



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:48 PM UTC

PDB ID : 1J7N / pdb_00001j7n
Title : Anthrax Toxin Lethal factor
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Deposited on : 2001-05-17
Resolution : 2.30 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
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

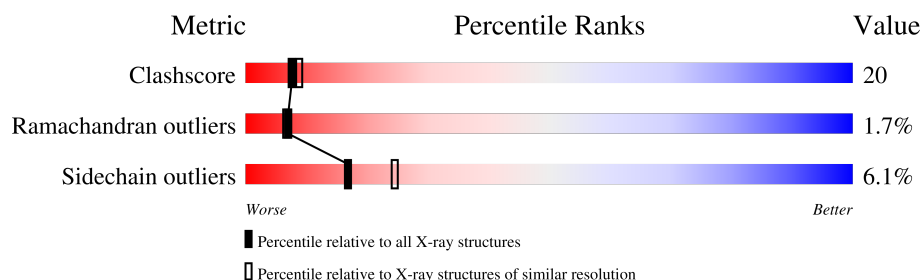
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	776	
1	B	776	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 12924 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 Lethal Factor precursor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	725	Total	C	N	O	S	0	0	0
			5947	3785	1003	1152	7			
1	B	736	Total	C	N	O	S	0	0	0
			6031	3832	1017	1175	7			

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total 1	Zn 1	0	0
3	B	1	Total 1	Zn 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	436	Total 436	O 436	0	0
4	B	498	Total 498	O 498	0	0

M744	S612	D495	K373	L185	I77	ALA
H745	D613	N496	K377	Q297	V84	GLY
S746	L614	L499	K378	K304	D85	HIS
T747	K616	K500	L379	S312	I88	GLY
H749	F629	W501		Q313	T89	ASP
A750	R502	R503	I388	I177	T166	VAL
E751	I503	I503	K389	E314	K178	GLY
R752	Q632	Q504	Q390	E315	H91	MET
L753	D633	L505	K391	K316	I92	HIS
	I634	S506	L392	E317	S93	VAL
A759				I318	L94	LVS
P760	I639	T509	L398	L319	E95	LVS
K761	Y643	R510			A96	GLU
F765	Y513		P402	I322	E99	GLU
T766	L514	Y514	Y408	Q323	K195	LVS
N767	E515	E515		I324	F201	ASN
D768	Y659	N516		D325	K102	LVS
Q769	G517	G517	Q411	S326	S202	ASP
I770	E662	K618	I413	S327	I104	GLU
		L519	R414	S331	L206	ASN
I773	I666	I520	D415	T332	D106	LVS
I774	K673	L521	I416	E333	I107	ARG
N775	E675	Q522	D420	E334	E212	LVS
S776	L677	R523		K335	V213	ASP
	E676			E336	V216	GLU
	L677	Q537			F217	
	R678	T535	H424	K339	F221	
		K536	Q425	K340	V119	
		Q537	S426	L341	I120	
	H690	R544	I427	Q342	A121	
			D428	I343	E226	
	D693	A547	L431	D344	P227	
D694			Y432	I345	Q228	
		P551			G124	
L700			Y439	S348	I125	E38
D701	K554	K554		LEU	E126	I39
K702			N441	SER	P127	M40
Q563	L703	Q563		GLU	V128	K41
N704	L564	L564	M444	GLU	L129	
Q704			M444	GLU	V130	
S705			N445	GLU	I131	E47
D706	Q568	Q568	L446	LYS	Q132	V48
L707			T447	GLU	S133	G50
			A448	LEU	S134	
	N571	N571		LEU	E135	E51
K712			D456	ASN	D136	E52
K713	K578	K578	S457	ARG		A53
	Y579	Y579		ILE	M140	V54
I717	F585	F585	N464	GLN	K143	K56
G722	N586	N586		VAL	E249	
S723	Y587	Y587	I467	D363	A144	
N724	H588	H588			L145	
	N589	N589	M482	K366	H146	
R730	R590	R590		P367	V147	E60
E733			I488	L368		L63
				S369	E150	E64
	K607	K607	R491	E370	L256	
F741			P492	K371	L265	L71
				E372	Y776	

4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	96.20Å 137.46Å 98.55Å 90.00° 98.35° 90.00°	Depositor
Resolution (Å)	15.00 – 2.30	Depositor
% Data completeness (in resolution range)	5.0 (15.00-2.30)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.229 , 0.261	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	12924	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, ZN

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	0.40	1/6053 (0.0%)	0.90	20/8153 (0.2%)
1	B	0.43	1/6139 (0.0%)	0.91	20/8272 (0.2%)
All	All	0.41	2/12192 (0.0%)	0.90	40/16425 (0.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	615	ILE	CG1-CD1	-10.06	1.12	1.51
1	A	615	ILE	CG1-CD1	5.90	1.74	1.51

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	615	ILE	CB-CG1-CD1	11.59	138.14	113.80
1	A	615	ILE	CB-CG1-CD1	-9.59	93.67	113.80
1	B	590	ARG	N-CA-C	8.96	123.32	112.38
1	A	639	ILE	N-CA-C	8.36	118.39	110.53
1	B	629	PHE	N-CA-C	-7.84	95.95	108.73
1	A	589	ASN	N-CA-C	7.33	120.25	109.69
1	A	590	ARG	N-CA-C	7.24	121.21	112.38
1	B	124	GLY	N-CA-C	-6.94	105.36	111.95
1	B	126	GLU	CA-C-N	6.64	126.61	119.78
1	B	126	GLU	C-N-CA	6.64	126.61	119.78
1	A	503	ILE	N-CA-C	6.59	117.40	108.17
1	B	587	VAL	N-CA-C	6.40	117.08	107.80
1	A	373	LYS	N-CA-C	-6.25	105.62	113.18
1	B	571	ASN	N-CA-C	-5.98	104.76	111.28
1	B	643	TYR	N-CA-C	5.96	119.64	112.38
1	B	589	ASN	N-CA-C	5.84	119.18	109.96
1	B	506	SER	N-CA-C	-5.64	102.50	110.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	578	LYS	N-CA-C	5.64	117.88	111.11
1	B	104	ILE	N-CA-C	5.60	115.65	108.82
1	A	632	THR	N-CA-C	5.54	117.39	109.14
1	A	571	ASN	N-CA-C	-5.53	105.33	111.36
1	B	42	HIS	N-CA-C	5.47	118.07	111.40
1	A	43	ILE	N-CA-C	5.39	119.86	113.22
1	A	630	VAL	N-CA-C	5.36	115.50	107.51
1	A	321	ARG	N-CA-C	5.28	115.98	108.54
1	A	197	HIS	CA-C-N	5.28	124.78	119.19
1	A	197	HIS	C-N-CA	5.28	124.78	119.19
1	A	587	VAL	N-CA-C	5.25	115.41	107.80
1	B	126	GLU	N-CA-C	-5.20	98.32	109.81
1	A	374	GLU	N-CA-C	-5.18	105.70	112.23
1	B	515	GLU	N-CA-C	5.17	117.66	111.71
1	A	643	TYR	N-CA-C	5.13	117.78	111.82
1	A	473	LYS	N-CA-C	5.11	119.75	111.37
1	B	503	ILE	N-CA-C	5.10	115.20	107.80
1	B	759	ALA	CA-C-N	5.08	125.12	119.32
1	B	759	ALA	C-N-CA	5.08	125.12	119.32
1	A	670	GLY	CA-C-N	5.07	125.09	119.32
1	A	670	GLY	C-N-CA	5.07	125.09	119.32
1	B	191	THR	N-CA-C	-5.06	103.36	110.35
1	B	438	TYR	N-CA-C	5.01	117.76	109.85

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	5947	0	5938	256	0
1	B	6031	0	5992	235	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	436	0	0	16	0
4	B	498	0	0	17	0
All	All	12924	0	11930	484	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 20.

