



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 10:34 AM UTC

PDB ID : 1XF1 / pdb_00001xf1
Title : Structure of C5a peptidase- a key virulence factor from Streptococcus
Authors : Brown, C.K.; Gu, Z.Y.; Cleary, P.P.; Matsuka, Y.; Olmstead, S.; Ohlendorf, D.H.; Earhart, C.A.
Deposited on : 2004-09-13
Resolution : 1.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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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

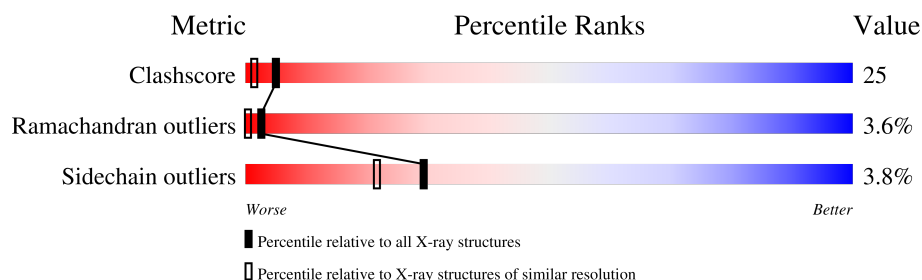
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)

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	926	 65% 29% 5%
1	B	926	 58% 36% 6%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	CIT	A	1101	-	X	-	-
4	CIT	A	1103	-	X	-	-
4	CIT	B	1102	-	X	-	-
4	CIT	B	1104	-	X	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	CIT	B	1106	-	X	-	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 15509 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 C5a peptidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	926	Total	C	N	O	Se	0	0	0
			7182	4510	1211	1445	16			
1	B	926	Total	C	N	O	Se	4	0	0
			7182	4510	1211	1445	16			

There are 38 discrepancies between the modelled and reference sequences:

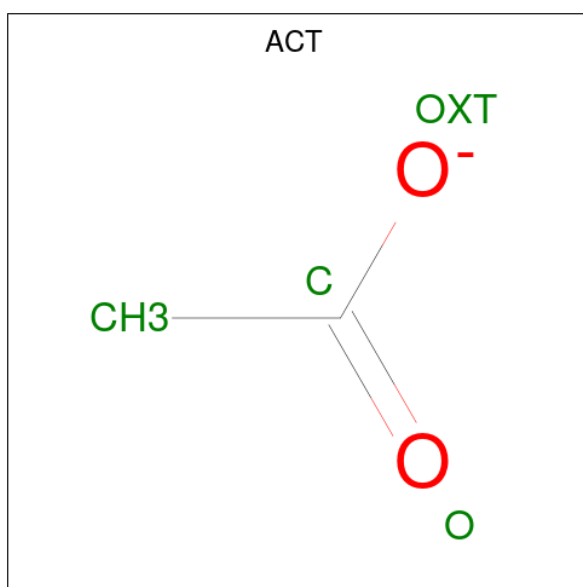
Chain	Residue	Modelled	Actual	Comment	Reference
A	219	MSE	MET	modified residue	UNP P15926
A	227	MSE	MET	modified residue	UNP P15926
A	259	MSE	MET	modified residue	UNP P15926
A	353	MSE	MET	modified residue	UNP P15926
A	433	MSE	MET	modified residue	UNP P15926
A	513	MSE	MET	modified residue	UNP P15926
A	522	MSE	MET	modified residue	UNP P15926
A	536	MSE	MET	modified residue	UNP P15926
A	550	MSE	MET	modified residue	UNP P15926
A	585	MSE	MET	modified residue	UNP P15926
A	648	THR	ALA	SEE REMARK 999	UNP P15926
A	680	MSE	MET	modified residue	UNP P15926
A	697	THR	LYS	SEE REMARK 999	UNP P15926
A	702	MSE	MET	modified residue	UNP P15926
A	794	PHE	LEU	SEE REMARK 999	UNP P15926
A	969	MSE	MET	modified residue	UNP P15926
A	996	MSE	THR	engineered mutation	UNP P15926
A	1005	MSE	MET	modified residue	UNP P15926
A	1015	MSE	MET	modified residue	UNP P15926
B	219	MSE	MET	modified residue	UNP P15926
B	227	MSE	MET	modified residue	UNP P15926
B	259	MSE	MET	modified residue	UNP P15926
B	353	MSE	MET	modified residue	UNP P15926
B	433	MSE	MET	modified residue	UNP P15926
B	513	MSE	MET	modified residue	UNP P15926

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Chain	Residue	Modelled	Actual	Comment	Reference
B	522	MSE	MET	modified residue	UNP P15926
B	536	MSE	MET	modified residue	UNP P15926
B	550	MSE	MET	modified residue	UNP P15926
B	585	MSE	MET	modified residue	UNP P15926
B	648	THR	ALA	SEE REMARK 999	UNP P15926
B	680	MSE	MET	modified residue	UNP P15926
B	697	THR	LYS	SEE REMARK 999	UNP P15926
B	702	MSE	MET	modified residue	UNP P15926
B	794	PHE	LEU	SEE REMARK 999	UNP P15926
B	969	MSE	MET	modified residue	UNP P15926
B	996	MSE	THR	engineered mutation	UNP P15926
B	1005	MSE	MET	modified residue	UNP P15926
B	1015	MSE	MET	modified residue	UNP P15926

- Molecule 2 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2^-$).

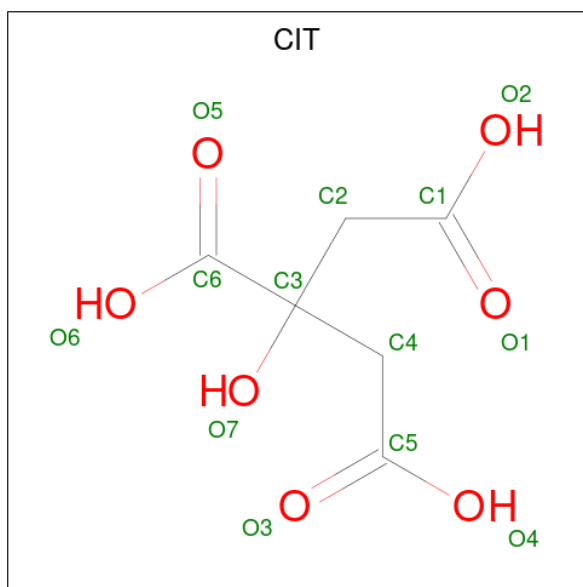


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

- Molecule 4 is CITRIC ACID (CCD ID: CIT) (formula: $C_6H_8O_7$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 13 6 7	0	0
4	A	1	Total C O 13 6 7	0	0
4	A	1	Total C O 13 6 7	0	0
4	B	1	Total C O 13 6 7	0	0
4	B	1	Total C O 13 6 7	0	0
4	B	1	Total C O 13 6 7	0	0

- Molecule 5 is water.

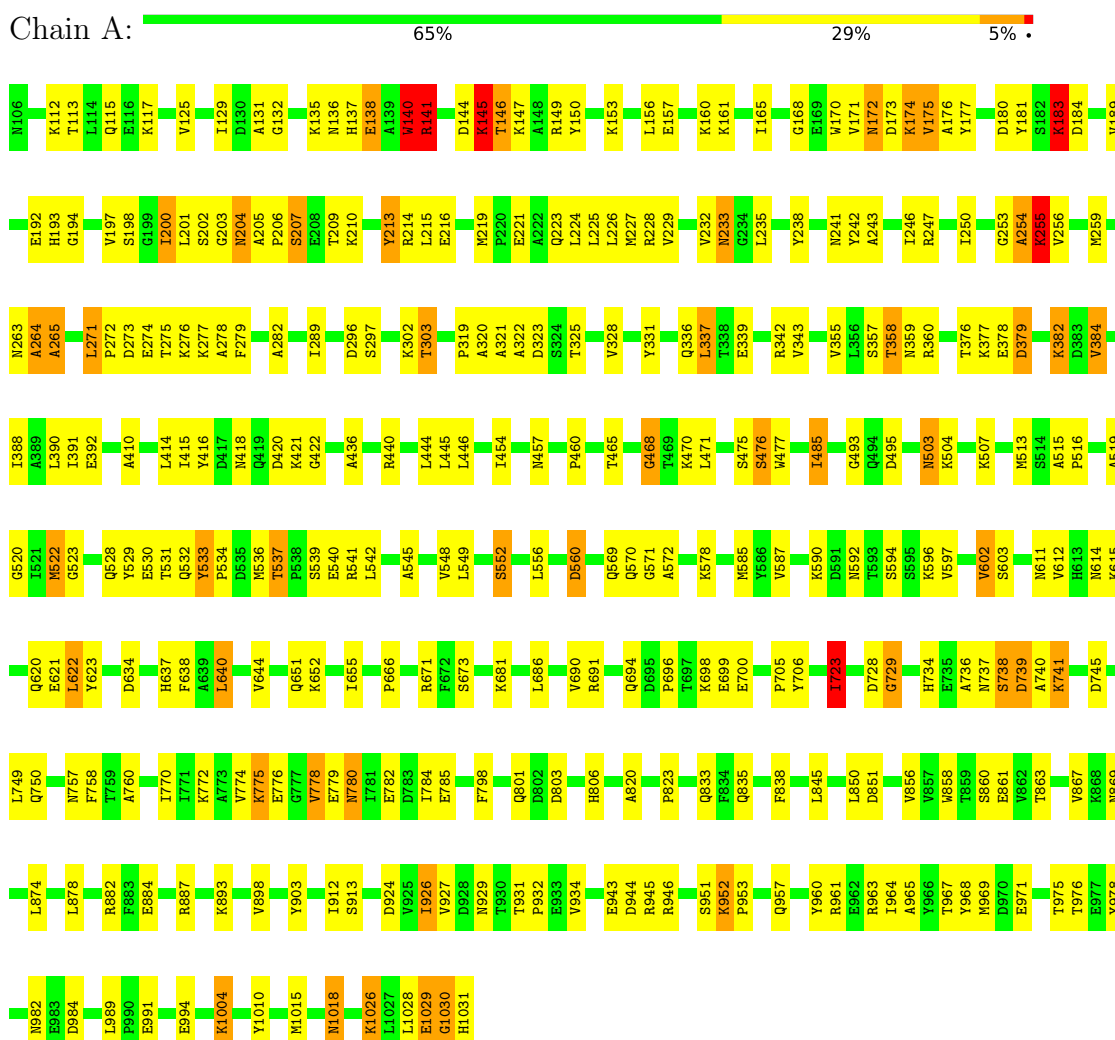
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	544	Total O 544 544	0	0
5	B	513	Total O 513 513	0	0

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. 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. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

