



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 02:31 AM UTC

PDB ID : 1LT8 / pdb_00001lt8
Title : Reduced Homo sapiens Betaine-Homocysteine S-Methyltransferase in Complex with S-(delta-carboxybutyl)-L-Homocysteine
Authors : Evans, J.C.; Huddler, D.P.; Jiracek, J.; Castro, C.; Millian, N.S.; Garrow, T.A.; Ludwig, M.L.
Deposited on : 2002-05-20
Resolution : 2.05 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) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

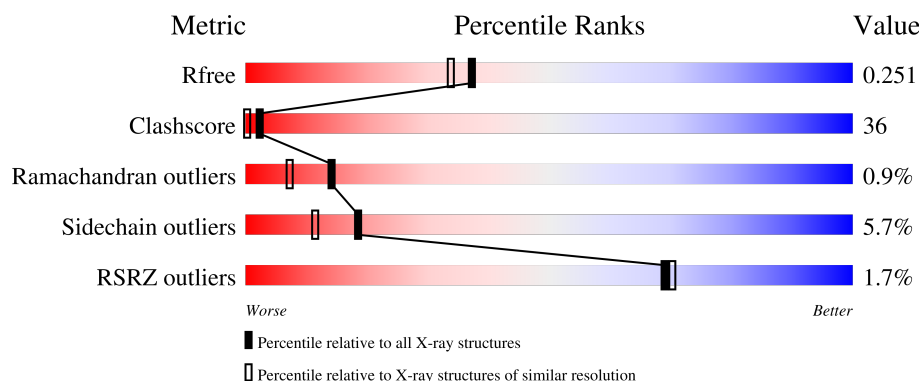
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

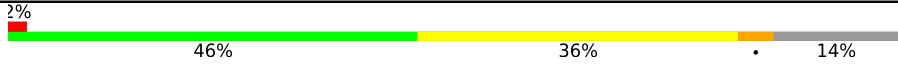
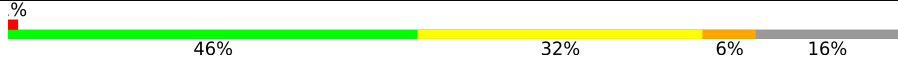
The reported resolution of this entry is 2.05 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2260 (2.04-2.04)
Clashscore	190562	2333 (2.04-2.04)
Ramachandran outliers	187476	2318 (2.04-2.04)
Sidechain outliers	187428	2318 (2.04-2.04)
RSRZ outliers	180081	2260 (2.04-2.04)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	406	
1	B	406	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5826 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 BETAINE-HOMOCYSTEINE METHYLTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	348	Total	C	N	O	S	0	0	0
			2700	1722	469	499	10			
1	B	340	Total	C	N	O	S	0	0	0
			2637	1686	458	483	10			

There are 14 discrepancies between the modelled and reference sequences:

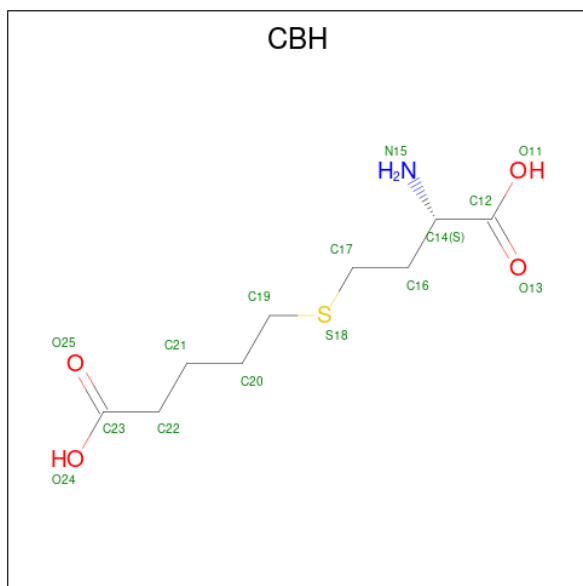
Chain	Residue	Modelled	Actual	Comment	Reference
A	2	ALA	PRO	engineered mutation	UNP Q93088
A	104	ALA	CYS	engineered mutation	UNP Q93088
A	131	ALA	CYS	engineered mutation	UNP Q93088
A	186	ALA	CYS	engineered mutation	UNP Q93088
A	201	ALA	CYS	engineered mutation	UNP Q93088
A	239	GLN	ARG	SEE REMARK 999	UNP Q93088
A	256	ALA	CYS	engineered mutation	UNP Q93088
B	2	ALA	PRO	engineered mutation	UNP Q93088
B	104	ALA	CYS	engineered mutation	UNP Q93088
B	131	ALA	CYS	engineered mutation	UNP Q93088
B	186	ALA	CYS	engineered mutation	UNP Q93088
B	201	ALA	CYS	engineered mutation	UNP Q93088
B	239	GLN	ARG	SEE REMARK 999	UNP Q93088
B	256	ALA	CYS	engineered mutation	UNP Q93088

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

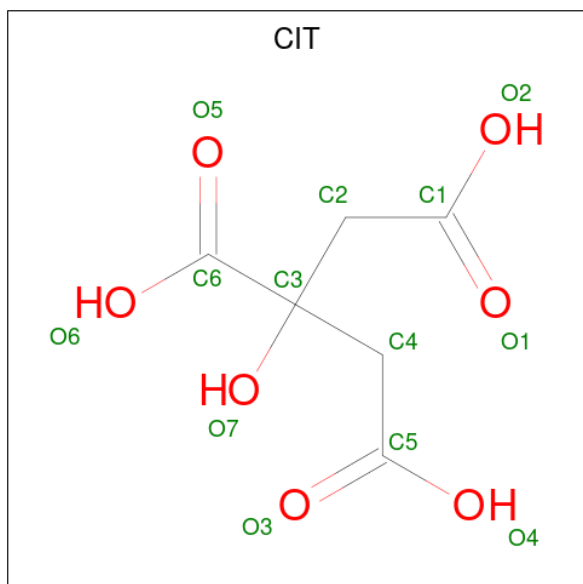
- Molecule 3 is S-(D-CARBOXYBUTYL)-L-HOMOCYSTEINE (CCD ID: CBH) (formula:

C₉H₁₇NO₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			15	9	1	4	1		
3	B	1	Total	C	N	O	S	0	0
			15	9	1	4	1		

- Molecule 4 is CITRIC ACID (CCD ID: CIT) (formula: C₆H₈O₇).