All (484) 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:615:ILE:CD1	1:A:615:ILE:CG1	1.74	1.58
1:A:268:TYR:HB3	1:B:125:TYR:CE2	1.87	1.09
1:B:704:GLN:NE2	1:B:706:ASP:H	1.52	1.07
1:A:92:ILE:HD12	1:A:92:ILE:H	1.25	1.01
1:A:677:LEU:HD13	1:A:683:GLY:HA2	1.43	1.01
1:A:119:VAL:HG21	1:A:147:VAL:HG22	1.43	1.00
1:A:615:ILE:CD1	1:A:615:ILE:CB	2.39	1.00
1:B:304:LYS:HD3	1:B:304:LYS:H	1.27	0.96
1:A:615:ILE:HD13	1:A:615:ILE:HG21	1.46	0.96
1:B:510:ARG:H	1:B:522:GLN:HE21	1.05	0.95
1:B:632:THR:HG21	1:B:639:ILE:HD11	1.50	0.93
1:B:176:THR:HG21	1:B:239:GLU:HG3	1.53	0.89
1:A:268:TYR:HB3	1:B:125:TYR:HE2	1.38	0.88
1:B:712:LYS:H	1:B:712:LYS:HD2	1.35	0.88
1:B:606:TRP:CE2	1:B:615:ILE:HD12	2.10	0.86
1:A:107:ILE:HD11	1:A:219:LYS:HG3	1.56	0.85
1:A:567:ASN:HD21	1:A:583:ILE:H	1.19	0.85
1:B:366:ASN:H	1:B:367:PRO:HD2	1.42	0.84
1:A:636:LEU:HA	1:A:639:ILE:HD13	1.60	0.83
1:A:615:ILE:CD1	1:A:615:ILE:HG21	2.09	0.82
1:A:615:ILE:CD1	1:A:615:ILE:CG2	2.58	0.81
1:B:516:ASN:H	1:B:516:ASN:HD22	1.29	0.81
1:A:298:ILE:O	1:A:298:ILE:HD12	1.81	0.80
1:B:104:ILE:HG13	1:B:105:LYS:H	1.46	0.79
1:B:304:LYS:HD3	1:B:304:LYS:N	1.96	0.79
1:A:563:GLN:HE21	1:A:585:PHE:H	1.28	0.79
1:B:186:GLN:HG2	1:B:195:LYS:HG2	1.65	0.78
1:B:516:ASN:H	1:B:516:ASN:ND2	1.80	0.78
1:A:615:ILE:HD13	1:A:615:ILE:CG2	2.14	0.78
1:B:370:GLU:HG2	1:B:371:LYS:HG3	1.66	0.78
1:A:714:PHE:HA	1:A:717:ILE:HD13	1.67	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:516:ASN:HD22	1:B:516:ASN:N	1.80	0.77
1:A:290:ARG:O	1:A:294:LYS:HE2	1.85	0.76
1:B:678:ARG:NH1	1:B:678:ARG:HB3	2.01	0.76
1:A:66:VAL:CG1	1:A:70:VAL:HG21	2.15	0.76
1:B:391:ARG:HG3	1:B:412:TYR:CD1	2.21	0.75
1:A:656:LYS:HE3	1:A:669:HIS:O	1.87	0.75
1:A:761:LYS:HD3	1:A:761:LYS:C	2.12	0.75
1:B:606:TRP:CZ2	1:B:615:ILE:HD12	2.22	0.74
1:B:501:TRP:HB3	1:B:503:ILE:HD11	1.68	0.74
1:B:322:ILE:HD13	1:B:323:GLN:N	2.02	0.74
1:A:176:THR:HG21	1:A:239:GLU:HG3	1.69	0.74
1:A:577:PRO:O	1:A:580:THR:HG22	1.89	0.73
1:A:563:GLN:NE2	1:A:585:PHE:H	1.87	0.72
1:B:713:LYS:HD2	1:B:765:PHE:HE1	1.52	0.72
1:B:233:LEU:HD23	1:B:237:ALA:HB3	1.69	0.72
1:B:704:GLN:CD	1:B:706:ASP:H	1.97	0.72
1:B:611:GLN:HE22	1:B:613:ASP:HB2	1.54	0.72
1:B:510:ARG:H	1:B:522:GLN:NE2	1.85	0.72
1:B:244:MET:HE3	1:B:248:ASN:HD21	1.54	0.71
1:B:412:TYR:O	1:B:416:ILE:HG12	1.91	0.71
1:A:107:ILE:O	1:A:107:ILE:HD13	1.89	0.71
1:A:176:THR:CG2	1:A:239:GLU:HG3	2.21	0.71
1:B:704:GLN:NE2	1:B:706:ASP:N	2.35	0.71
1:A:256:LEU:HD22	1:A:260:LYS:HE3	1.73	0.70
1:A:605:GLU:HG3	4:A:9361:HOH:O	1.91	0.70
1:A:391:ARG:NH1	1:A:404:ILE:HD12	2.06	0.69
1:B:212:GLU:O	1:B:216:VAL:HG23	1.92	0.69
1:B:717:ILE:HD12	1:B:761:LYS:HB3	1.73	0.69
1:A:500:LYS:HE2	1:A:537:GLN:HE22	1.57	0.69
1:B:713:LYS:HD2	1:B:765:PHE:CE1	2.27	0.69
1:A:308:ILE:HD12	1:A:345:ILE:HD11	1.75	0.68
1:B:107:ILE:HG21	1:B:145:LEU:HD12	1.74	0.68
1:B:693:ASP:OD2	1:B:707:LEU:HB3	1.93	0.68
1:B:398:LEU:HD23	4:B:9209:HOH:O	1.94	0.68
1:A:712:LYS:HE3	1:A:712:LYS:H	1.59	0.68
1:B:121:ALA:HB1	1:B:154:ILE:HD11	1.75	0.67
1:B:221:PHE:HA	1:B:244:MET:HE2	1.75	0.67
1:B:369:SER:HB2	1:B:372:GLU:HG3	1.77	0.67
1:B:563:GLN:NE2	1:B:585:PHE:H	1.91	0.66
1:A:614:LEU:HD22	1:A:770:ILE:HD12	1.77	0.66
1:B:123:GLU:HG2	1:B:124:GLY:H	1.60	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:268:TYR:HB3	1:B:125:TYR:CD2	2.31	0.66
1:A:717:ILE:H	1:A:717:ILE:HD12	1.60	0.66
1:B:121:ALA:HB2	1:B:150:GLU:HG3	1.77	0.65
1:A:443:ILE:HD13	1:A:454:LEU:HD22	1.78	0.65
1:A:712:LYS:HE3	1:A:712:LYS:N	2.10	0.65
1:B:304:LYS:H	1:B:304:LYS:CD	2.07	0.65
1:B:378:LYS:HE3	4:B:9364:HOH:O	1.96	0.65
1:A:119:VAL:CG2	1:A:147:VAL:HG22	2.21	0.65
1:A:679:ASN:ND2	1:A:682:GLU:H	1.95	0.65
1:A:317:GLU:O	1:A:320:LYS:HB3	1.97	0.65
1:A:404:ILE:HD13	1:A:404:ILE:H	1.61	0.65
1:A:102:LYS:HA	1:A:114:LEU:HD12	1.79	0.65
1:A:330:LEU:HB2	1:A:335:LYS:HE3	1.78	0.64
1:B:28:ARG:NH1	1:B:30:LYS:HB2	2.11	0.64
1:B:704:GLN:HE22	1:B:706:ASP:H	1.41	0.64
1:A:28:ARG:HG2	1:A:28:ARG:HH11	1.63	0.64
1:A:500:LYS:HE2	1:A:537:GLN:NE2	2.13	0.64
1:B:704:GLN:HE21	1:B:705:SER:N	1.96	0.64
1:B:749:HIS:HA	1:B:752:ARG:HD3	1.79	0.64
1:B:107:ILE:HD13	1:B:107:ILE:O	1.99	0.63
1:A:28:ARG:HG3	1:A:29:ASN:H	1.62	0.63
1:A:221:PHE:HA	1:A:244:MET:HE2	1.79	0.63
1:A:107:ILE:HG21	1:A:145:LEU:HD12	1.81	0.62
1:A:639:ILE:O	1:A:640:ALA:CB	2.46	0.62