• Molecule 1: C5a peptidase



• Molecule 1: C5a peptidase



M969	N106	H179	L252	T358	F437	E530	L622	N737	K852	M969
L973	D107	D160	G253	M359	I438	T531	Y623	S738	K858	L973
P974	P108	Y181	A254	R360	S439	Q532	A626	D739	V858	P974
Y978	S109	G185	K255	F361	R440	Y533	A639	K741	T859	Y978
D984	Q110	K186	V256	E362	K441	D442	F638	D742	S860	D984
E991	V111	K186	M259	P363	N364	T537	A639	Q743	E861	E991
E994	K112	V189	N259	N365	L445	P538	L640	E744	V862	E994
T995	E116	G190	N263	K365	L446	S539	V644	D745	N869	T995
M996	G123	Q191	A264	A366	N449	E540	K651	L749	L874	M996
E997	T124	G194	A265	Y367	Q451	R541	K652	N757	L878	E997
A999	T125	H196	L266	D368	K452	E545	I653	F758	T759	A999
Y1010	V126	V197	N270	Y369	T453	K546	T654	A760	R882	Y1010
D1014	A127	S198	L271	A370	T455	K547	P656	K772	F883	D1014
M1015	V128	G199	L272	Y371	F456	L549	A657	K775	E884	M1015
N1018	F133	I200	E274	A372	N457	E554	K658	E776	K885	N1018
I1019	D134	L201	T275	N373	P460	A555	S659	E777	T886	I1019
T1020	K135	S202	F279	K377	V462	L556	Q662	G778	R887	T1020
K1026	K136	P206	K283	D380	T465	Y557	V663	E779	V888	K1026
E1029	H137	E208	V287	F381	Q468	K562	T664	E780	K893	E1029
G1030	E138	T209	S297	K382	L471	P567	V665	E781	D894	G1030
H1031	A139	K210	E211	D383	S475	M585	F666	E782	V898	H1031
	V140	E212	A308	V384	W477	M585	I667	D783	Y903	
	R141	P212	D309	G386	K485	D589	R671	E784	T910	
	L142	T143	L390	K387	K486	K590	Q694	E785	P911	
	K145	Y213	D399	I388	P492	D591	D695	S786	Q912	
	T146	R214	H310	A389	Q493	M592	K698	S787	E943	
	K147	L215	E216	L391	D495	T593	F699	E796	D944	
	A148	E217	Y313	E392	I496	K596	E700	F797	R945	
	R149	A218	A321	D397	V500	N601	I704	F798	R946	
	Y150	M219	V328	F398	N503	F606	P705	Q801	K952	
	Q151	P220	E221	K406	K504	T609	Y706	D804	P953	
	S152	A222	Y331	K407	Q493	V610	I707	S805	K954	
	K153	Q223	D334	A408	D495	M513	F713	H806	T955	
	E154	L224	L337	Q409	I496	S514	T723	S822	P958	
	L156	L226	T338	G412	V500	A515	Y724	R829	V959	
	E157	L226	E339	V413	V500	P516	Q833	Q835	Y960	
	K158	M227	V340	L414	N503	M522	F734	F838	R961	
	A159	R228	R342	I415	K504	G523	E735	E839	E962	
	K160	V229	V343	Y416	M513	L524	H736	E844	R963	
	R161	I231	K344	Q419	S514	K618	E737	V849	A965	
	E162	V232	T345	I425	A515	P619	E738			
	Y167	N233	A346	E426	P516	Q620				
	G168	A236	D347	L427	M522	E739				
	E169	R240	Q348	D431	G523	A736				
	W170	Y242	M353	Q432	L524					
	N172	I246	P354	M433	K618					
	D173	R247	V355	P434	P619					
	K174	D248	L356	A435	Q620					
	V175		S357	A436	Y529					
	A176									
	I177									
	Y178									

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	114.70Å 75.11Å 132.39Å 90.00° 104.95° 90.00°	Depositor
Resolution (Å)	50.00 – 1.90	Depositor
% Data completeness (in resolution range)	(Not available) (50.00-1.90)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.229 , 0.269	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	15509	wwPDB-VP
Average B, all atoms (Å ²)	51.0	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: ACT, CA, CIT

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	0.38	0/7312	0.90	37/9884 (0.4%)
1	B	0.37	0/7312	0.89	23/9884 (0.2%)
All	All	0.38	0/14624	0.90	60/19768 (0.3%)

There are no bond length outliers.

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	140	TRP	N-CA-C	-8.98	101.90	112.86
1	A	265	ALA	N-CA-C	-7.78	101.96	113.40
1	A	729	GLY	N-CA-C	-7.49	104.71	115.27
1	B	861	GLU	N-CA-C	-7.21	100.81	110.55
1	A	339	GLU	N-CA-C	-7.08	101.19	110.53
1	B	694	GLN	N-CA-C	-6.98	103.75	111.36
1	A	690	VAL	N-CA-C	-6.56	97.74	107.51
1	A	297	SER	N-CA-C	6.55	120.98	112.92
1	B	339	GLU	N-CA-C	-6.55	102.07	110.53
1	B	328	VAL	N-CA-C	6.43	117.11	108.11
1	B	638	PHE	N-CA-C	-6.34	100.18	110.20
1	B	690	VAL	N-CA-C	-6.33	98.08	107.51
1	A	328	VAL	N-CA-C	6.32	117.40	108.36
1	A	325	THR	N-CA-C	-6.18	104.62	111.36
1	B	533	TYR	CA-C-N	6.14	126.59	119.47
1	B	533	TYR	C-N-CA	6.14	126.59	119.47
1	A	420	ASP	N-CA-C	6.12	118.04	111.36
1	A	485	ILE	N-CA-C	-6.00	101.84	109.58
1	A	476	SER	N-CA-C	5.98	123.55	110.80
1	B	476	SER	N-CA-C	5.98	123.55	110.80
1	A	418	ASN	N-CA-C	-5.83	105.50	113.30
1	B	310	HIS	CA-C-N	5.82	125.93	119.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	310	HIS	C-N-CA	5.82	125.93	119.87
1	A	475	SER	N-CA-C	5.82	119.13	110.52
1	B	475	SER	N-CA-C	5.78	119.51	110.32
1	B	485	ILE	N-CA-C	-5.77	102.14	109.58
1	A	173	ASP	N-CA-C	-5.65	105.65	112.54
1	A	533	TYR	CA-C-N	5.65	125.32	119.05
1	A	533	TYR	C-N-CA	5.65	125.32	119.05
1	A	694	GLN	N-CA-C	-5.60	106.45	113.28
1	A	681	LYS	N-CA-C	5.56	119.16	112.38
1	A	357	SER	N-CA-C	5.55	118.53	109.59
1	A	723	ILE	CB-CA-C	-5.55	103.56	112.16
1	B	787	SER	N-CA-C	5.52	120.17	113.38
1	A	957	GLN	N-CA-C	-5.51	103.18	110.40
1	B	373	ASN	CB-CA-C	-5.47	109.79	117.23
1	A	638	PHE	N-CA-C	-5.45	101.60	110.20
1	B	107	ASP	CA-C-N	5.38	125.46	119.32
1	B	107	ASP	C-N-CA	5.38	125.46	119.32
1	B	686	LEU	N-CA-C	-5.38	98.44	108.02
1	B	313	TYR	N-CA-C	5.38	119.81	112.88
1	A	861	GLU	N-CA-C	-5.31	103.01	110.50
1	A	686	LEU	N-CA-C	-5.29	98.60	108.02
1	A	358	THR	N-CA-C	-5.28	100.56	109.07
1	A	337	LEU	N-CA-C	-5.27	101.88	110.20
1	A	468	GLY	N-CA-C	-5.23	102.84	112.62
1	B	358	THR	N-CA-C	-5.21	100.69	109.07
1	A	422	GLY	N-CA-C	5.20	118.85	112.14
1	A	738	SER	N-CA-C	-5.17	102.62	110.28
1	A	470	LYS	N-CA-C	5.17	117.59	108.75
1	A	523	GLY	N-CA-C	-5.16	106.54	112.73
1	A	161	LYS	N-CA-C	-5.15	105.74	111.36
1	A	360	ARG	N-CA-C	5.11	117.74	109.06
1	A	382	LYS	N-CA-C	5.09	116.83	111.28
1	B	297	SER	N-CA-C	5.08	119.43	112.88
1	B	567	PRO	N-CA-C	-5.07	107.53	113.86
1	A	673	SER	N-CA-C	5.06	117.19	111.11
1	A	594	SER	N-CA-C	5.04	117.07	109.41
1	A	1018	ASN	N-CA-C	-5.03	102.83	110.28
1	A	174	LYS	N-CA-C	-5.03	101.50	109.59

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	7182	0	7004	327	0
1	B	7182	0	7005	400	0
2	A	4	0	3	0	0
2	B	4	0	3	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	39	0	15	0	0
4	B	39	0	15	2	0
5	A	544	0	0	34	0
5	B	513	0	0	23	0
All	All	15509	0	14045	712	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 25.