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

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

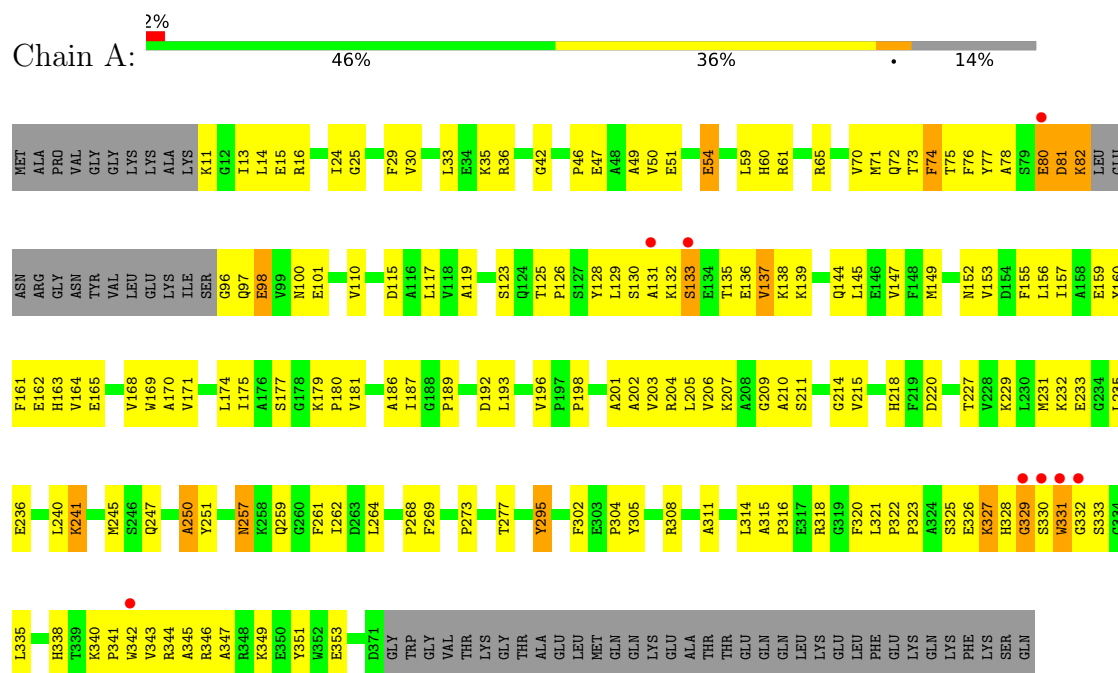
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	240	Total	O	0	0
			240	240		
5	B	191	Total	O	0	0
			191	191		