1:B:678:ARG:HB3	1:B:678:ARG:HH11	1.65	0.62
1:B:704:GLN:OE1	1:B:706:ASP:C	2.43	0.62
1:A:66:VAL:HG12	1:A:70:VAL:HG21	1.81	0.61
1:B:244:MET:HE3	1:B:248:ASN:ND2	2.15	0.61
4:A:9302:HOH:O	1:B:491:ARG:HD3	2.01	0.61
1:B:56:LYS:O	1:B:60:GLU:HG3	2.00	0.61
1:A:66:VAL:HG11	1:A:70:VAL:HG21	1.83	0.60
1:B:488:ILE:HD13	1:B:517:GLY:O	2.00	0.60
1:A:717:ILE:HD12	1:A:717:ILE:N	2.16	0.60
1:B:319:LEU:HD23	1:B:345:ILE:HD11	1.82	0.60
1:B:722:GLY:HA3	1:B:730:ARG:HH11	1.64	0.60
1:B:119:VAL:HG23	1:B:131:ILE:HD13	1.82	0.60
1:B:104:ILE:HG13	1:B:105:LYS:N	2.16	0.60
1:B:510:ARG:N	1:B:522:GLN:HE21	1.89	0.60
1:A:322:ILE:HD11	1:A:376:LEU:HD11	1.84	0.60
1:B:178:LYS:HD2	1:B:201:PHE:CE1	2.36	0.60
1:A:677:LEU:CD1	1:A:683:GLY:HA2	2.27	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:118:TYR:CD2	1:A:119:VAL:HG23	2.37	0.59
1:A:679:ASN:HD21	1:A:682:GLU:H	1.48	0.59
1:A:311:LEU:HA	1:A:315:GLU:OE2	2.03	0.59
1:B:611:GLN:NE2	1:B:614:LEU:H	2.00	0.59
1:A:312:SER:N	1:A:316:LYS:HG3	2.18	0.59
1:A:607:LYS:HA	1:A:615:ILE:HD11	1.84	0.59
1:B:370:GLU:HG2	1:B:371:LYS:N	2.17	0.59
1:B:733:GLU:CD	1:B:733:GLU:H	2.09	0.59
1:A:256:LEU:CD2	1:A:260:LYS:HE3	2.31	0.59
1:A:614:LEU:HD22	1:A:770:ILE:HG23	1.83	0.59
1:A:370:GLU:HG2	1:A:371:LYS:N	2.18	0.58
1:A:456:ASP:HB3	1:A:459:ASP:O	2.03	0.58
1:A:92:ILE:H	1:A:92:ILE:CD1	2.03	0.58
1:A:598:SER:O	1:A:602:ILE:HG13	2.03	0.58
1:B:693:ASP:CG	1:B:707:LEU:HB3	2.29	0.58
1:A:717:ILE:HG23	1:A:761:LYS:HD2	1.86	0.58
1:B:245:ASP:O	1:B:249:GLU:HG2	2.04	0.58
1:A:496:ASN:C	1:A:496:ASN:HD22	2.10	0.58
1:B:29:ASN:HA	1:B:32:GLN:HB3	1.85	0.58
1:A:46:ILE:HD12	1:A:46:ILE:N	2.18	0.58
1:A:733:GLU:H	1:A:733:GLU:CD	2.12	0.58
1:A:608:ASN:N	1:A:608:ASN:HD22	2.00	0.58
1:A:753:LEU:O	1:A:756:GLN:HB3	2.03	0.57
1:A:83:ILE:HD12	1:A:83:ILE:N	2.19	0.57
1:A:277:HIS:CD2	1:A:429:SER:HB2	2.39	0.57
1:A:303:LYS:HE3	1:A:306:ASP:OD1	2.04	0.57
1:A:314:GLU:O	1:A:318:LEU:HG	2.04	0.57
1:B:28:ARG:H	1:B:28:ARG:HD3	1.70	0.57
1:A:204:GLU:O	1:A:208:GLN:HG2	2.05	0.57
1:A:244:MET:CE	1:A:248:ASN:HD21	2.18	0.57
1:A:733:GLU:CD	1:A:733:GLU:N	2.63	0.57
1:B:304:LYS:HD2	4:B:9411:HOH:O	2.04	0.57
1:A:268:TYR:CB	1:B:125:TYR:HE2	2.15	0.56
1:B:733:GLU:HG2	4:B:9233:HOH:O	2.05	0.56
1:A:94:LEU:HB3	1:A:97:LEU:HD12	1.87	0.56
1:A:584:THR:HG23	1:A:630:VAL:HG22	1.88	0.56
1:B:28:ARG:HH12	1:B:30:LYS:HD2	1.71	0.56
1:B:456:ASP:O	1:B:457:SER:CB	2.53	0.56
1:A:244:MET:HE3	1:A:248:ASN:ND2	2.21	0.56
1:A:488:ILE:HD13	1:A:517:GLY:C	2.31	0.56
1:B:39:ILE:HG21	1:B:71:LEU:HB3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:221:PHE:HD1	1:B:244:MET:HE1	1.71	0.56
1:A:27:GLU:N	1:A:30:LYS:HB3	2.20	0.56
1:B:456:ASP:O	1:B:457:SER:HB3	2.06	0.56
1:A:244:MET:HE3	1:A:248:ASN:HD21	1.70	0.56
1:A:717:ILE:CG2	1:A:761:LYS:HD2	2.36	0.56
1:A:757:LYS:HD3	4:A:9240:HOH:O	2.06	0.56
1:B:60:GLU:O	1:B:64:GLU:HB2	2.06	0.56
1:B:523:ARG:HG2	4:B:9025:HOH:O	2.06	0.56
1:A:28:ARG:HG3	1:A:29:ASN:N	2.21	0.56
1:A:184:ASP:HB3	1:A:236:TYR:HB3	1.87	0.56
1:A:212:GLU:O	1:A:216:VAL:HG23	2.06	0.56
1:A:614:LEU:CD2	1:A:770:ILE:HD12	2.35	0.56
1:A:712:LYS:H	1:A:712:LYS:CE	2.18	0.56
1:B:366:ASN:H	1:B:367:PRO:CD	2.16	0.56
1:A:741:PHE:O	1:A:745:HIS:HD2	1.89	0.55
1:A:449:THR:HG21	4:A:9251:HOH:O	2.05	0.55
1:A:272:GLU:HG3	1:B:125:TYR:CE1	2.41	0.55
4:A:9170:HOH:O	1:B:124:GLY:HA2	2.06	0.55
1:B:391:ARG:HG3	1:B:412:TYR:CE1	2.41	0.55
1:A:495:ASP:OD2	1:B:495:ASP:HB2	2.07	0.55
1:A:368:LEU:HD22	1:A:372:GLU:CD	2.32	0.55
1:A:488:ILE:HD13	1:A:517:GLY:O	2.07	0.55
1:A:178:LYS:HB3	1:A:190:PHE:HE1	1.71	0.54
1:A:643:TYR:HA	1:A:646:GLN:HG3	1.90	0.54
1:B:431:LEU:HG	4:B:9306:HOH:O	2.06	0.54
1:A:460:ASN:HD22	1:A:461:THR:N	2.05	0.54
1:B:28:ARG:O	1:B:32:GLN:HB2	2.07	0.54
1:A:247:PHE:HA	1:A:251:GLU:HB2	1.89	0.54
1:A:615:ILE:O	1:A:619:THR:HG23	2.08	0.54
1:B:704:GLN:NE2	1:B:705:SER:N	2.55	0.54
1:B:244:MET:CE	1:B:248:ASN:HD21	2.18	0.54
1:A:524:ASN:ND2	4:A:9004:HOH:O	2.41	0.53
1:B:368:LEU:HB2	1:B:373:LYS:HG2	1.90	0.53
1:A:322:ILE:HA	1:A:368:LEU:HD13	1.89	0.53
1:A:154:ILE:HG22	1:A:159:ILE:HD13	1.91	0.53
1:A:748:ASP:OD2	1:A:750:ALA:HB3	2.09	0.53
1:B:31:THR:HA	1:B:34:GLU:HB3	1.89	0.53
1:A:712:LYS:H	1:A:712:LYS:CD	2.21	0.53
1:A:611:GLN:NE2	1:A:770:ILE:HG21	2.24	0.53
1:B:722:GLY:HA3	1:B:730:ARG:NH1	2.24	0.53