All (712) 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:778:VAL:HG21	1:A:784:ILE:HD11	1.40	1.03
1:A:210:LYS:HA	1:A:337:LEU:HD12	1.40	1.03
1:B:343:VAL:HG12	1:B:454:ILE:HG22	1.41	1.02
1:A:465:THR:HG23	1:A:468:GLY:H	1.23	1.01
1:B:465:THR:HG23	1:B:468:GLY:H	1.25	1.00
1:A:271:LEU:HD23	1:A:271:LEU:H	1.26	1.00
1:B:271:LEU:HD23	1:B:271:LEU:H	1.27	1.00
1:A:952:LYS:HB3	1:A:953:PRO:HA	1.43	1.00
1:A:343:VAL:HG12	1:A:454:ILE:HG22	1.41	0.99
1:B:536:MSE:HE2	1:B:540:GLU:HB3	1.41	0.99
1:B:958:PRO:HG2	1:B:1015:MSE:HG3	1.43	0.99
1:A:440:ARG:NH1	1:A:444:LEU:HD11	1.78	0.99
1:A:219:MSE:HE2	1:A:520:GLY:HA2	1.44	0.98
1:A:246:ILE:HD11	1:A:278:ALA:HB1	1.48	0.96
1:B:995:THR:HG23	1:B:997:GLU:H	1.31	0.95
1:B:360:ARG:HH11	1:B:360:ARG:HB3	1.31	0.95
1:B:556:LEU:H	1:B:570:GLN:HE22	1.05	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:556:LEU:H	1:A:570:GLN:HE22	1.04	0.93
1:A:216:GLU:HG2	1:A:224:LEU:HD21	1.51	0.92
1:A:141:ARG:HE	1:A:141:ARG:HA	1.37	0.90
1:B:835:GLN:HE21	1:B:882:ARG:HE	1.20	0.89
1:B:522:MSE:HG3	1:B:549:LEU:HD22	1.54	0.89
1:B:749:LEU:HD23	1:B:749:LEU:H	1.37	0.89
1:A:160:LYS:HB2	1:A:165:ILE:HB	1.54	0.88
1:B:528:GLN:HE21	1:B:532:GLN:HE22	1.23	0.87
1:A:960:TYR:HA	1:A:1015:MSE:HE3	1.56	0.87
1:B:139:ALA:HB1	1:B:206:PRO:HA	1.56	0.87
1:B:838:PHE:H	1:B:869:ASN:HD22	1.19	0.87
1:B:944:ASP:OD2	1:B:946:ARG:HD3	1.76	0.86
1:B:611:ASN:ND2	1:B:662:GLN:HG2	1.91	0.85
1:A:522:MSE:HG3	1:A:549:LEU:HD22	1.57	0.85
1:A:622:LEU:HD21	1:A:655:ILE:HD13	1.60	0.84
1:B:749:LEU:H	1:B:749:LEU:CD2	1.90	0.84
1:A:835:GLN:NE2	1:A:882:ARG:HE	1.76	0.82
1:A:991:GLU:OE2	1:B:263:ASN:HB3	1.80	0.82
1:A:536:MSE:O	1:A:537:THR:HB	1.79	0.81
1:A:150:TYR:H	1:A:223:GLN:HE22	1.29	0.81
1:B:522:MSE:HE1	1:B:542:LEU:HD12	1.63	0.81
1:B:200:ILE:HG22	1:B:201:LEU:HG	1.63	0.81
1:B:585:MSE:HG2	1:B:614:ASN:HA	1.64	0.80
1:A:226:LEU:C	1:A:227:MSE:HE3	2.06	0.80
1:A:835:GLN:HE21	1:A:882:ARG:HE	1.26	0.79
1:A:421:LYS:HG3	1:A:560:ASP:OD2	1.82	0.79
1:B:160:LYS:HE3	1:B:168:GLY:H	1.47	0.79
1:A:644:VAL:HG12	5:A:1124:HOH:O	1.83	0.79
1:B:835:GLN:NE2	1:B:882:ARG:HE	1.80	0.79
1:B:145:LYS:N	1:B:145:LYS:HD2	2.00	0.77
1:B:139:ALA:HB2	1:B:208:GLU:HG3	1.66	0.77
1:B:209:THR:HG22	1:B:210:LYS:HG3	1.67	0.77
1:B:780:ASN:ND2	1:B:783:ASP:H	1.83	0.77
1:B:621:GLU:HG2	1:B:654:THR:HG22	1.65	0.77
1:A:644:VAL:HG23	5:A:1332:HOH:O	1.83	0.77
1:B:353:MSE:HE1	1:B:446:LEU:HD11	1.66	0.76
1:A:823:PRO:HG2	1:A:929:ASN:HD21	1.50	0.76
1:B:271:LEU:HD21	1:B:321:ALA:HB3	1.67	0.76
1:B:656:PRO:HG2	1:B:659:SER:OG	1.86	0.75
1:B:137:HIS:HD1	1:B:513:MSE:HE3	1.52	0.75
1:A:698:LYS:HG2	1:A:699:GLU:H	1.50	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:995:THR:HG22	1:B:999:ALA:H	1.51	0.75
1:A:838:PHE:H	1:A:869:ASN:HD22	1.31	0.75
1:B:124:THR:HG21	1:B:219:MSE:HE1	1.69	0.75
1:A:952:LYS:CB	1:A:953:PRO:HA	2.16	0.75
1:A:952:LYS:HB3	1:A:953:PRO:CA	2.17	0.75
1:B:337:LEU:HD21	1:B:460:PRO:HB2	1.65	0.75
1:B:503:ASN:HD22	1:B:504:LYS:HD2	1.52	0.74
1:A:898:VAL:HG12	1:A:903:TYR:OH	1.86	0.74
1:A:343:VAL:CG1	1:A:454:ILE:HG22	2.15	0.74
1:A:271:LEU:H	1:A:271:LEU:CD2	1.99	0.74
1:B:781:ILE:HA	1:B:784:ILE:HG23	1.69	0.74
1:B:147:LYS:HB2	1:B:147:LYS:NZ	2.03	0.74
1:B:271:LEU:HB2	1:B:272:PRO:HD2	1.69	0.74
1:B:838:PHE:H	1:B:869:ASN:ND2	1.85	0.74
1:B:691:ARG:HD2	1:B:700:GLU:OE2	1.88	0.73
1:A:246:ILE:HD11	1:A:278:ALA:CB	2.19	0.73
1:A:378:GLU:O	1:A:379:ASP:HB2	1.88	0.72
1:A:780:ASN:HD21	1:A:782:GLU:HG3	1.54	0.72
1:A:379:ASP:HA	1:A:382:LYS:HG3	1.70	0.71
1:B:610:VAL:C	1:B:611:ASN:HD22	1.97	0.71
1:B:355:VAL:HG12	1:B:438:ILE:HG22	1.71	0.71
1:B:171:VAL:O	1:B:172:ASN:HB3	1.90	0.71
1:A:303:THR:HB	5:A:1144:HOH:O	1.90	0.71
1:A:536:MSE:O	1:A:540:GLU:HB2	1.89	0.71
1:A:967:THR:HG23	5:A:1535:HOH:O	1.91	0.71
1:B:742:ASP:HB3	1:B:809:ILE:HB	1.73	0.71
1:B:167:TYR:HB2	1:B:179:HIS:CD2	2.26	0.70
1:A:388:ILE:HD12	1:A:454:ILE:HD11	1.73	0.70
1:A:254:ALA:O	1:A:255:LYS:HB2	1.91	0.70
1:B:671:ARG:HG2	5:B:1162:HOH:O	1.90	0.70
5:A:1173:HOH:O	1:B:996:MSE:HE3	1.91	0.70
1:A:168:GLY:HA3	1:A:177:TYR:CE1	2.27	0.69
1:B:342:ARG:HG3	1:B:457:ASN:HD21	1.58	0.69
1:B:384:VAL:C	1:B:409:GLY:HA3	2.17	0.69
1:A:440:ARG:HH12	1:A:444:LEU:HD11	1.54	0.69
1:A:465:THR:HG23	1:A:468:GLY:N	2.03	0.69
1:B:337:LEU:CD2	1:B:460:PRO:HB2	2.22	0.69
1:A:384:VAL:HG13	1:A:410:ALA:HB2	1.75	0.68
1:B:123:GLY:HA2	1:B:148:ALA:HB3	1.75	0.68
1:B:528:GLN:HE21	1:B:532:GLN:NE2	1.91	0.68
1:B:932:PRO:HD2	1:B:1020:THR:HG23	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:622:LEU:HD23	1:A:622:LEU:N	2.09	0.68
1:B:242:TYR:O	1:B:246:ILE:HG23	1.93	0.68
1:A:150:TYR:H	1:A:223:GLN:NE2	1.90	0.68
1:A:205:ALA:N	1:A:206:PRO:HD3	2.09	0.68
1:A:838:PHE:H	1:A:869:ASN:ND2	1.91	0.68
1:B:522:MSE:CE	1:B:542:LEU:HD12	2.23	0.68
1:B:264:ALA:HB1	5:B:1395:HOH:O	1.93	0.67
1:B:271:LEU:H	1:B:271:LEU:CD2	2.04	0.67
1:B:144:ASP:C	1:B:145:LYS:HD2	2.19	0.67
1:A:440:ARG:HH11	1:A:444:LEU:HD11	1.55	0.67
1:B:644:VAL:HG12	5:B:1128:HOH:O	1.95	0.67
1:B:1020:THR:HG22	5:B:1251:HOH:O	1.95	0.66
1:A:172:ASN:HB2	1:A:174:LYS:O	1.96	0.66
1:B:173:ASP:O	1:B:175:VAL:N	2.28	0.66
1:B:522:MSE:HG3	1:B:549:LEU:CD2	2.25	0.66
1:B:556:LEU:H	1:B:570:GLN:NE2	1.88	0.66
1:B:745:ASP:OD2	1:B:806:HIS:HD2	1.78	0.66
1:A:140:TRP:O	1:A:141:ARG:HB2	1.95	0.66
1:B:433:MSE:HA	1:B:433:MSE:HE2	1.77	0.66
1:A:960:TYR:CA	1:A:1015:MSE:HE3	2.24	0.66
1:B:232:VAL:O	1:B:233:ASN:HB2	1.96	0.65
1:B:958:PRO:HG2	1:B:1015:MSE:CG	2.21	0.65
1:A:749:LEU:HD12	1:B:749:LEU:HG	1.77	0.65
1:A:931:THR:HG22	5:A:1249:HOH:O	1.95	0.65
1:B:515:ALA:HB3	1:B:516:PRO:HD3	1.77	0.65
1:B:844:ASN:HB3	5:B:1610:HOH:O	1.96	0.65
1:A:200:ILE:HG22	1:A:201:LEU:HG	1.77	0.65
1:A:503:ASN:HD22	1:A:503:ASN:H	1.45	0.65
1:B:590:LYS:HD3	1:B:609:THR:HG21	1.77	0.65
1:B:644:VAL:HG23	5:B:1347:HOH:O	1.97	0.65
1:B:780:ASN:C	1:B:782:GLU:H	2.04	0.65
1:A:209:THR:HG22	1:A:210:LYS:HG3	1.78	0.64
1:B:213:TYR:HA	5:B:1416:HOH:O	1.96	0.64
1:B:360:ARG:HB3	1:B:360:ARG:NH1	2.09	0.64
1:B:893:LYS:O	1:B:894:ASP:C	2.40	0.64
1:A:556:LEU:H	1:A:570:GLN:NE2	1.87	0.64
1:B:153:LYS:O	1:B:157:GLU:HG2	1.97	0.64
1:B:671:ARG:HG2	1:B:671:ARG:HH11	1.63	0.64
1:B:137:HIS:ND1	1:B:513:MSE:HE3	2.13	0.64
1:B:601:ASN:HD21	1:B:713:PHE:H	1.45	0.64
1:A:140:TRP:HA	1:A:174:LYS:HD2	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:528:GLN:HE21	1:A:532:GLN:NE2	1.95	0.63
1:B:562:LYS:HE2	1:B:562:LYS:HA	1.80	0.63
1:A:135:LYS:HB2	1:B:943:GLU:OE1	1.99	0.63
1:B:952:LYS:HD2	1:B:952:LYS:C	2.22	0.63
1:B:384:VAL:O	1:B:409:GLY:HA3	1.98	0.63
1:B:124:THR:HG22	1:B:125:VAL:N	2.14	0.63
1:B:359:ASN:HB2	1:B:434:PRO:HA	1.80	0.63
1:A:174:LYS:O	1:A:175:VAL:HB	1.99	0.63
1:B:389:ALA:HB3	1:B:413:VAL:HG12	1.81	0.63
1:A:149:ARG:HH12	1:A:253:GLY:HA3	1.63	0.63
1:B:427:LEU:CD2	1:B:437:PHE:HB2	2.29	0.62
1:B:219:MSE:HE3	1:B:527:LYS:NZ	2.13	0.62
1:B:995:THR:HG21	5:B:1345:HOH:O	1.99	0.62
1:A:485:ILE:HD12	1:A:571:GLY:HA2	1.82	0.62
1:B:898:VAL:HG22	1:B:903:TYR:OH	2.00	0.62
1:B:112:LYS:O	1:B:116:GLU:HG3	1.99	0.62
1:B:749:LEU:HD23	1:B:749:LEU:N	2.12	0.62
1:B:219:MSE:HE3	1:B:527:LYS:HZ2	1.63	0.62
1:B:829:ARG:NH1	5:B:1173:HOH:O	2.31	0.62
1:A:379:ASP:CG	1:A:382:LYS:HE3	2.25	0.62
1:A:530:GLU:HA	1:A:541:ARG:HE	1.65	0.62
1:B:433:MSE:HE2	1:B:434:PRO:HD2	1.82	0.62
1:A:193:HIS:HB2	1:A:197:VAL:HA	1.82	0.61
1:A:522:MSE:HE3	1:A:545:ALA:HB3	1.82	0.61
1:B:462:VAL:HG23	1:B:462:VAL:O	2.00	0.61
1:A:515:ALA:HB3	1:A:516:PRO:HD3	1.83	0.61
1:A:729:GLY:C	1:A:736:ALA:HB2	2.24	0.61
1:B:485:ILE:CG1	1:B:596:LYS:HD2	2.30	0.61
1:A:738:SER:O	1:A:739:ASP:HB2	1.99	0.61
1:A:964:ILE:HD13	1:A:1010:TYR:HA	1.81	0.61
1:B:365:LYS:H	1:B:455:THR:HG23	1.65	0.61
1:B:737:ASN:HD22	1:B:743:GLN:NE2	1.99	0.61
1:A:343:VAL:HG11	1:A:446:LEU:CD2	2.30	0.61
1:A:548:VAL:O	1:A:552:SER:HB2	2.00	0.61
1:A:271:LEU:CD2	1:A:321:ALA:HB3	2.31	0.61
1:A:216:GLU:CG	1:A:224:LEU:HD21	2.28	0.60
1:A:507:LYS:HD3	5:A:1436:HOH:O	2.01	0.60
1:B:215:LEU:O	1:B:216:GLU:HG3	2.01	0.60
1:A:882:ARG:NH1	1:B:996:MSE:HE1	2.17	0.60
1:B:343:VAL:CG1	1:B:454:ILE:HG22	2.26	0.60
1:A:331:TYR:HB2	1:A:471:LEU:HD22	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:867:VAL:HG13	5:A:1115:HOH:O	2.02	0.60
1:B:522:MSE:HE3	1:B:545:ALA:HB3	1.82	0.60
1:B:780:ASN:HD21	1:B:783:ASP:H	1.50	0.60
1:B:958:PRO:O	1:B:1015:MSE:HG2	2.02	0.60
1:A:144:ASP:O	1:A:145:LYS:HB2	2.02	0.60
1:B:136:ASN:O	1:B:137:HIS:HB3	2.02	0.59
1:A:384:VAL:CG1	1:A:410:ALA:HB2	2.31	0.59
1:A:379:ASP:OD2	1:A:382:LYS:HE3	2.01	0.59
1:B:852:LYS:HE3	5:B:1324:HOH:O	2.00	0.59
1:B:126:VAL:HG22	1:B:256:VAL:HG11	1.84	0.59
1:A:180:ASP:O	1:A:183:LYS:HD2	2.03	0.59
1:A:912:ILE:HD12	1:A:912:ILE:C	2.27	0.59
1:B:124:THR:HG21	1:B:219:MSE:CE	2.32	0.59
1:B:465:THR:HG23	1:B:468:GLY:N	2.08	0.59
1:A:214:ARG:HG2	5:A:1578:HOH:O	2.03	0.59
1:A:536:MSE:HE2	1:A:540:GLU:HB3	1.85	0.59
1:B:414:LEU:HD23	1:B:436:ALA:HB3	1.86	0.58
1:A:723:ILE:HD11	1:A:760:ALA:HB2	1.86	0.58
1:B:107:ASP:OD2	1:B:110:GLN:HA	2.02	0.58
1:B:338:THR:HG21	1:B:354:PRO:HB3	1.85	0.58
1:B:454:ILE:O	1:B:454:ILE:HD12	2.02	0.58
1:B:838:PHE:N	1:B:869:ASN:HD22	1.96	0.58
1:A:960:TYR:CB	1:A:1015:MSE:HE3	2.33	0.58
1:A:533:TYR:N	1:A:534:PRO:HD3	2.18	0.58
1:B:655:ILE:N	1:B:655:ILE:HD12	2.18	0.58
1:A:585:MSE:HG3	5:A:1620:HOH:O	2.04	0.58
1:A:602:VAL:HG13	1:A:603:SER:O	2.03	0.58
1:A:926:ILE:C	1:A:926:ILE:HD12	2.29	0.58
1:B:213:TYR:C	1:B:214:ARG:HD2	2.28	0.58
1:B:590:LYS:HD3	1:B:609:THR:CG2	2.34	0.58
1:B:557:TYR:OH	1:B:562:LYS:HE2	2.03	0.58
1:B:995:THR:HG23	1:B:997:GLU:N	2.11	0.58
1:A:273:ASP:HA	1:A:276:LYS:NZ	2.19	0.57
1:B:171:VAL:O	1:B:172:ASN:CB	2.51	0.57
1:A:183:LYS:HD3	1:A:183:LYS:H	1.69	0.57
1:B:367:TYR:HB2	1:B:454:ILE:CD1	2.34	0.57
1:A:355:VAL:CG2	1:A:436:ALA:HB1	2.33	0.57
1:B:932:PRO:HB3	1:B:955:THR:HG22	1.86	0.57
1:B:228:ARG:HG3	1:B:228:ARG:HH11	1.69	0.57
1:B:148:ALA:O	1:B:149:ARG:O	2.22	0.57
1:B:440:ARG:HG3	1:B:440:ARG:HH11	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:536:MSE:O	1:A:537:THR:CB	2.52	0.57
1:B:723:ILE:HD11	1:B:760:ALA:HB2	1.85	0.57
1:A:775:LYS:HE3	1:A:775:LYS:N	2.19	0.57
1:A:833:GLN:HE22	1:A:887:ARG:HH21	1.52	0.57
1:B:138:GLU:C	1:B:140:TRP:H	2.13	0.57
1:B:427:LEU:HD21	1:B:437:PHE:HB2	1.87	0.57
1:A:376:THR:HG22	5:A:1342:HOH:O	2.04	0.57
1:A:302:LYS:NZ	1:A:302:LYS:HB3	2.20	0.57
1:B:945:ARG:CZ	1:B:991:GLU:HG2	2.35	0.57
1:A:691:ARG:HD2	1:A:700:GLU:OE2	2.05	0.56
1:A:850:LEU:CD2	1:A:856:VAL:HG22	2.36	0.56
1:B:150:TYR:HB2	1:B:223:GLN:HE22	1.70	0.56
1:B:153:LYS:HB2	5:B:1253:HOH:O	2.03	0.56
1:B:383:ASP:C	1:B:385:LYS:H	2.11	0.56