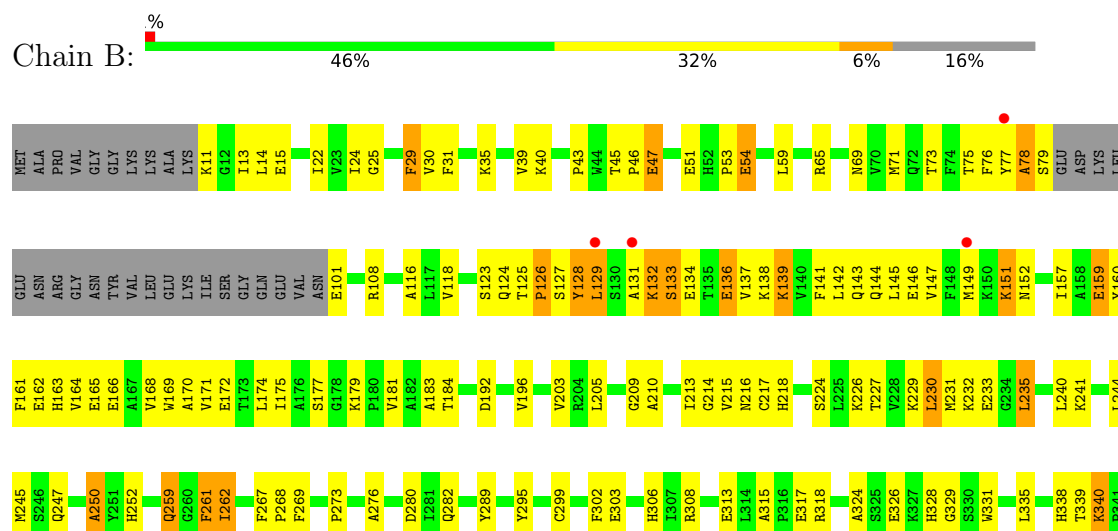
3 Residue-property plots

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

• Molecule 1: BETAINE-HOMOCYSTEINE METHYLTRANSFERASE



• Molecule 1: BETAINE-HOMOCYSTEINE METHYLTRANSFERASE



V342	V343	R346	R347	R348	R349	R350	R351	R352	R353	R354	R355	R356	R357	R358	R359	R360	R361	R362	R363	R364	R365	R366	R367	R368	R369	R370	R371	R372	R373	R374	R375	R376	R377	R378	R379	R380	R381	R382	R383	R384	R385	R386	R387	R388	R389	R390	R391	R392	R393	R394	R395	R396	R397	R398	R399	R400	R401	R402	R403	R404	R405	R406	R407	R408	R409	R410	R411	R412	R413	R414	R415	R416	R417	R418	R419	R420	R421	R422	R423	R424	R425	R426	R427	R428	R429	R430	R431	R432	R433	R434	R435	R436	R437	R438	R439	R440	R441	R442	R443	R444	R445	R446	R447	R448	R449	R450	R451	R452	R453	R454	R455	R456	R457	R458	R459	R460	R461	R462	R463	R464	R465	R466	R467	R468	R469	R470	R471	R472	R473	R474	R475	R476	R477	R478	R479	R480	R481	R482	R483	R484	R485	R486	R487	R488	R489	R490	R491	R492	R493	R494	R495	R496	R497	R498	R499	R500	R501	R502	R503	R504	R505	R506	R507	R508	R509	R510	R511	R512	R513	R514	R515	R516	R517	R518	R519	R520	R521	R522	R523	R524	R525	R526	R527	R528	R529	R530	R531	R532	R533	R534	R535	R536	R537	R538	R539	R540	R541	R542	R543	R544	R545	R546	R547	R548	R549	R550	R551	R552	R553	R554	R555	R556	R557	R558	R559	R560	R561	R562	R563	R564	R565	R566	R567	R568	R569	R570	R571	R572	R573	R574	R575	R576	R577	R578	R579	R580	R581	R582	R583	R584	R585	R586	R587	R588	R589	R590	R591	R592	R593	R594	R595	R596	R597	R598	R599	R600	R601	R602	R603	R604	R605	R606	R607	R608	R609	R610	R611	R612	R613	R614	R615	R616	R617	R618	R619	R620	R621	R622	R623	R624	R625	R626	R627	R628	R629	R630	R631	R632	R633	R634	R635	R636	R637	R638	R639	R640	R641	R642	R643	R644	R645	R646	R647	R648	R649	R650	R651	R652	R653	R654	R655	R656	R657	R658	R659	R660	R661	R662	R663	R664	R665	R666	R667	R668	R669	R670	R671	R672	R673	R674	R675	R676	R677	R678	R679	R680	R681	R682	R683	R684	R685	R686	R687	R688	R689	R690	R691	R692	R693	R694	R695	R696	R697	R698	R699	R700	R701	R702	R703	R704	R705	R706	R707	R708	R709	R710	R711	R712	R713	R714	R715	R716	R717	R718	R719	R720	R721	R722	R723	R724	R725	R726	R727	R728	R729	R730	R731	R732	R733	R734	R735	R736	R737	R738	R739	R740	R741	R742	R743	R744	R745	R746	R747	R748	R749	R750	R751	R752	R753	R754	R755	R756	R757	R758	R759	R760	R761	R762	R763	R764	R765	R766	R767	R768	R769	R770	R771	R772	R773	R774	R775	R776	R777	R778	R779	R780	R781	R782	R783	R784	R785	R786	R787	R788	R789	R790	R791	R792	R793	R794	R795	R796	R797	R798	R799	R800	R801	R802	R803	R804	R805	R806	R807	R808	R809	R810	R811	R812	R813	R814	R815	R816	R817	R818	R819	R820	R821	R822	R823	R824	R825	R826	R827	R828	R829	R830	R831	R832	R833	R834	R835	R836	R837	R838	R839	R840	R841	R842	R843	R844	R845	R846	R847	R848	R849	R850	R851	R852	R853	R854	R855	R856	R857	R858	R859	R860	R861	R862	R863	R864	R865	R866	R867	R868	R869	R870	R871	R872	R873	R874	R875	R876	R877	R878	R879	R880	R881	R882	R883	R884	R885	R886	R887	R888	R889	R890	R891	R892	R893	R894	R895	R896	R897	R898	R899	R900	R901	R902	R903	R904	R905	R906	R907	R908	R909	R910	R911	R912	R913	R914	R915	R916	R917	R918	R919	R920	R921	R922	R923	R924	R925	R926	R927	R928	R929	R930	R931	R932	R933	R934	R935	R936	R937	R938	R939	R940	R941	R942	R943	R944	R945	R946	R947	R948	R949	R950	R951	R952	R953	R954	R955	R956	R957	R958	R959	R960	R961	R962	R963	R964	R965	R966	R967	R968	R969	R970	R971	R972	R973	R974	R975	R976	R977	R978	R979	R980	R981	R982	R983	R984	R985	R986	R987	R988	R989	R990	R991	R992	R993	R994	R995	R996	R997	R998	R999	R1000
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4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	109.70Å 90.84Å 88.40Å 90.00° 122.28° 90.00°	Depositor
Resolution (Å)	10.00 – 2.05 10.00 – 2.05	Depositor EDS
% Data completeness (in resolution range)	99.9 (10.00-2.05) 99.0 (10.00-2.05)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.04 (at 2.06Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.226 , 0.255 0.225 , 0.251	Depositor DCC
R_{free} test set	2317 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	30.3	Xtriage
Anisotropy	0.460	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.44 , 79.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5826	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.99% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CBH, CIT, 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	0.41	0/2768	0.94	8/3750 (0.2%)
1	B	0.39	0/2705	0.99	15/3666 (0.4%)
All	All	0.40	0/5473	0.97	23/7416 (0.3%)

There are no bond length outliers.

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	29	PHE	N-CA-C	6.87	118.42	111.07
1	B	126	PRO	N-CA-C	-6.58	105.93	114.03
1	B	159	GLU	N-CA-C	6.58	120.42	109.95
1	B	340	LYS	CA-C-N	6.25	125.46	118.97
1	B	340	LYS	C-N-CA	6.25	125.46	118.97
1	B	29	PHE	N-CA-C	6.07	117.69	111.14
1	B	250	ALA	N-CA-C	-5.91	105.98	112.72
1	B	226	LYS	N-CA-C	-5.83	105.01	111.36
1	B	128	TYR	N-CA-C	-5.82	105.06	111.82
1	A	250	ALA	N-CA-C	-5.72	106.19	112.72
1	B	196	VAL	CA-C-N	5.62	123.76	119.66
1	B	196	VAL	C-N-CA	5.62	123.76	119.66
1	B	78	ALA	CB-CA-C	-5.49	110.22	116.54
1	A	277	THR	N-CA-C	-5.47	103.47	110.53
1	A	269	PHE	N-CA-C	5.42	120.00	113.17
1	B	339	THR	N-CA-C	5.31	117.07	111.28
1	B	326	GLU	N-CA-C	-5.25	106.72	113.01
1	A	81	ASP	N-CA-C	-5.15	99.83	110.80
1	B	269	PHE	N-CA-C	5.14	119.70	113.38
1	A	137	VAL	N-CA-C	5.06	115.67	110.36
1	A	264	LEU	CA-C-N	5.03	125.30	119.47
1	A	264	LEU	C-N-CA	5.03	125.30	119.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	129	LEU	N-CA-C	-5.01	104.91	111.02

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	2700	0	2653	188	0
1	B	2637	0	2598	197	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	15	0	15	3	0
3	B	15	0	15	5	0
4	A	13	0	5	0	0
4	B	13	0	5	0	0
5	A	240	0	0	90	0
5	B	191	0	0	82	0
All	All	5826	0	5291	383	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 36.