1:A:31:THR:O	1:A:35:HIS:HB2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:404:ILE:HD13	1:A:404:ILE:N	2.24	0.52
1:A:570:TRP:O	1:A:574:LEU:HB2	2.09	0.52
1:A:694:ASP:HA	1:A:707:LEU:HD23	1.91	0.52
1:A:272:GLU:HG3	1:B:125:TYR:CD1	2.44	0.52
1:B:578:LYS:O	1:B:579:TYR:HB2	2.10	0.52
1:B:38:GLU:O	1:B:41:LYS:HB3	2.09	0.52
1:B:392:LEU:HD11	1:B:416:ILE:HD12	1.92	0.52
1:B:312:SER:OG	1:B:315:GLU:HG3	2.10	0.52
1:A:491:ARG:HB3	1:A:492:PRO:HD2	1.92	0.52
1:A:66:VAL:HG12	1:A:70:VAL:CG2	2.39	0.51
1:A:107:ILE:HG21	1:A:145:LEU:CD1	2.40	0.51
1:A:322:ILE:HD12	1:A:372:GLU:OE1	2.10	0.51
1:B:114:LEU:HD21	1:B:120:TYR:HB2	1.92	0.51
1:B:496:ASN:C	1:B:496:ASN:HD22	2.18	0.51
1:A:104:ILE:HG22	1:A:105:LYS:N	2.25	0.51
1:B:47:GLU:O	1:B:84:VAL:HG23	2.11	0.51
1:B:206:LEU:C	1:B:206:LEU:HD13	2.35	0.51
1:A:577:PRO:O	1:A:580:THR:CG2	2.58	0.51
1:B:126:GLU:N	1:B:127:PRO:CD	2.72	0.51
1:A:413:LYS:O	1:A:417:GLN:HG3	2.11	0.51
1:B:206:LEU:HD13	1:B:206:LEU:O	2.11	0.51
1:B:317:GLU:HB2	4:B:9189:HOH:O	2.10	0.51
1:A:766:ILE:O	1:A:770:ILE:HG12	2.11	0.51
1:B:140:ASN:ND2	1:B:143:LYS:NZ	2.59	0.51
1:B:515:GLU:O	1:B:515:GLU:CD	2.54	0.51
1:A:49:LYS:HD2	1:A:51:GLU:OE1	2.11	0.50
1:A:264:MET:HE3	1:A:265:LEU:HD13	1.93	0.50
1:A:329:PHE:HE2	1:A:377:LYS:HA	1.75	0.50
1:A:627:GLY:HA3	1:A:664:ARG:O	2.12	0.50
1:B:121:ALA:HB1	1:B:154:ILE:CD1	2.41	0.50
1:A:28:ARG:CG	1:A:29:ASN:H	2.25	0.50
1:B:759:ALA:N	1:B:760:PRO:HD3	2.26	0.50
1:B:704:GLN:CD	1:B:706:ASP:N	2.67	0.50
1:A:426:SER:HA	1:A:510:ARG:HA	1.94	0.50
1:A:717:ILE:H	1:A:717:ILE:CD1	2.23	0.50
1:A:725:LEU:HD12	1:A:736:PHE:CE1	2.47	0.50
1:B:702:LYS:N	1:B:702:LYS:HD2	2.26	0.50
1:A:368:LEU:HB3	1:A:370:GLU:OE1	2.11	0.50
1:A:330:LEU:HD13	1:A:338:LEU:HD12	1.94	0.49
1:A:704:GLN:NE2	1:A:705:SER:HB3	2.27	0.49
1:A:433:ASN:O	1:A:435:ILE:HD12	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:502:ARG:C	1:B:503:ILE:HD13	2.37	0.49
1:B:611:GLN:HE22	1:B:613:ASP:CB	2.23	0.49
1:A:70:VAL:CG2	1:A:71:LEU:N	2.75	0.49
1:A:322:ILE:HA	1:A:368:LEU:CD1	2.42	0.49
1:A:341:LEU:O	1:A:345:ILE:HG12	2.12	0.49
1:A:606:TRP:CH2	1:A:615:ILE:HG23	2.47	0.49
1:B:319:LEU:O	1:B:322:ILE:HG22	2.12	0.49
1:B:373:LYS:O	1:B:377:LYS:HG3	2.12	0.49
1:B:427:ILE:O	1:B:428:GLY:C	2.55	0.49
1:B:500:LYS:HD3	1:B:537:GLN:HE22	1.77	0.49
1:A:57:GLU:O	1:A:61:LYS:HG2	2.12	0.49
1:A:322:ILE:HG13	1:A:368:LEU:HD13	1.93	0.49
1:A:576:LEU:HB3	1:A:580:THR:HG21	1.95	0.49
1:A:723:SER:HB3	1:A:730:ARG:NH1	2.27	0.49
1:B:47:GLU:OE1	1:B:91:HIS:HE1	1.95	0.49
1:B:441:MET:O	1:B:499:LEU:HB2	2.13	0.49
1:B:278:TYR:HE2	1:B:425:GLN:HB3	1.76	0.49
1:A:70:VAL:HG23	1:A:71:LEU:N	2.27	0.49
1:A:701:ASP:C	1:A:703:ASN:H	2.20	0.49
1:B:659:TYR:HD1	1:B:666:ILE:HD13	1.77	0.49
1:A:432:TYR:CD1	1:A:435:ILE:HD11	2.48	0.48
1:A:707:LEU:HB3	1:A:709:THR:HG22	1.95	0.48
1:B:150:GLU:OE2	1:B:153:LYS:NZ	2.46	0.48
1:A:537:GLN:NE2	4:A:9115:HOH:O	2.46	0.48
1:B:34:GLU:O	1:B:38:GLU:HG3	2.13	0.48
1:B:54:VAL:HA	1:B:57:GLU:OE2	2.12	0.48
1:B:176:THR:CG2	1:B:239:GLU:HG3	2.34	0.48
1:B:129:LEU:HD11	1:B:131:ILE:HD11	1.96	0.48
1:B:113:LEU:N	1:B:113:LEU:HD22	2.28	0.48
1:B:133:SER:O	1:B:134:SER:OG	2.30	0.48
1:A:28:ARG:HG3	1:A:29:ASN:OD1	2.13	0.48
1:A:159:ILE:HD12	1:A:159:ILE:N	2.27	0.48
1:A:331:SER:O	1:A:335:LYS:HG2	2.14	0.48
1:B:85:ASP:HB3	1:B:133:SER:OG	2.12	0.48
1:A:49:LYS:HB2	1:A:51:GLU:OE1	2.13	0.48
1:A:329:PHE:CE2	1:A:377:LYS:HA	2.49	0.48
1:B:551:PRO:HD2	1:B:554:LYS:HE3	1.95	0.48
1:B:607:LYS:HE2	4:B:9155:HOH:O	2.14	0.48
1:B:632:THR:OG1	1:B:634:ILE:HG12	2.14	0.48
1:B:744:MET:C	1:B:752:ARG:HG2	2.38	0.48
1:B:28:ARG:C	1:B:30:LYS:H	2.20	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:701:ASP:OD1	1:A:704:GLN:HB3	2.13	0.48
1:B:704:GLN:NE2	1:B:704:GLN:C	2.72	0.48
1:A:61:LYS:O	1:A:64:GLU:HB3	2.12	0.47
1:A:67:PRO:O	1:A:70:VAL:HG22	2.13	0.47
1:A:656:LYS:HE2	1:A:680:ASP:OD2	2.13	0.47
1:A:104:ILE:CG2	1:A:105:LYS:N	2.77	0.47
1:B:89:THR:O	1:B:89:THR:HG22	2.15	0.47
1:B:331:SER:OG	1:B:334:GLU:HG3	2.14	0.47
1:A:608:ASN:N	1:A:608:ASN:ND2	2.62	0.47
1:A:705:SER:O	1:A:706:ASP:HB2	2.14	0.47
1:B:143:LYS:O	1:B:147:VAL:HG23	2.14	0.47
1:B:178:LYS:HD2	1:B:201:PHE:CZ	2.50	0.47
1:A:154:ILE:O	1:A:159:ILE:HD13	2.15	0.47
1:B:77:ILE:HG23	1:B:77:ILE:O	2.15	0.47
1:B:408:VAL:HA	1:B:411:GLN:HG2	1.97	0.47