1:B:272:PRO:HB2	1:B:274:GLU:OE1	2.05	0.56
1:B:160:LYS:CE	1:B:168:GLY:H	2.18	0.56
1:B:388:ILE:HD12	1:B:454:ILE:HD11	1.88	0.56
1:B:738:SER:O	1:B:739:ASP:HB2	2.06	0.56
1:B:933:GLU:OE2	1:B:954:LYS:HE3	2.06	0.56
1:A:146:THR:O	1:A:146:THR:HG22	2.06	0.56
1:B:137:HIS:HD1	1:B:513:MSE:CE	2.18	0.56
1:B:168:GLY:HA2	1:B:177:TYR:CE1	2.40	0.56
1:A:254:ALA:O	1:A:255:LYS:CB	2.54	0.56
1:B:410:ALA:O	1:B:411:VAL:HB	2.06	0.56
1:B:621:GLU:HG2	1:B:654:THR:CG2	2.35	0.56
1:A:271:LEU:HD21	1:A:321:ALA:HB3	1.87	0.56
1:A:634:ASP:HB2	5:A:1583:HOH:O	2.05	0.56
1:A:734:HIS:HD2	5:A:1116:HOH:O	1.88	0.56
1:A:912:ILE:HD12	1:A:913:SER:N	2.21	0.56
1:A:177:TYR:CD2	1:A:227:MSE:HE2	2.41	0.56
1:B:893:LYS:HD2	5:B:1550:HOH:O	2.06	0.56
1:A:637:HIS:HD2	5:A:1250:HOH:O	1.88	0.55
1:B:137:HIS:NE2	1:B:211:GLU:HG2	2.21	0.55
1:A:171:VAL:O	1:A:172:ASN:O	2.23	0.55
1:B:611:ASN:HD22	1:B:611:ASN:N	2.03	0.55
1:A:145:LYS:C	1:A:147:LYS:H	2.15	0.55
1:A:738:SER:O	1:A:739:ASP:CB	2.54	0.55
1:A:343:VAL:HG11	1:A:446:LEU:HD21	1.88	0.55
1:B:206:PRO:O	1:B:207:SER:HB3	2.07	0.55
1:A:210:LYS:HA	1:A:337:LEU:CD1	2.26	0.55
1:A:263:ASN:HB2	1:B:991:GLU:OE1	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:503:ASN:H	1:A:503:ASN:ND2	2.04	0.55
1:B:353:MSE:SE	1:B:442:ASP:HB3	2.57	0.55
1:A:132:GLY:HA3	1:B:942:THR:HG23	1.88	0.54
1:A:944:ASP:OD1	1:A:946:ARG:HD2	2.08	0.54
1:B:454:ILE:HD13	1:B:456:PHE:HE1	1.72	0.54
1:A:113:THR:HG21	1:A:578:LYS:HG3	1.89	0.54
1:A:141:ARG:HE	1:A:141:ARG:CA	2.14	0.54
1:A:181:TYR:O	1:A:241:ASN:ND2	2.41	0.54
1:A:602:VAL:HG22	5:A:1453:HOH:O	2.06	0.54
1:A:587:VAL:HG22	1:A:612:VAL:HG22	1.90	0.54
1:A:171:VAL:HG12	1:A:172:ASN:OD1	2.08	0.54
1:A:737:ASN:ND2	1:A:740:ALA:HB3	2.23	0.54
1:A:772:LYS:O	1:A:776:GLU:HG3	2.07	0.54
1:A:838:PHE:N	1:A:869:ASN:HD22	2.03	0.54
1:A:926:ILE:HD12	1:A:927:VAL:N	2.22	0.54
1:A:264:ALA:O	1:A:265:ALA:HB3	2.07	0.54
1:A:537:THR:HG22	1:A:539:SER:H	1.71	0.54
1:B:216:GLU:O	1:B:218:ALA:N	2.39	0.54
1:B:537:THR:HG23	1:B:540:GLU:H	1.72	0.54
1:B:141:ARG:HH12	1:B:216:GLU:CD	2.16	0.54
1:A:833:GLN:NE2	1:A:887:ARG:HH21	2.06	0.54
1:A:932:PRO:HD3	1:A:1018:ASN:HB3	1.88	0.54
1:A:542:LEU:HD23	1:A:542:LEU:C	2.34	0.53
1:A:655:ILE:HD12	1:A:655:ILE:N	2.23	0.53
1:A:296:ASP:OD2	1:A:302:LYS:HG3	2.07	0.53
1:B:213:TYR:CD1	1:B:513:MSE:HB3	2.43	0.53
1:A:823:PRO:HG2	1:A:929:ASN:ND2	2.22	0.53
1:A:952:LYS:CB	1:A:953:PRO:CA	2.81	0.53
1:B:785:GLU:HG3	1:B:969:MSE:CE	2.39	0.53
1:B:158:LYS:O	1:B:162:GLU:HG3	2.09	0.53
1:B:346:ALA:C	1:B:348:GLN:H	2.16	0.53
1:B:362:GLU:OE1	1:B:365:LYS:HE3	2.08	0.53
1:B:178:TYR:HA	1:B:226:LEU:O	2.08	0.53
1:B:749:LEU:CD2	1:B:749:LEU:N	2.67	0.53
1:A:271:LEU:CD2	1:A:319:PRO:HB2	2.39	0.53
1:A:150:TYR:N	1:A:223:GLN:HE22	2.03	0.53
1:A:798:PHE:HB3	1:A:960:TYR:CE1	2.44	0.53
1:A:882:ARG:CZ	1:B:996:MSE:HE1	2.38	0.53
1:A:585:MSE:HG2	1:A:614:ASN:HA	1.91	0.53
1:A:1029:GLU:O	1:A:1030:GLY:C	2.52	0.53
1:B:360:ARG:HH11	1:B:360:ARG:CB	2.15	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:503:ASN:HD22	1:A:503:ASN:N	2.05	0.53
1:A:698:LYS:HG2	1:A:699:GLU:N	2.22	0.53
1:A:779:GLU:O	1:A:780:ASN:HB3	2.07	0.53
1:A:801:GLN:NE2	1:A:963:ARG:HG2	2.23	0.53
1:B:231:ILE:HD11	1:B:266:LEU:HD21	1.89	0.53
1:B:775:LYS:HE3	5:B:1431:HOH:O	2.07	0.53
1:B:652:LYS:NZ	1:B:654:THR:HG23	2.23	0.53
1:B:801:GLN:NE2	1:B:963:ARG:HG2	2.24	0.53
1:A:273:ASP:HA	1:A:276:LYS:HZ3	1.73	0.52
1:B:912:ILE:HD12	1:B:913:SER:N	2.23	0.52
1:A:738:SER:HA	1:A:741:LYS:HE3	1.90	0.52
1:A:440:ARG:CZ	5:A:1614:HOH:O	2.57	0.52
1:B:358:THR:O	1:B:359:ASN:HB2	2.10	0.52
1:A:115:GLN:C	1:A:117:LYS:H	2.18	0.52
1:A:145:LYS:CD	1:A:147:LYS:HB2	2.40	0.52
1:A:168:GLY:HA3	1:A:177:TYR:HE1	1.74	0.52
1:A:867:VAL:HG12	5:A:1229:HOH:O	2.08	0.52
1:B:530:GLU:HA	1:B:541:ARG:NE	2.25	0.52
1:B:801:GLN:HE22	1:B:963:ARG:HG2	1.74	0.52
1:A:129:ILE:HG21	1:A:242:TYR:CE2	2.45	0.52
1:A:597:VAL:O	1:A:706:TYR:HA	2.08	0.52
1:B:912:ILE:HD12	1:B:912:ILE:C	2.35	0.52
1:B:995:THR:CG2	1:B:999:ALA:H	2.21	0.52
1:B:729:GLY:C	1:B:736:ALA:HB2	2.35	0.52
1:A:858:TRP:CH2	1:A:860:SER:HB3	2.45	0.52
1:B:123:GLY:CA	1:B:148:ALA:HB3	2.38	0.52
1:A:140:TRP:HZ2	1:A:205:ALA:HB3	1.75	0.52
1:B:223:GLN:HG3	5:B:1314:HOH:O	2.09	0.52
1:A:414:LEU:HD11	1:A:454:ILE:HD13	1.92	0.51
1:A:271:LEU:HB2	1:A:272:PRO:HD2	1.92	0.51
1:A:271:LEU:HG	1:A:321:ALA:HB3	1.92	0.51
1:A:445:LEU:C	1:A:445:LEU:HD23	2.35	0.51
1:B:123:GLY:HA2	1:B:148:ALA:CB	2.40	0.51
1:B:414:LEU:CD2	1:B:436:ALA:HB3	2.40	0.51
1:A:943:GLU:OE2	1:B:135:LYS:HB2	2.10	0.51
1:B:781:ILE:HA	1:B:784:ILE:CG2	2.38	0.51
1:B:419:GLN:HE22	4:B:1104:CIT:H41	1.75	0.51
1:B:964:ILE:HD13	1:B:1010:TYR:HA	1.93	0.51
1:A:246:ILE:CD1	1:A:278:ALA:HB1	2.31	0.51
1:A:666:PRO:HG2	5:A:1324:HOH:O	2.11	0.51
1:B:242:TYR:OH	1:B:259:MSE:HB3	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:618:LYS:NZ	1:B:620:GLN:HE22	2.09	0.51
1:B:125:VAL:HB	1:B:253:GLY:O	2.11	0.51
1:B:368:ASP:CB	1:B:387:LYS:HD3	2.41	0.51
1:A:503:ASN:ND2	1:A:504:LYS:HD3	2.26	0.51
1:B:371:TYR:HD1	1:B:390:LEU:HD22	1.76	0.50
1:B:1026:LYS:O	1:B:1029:GLU:HG2	2.12	0.50
1:B:653:ILE:HD13	1:B:663:VAL:HG22	1.93	0.50
5:A:1173:HOH:O	1:B:996:MSE:HG2	2.10	0.50
1:B:361:PHE:CE1	1:B:434:PRO:HB2	2.46	0.50
1:B:384:VAL:O	1:B:385:LYS:C	2.55	0.50
1:B:112:LYS:HG2	1:B:116:GLU:OE2	2.10	0.50
1:B:181:TYR:HE2	1:B:227:MSE:HG2	1.76	0.50
1:B:271:LEU:HD11	1:B:275:THR:HG21	1.94	0.50
1:B:345:THR:HG22	1:B:346:ALA:N	2.26	0.50
1:B:777:GLY:O	1:B:778:VAL:C	2.54	0.50
1:B:860:SER:HB2	1:B:885:LYS:O	2.12	0.50
1:A:528:GLN:HE21	1:A:532:GLN:HE22	1.56	0.50
1:B:213:TYR:H	1:B:213:TYR:HD2	1.58	0.50
1:B:367:TYR:HB2	1:B:454:ILE:HD11	1.93	0.50
1:B:371:TYR:CZ	1:B:373:ASN:HA	2.46	0.50
1:B:147:LYS:HB2	1:B:147:LYS:HZ2	1.74	0.50
1:A:271:LEU:HD22	1:A:319:PRO:HB2	1.94	0.50
1:A:358:THR:O	1:A:359:ASN:HB2	2.12	0.50
1:A:590:LYS:HA	1:A:611:ASN:OD1	2.12	0.50
1:B:173:ASP:O	1:B:174:LYS:C	2.55	0.50
1:B:254:ALA:C	1:B:256:VAL:H	2.20	0.50
1:B:584:THR:OG1	1:B:616:SER:HB3	2.11	0.50
1:A:157:GLU:CD	1:A:160:LYS:HE3	2.37	0.49
1:A:476:SER:O	1:A:477:TRP:C	2.55	0.49
1:B:213:TYR:N	1:B:213:TYR:CD2	2.79	0.49
1:B:849:VAL:HG23	1:B:858:TRP:HE3	1.77	0.49
1:B:178:TYR:CG	1:B:178:TYR:O	2.65	0.49
1:B:364:ASN:C	1:B:364:ASN:HD22	2.20	0.49
1:B:440:ARG:HG3	1:B:440:ARG:NH1	2.27	0.49
1:A:532:GLN:O	1:A:533:TYR:HB2	2.13	0.49
1:B:228:ARG:HH21	1:B:230:GLU:CD	2.20	0.49
1:A:893:LYS:HE2	5:A:1334:HOH:O	2.12	0.49
1:A:945:ARG:HG3	1:A:989:LEU:O	2.12	0.49
1:B:210:LYS:O	1:B:212:PRO:HD3	2.12	0.49
1:B:331:TYR:HB2	1:B:471:LEU:HD22	1.94	0.49
1:B:496:ILE:HD11	5:B:1350:HOH:O	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:639:ALA:O	1:B:640:LEU:HB2	2.12	0.49
1:A:770:ILE:O	1:A:774:VAL:HG23	2.13	0.49
1:B:147:LYS:HB2	1:B:147:LYS:HZ3	1.76	0.49
1:A:250:ILE:HD11	1:A:282:ALA:HB2	1.95	0.49
1:A:671:ARG:HB2	5:A:1514:HOH:O	2.13	0.49
1:B:606:PHE:CE1	1:B:667:ILE:HD12	2.48	0.49
1:B:149:ARG:O	1:B:223:GLN:NE2	2.46	0.49
1:B:283:LYS:NZ	1:B:283:LYS:HB2	2.28	0.49
1:B:1029:GLU:O	1:B:1030:GLY:C	2.55	0.49
1:A:924:ASP:HB3	5:A:1407:HOH:O	2.12	0.49
1:B:138:GLU:C	1:B:140:TRP:N	2.70	0.49
1:B:833:GLN:HE21	1:B:887:ARG:HB2	1.78	0.49
1:A:125:VAL:O	1:A:254:ALA:O	2.30	0.49
1:A:141:ARG:HA	1:A:172:ASN:HD22	1.77	0.49
1:A:898:VAL:HG11	1:A:903:TYR:CE2	2.48	0.49
1:B:128:VAL:HB	1:B:226:LEU:HD23	1.94	0.49
1:A:414:LEU:HD11	1:A:454:ILE:CD1	2.43	0.48
1:A:414:LEU:HD23	1:A:436:ALA:HB3	1.95	0.48
1:B:136:ASN:C	1:B:138:GLU:H	2.21	0.48
1:B:345:THR:HB	1:B:347:ASP:OD1	2.12	0.48
1:B:887:ARG:HG2	1:B:887:ARG:HH11	1.77	0.48
1:A:213:TYR:CE1	1:A:493:GLY:HA2	2.48	0.48
1:B:391:ILE:O	1:B:415:ILE:HA	2.13	0.48
1:A:215:LEU:O	1:A:216:GLU:CB	2.62	0.48
1:A:623:TYR:CD2	1:A:696:PRO:HD3	2.49	0.48
1:A:745:ASP:OD2	1:A:806:HIS:HD2	1.97	0.48
1:B:1014:ASP:OD1	1:B:1014:ASP:C	2.57	0.48
1:A:129:ILE:CD1	1:A:246:ILE:HG22	2.44	0.48
1:B:124:THR:CG2	1:B:125:VAL:N	2.76	0.48
1:B:503:ASN:ND2	1:B:504:LYS:HD2	2.24	0.48
1:B:344:LYS:HB2	1:B:451:GLN:CD	2.39	0.48
1:B:782:GLU:HG3	1:B:783:ASP:OD1	2.13	0.48
1:A:174:LYS:O	1:A:175:VAL:CB	2.61	0.48
1:A:757:ASN:ND2	5:A:1129:HOH:O	2.47	0.48
1:A:845:LEU:HB3	1:A:863:THR:HB	1.96	0.48
1:A:898:VAL:CG1	1:A:903:TYR:OH	2.61	0.48
1:A:934:VAL:C	1:A:952:LYS:HG3	2.39	0.48
1:A:1004:LYS:NZ	1:A:1004:LYS:HB3	2.29	0.48
1:B:695:ASP:HB3	1:B:698:LYS:HD2	1.96	0.48
1:A:171:VAL:O	1:A:175:VAL:O	2.31	0.48
1:A:1015:MSE:HA	1:A:1015:MSE:HE2	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:171:VAL:O	1:B:171:VAL:HG12	2.13	0.48
1:A:203:GLY:O	1:A:204:ASN:HB2	2.13	0.48
1:A:533:TYR:H	1:A:534:PRO:HD3	1.79	0.48
5:A:1129:HOH:O	1:B:996:MSE:HE3	2.14	0.48
1:A:485:ILE:HG12	1:A:596:LYS:HE3	1.96	0.47
1:B:397:ASP:HB2	4:B:1106:CIT:O3	2.14	0.47
1:B:528:GLN:NE2	1:B:532:GLN:HE22	2.03	0.47
1:A:213:TYR:HE1	1:A:493:GLY:HA2	1.79	0.47
1:B:198:SER:HB2	1:B:202:SER:OG	2.14	0.47
1:B:849:VAL:HG23	1:B:858:TRP:CE3	2.49	0.47
1:B:946:ARG:NH2	1:B:984:ASP:OD2	2.47	0.47
1:A:391:ILE:O	1:A:415:ILE:HA	2.14	0.47
1:B:197:VAL:HG12	1:B:197:VAL:O	2.13	0.47
1:B:213:TYR:CE1	1:B:513:MSE:HB3	2.49	0.47
1:B:476:SER:O	1:B:477:TRP:C	2.57	0.47
1:A:255:LYS:HA	1:A:255:LYS:HZ3	1.78	0.47
1:A:882:ARG:CZ	1:B:996:MSE:CE	2.92	0.47
1:B:383:ASP:CG	1:B:384:VAL:H	2.23	0.47
1:B:591:ASP:OD1	1:B:593:THR:N	2.33	0.47
1:A:621:GLU:C	1:A:622:LEU:HD23	2.40	0.47
1:B:142:LEU:HD13	1:B:143:THR:H	1.79	0.47
1:A:180:ASP:OD2	1:A:228:ARG:HD3	2.14	0.47
1:A:192:GLU:C	1:A:194:GLY:H	2.23	0.47
1:B:141:ARG:O	1:B:142:LEU:O	2.32	0.47
1:A:226:LEU:O	1:A:227:MSE:HE3	2.14	0.47
1:A:750:GLN:HA	5:A:1616:HOH:O	2.14	0.47
1:B:172:ASN:C	1:B:173:ASP:O	2.57	0.47
1:B:213:TYR:CE1	1:B:493:GLY:HA2	2.50	0.47
1:B:833:GLN:NE2	1:B:884:GLU:HA	2.30	0.47
1:B:874:LEU:HD23	1:B:878:LEU:HD21	1.97	0.47
1:A:215:LEU:C	1:A:216:GLU:HG3	2.40	0.47
1:A:265:ALA:HB3	5:A:1533:HOH:O	2.14	0.47
1:A:833:GLN:HE21	1:A:887:ARG:HE	1.62	0.47
1:B:398:PHE:CE1	1:B:425:ILE:HG21	2.50	0.47
1:A:198:SER:HB3	1:A:202:SER:OG	2.15	0.47
1:A:778:VAL:O	1:A:778:VAL:CG2	2.62	0.47
1:A:177:TYR:HB3	1:A:225:LEU:HD22	1.97	0.46
1:A:200:ILE:O	1:A:201:LEU:HB2	2.15	0.46
1:A:342:ARG:CD	1:A:457:ASN:HD21	2.28	0.46
1:A:820:ALA:CB	1:A:926:ILE:HG13	2.45	0.46
1:A:1028:LEU:O	1:A:1029:GLU:C	2.58	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:611:ASN:HD21	1:B:662:GLN:HG2	1.72	0.46
1:A:149:ARG:HG2	1:A:149:ARG:HH11	1.80	0.46
1:B:200:ILE:O	1:B:201:LEU:HB2	2.16	0.46
1:B:111:VAL:HG11	1:B:218:ALA:HB1	1.98	0.46
1:A:145:LYS:O	1:A:147:LYS:N	2.49	0.46
1:A:392:GLU:HB2	1:A:416:TYR:CZ	2.50	0.46
1:B:337:LEU:HA	1:B:462:VAL:HA	1.97	0.46
