	167 (15%)	3	1

All (167) 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	47	GLU
1	A	67	LYS
1	A	70	GLU
1	A	72	LYS
1	A	81	LYS
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	299	VAL
1	A	314	GLU
1	A	320	LYS
1	A	323	GLN
1	A	332	THR
1	A	333	LYS
1	A	343	LYS
1	A	352	SER
1	A	353	GLU
1	A	355	ARG
1	A	358	ASN
1	A	361	SER

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Mol	Chain	Res	Type
1	A	391	ARG
1	A	392	LEU
1	A	432	SER
1	A	433	LEU
1	A	455	LEU
1	A	457	LEU
1	A	461	LYS
1	A	495	ARG
1	A	511	LEU
1	A	513	GLN
1	A	518	SER
1	A	519	ARG
1	A	530	SER
1	A	534	ASP
1	A	535	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	564	VAL
1	A	567	LYS
1	A	573	LEU
1	A	574	LYS
1	A	576	GLU
1	A	577	SER
1	A	579	LYS
1	A	582	LEU
1	A	589	LEU
1	A	590	ILE
1	A	593	LEU
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

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Mol	Chain	Res	Type
1	B	47	GLU
1	B	59	GLU
1	B	60	LYS
1	B	67	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
1	B	92	ARG
1	B	97	LEU
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	226	ARG
1	B	227	VAL
1	B	264	ASP
1	B	265	SER
1	B	272	LEU
1	B	278	LEU
1	B	284	LYS
1	B	301	LEU
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	388	ASN
1	B	392	LEU
1	B	395	LYS
1	B	408	GLN

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Mol	Chain	Res	Type
1	B	435	HIS
1	B	447	GLN
1	B	459	SER
1	B	460	LYS
1	B	464	ARG
1	B	466	VAL
1	B	495	ARG
1	B	513	GLN
1	B	515	GLU
1	B	537	LYS
1	B	541	ARG
1	B	542	GLN
1	B	550	THR
1	B	552	GLU
1	B	557	GLN
1	B	558	LYS
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	576	GLU
1	B	577	SER
1	B	579	LYS
1	B	582	LEU
1	B	585	ARG
1	B	586	LYS
1	B	587	ASN
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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	HIS
1	A	28	ASN
1	A	116	HIS
1	A	128	ASN
1	A	323	GLN
1	A	338	ASN
1	A	471	ASN
1	A	513	GLN
1	A	542	GLN
1	A	557	GLN
1	A	592	ASN
1	B	13	HIS
1	B	108	ASN
1	B	308	ASN
1	B	318	HIS
1	B	331	HIS
1	B	338	ASN
1	B	364	ASN
1	B	401	GLN
1	B	408	GLN
1	B	447	GLN
1	B	463	ASN
1	B	471	ASN
1	B	513	GLN
1	B	547	HIS
1	B	570	ASN
1	B	602	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides 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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	622/663 (93%)	0.09	27 (4%) 40 39	13, 36, 81, 100	0
1	B	622/663 (93%)	-0.00	36 (5%) 29 27	8, 29, 85, 100	0
All	All	1244/1326 (93%)	0.04	63 (5%) 33 32	8, 33, 84, 100	0

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	200	PRO	6.5
1	A	628	VAL	5.2
1	B	537	LYS	4.7
1	A	327	VAL	3.9
1	A	517	PRO	3.6
1	A	514	THR	3.5
1	B	577	SER	3.4
1	B	327	VAL	3.4
1	B	584	GLY	3.3
1	A	627	VAL	3.3
1	A	199	SER	3.3
1	B	200	PRO	3.3
1	A	283	LEU	3.2
1	B	459	SER	3.2
1	B	599	GLY	3.2
1	A	343	LYS	3.1
1	A	326	THR	3.0
1	A	583	MET	3.0
1	B	625	VAL	3.0
1	A	515	GLU	3.0
1	A	198	LYS	3.0
1	A	344	PRO	2.9
1	B	199	SER	2.9
1	A	205	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	590	ILE	2.8
1	B	544	PHE	2.8
1	B	609	VAL	2.7
1	B	600	VAL	2.7
1	B	551	ALA	2.7
1	A	280	SER	2.6
1	B	627	VAL	2.5
1	B	71	ASP	2.5
1	B	578	PRO	2.5
1	B	583	MET	2.5
1	B	582	LEU	2.5
1	A	520	GLY	2.4
1	B	581	GLY	2.4
1	B	624	GLU	2.4
1	B	623	LEU	2.4
1	B	538	GLY	2.4
1	B	572	VAL	2.4
1	B	580	TYR	2.3
1	B	283	LEU	2.3
1	A	518	SER	2.3
1	B	622	VAL	2.3
1	B	343	LYS	2.3
1	B	84	GLN	2.3
1	B	76	CYS	2.3
1	A	575	ALA	2.3
1	A	537	LYS	2.2
1	B	596	GLY	2.2
1	B	545	PHE	2.1
1	A	172	SER	2.1
1	B	592	ASN	2.1
1	B	37	ASP	2.1
1	A	173	HIS	2.1
1	A	582	LEU	2.1
1	A	330	SER	2.1
1	A	281	PRO	2.1
1	A	512	HIS	2.1
1	B	550	THR	2.1
1	B	282	GLY	2.0
1	A	532	CYS	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 oligosaccharides 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.