1:A:29:ASN:HA	1:A:32:GLN:HB2	1.97	0.47
1:A:679:ASN:HD22	1:A:679:ASN:H	1.63	0.47
1:B:125:TYR:CD1	1:B:125:TYR:N	2.83	0.47
1:B:564:LEU:O	1:B:568:GLN:HG3	2.14	0.47
1:B:706:ASP:O	1:B:707:LEU:HD23	2.15	0.47
1:B:304:LYS:HA	1:B:341:LEU:HD21	1.97	0.47
1:B:741:PHE:O	1:B:745:HIS:HD2	1.98	0.47
1:B:119:VAL:HG23	1:B:131:ILE:CD1	2.45	0.47
1:A:611:GLN:HE22	1:A:770:ILE:HG21	1.80	0.46
1:B:52:GLU:HG3	1:B:52:GLU:O	2.14	0.46
1:B:675:VAL:O	1:B:676:GLU:HB2	2.15	0.46
1:A:28:ARG:HG2	1:A:28:ARG:NH1	2.26	0.46
1:B:535:ILE:HD13	1:B:544:ARG:HB2	1.96	0.46
1:B:368:LEU:HA	4:B:9278:HOH:O	2.14	0.46
1:A:342:GLN:C	1:A:344:ASP:H	2.24	0.46
1:A:411:GLN:HE21	1:A:411:GLN:HA	1.80	0.46
1:B:319:LEU:HD23	1:B:345:ILE:CD1	2.44	0.46
1:A:454:LEU:HG	1:A:463:ILE:HD12	1.97	0.46
1:A:460:ASN:ND2	1:A:460:ASN:C	2.73	0.46
1:A:721:GLU:OE1	1:A:761:LYS:HB3	2.15	0.46
1:A:560:GLN:HG2	4:A:9041:HOH:O	2.16	0.46
1:A:501:TRP:HB3	1:A:503:ILE:HD11	1.97	0.46
1:B:221:PHE:HD1	1:B:244:MET:CE	2.29	0.46
1:B:704:GLN:HE21	1:B:704:GLN:C	2.24	0.46
1:A:557:THR:O	1:A:561:GLU:HG3	2.15	0.46
1:A:656:LYS:O	1:A:656:LYS:HD3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:402:PRO:O	1:B:649:ILE:HD12	2.16	0.46
1:B:703:ASN:O	1:B:704:GLN:CB	2.62	0.46
1:A:36:LEU:O	1:A:40:MET:HG2	2.15	0.46
1:B:95:GLU:O	1:B:96:ALA:HB2	2.16	0.46
1:B:140:ASN:ND2	1:B:143:LYS:HZ2	2.14	0.46
1:B:488:ILE:HD13	1:B:517:GLY:C	2.40	0.46
1:A:124:GLY:O	1:A:127:PRO:HD3	2.16	0.46
1:A:322:ILE:HD13	1:A:376:LEU:HD21	1.98	0.46
1:A:434:LYS:HB3	1:A:434:LYS:NZ	2.30	0.46
1:B:388:ILE:HG23	1:B:416:ILE:HD11	1.97	0.46
1:B:464:ASN:HB3	4:B:9084:HOH:O	2.15	0.46
1:B:690:HIS:O	1:B:693:ASP:HB3	2.15	0.46
1:A:51:GLU:CD	1:A:51:GLU:H	2.24	0.45
1:A:323:GLN:HB3	1:A:326:SER:OG	2.15	0.45
1:B:388:ILE:HG23	1:B:416:ILE:CD1	2.46	0.45
1:A:193:GLN:HE21	1:A:193:GLN:HA	1.80	0.45
1:A:480:SER:HB3	1:A:525:ILE:HB	1.98	0.45
1:A:169:LYS:HB3	4:A:9056:HOH:O	2.16	0.45
1:B:370:GLU:HG2	1:B:371:LYS:H	1.80	0.45
1:B:420:ASP:OD1	1:B:523:ARG:HD3	2.17	0.45
1:A:269:GLU:HB2	4:A:9290:HOH:O	2.17	0.45
1:A:433:ASN:O	1:A:435:ILE:CD1	2.65	0.45
1:B:88:ILE:O	1:B:94:LEU:HD12	2.17	0.45
1:B:389:ASN:OD1	1:B:482:ASN:HB2	2.17	0.45
1:B:426:SER:HA	1:B:510:ARG:HA	1.99	0.45
1:B:611:GLN:HE21	1:B:614:LEU:H	1.65	0.45
1:A:87:ASP:OD1	1:A:115:HIS:HB2	2.17	0.45
1:A:538:SER:O	1:A:539:GLU:HB2	2.17	0.45
1:A:758:ASN:HB3	4:A:9183:HOH:O	2.16	0.45
1:A:467:ILE:N	1:A:467:ILE:HD12	2.32	0.44
1:A:141:THR:HG21	1:A:228:GLN:HG3	1.99	0.44
1:A:768:ASP:O	1:A:771:LYS:HB3	2.17	0.44
1:A:149:TYR:HA	1:A:222:ALA:HB2	1.98	0.44
1:A:765:PHE:HD2	1:A:766:ILE:HD12	1.82	0.44
1:B:700:LEU:O	1:B:701:ASP:HB3	2.18	0.44
1:B:769:GLN:O	1:B:773:ILE:HD13	2.18	0.44
1:A:121:ALA:HB2	1:A:150:GLU:HG3	1.98	0.44
1:B:327:SER:HA	4:B:9214:HOH:O	2.17	0.44
1:A:584:THR:CG2	1:A:630:VAL:HG22	2.48	0.44
1:A:687:GLU:O	1:A:690:HIS:HB2	2.17	0.44
1:B:505:LEU:HD22	1:B:509:THR:HG21	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:409:ARG:HD2	4:A:9119:HOH:O	2.17	0.44
1:A:679:ASN:ND2	1:A:682:GLU:HB2	2.32	0.44
1:B:91:HIS:CD2	1:B:93:SER:H	2.36	0.44
1:A:338:LEU:HD23	1:A:341:LEU:HD12	1.98	0.44
1:A:412:TYR:O	1:A:416:ILE:HG13	2.18	0.44
1:B:49:LYS:C	1:B:49:LYS:HD2	2.43	0.44
1:B:125:TYR:N	1:B:125:TYR:HD1	2.16	0.44
1:B:444:ASN:HD22	1:B:448:ALA:HA	1.82	0.44
1:A:496:ASN:C	1:A:496:ASN:ND2	2.76	0.43
1:B:226:GLU:OE1	1:B:228:GLN:HB2	2.18	0.43
1:B:414:ARG:NH2	4:B:9146:HOH:O	2.50	0.43
1:A:51:GLU:CD	1:A:51:GLU:N	2.76	0.43
1:A:675:VAL:HG22	1:A:675:VAL:O	2.18	0.43
1:B:611:GLN:NE2	1:B:613:ASP:HB2	2.29	0.43
1:A:373:LYS:HD2	1:A:377:LYS:HE3	2.00	0.43
1:B:206:LEU:HD23	1:B:213:VAL:HG21	2.00	0.43
1:B:366:ASN:N	1:B:367:PRO:HD2	2.20	0.43
1:A:50:GLY:C	1:A:52:GLU:H	2.26	0.43
1:B:713:LYS:O	1:B:717:ILE:HG12	2.18	0.43
1:A:490:GLU:OE2	1:A:500:LYS:HE3	2.18	0.43
1:B:444:ASN:ND2	1:B:448:ALA:HA	2.34	0.43
1:A:294:LYS:NZ	4:A:9167:HOH:O	2.51	0.43
1:B:339:LYS:O	1:B:343:ILE:HG12	2.17	0.43
1:B:370:GLU:OE2	1:B:370:GLU:N	2.49	0.43
1:B:678:ARG:HB3	1:B:678:ARG:CZ	2.48	0.43
1:B:297:GLN:NE2	1:B:514:LEU:HD13	2.33	0.43
1:A:370:GLU:OE1	1:A:370:GLU:N	2.44	0.43
1:A:639:ILE:HG22	1:A:641:GLU:H	1.84	0.43
1:B:408:VAL:HA	1:B:411:GLN:CG	2.49	0.43
1:B:491:ARG:HB3	1:B:492:PRO:HD2	2.00	0.43
1:A:460:ASN:HD22	1:A:460:ASN:C	2.25	0.43
1:B:212:GLU:HG2	4:B:9135:HOH:O	2.18	0.43