All (383) 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:156:LEU:HD13	1:A:174:LEU:HD12	1.23	1.09
1:A:241:LYS:HA	1:A:241:LYS:HE2	1.46	0.97
1:A:24:ILE:HG13	5:A:840:HOH:O	1.63	0.97
1:B:151:LYS:HE2	1:B:151:LYS:HA	1.52	0.92
1:B:77:TYR:HB2	5:B:851:HOH:O	1.70	0.91
1:A:170:ALA:O	1:A:174:LEU:HD23	1.70	0.89
1:B:215:VAL:HG21	5:B:841:HOH:O	1.73	0.89
1:B:24:ILE:H	1:B:69:ASN:HD22	1.19	0.89
1:B:303:GLU:H	1:B:306:HIS:HD2	1.11	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:116:ALA:HB1	5:B:855:HOH:O	1.74	0.86
1:A:227:THR:HG23	5:A:900:HOH:O	1.75	0.86
1:A:33:LEU:HA	5:A:781:HOH:O	1.76	0.85
1:B:149:MET:HE1	1:B:177:SER:HB2	1.58	0.85
1:A:327:LYS:HE3	1:A:327:LYS:HA	1.59	0.85
1:A:80:GLU:OE2	1:A:80:GLU:HA	1.75	0.84
1:B:45:THR:HA	5:B:851:HOH:O	1.76	0.84
1:B:125:THR:HG23	1:B:128:TYR:H	1.43	0.82
1:B:73:THR:HB	5:B:826:HOH:O	1.79	0.82
1:A:156:LEU:HD13	1:A:174:LEU:CD1	2.08	0.82
1:A:70:VAL:HG11	5:A:941:HOH:O	1.78	0.81
1:B:151:LYS:HA	1:B:151:LYS:CE	2.10	0.81
1:A:145:LEU:HG	1:A:149:MET:HE2	1.64	0.80
1:A:330:SER:HB2	1:A:333:SER:OG	1.83	0.79
1:B:126:PRO:O	1:B:129:LEU:HB3	1.82	0.79
1:B:262:ILE:HD13	1:B:262:ILE:H	1.49	0.78
1:B:213:ILE:HG13	5:B:877:HOH:O	1.82	0.77
1:A:110:VAL:HG13	5:A:891:HOH:O	1.84	0.77
1:B:73:THR:HG22	1:B:75:THR:HG23	1.67	0.77
1:A:33:LEU:HD23	5:A:781:HOH:O	1.84	0.77
1:A:157:ILE:HD11	5:A:941:HOH:O	1.85	0.77
1:A:125:THR:HG23	1:A:128:TYR:H	1.50	0.77
1:A:54:GLU:CD	1:A:54:GLU:H	1.94	0.76
1:A:82:LYS:HA	1:A:82:LYS:HE2	1.67	0.75
1:A:132:LYS:HB2	5:A:784:HOH:O	1.86	0.75
1:B:217:CYS:HB2	5:B:864:HOH:O	1.86	0.75
1:B:159:GLU:HA	5:B:829:HOH:O	1.87	0.75
1:A:80:GLU:CD	1:A:81:ASP:H	1.94	0.74
1:B:370:PRO:O	1:B:371:ASP:HB2	1.87	0.74
1:B:229:LYS:O	1:B:233:GLU:HG3	1.88	0.73
1:B:227:THR:HB	5:B:841:HOH:O	1.89	0.72
1:B:125:THR:HG22	1:B:166:GLU:OE2	1.89	0.72
1:B:136:GLU:HB2	5:B:839:HOH:O	1.89	0.72
1:B:303:GLU:H	1:B:306:HIS:CD2	2.01	0.72
1:B:308:ARG:HG3	5:B:853:HOH:O	1.89	0.72
1:A:332:GLY:HA3	5:A:844:HOH:O	1.90	0.71
1:A:210:ALA:N	5:A:852:HOH:O	2.23	0.71
1:A:36:ARG:HD2	5:A:781:HOH:O	1.90	0.71
1:A:82:LYS:HB2	5:A:932:HOH:O	1.90	0.70
1:B:137:VAL:HG11	1:B:169:TRP:CE3	2.27	0.70
1:B:340:LYS:HB3	5:B:825:HOH:O	1.92	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:128:TYR:CD2	1:B:166:GLU:HB2	2.26	0.70
1:B:24:ILE:H	1:B:69:ASN:ND2	1.89	0.70
1:B:123:SER:HA	1:B:159:GLU:O	1.90	0.70
1:A:132:LYS:HE2	5:A:784:HOH:O	1.92	0.69
1:A:257:ASN:C	1:A:257:ASN:HD22	1.97	0.69
1:B:168:VAL:O	1:B:172:GLU:HG3	1.91	0.69
1:A:218:HIS:HD2	5:A:707:HOH:O	1.76	0.69
1:B:299:CYS:SG	5:B:864:HOH:O	2.50	0.69
1:A:206:VAL:HA	5:A:852:HOH:O	1.91	0.69
1:A:163:HIS:HB3	5:A:930:HOH:O	1.93	0.68
1:A:130:SER:HB2	5:A:784:HOH:O	1.92	0.68
1:B:203:VAL:HG22	5:B:830:HOH:O	1.93	0.68
1:A:100:ASN:HD21	1:A:144:GLN:HE21	1.42	0.68
1:A:61:ARG:HG2	5:A:891:HOH:O	1.94	0.67
1:A:257:ASN:HD21	1:A:259:GLN:HB2	1.59	0.67
1:B:164:VAL:O	1:B:168:VAL:HG23	1.95	0.67
1:A:73:THR:HG23	5:A:893:HOH:O	1.95	0.67
1:B:25:GLY:HA2	5:B:880:HOH:O	1.94	0.66
1:A:165:GLU:HB2	5:A:930:HOH:O	1.96	0.66
1:B:69:ASN:HD21	1:B:318:ARG:HH12	1.43	0.66
1:B:128:TYR:HA	1:B:131:ALA:O	1.95	0.66
1:A:168:VAL:HA	5:A:909:HOH:O	1.95	0.66
1:A:257:ASN:ND2	1:A:259:GLN:H	1.93	0.66
1:A:137:VAL:HG11	1:A:169:TRP:CE3	2.31	0.66
1:A:314:LEU:O	1:A:318:ARG:HG3	1.95	0.66
1:A:49:ALA:HB2	5:A:914:HOH:O	1.95	0.65
1:A:333:SER:HA	1:A:347:ALA:HB1	1.78	0.65
1:A:245:MET:HE3	1:A:295:TYR:CE2	2.30	0.65
1:B:137:VAL:HG13	1:B:138:LYS:N	2.10	0.65
1:B:184:THR:OG1	5:B:829:HOH:O	2.15	0.65
1:A:137:VAL:HG11	1:A:169:TRP:HE3	1.62	0.64
1:A:331:TRP:HE3	1:A:331:TRP:H	1.46	0.64
1:A:60:HIS:HB3	1:A:110:VAL:HG11	1.80	0.64
1:B:170:ALA:O	1:B:174:LEU:HG	1.98	0.64
1:A:42:GLY:HA2	5:B:776:HOH:O	1.98	0.64
1:A:179:LYS:HD2	5:A:850:HOH:O	1.98	0.64
1:B:171:VAL:HG21	5:B:860:HOH:O	1.97	0.63
1:B:216:ASN:ND2	5:B:864:HOH:O	2.30	0.63
1:B:230:LEU:HD13	5:B:889:HOH:O	1.99	0.63
1:B:152:ASN:HD22	1:B:179:LYS:NZ	1.97	0.63
1:B:259:GLN:O	1:B:262:ILE:HD11	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:145:LEU:O	1:B:149:MET:HB2	1.98	0.63
1:A:196:VAL:HG11	5:A:934:HOH:O	1.99	0.62
1:A:162:GLU:O	1:A:192:ASP:HB2	1.99	0.62
1:B:315:ALA:HB1	5:B:842:HOH:O	1.99	0.62
1:B:46:PRO:HD3	5:B:851:HOH:O	1.99	0.61
1:A:210:ALA:HB2	5:A:912:HOH:O	1.98	0.61
1:A:169:TRP:HB3	5:A:939:HOH:O	2.00	0.61
1:B:71:MET:HG2	5:B:855:HOH:O	1.99	0.61
1:A:137:VAL:HG12	5:A:783:HOH:O	1.99	0.61
1:A:11:LYS:HE2	5:A:876:HOH:O	2.00	0.60
1:A:119:ALA:HA	5:A:866:HOH:O	2.01	0.60
1:A:331:TRP:HB3	1:A:349:LYS:HD2	1.82	0.60
1:B:152:ASN:HD22	1:B:179:LYS:HZ1	1.48	0.60
1:A:153:VAL:HB	5:A:866:HOH:O	2.01	0.60
1:B:331:TRP:HB3	1:B:349:LYS:HA	1.83	0.60
1:A:147:VAL:HG23	5:A:851:HOH:O	2.01	0.60
1:A:304:PRO:HD2	5:B:890:HOH:O	2.01	0.60
1:A:25:GLY:N	5:A:896:HOH:O	2.35	0.60
1:A:164:VAL:HG11	5:A:934:HOH:O	2.02	0.59
1:B:245:MET:HE3	1:B:295:TYR:CE1	2.37	0.59
1:B:76:PHE:HB3	5:B:821:HOH:O	2.02	0.59
1:B:138:LYS:HB3	5:B:886:HOH:O	2.01	0.59
1:A:138:LYS:HG2	5:A:939:HOH:O	2.01	0.59
1:A:320:PHE:HD1	5:A:857:HOH:O	1.84	0.59
1:B:352:TRP:HB2	5:B:813:HOH:O	2.03	0.58
1:A:180:PRO:HB3	5:A:864:HOH:O	2.02	0.58
1:B:138:LYS:HE2	1:B:169:TRP:HB3	1.84	0.58
1:B:210:ALA:HB2	5:B:860:HOH:O	2.03	0.58
1:B:241:LYS:NZ	1:B:241:LYS:HB3	2.19	0.58
1:B:210:ALA:HA	5:B:763:HOH:O	2.03	0.58
1:A:341:PRO:HG3	1:A:344:ARG:HH22	1.67	0.57
1:A:138:LYS:N	5:A:780:HOH:O	2.30	0.57
1:A:73:THR:O	1:A:75:THR:N	2.36	0.57
1:A:232:LYS:O	1:A:236:GLU:HG3	2.05	0.57
1:A:245:MET:HE3	1:A:295:TYR:CZ	2.40	0.56
1:A:189:PRO:HA	5:A:900:HOH:O	2.05	0.56
1:A:349:LYS:HG3	5:A:872:HOH:O	2.05	0.56