1:B:341:VAL:HA	1:B:455:THR:O	2.16	0.46
1:B:228:ARG:HG3	1:B:228:ARG:NH1	2.31	0.46
1:B:390:LEU:C	1:B:390:LEU:HD23	2.41	0.46
1:A:183:LYS:HB2	1:A:183:LYS:NZ	2.31	0.46
1:B:141:ARG:HG2	1:B:141:ARG:HH11	1.80	0.46
1:A:137:HIS:O	1:A:138:GLU:O	2.34	0.46
1:A:156:LEU:HD13	1:A:156:LEU:C	2.41	0.46
1:A:263:ASN:ND2	1:B:945:ARG:HG2	2.30	0.46
1:A:723:ILE:HG12	1:A:758:PHE:CD2	2.51	0.46
1:B:367:TYR:HB2	1:B:454:ILE:HD12	1.98	0.46
1:A:215:LEU:O	1:A:216:GLU:HB2	2.16	0.45
1:A:529:TYR:O	1:A:532:GLN:O	2.33	0.45
1:A:960:TYR:CD1	1:A:961:ARG:HG3	2.52	0.45
1:A:1026:LYS:HA	1:A:1029:GLU:HG2	1.97	0.45
1:B:364:ASN:C	1:B:364:ASN:ND2	2.73	0.45
1:B:780:ASN:HD21	1:B:783:ASP:N	2.12	0.45
1:B:898:VAL:HG21	1:B:903:TYR:CE2	2.51	0.45
1:A:153:LYS:HE3	5:A:1622:HOH:O	2.17	0.45
1:B:780:ASN:HD21	1:B:783:ASP:HB2	1.81	0.45
1:A:213:TYR:CE1	1:A:513:MSE:HB2	2.52	0.45
1:A:728:ASP:O	1:A:741:LYS:HG3	2.17	0.45
1:A:729:GLY:O	1:A:736:ALA:HB2	2.17	0.45
1:A:960:TYR:HB2	1:A:1015:MSE:HE3	1.98	0.45
1:B:125:VAL:CG1	1:B:225:LEU:HG	2.46	0.45
1:B:454:ILE:HD13	1:B:456:PHE:CE1	2.50	0.45
1:B:734:HIS:HE1	5:B:1328:HOH:O	1.98	0.45
1:A:528:GLN:HG2	1:A:532:GLN:NE2	2.32	0.45
1:A:775:LYS:NZ	5:A:1322:HOH:O	2.49	0.45
1:B:368:ASP:HB3	1:B:387:LYS:HD3	1.96	0.45
1:B:601:ASN:ND2	1:B:713:PHE:H	2.13	0.45
1:B:671:ARG:HG2	1:B:671:ARG:NH1	2.29	0.45
1:A:271:LEU:HD23	1:A:271:LEU:N	2.09	0.45
1:A:302:LYS:HB3	1:A:302:LYS:HZ3	1.80	0.45
1:A:337:LEU:CD1	1:A:460:PRO:HB2	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:381:PHE:O	1:B:382:LYS:C	2.59	0.45
1:A:803:ASP:HB2	5:A:1141:HOH:O	2.17	0.45
1:B:383:ASP:C	1:B:385:LYS:N	2.74	0.45
1:A:242:TYR:OH	1:A:259:MSE:HB3	2.17	0.45
1:A:850:LEU:HD21	1:A:856:VAL:HG22	1.99	0.45
1:B:626:ALA:CB	1:B:665:VAL:HG11	2.47	0.45
1:A:271:LEU:CG	1:A:321:ALA:HB3	2.46	0.44
1:A:149:ARG:HG2	1:A:149:ARG:NH1	2.33	0.44
1:B:263:ASN:O	1:B:264:ALA:O	2.35	0.44
1:B:265:ALA:HB2	5:B:1597:HOH:O	2.17	0.44
1:A:556:LEU:N	1:A:570:GLN:HE22	1.89	0.44
1:B:108:PRO:HB2	1:B:492:PRO:HG2	1.99	0.44
1:B:111:VAL:HG11	1:B:218:ALA:CB	2.47	0.44
1:B:172:ASN:OD1	1:B:173:ASP:N	2.50	0.44
1:B:346:ALA:C	1:B:348:GLN:N	2.74	0.44
1:B:965:ALA:HB2	1:B:978:TYR:CE1	2.52	0.44
1:B:308:ALA:HA	1:B:638:PHE:CE1	2.53	0.44
1:B:969:MSE:HE1	1:B:974:PRO:HB3	2.00	0.44
1:A:378:GLU:HG2	1:A:379:ASP:N	2.33	0.44
1:A:471:LEU:HD21	1:A:556:LEU:HD13	1.99	0.44
1:A:528:GLN:NE2	1:A:532:GLN:NE2	2.65	0.44
1:B:454:ILE:HD12	1:B:454:ILE:C	2.42	0.44
1:B:786:SER:HB2	5:B:1581:HOH:O	2.18	0.44
1:A:125:VAL:CG1	1:A:225:LEU:HG	2.48	0.44
1:B:406:LYS:NZ	1:B:431:ASP:HB3	2.32	0.44
1:B:532:GLN:HG2	1:B:533:TYR:CE1	2.52	0.44
1:B:960:TYR:CD1	1:B:961:ARG:HG3	2.53	0.44
1:A:536:MSE:O	1:A:540:GLU:OE2	2.36	0.44
1:A:898:VAL:CG1	1:A:903:TYR:CZ	3.00	0.44
1:B:264:ALA:O	1:B:265:ALA:HB3	2.17	0.44
1:B:377:LYS:HB2	1:B:380:ASP:OD2	2.18	0.44
1:A:131:ALA:HA	1:A:229:VAL:O	2.18	0.44
1:A:378:GLU:O	1:A:379:ASP:CB	2.61	0.44
1:A:476:SER:HB2	1:A:569:GLN:HA	1.98	0.44
1:A:850:LEU:HD22	1:A:856:VAL:HA	2.00	0.44
1:A:982:ASN:ND2	5:A:1191:HOH:O	2.50	0.44
1:B:137:HIS:CE1	1:B:513:MSE:HE3	2.53	0.44
1:B:156:LEU:C	1:B:156:LEU:HD13	2.43	0.44
1:B:356:LEU:O	1:B:436:ALA:HA	2.17	0.44
1:B:849:VAL:HG21	1:B:888:TRP:CD2	2.53	0.44
1:A:264:ALA:HB3	5:A:1500:HOH:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:623:TYR:CE1	1:A:652:LYS:HG2	2.53	0.44
1:A:723:ILE:HG12	1:A:758:PHE:CE2	2.53	0.44
1:A:965:ALA:HB2	1:A:978:TYR:CE1	2.53	0.44
1:B:126:VAL:HA	1:B:256:VAL:HG13	2.00	0.44
1:B:139:ALA:C	1:B:141:ARG:N	2.70	0.44
1:B:734:HIS:HD2	5:B:1138:HOH:O	2.00	0.44
1:A:585:MSE:HE2	1:A:620:GLN:NE2	2.33	0.43
1:A:622:LEU:HD21	1:A:655:ILE:CD1	2.40	0.43
1:A:801:GLN:HE22	1:A:963:ARG:HG2	1.83	0.43
1:A:874:LEU:HD23	1:A:878:LEU:HD21	1.99	0.43
1:B:126:VAL:HG22	1:B:256:VAL:CG1	2.48	0.43
1:A:256:VAL:CG1	1:A:519:ALA:HB1	2.48	0.43
1:A:528:GLN:HG2	1:A:532:GLN:HE21	1.82	0.43
1:B:142:LEU:HD13	1:B:143:THR:O	2.18	0.43
1:B:409:GLY:O	1:B:410:ALA:HB3	2.18	0.43
1:B:570:GLN:HE21	1:B:573:GLY:HA2	1.83	0.43
1:B:618:LYS:CE	1:B:620:GLN:HE22	2.31	0.43
1:A:170:TRP:CD1	1:A:170:TRP:C	2.96	0.43
1:A:242:TYR:CE2	1:A:259:MSE:SE	3.21	0.43
1:A:337:LEU:HD11	1:A:460:PRO:HB2	2.00	0.43
1:A:946:ARG:NH2	1:A:984:ASP:OD2	2.51	0.43
1:B:152:SER:O	1:B:153:LYS:C	2.61	0.43
1:B:589:ASP:OD1	1:B:591:ASP:OD1	2.36	0.43
1:A:835:GLN:HE21	1:A:882:ARG:NE	2.04	0.43
1:A:898:VAL:HG11	1:A:903:TYR:CZ	2.54	0.43
1:B:145:LYS:HE3	1:B:221:GLU:OE1	2.17	0.43
1:B:445:LEU:HD23	1:B:445:LEU:C	2.44	0.43
1:A:206:PRO:O	1:A:207:SER:HB3	2.19	0.43
1:A:235:LEU:HD22	1:A:235:LEU:N	2.33	0.43
1:A:528:GLN:NE2	1:A:532:GLN:HE22	2.16	0.43
1:A:749:LEU:CD1	1:B:749:LEU:HG	2.46	0.43
1:B:111:VAL:HG12	1:B:111:VAL:O	2.18	0.43
1:B:410:ALA:O	1:B:411:VAL:CB	2.67	0.43
1:B:142:LEU:HD13	1:B:143:THR:N	2.33	0.43
1:B:145:LYS:O	1:B:146:THR:C	2.62	0.43
1:B:214:ARG:HD2	1:B:214:ARG:N	2.34	0.43
1:A:485:ILE:CG1	1:A:596:LYS:HE3	2.48	0.43
1:A:728:ASP:HB2	5:A:1636:HOH:O	2.19	0.43
1:A:785:GLU:HG3	1:A:969:MSE:HE1	2.00	0.43
1:A:967:THR:HG22	1:A:976:THR:HA	2.00	0.43
1:A:1031:HIS:O	1:B:191:GLN:HG2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:353:MSE:CE	1:B:446:LEU:HD11	2.44	0.43
1:B:392:GLU:HB2	1:B:416:TYR:CZ	2.53	0.43
1:B:503:ASN:HD22	1:B:503:ASN:C	2.27	0.43
1:B:623:TYR:HA	1:B:651:GLN:O	2.18	0.43
1:B:796:GLY:HA2	1:B:818:TYR:O	2.18	0.43
1:B:723:ILE:HG12	1:B:758:PHE:CD2	2.53	0.43
1:B:1014:ASP:OD2	1:B:1018:ASN:HB2	2.18	0.43
1:A:197:VAL:O	1:A:197:VAL:HG12	2.18	0.43
1:A:232:VAL:O	1:A:233:ASN:HB3	2.19	0.43
1:B:275:THR:O	1:B:279:PHE:HD1	2.01	0.43
1:A:209:THR:HG22	1:A:210:LYS:N	2.33	0.42
1:A:968:TYR:O	1:A:975:THR:HG22	2.19	0.42
1:B:944:ASP:CG	1:B:946:ARG:HD3	2.43	0.42
1:B:194:GLY:O	1:B:198:SER:HA	2.19	0.42
1:B:485:ILE:HD12	1:B:571:GLY:HA2	2.00	0.42
1:B:556:LEU:N	1:B:570:GLN:HE22	1.90	0.42
1:B:610:VAL:HG11	1:B:704:ILE:HG21	2.01	0.42
1:B:804:ASP:O	1:B:805:SER:OG	2.35	0.42
1:A:205:ALA:N	1:A:206:PRO:CD	2.79	0.42
1:A:926:ILE:HD12	1:A:927:VAL:C	2.43	0.42
1:A:944:ASP:OD2	1:B:135:LYS:HE3	2.19	0.42
1:B:154:GLU:O	1:B:155:ASP:C	2.63	0.42
1:B:341:VAL:CG1	1:B:454:ILE:HB	2.49	0.42
1:B:384:VAL:O	1:B:384:VAL:HG12	2.19	0.42
1:B:451:GLN:O	1:B:453:THR:N	2.52	0.42
1:A:138:GLU:HG3	1:A:215:LEU:HD12	2.01	0.42
1:A:741:LYS:HE2	1:A:741:LYS:N	2.33	0.42
1:B:494:GLN:O	1:B:496:ILE:HD12	2.18	0.42
1:B:585:MSE:HE1	1:B:622:LEU:HD21	2.00	0.42
1:A:210:LYS:HD2	5:A:1303:HOH:O	2.19	0.42
1:B:369:TYR:CE1	1:B:452:LYS:HD2	2.55	0.42
1:B:554:THR:HA	1:B:700:GLU:OE1	2.19	0.42
1:A:145:LYS:C	1:A:147:LYS:N	2.77	0.42
1:A:388:ILE:CD1	1:A:454:ILE:HD11	2.46	0.42
1:A:537:THR:HG22	1:A:539:SER:N	2.35	0.42
1:B:780:ASN:O	1:B:782:GLU:N	2.52	0.42
1:B:858:TRP:CH2	1:B:860:SER:HB3	2.55	0.42
1:B:135:LYS:O	1:B:136:ASN:C	2.63	0.42
1:B:369:TYR:O	1:B:452:LYS:HB3	2.18	0.42
1:B:503:ASN:ND2	1:B:503:ASN:H	2.17	0.42
1:A:572:ALA:HA	1:A:705:PRO:HD3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:441:LYS:HE2	5:B:1498:HOH:O	2.19	0.42
1:B:932:PRO:HD3	1:B:1018:ASN:HB3	2.02	0.42
1:A:229:VAL:HG12	1:A:238:TYR:CE1	2.55	0.42
1:B:137:HIS:CD2	1:B:211:GLU:HG2	2.55	0.42
1:B:136:ASN:C	1:B:138:GLU:N	2.78	0.41
1:B:218:ALA:O	1:B:524:LEU:HD11	2.20	0.41
1:B:584:THR:HG22	5:B:1386:HOH:O	2.20	0.41
1:A:175:VAL:O	1:A:175:VAL:HG12	2.21	0.41
1:B:440:ARG:O	1:B:441:LYS:C	2.63	0.41
1:B:537:THR:HG22	1:B:540:GLU:CG	2.49	0.41
1:B:611:ASN:ND2	1:B:611:ASN:N	2.68	0.41
1:B:740:ALA:HB1	1:B:743:GLN:HE21	1.85	0.41
1:A:272:PRO:C	1:A:274:GLU:H	2.28	0.41
1:A:833:GLN:NE2	1:A:884:GLU:HA	2.36	0.41
1:B:218:ALA:HB1	1:B:524:LEU:HD12	2.02	0.41
1:B:345:THR:HA	1:B:449:ASN:OD1	2.20	0.41
1:B:738:SER:O	1:B:739:ASP:CB	2.69	0.41
1:B:757:ASN:ND2	5:B:1122:HOH:O	2.53	0.41
1:B:135:LYS:O	1:B:137:HIS:N	2.53	0.41
1:B:331:TYR:HB3	1:B:471:LEU:HD13	2.03	0.41
1:B:334:ASP:C	1:B:465:THR:HG22	2.46	0.41
1:B:398:PHE:HE1	1:B:425:ILE:HG21	1.84	0.41
1:A:833:GLN:NE2	1:A:887:ARG:HE	2.18	0.41
1:A:951:SER:OG	1:A:952:LYS:HG2	2.21	0.41
1:B:940:PHE:CZ	1:B:945:ARG:HA	2.55	0.41
1:A:275:THR:O	1:A:279:PHE:HD1	2.02	0.41
1:A:440:ARG:HD3	5:A:1624:HOH:O	2.20	0.41
1:B:141:ARG:HA	1:B:141:ARG:HD2	1.83	0.41
1:B:178:TYR:O	1:B:178:TYR:CD2	2.73	0.41
1:B:614:ASN:ND2	1:B:657:ALA:HA	2.36	0.41
1:B:679:GLN:HE21	1:B:679:GLN:HB2	1.67	0.41
1:A:232:VAL:O	1:A:233:ASN:CB	2.69	0.41
1:B:106:ASN:C	1:B:108:PRO:HD3	2.46	0.41
1:B:139:ALA:HB1	1:B:206:PRO:CA	2.38	0.41
1:B:255:LYS:HA	1:B:287:VAL:HG22	2.03	0.41
1:B:537:THR:OG1	1:B:538:PRO:HD2	2.21	0.41
1:B:801:GLN:HE22	1:B:963:ARG:CG	2.33	0.41
1:A:174:LYS:NZ	1:A:216:GLU:OE1	2.53	0.41
1:A:221:GLU:OE2	1:A:221:GLU:HA	2.20	0.41
1:A:503:ASN:ND2	1:A:503:ASN:N	2.64	0.41
1:A:851:ASP:C	1:A:851:ASP:OD1	2.64	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:248:ASP:O	1:B:252:LEU:HG	2.21	0.41
1:B:431:ASP:C	1:B:433:MSE:H	2.28	0.41
1:B:685:PHE:CD2	1:B:707:ILE:HD11	2.54	0.41
1:B:780:ASN:C	1:B:782:GLU:N	2.71	0.41
1:A:259:MSE:HG3	1:A:289:ILE:HG23	2.02	0.41
1:A:640:LEU:HD12	1:A:640:LEU:HA	1.89	0.41
1:A:1028:LEU:O	1:A:1030:GLY:N	2.54	0.41
1:B:133:PHE:CD1	1:B:133:PHE:N	2.89	0.41
1:B:416:TYR:HA	1:B:438:ILE:O	2.21	0.41
1:B:442:ASP:O	1:B:445:LEU:HB3	2.21	0.41
1:B:547:LYS:NZ	1:B:593:THR:O	2.54	0.41
1:A:243:ALA:O	1:A:246:ILE:HG12	2.20	0.40
1:A:320:ALA:C	1:A:322:ALA:H	2.29	0.40
1:A:946:ARG:HH21	1:B:500:VAL:HB	1.86	0.40
1:B:236:ALA:O	1:B:240:ARG:HG3	2.21	0.40
1:B:355:VAL:HG12	1:B:438:ILE:CG2	2.47	0.40
1:B:365:LYS:HB3	1:B:366:ALA:H	1.60	0.40
1:B:1029:GLU:O	1:B:1031:HIS:N	2.53	0.40
1:A:247:ARG:NH2	1:A:277:LYS:NZ	2.69	0.40
1:B:171:VAL:O	1:B:172:ASN:ND2	2.53	0.40
1:B:206:PRO:O	1:B:207:SER:CB	2.68	0.40
1:B:369:TYR:CZ	1:B:452:LYS:HA	2.57	0.40
1:B:527:LYS:HE3	1:B:527:LYS:HB2	1.94	0.40
1:B:772:LYS:O	1:B:776:GLU:HG3	2.21	0.40
1:B:910:THR:HA	1:B:911:PRO:HD3	1.98	0.40
1:A:192:GLU:C	1:A:194:GLY:N	2.79	0.40
1:A:944:ASP:O	1:A:945:ARG:CB	2.68	0.40
1:A:946:ARG:NH2	1:B:500:VAL:HB	2.36	0.40
1:B:137:HIS:CD2	1:B:137:HIS:C	2.98	0.40
1:B:572:ALA:HA	1:B:705:PRO:HD3	2.03	0.40
1:B:626:ALA:HB3	1:B:665:VAL:HG11	2.03	0.40
1:B:723:ILE:HD12	1:B:724:TYR:H	1.86	0.40
1:B:737:ASN:ND2	1:B:743:GLN:HE22	2.20	0.40
1:B:798:PHE:HB3	1:B:960:TYR:CE1	2.56	0.40
1:A:156:LEU:HG	1:A:176:ALA:O	2.21	0.40
1:A:377:LYS:O	1:A:378:GLU:C	2.64	0.40
1:A:850:LEU:HD22	1:A:856:VAL:HG22	2.03	0.40
1:B:264:ALA:HB3	5:B:1406:HOH:O	2.20	0.40
1:B:368:ASP:HB2	1:B:387:LYS:HD3	2.03	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	924/926 (100%)	830 (90%)	64 (7%)	30 (3%)	3	0
1	B	924/926 (100%)	818 (88%)	70 (8%)	36 (4%)	2	0
All	All	1848/1852 (100%)	1648 (89%)	134 (7%)	66 (4%)	2	0