1:B:322:ILE:HD13	1:B:322:ILE:C	2.44	0.43
1:A:107:ILE:HD13	1:A:107:ILE:C	2.43	0.42
1:B:712:LYS:H	1:B:712:LYS:CD	2.07	0.42
1:A:322:ILE:HD12	1:A:372:GLU:CD	2.44	0.42
1:A:741:PHE:O	1:A:745:HIS:CD2	2.72	0.42
1:B:28:ARG:HH11	1:B:30:LYS:HB2	1.83	0.42
1:B:513:TYR:HA	1:B:519:LEU:HD23	2.01	0.42
1:B:767:ASN:HD22	1:B:767:ASN:HA	1.59	0.42
1:A:49:LYS:HG3	1:A:85:ASP:OD1	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:159:ILE:N	1:A:159:ILE:CD1	2.82	0.42
1:A:639:ILE:O	1:A:640:ALA:HB3	2.20	0.42
1:A:226:GLU:HB3	1:A:229:HIS:HB2	2.00	0.42
1:A:370:GLU:C	1:A:372:GLU:H	2.26	0.42
1:B:724:ASN:CG	4:B:9367:HOH:O	2.61	0.42
1:A:410:LYS:HG3	4:A:9333:HOH:O	2.18	0.42
1:A:719:LYS:N	1:A:719:LYS:HE2	2.35	0.42
1:B:55:LYS:HD3	1:B:133:SER:HB2	2.01	0.42
1:B:156:SER:HB2	1:B:217:PHE:CD2	2.54	0.42
1:A:119:VAL:HG12	1:A:120:TYR:N	2.35	0.42
1:A:182:ASP:OD1	1:A:184:ASP:N	2.51	0.42
1:A:389:ASN:OD1	1:A:482:ASN:HB2	2.19	0.42
1:A:79:GLY:O	1:A:80:LYS:HD2	2.19	0.42
1:A:639:ILE:O	1:A:640:ALA:HB2	2.19	0.42
1:B:748:ASP:OD1	1:B:750:ALA:HB3	2.20	0.42
1:A:309:HIS:O	1:A:309:HIS:ND1	2.52	0.42
1:A:640:ALA:C	1:A:642:GLN:N	2.73	0.42
1:B:237:ALA:N	1:B:238:PRO:HD3	2.35	0.42
1:B:746:SER:O	1:B:752:ARG:HD2	2.19	0.42
1:B:775:ASN:HA	4:B:9476:HOH:O	2.20	0.42
1:A:303:LYS:HE3	1:A:306:ASP:CG	2.45	0.42
1:B:126:GLU:N	1:B:127:PRO:HD3	2.34	0.42
1:B:234:GLN:HB2	1:B:241:PHE:CD2	2.55	0.42
1:A:106:ASP:OD1	1:A:110:LYS:HE3	2.20	0.41
1:A:178:LYS:HD2	1:A:201:PHE:CE1	2.55	0.41
1:A:368:LEU:HD12	1:A:368:LEU:N	2.34	0.41
1:A:427:ILE:O	1:A:428:GLY:C	2.63	0.41
1:A:581:LYS:HE3	1:A:628:ARG:HH21	1.84	0.41
1:B:231:ASP:O	1:B:235:LEU:HB2	2.20	0.41
1:B:503:ILE:HD12	1:B:547:ALA:HB3	2.01	0.41
1:B:673:LYS:NZ	1:B:677:LEU:O	2.49	0.41
1:B:694:ASP:C	1:B:694:ASP:OD1	2.63	0.41
1:A:70:VAL:HG23	1:A:71:LEU:HD12	2.01	0.41
1:A:679:ASN:HD22	1:A:679:ASN:N	2.17	0.41
1:A:723:SER:HB3	1:A:730:ARG:HH12	1.85	0.41
1:B:611:GLN:NE2	1:B:613:ASP:N	2.69	0.41
1:B:49:LYS:HD2	1:B:50:GLY:N	2.35	0.41
1:A:678:ARG:HD3	4:A:9226:HOH:O	2.20	0.41
1:B:235:LEU:HD23	1:B:236:TYR:CE2	2.55	0.41
1:A:313:GLN:HB2	4:A:9248:HOH:O	2.20	0.41
1:B:332:THR:HG22	1:B:336:GLU:OE2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:49:LYS:HG3	1:A:49:LYS:H	1.69	0.41
1:B:40:MET:HE1	1:B:63:LEU:HB2	2.03	0.41
1:B:136:ASP:O	1:B:140:ASN:N	2.54	0.41
1:B:278:TYR:CE2	1:B:425:GLN:HB3	2.54	0.41
1:B:388:ILE:HD13	1:B:412:TYR:CD2	2.56	0.41
1:B:388:ILE:HD13	1:B:412:TYR:HD2	1.86	0.41
1:B:457:SER:CA	4:B:9182:HOH:O	2.68	0.41
1:B:112:ALA:C	1:B:113:LEU:HD22	2.46	0.41
1:B:703:ASN:O	1:B:704:GLN:HB2	2.20	0.41
1:A:586:ASN:OD1	1:A:588:HIS:CE1	2.74	0.41
1:B:424:HIS:HA	1:B:510:ARG:HD2	2.03	0.41
1:A:92:ILE:HD12	1:A:92:ILE:N	2.10	0.41
1:A:711:SER:HA	1:A:712:LYS:HE3	2.03	0.41
1:B:28:ARG:C	1:B:30:LYS:N	2.79	0.41
1:B:121:ALA:CB	1:B:150:GLU:HG3	2.47	0.41
1:B:165:GLN:HA	1:B:166:PRO:C	2.46	0.41
1:B:236:TYR:C	1:B:238:PRO:HD3	2.46	0.41
1:A:31:THR:O	1:A:31:THR:HG22	2.21	0.41
1:A:221:PHE:HD1	1:A:244:MET:HE1	1.85	0.41
1:A:606:TRP:CZ2	1:A:615:ILE:HG23	2.56	0.41
1:B:228:GLN:N	1:B:228:GLN:CD	2.78	0.41
1:B:457:SER:HA	4:B:9182:HOH:O	2.21	0.41
1:A:94:LEU:O	1:A:97:LEU:HB2	2.21	0.40
1:A:739:GLU:OE1	1:A:739:GLU:HA	2.21	0.40
1:B:107:ILE:HG21	1:B:145:LEU:CD1	2.45	0.40
1:B:226:GLU:OE2	1:B:227:PRO:HD2	2.21	0.40
1:B:662:GLU:H	1:B:662:GLU:CD	2.29	0.40
1:B:770:ILE:O	1:B:774:ILE:HG13	2.22	0.40
1:A:437:LEU:HD11	1:A:519:LEU:HD12	2.03	0.40
1:A:501:TRP:CE3	1:A:503:ILE:HD11	2.56	0.40
1:A:719:LYS:HE2	1:A:719:LYS:CA	2.52	0.40
1:B:54:VAL:HA	1:B:57:GLU:HG2	2.03	0.40
1:A:219:LYS:HE3	1:A:219:LYS:HB2	1.94	0.40
1:A:399:ILE:HD12	1:A:400:ASP:N	2.36	0.40
1:A:463:ILE:HD13	1:A:463:ILE:HA	1.93	0.40
1:A:226:GLU:OE1	1:A:228:GLN:HB2	2.22	0.40
1:A:762:THR:HG23	1:A:766:ILE:HD13	2.02	0.40
1:B:467:ILE:HD12	1:B:467:ILE:N	2.36	0.40
1:B:706:ASP:C	1:B:707:LEU:HG	2.46	0.40
1:A:36:LEU:O	1:A:36:LEU:HD23	2.22	0.40
1:A:754:LYS:HE2	1:A:754:LYS:HB3	1.97	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:456:ASP:HA	1:B:464:ASN:OD1	2.22	0.40
1:B:611:GLN:HE22	1:B:613:ASP:CA	2.35	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	721/776 (93%)	670 (93%)	38 (5%)	13 (2%)	6	6
1	B	732/776 (94%)	685 (94%)	35 (5%)	12 (2%)	7	7
All	All	1453/1552 (94%)	1355 (93%)	73 (5%)	25 (2%)	7	7