1:A:82:LYS:HE2	1:A:82:LYS:CA	2.35	0.56
1:B:181:VAL:HB	5:B:763:HOH:O	2.04	0.56
1:A:325:SER:O	1:A:329:GLY:N	2.39	0.56
1:A:341:PRO:HG3	1:A:344:ARG:NH2	2.21	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:119:ALA:HB1	5:A:923:HOH:O	2.05	0.56
1:A:315:ALA:HB3	1:A:316:PRO:HD3	1.87	0.56
1:A:50:VAL:HG11	5:A:865:HOH:O	2.05	0.56
1:B:245:MET:HG3	1:B:295:TYR:CD1	2.41	0.56
1:A:47:GLU:HB2	5:A:901:HOH:O	2.04	0.56
1:A:211:SER:HB2	5:A:864:HOH:O	2.04	0.55
1:B:152:ASN:ND2	1:B:179:LYS:NZ	2.53	0.55
1:B:79:SER:CB	1:B:144:GLN:HG2	2.37	0.55
1:B:149:MET:CE	1:B:177:SER:HB2	2.33	0.55
1:B:338:HIS:ND1	5:B:776:HOH:O	2.33	0.55
1:B:343:VAL:N	5:B:825:HOH:O	2.28	0.55
1:A:137:VAL:HG13	1:A:138:LYS:N	2.21	0.55
1:B:137:VAL:HG11	1:B:169:TRP:HE3	1.71	0.55
1:A:36:ARG:HB2	5:A:781:HOH:O	2.05	0.55
1:A:11:LYS:HB3	5:A:876:HOH:O	2.06	0.55
1:A:203:VAL:O	1:A:206:VAL:HG22	2.07	0.55
1:A:157:ILE:HG13	5:A:923:HOH:O	2.05	0.55
1:B:137:VAL:HG13	1:B:138:LYS:H	1.72	0.54
1:A:80:GLU:OE2	1:A:80:GLU:CA	2.52	0.54
1:B:371:ASP:HA	5:B:820:HOH:O	2.07	0.54
1:B:127:SER:HA	1:B:132:LYS:HE2	1.89	0.54
1:B:240:LEU:HD12	5:B:830:HOH:O	2.08	0.54
1:B:261:PHE:HD1	5:B:847:HOH:O	1.91	0.54
1:B:276:ALA:O	1:B:306:HIS:HE1	1.90	0.54
1:B:138:LYS:NZ	5:B:852:HOH:O	2.41	0.54
1:B:147:VAL:HG12	5:B:844:HOH:O	2.07	0.54
1:B:338:HIS:HD2	1:B:340:LYS:H	1.56	0.54
1:A:125:THR:HG21	1:A:137:VAL:HG23	1.90	0.54
1:B:342:TRP:N	5:B:825:HOH:O	2.41	0.54
5:A:917:HOH:O	1:B:40:LYS:HE3	2.09	0.53
1:A:175:ILE:HG21	1:A:209:GLY:HA3	1.90	0.53
1:A:345:ALA:HB2	5:A:764:HOH:O	2.09	0.53
1:B:124:GLN:HA	1:B:161:PHE:CE1	2.44	0.53
1:B:128:TYR:CE2	1:B:166:GLU:HB2	2.44	0.53
1:B:139:LYS:HA	1:B:139:LYS:HZ2	1.73	0.53
1:A:181:VAL:HG21	5:A:863:HOH:O	2.08	0.53
1:A:187:ILE:HD12	5:A:908:HOH:O	2.08	0.52
1:A:353:GLU:HB2	5:A:793:HOH:O	2.07	0.52
1:A:262:ILE:HG21	5:B:823:HOH:O	2.08	0.52
1:A:338:HIS:CD2	1:A:343:VAL:HG11	2.44	0.52
1:B:159:GLU:HG3	5:B:829:HOH:O	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:183:ALA:O	1:B:213:ILE:HA	2.09	0.52
1:A:97:GLN:O	1:A:101:GLU:HG3	2.09	0.52
1:A:321:LEU:HD11	1:A:331:TRP:HH2	1.75	0.52
1:B:157:ILE:HG22	1:B:159:GLU:HB2	1.91	0.52
1:A:76:PHE:HB3	5:A:884:HOH:O	2.09	0.52
1:A:257:ASN:C	1:A:257:ASN:ND2	2.68	0.52
1:A:132:LYS:HG2	1:A:136:GLU:HG2	1.93	0.51
1:A:231:MET:SD	5:A:853:HOH:O	2.59	0.51
1:B:218:HIS:HD2	5:B:717:HOH:O	1.94	0.51
1:B:143:GLN:O	1:B:147:VAL:HG23	2.11	0.51
1:B:172:GLU:HB2	5:B:852:HOH:O	2.09	0.51
1:A:54:GLU:CD	1:A:54:GLU:N	2.68	0.51
1:A:100:ASN:ND2	1:A:144:GLN:HE21	2.07	0.51
1:A:201:ALA:HA	5:A:934:HOH:O	2.10	0.51
1:B:78:ALA:HB3	5:B:862:HOH:O	2.10	0.51
1:B:172:GLU:HG2	5:B:881:HOH:O	2.11	0.51
1:B:160:TYR:CE2	3:B:602:CBH:H102	2.46	0.51
1:A:160:TYR:HB2	5:A:858:HOH:O	2.11	0.51
1:B:214:GLY:HA3	1:B:245:MET:O	2.11	0.50
1:A:171:VAL:HG22	5:A:912:HOH:O	2.11	0.50
1:A:204:ARG:HD3	5:A:934:HOH:O	2.11	0.50
1:B:79:SER:HB2	1:B:144:GLN:HG2	1.93	0.50
1:A:47:GLU:HG3	1:A:51:GLU:OE2	2.10	0.50
1:A:203:VAL:HG23	5:A:883:HOH:O	2.11	0.50
1:B:124:GLN:NE2	1:B:162:GLU:H	2.08	0.50
1:B:308:ARG:HD2	5:B:707:HOH:O	2.10	0.50
1:A:80:GLU:CD	1:A:81:ASP:N	2.68	0.50
1:A:136:GLU:O	1:A:139:LYS:HB2	2.11	0.50
1:B:73:THR:O	1:B:75:THR:N	2.44	0.50
1:A:135:THR:C	5:A:780:HOH:O	2.55	0.49
1:B:134:GLU:OE1	1:B:138:LYS:HE3	2.10	0.49
1:B:139:LYS:O	1:B:143:GLN:HG3	2.12	0.49
1:B:349:LYS:HA	5:B:813:HOH:O	2.11	0.49
1:A:250:ALA:HB2	1:A:302:PHE:CD1	2.47	0.49
1:A:46:PRO:HG3	1:A:78:ALA:HB2	1.95	0.49
1:A:72:GLN:HE22	1:A:247:GLN:HE22	1.58	0.49
1:A:198:PRO:HG3	5:A:900:HOH:O	2.12	0.49
1:B:11:LYS:HE2	5:B:866:HOH:O	2.12	0.49
1:B:224:SER:HA	5:B:841:HOH:O	2.13	0.49
1:B:354:ASN:N	5:B:824:HOH:O	2.42	0.49
1:B:134:GLU:HG2	1:B:138:LYS:HD2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:141:PHE:HB3	5:B:833:HOH:O	2.12	0.49
1:B:328:HIS:CG	1:B:329:GLY:H	2.31	0.49
1:B:151:LYS:HD2	5:B:836:HOH:O	2.11	0.49
1:A:15:GLU:C	5:A:876:HOH:O	2.55	0.49
1:A:153:VAL:O	1:A:179:LYS:NZ	2.43	0.49
1:B:126:PRO:C	1:B:129:LEU:HB3	2.38	0.49
1:B:159:GLU:HG3	1:B:216:ASN:ND2	2.27	0.48
1:B:131:ALA:HB3	5:B:786:HOH:O	2.11	0.48
1:A:123:SER:HA	1:A:159:GLU:O	2.13	0.48
1:A:137:VAL:HG13	1:A:138:LYS:H	1.78	0.48
1:A:181:VAL:HG11	5:A:863:HOH:O	2.12	0.48
1:B:276:ALA:HB1	1:B:280:ASP:HB2	1.95	0.48
1:B:152:ASN:ND2	1:B:179:LYS:HZ1	2.08	0.48
1:B:235:LEU:HD12	5:B:830:HOH:O	2.13	0.48
1:A:177:SER:HB2	5:A:892:HOH:O	2.12	0.48
1:A:202:ALA:O	1:A:206:VAL:HG13	2.14	0.48
1:B:349:LYS:HE3	5:B:882:HOH:O	2.13	0.48
3:B:602:CBH:O13	3:B:602:CBH:H172	2.14	0.48
1:A:126:PRO:HD2	5:A:843:HOH:O	2.14	0.48
1:A:51:GLU:HG3	5:A:901:HOH:O	2.13	0.48
1:A:241:LYS:HA	1:A:241:LYS:CE	2.29	0.48
1:B:108:ARG:HA	1:B:118:VAL:HG21	1.95	0.48
1:B:348:ARG:NH2	5:B:879:HOH:O	2.46	0.47
1:B:340:LYS:HD2	1:B:342:TRP:CZ2	2.49	0.47
1:A:308:ARG:NH1	5:A:890:HOH:O	2.40	0.47
1:B:151:LYS:NZ	5:B:856:HOH:O	2.48	0.47
1:B:160:TYR:OH	3:B:602:CBH:H222	2.14	0.47
1:B:346:ARG:HG2	1:B:351:TYR:CZ	2.49	0.47
1:B:370:PRO:O	1:B:371:ASP:CB	2.59	0.47
1:B:349:LYS:NZ	1:B:349:LYS:HB3	2.29	0.47
1:A:72:GLN:NE2	1:A:247:GLN:HE22	2.13	0.47
1:A:179:LYS:HB2	5:A:850:HOH:O	2.15	0.47
1:B:137:VAL:CG1	1:B:138:LYS:N	2.76	0.47
1:B:54:GLU:HB3	5:B:781:HOH:O	2.14	0.47
1:A:326:GLU:HB3	5:A:885:HOH:O	2.15	0.47
1:B:133:SER:N	5:B:839:HOH:O	2.48	0.47
1:A:65:ARG:O	1:A:323:PRO:HG2	2.14	0.47
1:A:165:GLU:CD	1:A:204:ARG:HH12	2.23	0.47
1:B:205:LEU:HB3	5:B:860:HOH:O	2.14	0.47
1:B:159:GLU:CA	5:B:829:HOH:O	2.57	0.47
1:B:331:TRP:HE3	5:B:813:HOH:O	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:13:ILE:HG23	1:B:14:LEU:N	2.29	0.47
1:A:100:ASN:HD21	1:A:144:GLN:NE2	2.12	0.46