All (66) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	138	GLU
1	A	140	TRP
1	A	145	LYS
1	A	172	ASN
1	A	184	ASP
1	A	207	SER
1	A	254	ALA
1	A	264	ALA
1	A	592	ASN
1	A	952	LYS
1	A	1029	GLU
1	A	1030	GLY
1	B	141	ARG
1	B	142	LEU
1	B	146	THR
1	B	149	ARG
1	B	172	ASN
1	B	174	LYS
1	B	189	VAL
1	B	217	GLY
1	B	264	ALA
1	B	384	VAL
1	B	741	LYS
1	B	778	VAL
1	B	781	ILE

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Mol	Chain	Res	Type
1	B	1030	GLY
1	A	146	THR
1	A	183	LYS
1	A	233	ASN
1	A	255	LYS
1	A	323	ASP
1	B	136	ASN
1	B	173	ASP
1	B	200	ILE
1	B	364	ASN
1	B	366	ALA
1	B	408	ALA
1	B	894	ASP
1	A	141	ARG
1	A	204	ASN
1	B	144	ASP
1	B	170	TRP
1	B	185	GLY
1	B	186	LYS
1	B	233	ASN
1	B	382	LYS
1	B	385	LYS
1	B	777	GLY
1	A	200	ILE
1	A	531	THR
1	A	739	ASP
1	A	971	GLU
1	B	207	SER
1	B	367	TYR
1	B	476	SER
1	A	136	ASN
1	A	495	ASP
1	A	780	ASN
1	B	206	PRO
1	A	175	VAL
1	A	379	ASP
1	B	195	THR
1	B	495	ASP
1	A	189	VAL
1	A	537	THR
1	B	411	VAL