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	49	LYS
1	A	313	GLN
1	A	640	ALA
1	B	28	ARG
1	B	96	ALA
1	B	704	GLN
1	A	701	ASP
1	A	706	ASP
1	A	772	PHE
1	B	30	LYS
1	B	51	GLU
1	B	140	ASN
1	B	251	GLU
1	B	366	ASN
1	B	457	SER
1	A	53	ALA

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Mol	Chain	Res	Type
1	A	250	GLN
1	A	702	LYS
1	B	53	ALA
1	A	52	GLU
1	A	312	SER
1	B	325	ASP
1	B	705	SER
1	A	343	ILE
1	A	50	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	660/710 (93%)	622 (94%)	38 (6%)	18	26
1	B	669/710 (94%)	626 (94%)	43 (6%)	16	23
All	All	1329/1420 (94%)	1248 (94%)	81 (6%)	17	24

All (81) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	92	ILE
1	A	107	ILE
1	A	125	TYR
1	A	192	ASN
1	A	215	GLU
1	A	233	LEU
1	A	256	LEU
1	A	259	LEU
1	A	265	LEU
1	A	296	LEU
1	A	301	GLU
1	A	319	LEU
1	A	370	GLU
1	A	373	LYS

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Mol	Chain	Res	Type
1	A	379	LEU
1	A	404	ILE
1	A	443	ILE
1	A	446	LEU
1	A	447	THR
1	A	458	THR
1	A	460	ASN
1	A	494	LEU
1	A	496	ASN
1	A	505	LEU
1	A	580	THR
1	A	582	LEU
1	A	584	THR
1	A	605	GLU
1	A	636	LEU
1	A	656	LYS
1	A	658	LEU
1	A	679	ASN
1	A	704	GLN
1	A	712	LYS
1	A	719	LYS
1	A	733	GLU
1	A	753	LEU
1	A	761	LYS
1	B	27	GLU
1	B	28	ARG
1	B	49	LYS
1	B	51	GLU
1	B	77	ILE
1	B	95	GLU
1	B	99	GLU
1	B	102	LYS
1	B	107	ILE
1	B	111	ASP
1	B	129	LEU
1	B	135	GLU
1	B	203	VAL
1	B	207	GLU
1	B	228	GLN
1	B	233	LEU
1	B	256	LEU
1	B	265	LEU