1:B:229:LYS:HB3	5:B:889:HOH:O	2.14	0.46
1:B:349:LYS:HG2	1:B:353:GLU:OE1	2.15	0.46
1:B:76:PHE:CE1	3:B:602:CBH:H191	2.50	0.46
1:A:311:ALA:HB2	5:A:840:HOH:O	2.14	0.46
1:B:101:GLU:N	5:B:812:HOH:O	2.49	0.46
1:B:69:ASN:HD21	1:B:318:ARG:NH1	2.10	0.46
1:A:165:GLU:OE1	1:A:165:GLU:N	2.46	0.46
1:B:127:SER:HB3	1:B:132:LYS:HE3	1.97	0.46
1:B:267:PHE:HZ	3:B:602:CBH:O24	1.98	0.46
1:A:98:GLU:HB3	5:A:849:HOH:O	2.15	0.46
5:A:913:HOH:O	1:B:54:GLU:HB2	2.16	0.46
1:B:45:THR:OG1	1:B:47:GLU:OE2	2.33	0.46
1:B:338:HIS:CD2	1:B:340:LYS:H	2.33	0.46
1:A:308:ARG:CZ	1:A:328:HIS:HB2	2.46	0.46
1:B:350:GLU:C	5:B:824:HOH:O	2.59	0.46
1:B:47:GLU:HB2	1:B:51:GLU:OE2	2.15	0.45
1:B:77:TYR:HE2	5:B:845:HOH:O	1.99	0.45
1:A:186:ALA:N	5:A:868:HOH:O	2.48	0.45
1:B:29:PHE:CD2	1:B:59:LEU:HD23	2.51	0.45
1:B:250:ALA:HB2	1:B:302:PHE:CD1	2.51	0.45
1:A:229:LYS:O	1:A:233:GLU:HG3	2.16	0.45
1:A:311:ALA:HB1	1:A:322:PRO:HD3	1.98	0.45
1:A:152:ASN:HA	5:A:897:HOH:O	2.14	0.45
1:A:257:ASN:HD22	1:A:259:GLN:H	1.63	0.45
1:B:262:ILE:HD13	5:B:847:HOH:O	2.16	0.45
1:B:53:PRO:HB3	5:B:857:HOH:O	2.17	0.45
1:A:46:PRO:HD3	1:A:76:PHE:O	2.16	0.45
1:B:125:THR:CG2	1:B:127:SER:HB2	2.46	0.45
1:A:145:LEU:HD13	1:A:174:LEU:HD13	1.99	0.45
1:B:134:GLU:O	1:B:137:VAL:HG12	2.16	0.45
1:A:77:TYR:HE1	5:A:928:HOH:O	1.99	0.45
1:B:75:THR:O	1:B:77:TYR:O	2.35	0.45
1:B:162:GLU:O	1:B:192:ASP:HB2	2.17	0.45
1:B:282:GLN:O	1:B:313:GLU:HG2	2.16	0.44
1:B:353:GLU:HG2	5:B:824:HOH:O	2.17	0.44
1:A:155:PHE:HB2	1:A:180:PRO:O	2.17	0.44
1:A:305:TYR:CE2	1:B:35:LYS:HD2	2.53	0.44
1:B:146:GLU:HA	1:B:149:MET:HB2	1.99	0.44
1:A:16:ARG:NH2	1:A:115:ASP:OD2	2.39	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:216:ASN:HA	1:B:247:GLN:O	2.18	0.44
1:B:252:HIS:HE1	1:B:280:ASP:OD2	2.00	0.44
1:B:139:LYS:HA	1:B:139:LYS:NZ	2.31	0.44
1:B:151:LYS:HE3	5:B:818:HOH:O	2.17	0.44
1:A:201:ALA:O	1:A:205:LEU:HG	2.18	0.44
1:A:133:SER:HB2	5:A:771:HOH:O	2.17	0.44
1:A:331:TRP:CE3	1:A:331:TRP:N	2.86	0.44
1:B:76:PHE:O	1:B:77:TYR:HB2	2.18	0.44
1:B:227:THR:O	1:B:231:MET:HG3	2.18	0.44
1:B:348:ARG:HD3	5:B:879:HOH:O	2.18	0.44
1:A:80:GLU:O	1:A:81:ASP:HB3	2.18	0.44
1:A:308:ARG:HD2	5:A:719:HOH:O	2.17	0.44
1:B:162:GLU:C	1:B:163:HIS:HD2	2.26	0.44
1:A:136:GLU:HB2	5:A:771:HOH:O	2.16	0.43
1:B:78:ALA:HB2	5:B:814:HOH:O	2.18	0.43
1:B:137:VAL:CG1	1:B:138:LYS:H	2.31	0.43
1:A:214:GLY:N	5:A:853:HOH:O	2.50	0.43
1:A:262:ILE:HD11	3:A:601:CBH:H221	1.99	0.43
1:B:124:GLN:HG2	5:B:845:HOH:O	2.18	0.43
1:A:235:LEU:HD23	5:A:883:HOH:O	2.18	0.43
1:B:289:TYR:CE2	1:B:317:GLU:HG2	2.52	0.43
1:A:181:VAL:O	1:A:210:ALA:HA	2.18	0.43
1:A:332:GLY:O	1:A:347:ALA:HA	2.18	0.43
1:B:273:PRO:HG3	1:B:361:ARG:NH2	2.32	0.43
1:A:30:VAL:HG22	3:A:601:CBH:O13	2.17	0.43
1:A:163:HIS:CE1	1:A:193:LEU:HD12	2.53	0.43
1:A:50:VAL:HG21	5:A:865:HOH:O	2.19	0.43
1:A:129:LEU:C	1:A:131:ALA:H	2.27	0.43
1:A:245:MET:HG3	1:A:295:TYR:CD2	2.53	0.43
1:A:340:LYS:HA	1:A:341:PRO:HD3	1.92	0.43
1:B:124:GLN:NE2	5:B:778:HOH:O	2.51	0.43
1:B:138:LYS:O	1:B:142:LEU:HB2	2.19	0.43
1:B:342:TRP:CD1	5:B:825:HOH:O	2.72	0.43
1:A:35:LYS:HE2	5:A:775:HOH:O	2.18	0.43
1:B:149:MET:HE3	5:B:784:HOH:O	2.19	0.43
1:A:174:LEU:HB2	5:A:863:HOH:O	2.18	0.43
1:A:202:ALA:HB3	5:A:883:HOH:O	2.19	0.43
1:A:273:PRO:HA	1:B:273:PRO:HA	2.00	0.43
1:B:73:THR:CG2	1:B:75:THR:HG23	2.45	0.42
1:A:73:THR:N	5:A:893:HOH:O	2.53	0.42
1:A:160:TYR:OH	3:A:601:CBH:H222	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:203:VAL:CG1	1:A:207:LYS:HE3	2.48	0.42
1:B:129:LEU:C	1:B:131:ALA:H	2.28	0.42
1:B:262:ILE:HD13	1:B:262:ILE:N	2.24	0.42
1:A:82:LYS:HA	1:A:82:LYS:CE	2.43	0.42
1:A:96:GLY:N	5:A:849:HOH:O	2.53	0.42
1:B:22:ILE:HD11	1:B:289:TYR:CE2	2.55	0.42
1:B:31:PHE:O	1:B:35:LYS:HG2	2.19	0.42
1:A:76:PHE:O	1:A:77:TYR:HB2	2.20	0.42
1:B:331:TRP:HB3	1:B:349:LYS:CA	2.49	0.42
1:A:33:LEU:HD12	1:A:74:PHE:CZ	2.54	0.42
1:A:161:PHE:HZ	5:A:848:HOH:O	2.02	0.42
1:A:331:TRP:C	1:A:333:SER:H	2.27	0.42
1:B:15:GLU:OE1	1:B:15:GLU:N	2.50	0.42
1:B:261:PHE:N	5:B:847:HOH:O	2.53	0.42
1:A:13:ILE:HG23	1:A:14:LEU:N	2.35	0.41
1:A:214:GLY:HA3	1:A:245:MET:O	2.19	0.41
1:B:39:VAL:HG12	1:B:40:LYS:N	2.35	0.41
1:B:232:LYS:HD2	1:B:244:LEU:CD1	2.50	0.41
1:A:175:ILE:HG23	5:A:863:HOH:O	2.21	0.41
1:B:241:LYS:HB3	1:B:241:LYS:HZ3	1.84	0.41
1:A:342:TRP:HA	1:A:342:TRP:CE3	2.54	0.41
1:A:164:VAL:HG23	1:A:192:ASP:OD1	2.21	0.41
1:B:232:LYS:HD2	1:B:244:LEU:HD11	2.02	0.41
1:B:30:VAL:HG11	5:B:821:HOH:O	2.19	0.41
1:A:220:ASP:HB3	1:A:251:TYR:O	2.21	0.41
1:A:346:ARG:HG2	1:A:351:TYR:CZ	2.56	0.41
1:B:349:LYS:CG	1:B:353:GLU:OE1	2.68	0.41
1:A:70:VAL:O	1:A:71:MET:HE2	2.21	0.41
1:A:164:VAL:HG21	5:A:934:HOH:O	2.20	0.41
1:A:273:PRO:HB2	1:B:359:SER:HA	2.03	0.41
1:B:77:TYR:HA	5:B:858:HOH:O	2.21	0.41
1:B:141:PHE:CE1	1:B:170:ALA:HB2	2.56	0.41
1:B:151:LYS:HB2	5:B:844:HOH:O	2.20	0.41
1:A:202:ALA:HB2	1:A:231:MET:HB3	2.03	0.40
1:B:160:TYR:OH	1:B:218:HIS:HE1	2.04	0.40
1:B:175:ILE:HG21	1:B:209:GLY:HA3	2.03	0.40
1:B:40:LYS:O	1:B:43:PRO:HD2	2.21	0.40
1:B:65:ARG:HG2	1:B:324:ALA:HB2	2.02	0.40
1:B:132:LYS:O	1:B:133:SER:O	2.38	0.40
1:B:342:TRP:CG	5:B:825:HOH:O	2.74	0.40
1:A:11:LYS:N	5:A:921:HOH:O	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:165:GLU:HA	5:A:910:HOH:O	2.21	0.40
1:B:262:ILE:HA	1:B:267:PHE:CG	2.57	0.40
1:B:308:ARG:NE	5:B:853:HOH:O	2.51	0.40
1:B:53:PRO:HD3	5:B:857:HOH:O	2.21	0.40
1:B:346:ARG:HG2	1:B:351:TYR:CE1	2.57	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	344/406 (85%)	323 (94%)	17 (5%)	4 (1%)	10	4
1	B	336/406 (83%)	313 (93%)	21 (6%)	2 (1%)	21	13
All	All	680/812 (84%)	636 (94%)	38 (6%)	6 (1%)	14	7