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	771/760 (101%)	742 (96%)	29 (4%)	29	21
1	B	771/760 (101%)	741 (96%)	30 (4%)	28	21
All	All	1542/1520 (101%)	1483 (96%)	59 (4%)	29	21

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	112	LYS
1	A	140	TRP
1	A	141	ARG
1	A	145	LYS
1	A	183	LYS
1	A	213	TYR
1	A	255	LYS
1	A	271	LEU
1	A	303	THR
1	A	336	GLN
1	A	384	VAL
1	A	390	LEU
1	A	503	ASN
1	A	522	MSE
1	A	552	SER
1	A	560	ASP
1	A	602	VAL
1	A	615	LYS
1	A	622	LEU
1	A	640	LEU
1	A	651	GLN
1	A	723	ILE
1	A	741	LYS
1	A	775	LYS
1	A	778	VAL
1	A	926	ILE
1	A	994	GLU

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Mol	Chain	Res	Type
1	A	1004	LYS
1	A	1026	LYS
1	B	142	LEU
1	B	145	LYS
1	B	147	LYS
1	B	155	ASP
1	B	213	TYR
1	B	227	MSE
1	B	246	ILE
1	B	256	VAL
1	B	270	ASN
1	B	271	LEU
1	B	283	LYS
1	B	328	VAL
1	B	337	LEU
1	B	360	ARG
1	B	476	SER
1	B	486	LYS
1	B	503	ASN
1	B	504	LYS
1	B	522	MSE
1	B	554	THR
1	B	640	LEU
1	B	694	GLN
1	B	723	ILE
1	B	749	LEU
1	B	785	GLU
1	B	822	SER
1	B	862	VAL
1	B	973	LEU
1	B	994	GLU
1	B	995	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (73) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	115	GLN
1	A	163	HIS
1	A	223	GLN
1	A	233	ASN
1	A	244	GLN
1	A	263	ASN