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Mol	Chain	Res	Type
1	B	304	LYS
1	B	314	GLU
1	B	322	ILE
1	B	323	GLN
1	B	379	LEU
1	B	391	ARG
1	B	425	GLN
1	B	432	TYR
1	B	446	LEU
1	B	447	THR
1	B	488	ILE
1	B	496	ASN
1	B	499	LEU
1	B	515	GLU
1	B	516	ASN
1	B	520	ILE
1	B	611	GLN
1	B	615	ILE
1	B	616	LYS
1	B	678	ARG
1	B	702	LYS
1	B	704	GLN
1	B	712	LYS
1	B	733	GLU
1	B	753	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (82) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	140	ASN
1	A	164	ASN
1	A	165	GLN
1	A	193	GLN
1	A	197	HIS
1	A	209	ASN
1	A	214	GLN
1	A	242	ASN
1	A	248	ASN
1	A	253	ASN
1	A	276	GLN
1	A	277	HIS
1	A	279	GLN

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Mol	Chain	Res	Type
1	A	297	GLN
1	A	390	GLN
1	A	393	GLN
1	A	411	GLN
1	A	440	ASN
1	A	445	ASN
1	A	460	ASN
1	A	496	ASN
1	A	524	ASN
1	A	533	GLN
1	A	537	GLN
1	A	563	GLN
1	A	567	ASN
1	A	571	ASN
1	A	588	HIS
1	A	589	ASN
1	A	608	ASN
1	A	611	GLN
1	A	652	GLN
1	A	679	ASN
1	A	704	GLN
1	A	710	ASN
1	A	745	HIS
1	A	767	ASN
1	B	29	ASN
1	B	32	GLN
1	B	35	HIS
1	B	91	HIS
1	B	117	HIS
1	B	140	ASN
1	B	164	ASN
1	B	165	GLN
1	B	186	GLN
1	B	193	GLN
1	B	197	HIS
1	B	208	GLN
1	B	209	ASN
1	B	242	ASN
1	B	248	ASN
1	B	262	GLN
1	B	297	GLN
1	B	323	GLN

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Mol	Chain	Res	Type
1	B	390	GLN
1	B	411	GLN
1	B	440	ASN
1	B	444	ASN
1	B	445	ASN
1	B	474	ASN
1	B	496	ASN
1	B	504	GLN
1	B	516	ASN
1	B	522	GLN
1	B	524	ASN
1	B	533	GLN
1	B	537	GLN
1	B	563	GLN
1	B	568	GLN
1	B	571	ASN
1	B	586	ASN
1	B	608	ASN
1	B	609	ASN
1	B	611	GLN
1	B	620	ASN
1	B	638	ASN
1	B	704	GLN
1	B	745	HIS
1	B	756	GLN
1	B	767	ASN
1	B	769	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

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	SO4	B	777	-	4,4,4	0.36	0	6,6,6	0.08	0
2	SO4	A	777	-	4,4,4	0.32	0	6,6,6	0.18	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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 is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.