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	133	SER
1	A	133	SER
1	A	329	GLY
1	B	132	LYS
1	A	331	TRP
1	A	74	PHE

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	275/323 (85%)	260 (94%)	15 (6%)	19	12
1	B	268/323 (83%)	252 (94%)	16 (6%)	17	10
All	All	543/646 (84%)	512 (94%)	31 (6%)	18	11

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	54	GLU
1	A	59	LEU
1	A	80	GLU
1	A	82	LYS
1	A	98	GLU
1	A	117	LEU
1	A	215	VAL
1	A	240	LEU
1	A	241	LYS
1	A	257	ASN
1	A	261	PHE
1	A	268	PRO
1	A	295	TYR
1	A	327	LYS
1	A	335	LEU
1	B	47	GLU
1	B	54	GLU
1	B	136	GLU
1	B	139	LYS
1	B	151	LYS
1	B	165	GLU
1	B	230	LEU
1	B	235	LEU
1	B	259	GLN
1	B	261	PHE
1	B	262	ILE
1	B	268	PRO
1	B	335	LEU
1	B	348	ARG
1	B	349	LYS
1	B	371	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	GLN
1	A	144	GLN
1	A	163	HIS
1	A	218	HIS
1	A	257	ASN
1	A	290	ASN
1	B	18	ASN
1	B	69	ASN
1	B	124	GLN
1	B	152	ASN
1	B	194	HIS
1	B	216	ASN
1	B	218	HIS
1	B	243	HIS
1	B	252	HIS
1	B	259	GLN
1	B	306	HIS
1	B	338	HIS
1	B	354	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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
3	CBH	B	602	2	13,14,14	0.89	0	12,16,16	1.05	0
4	CIT	B	702	-	12,12,12	1.57	2 (16%)	17,17,17	1.20	3 (17%)
4	CIT	A	701	-	12,12,12	1.53	1 (8%)	17,17,17	1.19	3 (17%)
3	CBH	A	601	2	13,14,14	0.88	0	12,16,16	1.03	0