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Mol	Chain	Res	Type
1	A	336	GLN
1	A	432	GLN
1	A	451	GLN
1	A	457	ASN
1	A	484	ASN
1	A	503	ASN
1	A	526	GLN
1	A	528	GLN
1	A	532	GLN
1	A	570	GLN
1	A	592	ASN
1	A	625	GLN
1	A	651	GLN
1	A	679	GLN
1	A	682	ASN
1	A	694	GLN
1	A	734	HIS
1	A	756	ASN
1	A	757	ASN
1	A	780	ASN
1	A	806	HIS
1	A	833	GLN
1	A	835	GLN
1	A	844	ASN
1	A	855	ASN
1	A	865	GLN
1	A	869	ASN
1	A	929	ASN
1	A	982	ASN
1	A	1018	ASN
1	B	115	GLN
1	B	136	ASN
1	B	163	HIS
1	B	204	ASN
1	B	223	GLN
1	B	233	ASN
1	B	241	ASN
1	B	244	GLN
1	B	295	ASN
1	B	349	GLN
1	B	364	ASN
1	B	419	GLN

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Mol	Chain	Res	Type
1	B	451	GLN
1	B	494	GLN
1	B	503	ASN
1	B	526	GLN
1	B	532	GLN
1	B	569	GLN
1	B	570	GLN
1	B	601	ASN
1	B	611	ASN
1	B	614	ASN
1	B	620	GLN
1	B	651	GLN
1	B	658	ASN
1	B	679	GLN
1	B	743	GLN
1	B	756	ASN
1	B	757	ASN
1	B	780	ASN
1	B	806	HIS
1	B	812	HIS
1	B	833	GLN
1	B	835	GLN
1	B	844	ASN
1	B	869	ASN
1	B	982	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 10 ligands modelled in this entry, 2 are monoatomic - leaving 8 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
4	CIT	B	1104	-	12,12,12	4.30	4 (33%)	17,17,17	5.71	10 (58%)
4	CIT	B	1106	-	12,12,12	4.24	5 (41%)	17,17,17	5.65	11 (64%)
2	ACT	A	1107	-	3,3,3	0.60	0	3,3,3	0.33	0
4	CIT	A	1105	-	12,12,12	4.45	5 (41%)	17,17,17	5.62	9 (52%)
4	CIT	B	1102	-	12,12,12	4.39	5 (41%)	17,17,17	5.66	11 (64%)
2	ACT	B	1108	-	3,3,3	0.58	0	3,3,3	0.36	0
4	CIT	A	1103	-	12,12,12	4.31	5 (41%)	17,17,17	5.76	10 (58%)
4	CIT	A	1101	-	12,12,12	4.55	5 (41%)	17,17,17	5.70	11 (64%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	CIT	B	1104	-	-	6/16/16/16	-
4	CIT	B	1106	-	-	4/16/16/16	-
4	CIT	B	1102	-	-	6/16/16/16	-
4	CIT	A	1105	-	-	3/16/16/16	-
4	CIT	A	1103	-	-	6/16/16/16	-
4	CIT	A	1101	-	-	5/16/16/16	-

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1101	CIT	C3-C6	14.20	1.68	1.53
4	A	1105	CIT	C3-C6	13.74	1.67	1.53
4	B	1102	CIT	C3-C6	13.67	1.67	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1103	CIT	C3-C6	13.19	1.67	1.53
4	B	1104	CIT	C3-C6	13.07	1.67	1.53
4	B	1106	CIT	C3-C6	12.93	1.66	1.53
4	B	1104	CIT	O5-C6	4.38	1.35	1.22
4	A	1103	CIT	O5-C6	4.21	1.35	1.22
4	B	1106	CIT	O5-C6	4.15	1.35	1.22
4	B	1102	CIT	O5-C6	4.15	1.35	1.22
4	A	1105	CIT	O5-C6	4.13	1.35	1.22
4	A	1101	CIT	O5-C6	4.11	1.35	1.22
4	B	1104	CIT	O3-C5	3.74	1.34	1.22
4	A	1105	CIT	O3-C5	3.64	1.34	1.22
4	A	1103	CIT	O3-C5	3.58	1.33	1.22
4	B	1106	CIT	O3-C5	3.49	1.33	1.22
4	B	1102	CIT	O3-C5	3.25	1.32	1.22
4	A	1101	CIT	O3-C5	3.05	1.32	1.22
4	A	1101	CIT	C2-C3	2.85	1.57	1.54
4	A	1103	CIT	O4-C5	-2.68	1.22	1.30
4	A	1105	CIT	O4-C5	-2.63	1.22	1.30
4	B	1104	CIT	O4-C5	-2.60	1.22	1.30
4	B	1106	CIT	O4-C5	-2.55	1.22	1.30
4	B	1106	CIT	C2-C3	2.54	1.57	1.54
4	A	1101	CIT	O4-C5	-2.54	1.22	1.30
4	B	1102	CIT	O4-C5	-2.49	1.22	1.30
4	A	1103	CIT	C4-C3	-2.15	1.51	1.54
4	A	1105	CIT	C2-C3	2.11	1.56	1.54
4	B	1102	CIT	C2-C3	2.09	1.56	1.54

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1103	CIT	O7-C3-C6	-15.42	87.09	108.96
4	B	1104	CIT	O7-C3-C6	-14.94	87.77	108.96
4	A	1101	CIT	O7-C3-C6	-14.11	88.95	108.96
4	A	1105	CIT	O7-C3-C6	-14.04	89.05	108.96
4	B	1102	CIT	O7-C3-C6	-13.96	89.16	108.96
4	B	1106	CIT	O7-C3-C6	-13.62	89.64	108.96
4	B	1106	CIT	C4-C3-C6	-12.16	83.14	110.03
4	A	1105	CIT	C4-C3-C6	-11.44	84.72	110.03
4	A	1101	CIT	C2-C3-C6	-11.26	85.14	110.03
4	B	1102	CIT	C2-C3-C6	-11.15	85.38	110.03
4	B	1104	CIT	C4-C3-C6	-11.09	85.50	110.03
4	B	1102	CIT	C4-C3-C6	-10.93	85.85	110.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1103	CIT	C2-C3-C6	-10.62	86.54	110.03
4	A	1101	CIT	C4-C3-C6	-10.58	86.64	110.03
4	A	1105	CIT	C2-C3-C6	-10.41	87.00	110.03
4	A	1103	CIT	C4-C3-C6	-10.38	87.08	110.03
4	B	1106	CIT	C2-C3-C6	-10.30	87.25	110.03
4	B	1104	CIT	C2-C3-C6	-10.26	87.35	110.03
4	B	1106	CIT	C4-C3-C2	6.40	125.72	109.31
4	A	1105	CIT	C4-C3-C2	6.32	125.52	109.31
4	B	1102	CIT	C4-C3-C2	5.87	124.37	109.31
4	A	1101	CIT	C4-C3-C2	5.84	124.29	109.31
4	B	1104	CIT	C4-C3-C2	5.77	124.11	109.31
4	A	1103	CIT	C4-C3-C2	5.31	122.93	109.31
4	A	1103	CIT	O7-C3-C2	3.93	118.34	109.38
4	B	1104	CIT	O5-C6-C3	-3.86	114.61	122.09
4	A	1103	CIT	O5-C6-C3	-3.85	114.64	122.09
4	A	1101	CIT	O5-C6-C3	-3.82	114.69	122.09
4	B	1104	CIT	O7-C3-C4	3.72	117.87	109.38
4	A	1103	CIT	O7-C3-C4	3.72	117.86	109.38
4	A	1101	CIT	O7-C3-C2	3.69	117.79	109.38
4	A	1105	CIT	O5-C6-C3	-3.63	115.06	122.09
4	A	1103	CIT	O6-C6-C3	3.62	120.08	113.14
4	B	1106	CIT	O7-C3-C4	3.61	117.62	109.38
4	B	1106	CIT	O5-C6-C3	-3.57	115.18	122.09
4	B	1104	CIT	O6-C6-C3	3.57	119.99	113.14
4	B	1102	CIT	O7-C3-C2	3.57	117.52	109.38
4	B	1102	CIT	O5-C6-C3	-3.57	115.18	122.09
4	A	1101	CIT	O6-C6-C3	3.57	119.98	113.14
4	A	1105	CIT	O6-C6-C3	3.52	119.89	113.14
4	A	1105	CIT	O7-C3-C4	3.42	117.17	109.38
4	B	1102	CIT	O7-C3-C4	3.41	117.15	109.38
4	B	1104	CIT	O7-C3-C2	3.40	117.12	109.38
4	B	1102	CIT	O6-C6-C3	3.36	119.58	113.14
4	A	1101	CIT	O7-C3-C4	3.35	117.03	109.38
4	B	1106	CIT	O6-C6-C3	3.30	119.47	113.14
4	A	1105	CIT	O7-C3-C2	3.08	116.41	109.38
4	A	1101	CIT	C3-C4-C5	3.06	122.29	113.92
4	A	1101	CIT	C3-C2-C1	2.91	121.89	113.92
4	B	1106	CIT	O7-C3-C2	2.72	115.59	109.38
4	A	1103	CIT	C3-C2-C1	2.71	121.34	113.92
4	B	1102	CIT	C3-C2-C1	2.71	121.33	113.92
4	B	1102	CIT	C3-C4-C5	2.58	120.97	113.92
4	A	1103	CIT	O3-C5-C4	-2.34	116.31	122.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1104	CIT	C3-C2-C1	2.34	120.31	113.92
4	B	1106	CIT	C3-C2-C1	2.30	120.20	113.92
4	B	1104	CIT	O3-C5-C4	-2.23	116.63	122.95
4	A	1105	CIT	C3-C2-C1	2.23	120.02	113.92
4	A	1101	CIT	O3-C5-C4	-2.15	116.85	122.95
4	B	1106	CIT	O3-C5-C4	-2.13	116.91	122.95
4	B	1102	CIT	O3-C5-C4	-2.10	117.00	122.95
4	B	1106	CIT	C3-C4-C5	2.04	119.50	113.92

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1101	CIT	C1-C2-C3-O7
4	A	1101	CIT	O7-C3-C4-C5
4	A	1103	CIT	C1-C2-C3-O7
4	A	1105	CIT	C1-C2-C3-O7
4	A	1105	CIT	C2-C3-C4-C5
4	B	1102	CIT	C1-C2-C3-O7
4	B	1102	CIT	O7-C3-C4-C5
4	B	1104	CIT	C1-C2-C3-O7
4	B	1104	CIT	C2-C3-C4-C5
4	B	1106	CIT	C1-C2-C3-O7
4	A	1103	CIT	O7-C3-C4-C5
4	B	1106	CIT	C2-C3-C4-C5
4	A	1101	CIT	C1-C2-C3-C6
4	A	1105	CIT	C1-C2-C3-C6
4	B	1102	CIT	C1-C2-C3-C6
4	B	1104	CIT	C1-C2-C3-C6
4	B	1104	CIT	O7-C3-C4-C5
4	B	1106	CIT	C1-C2-C3-C6
4	A	1103	CIT	C1-C2-C3-C6
4	B	1106	CIT	C6-C3-C4-C5
4	A	1103	CIT	C2-C3-C4-C5
4	B	1102	CIT	O2-C1-C2-C3
4	A	1101	CIT	O2-C1-C2-C3
4	B	1102	CIT	O1-C1-C2-C3
4	A	1101	CIT	O1-C1-C2-C3
4	A	1103	CIT	O1-C1-C2-C3
4	A	1103	CIT	O2-C1-C2-C3
4	B	1104	CIT	O1-C1-C2-C3
4	B	1102	CIT	C6-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
4	B	1104	CIT	O2-C1-C2-C3

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1104	CIT	1	0
4	B	1106	CIT	1	0

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

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.