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
3	CBH	B	602	2	-	2/14/14/14	-
4	CIT	B	702	-	-	8/16/16/16	-
4	CIT	A	701	-	-	8/16/16/16	-
3	CBH	A	601	2	-	2/14/14/14	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	702	CIT	O7-C3	-3.32	1.36	1.43
4	A	701	CIT	O7-C3	-3.16	1.37	1.43
4	B	702	CIT	C3-C6	2.03	1.55	1.53

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	702	CIT	O6-C6-C3	2.59	118.11	113.14
4	A	701	CIT	O6-C6-C3	2.44	117.81	113.14
4	B	702	CIT	O3-C5-C4	-2.26	116.55	122.95
4	A	701	CIT	O3-C5-C4	-2.24	116.60	122.95
4	A	701	CIT	O1-C1-C2	-2.19	116.76	122.95
4	B	702	CIT	O5-C6-C3	-2.01	118.19	122.09

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	701	CIT	C2-C3-C6-O5
4	A	701	CIT	C2-C3-C6-O6
4	A	701	CIT	O7-C3-C6-O5
4	A	701	CIT	O7-C3-C6-O6
4	B	702	CIT	O7-C3-C6-O5
4	B	702	CIT	C2-C3-C6-O5
4	B	702	CIT	C4-C3-C6-O6
4	B	702	CIT	O7-C3-C6-O6
4	B	702	CIT	C2-C3-C6-O6
3	B	602	CBH	C21-C22-C23-O25
3	B	602	CBH	C21-C22-C23-O24
4	B	702	CIT	C3-C4-C5-O4
4	B	702	CIT	C4-C3-C6-O5
3	A	601	CBH	C21-C22-C23-O24
4	A	701	CIT	C3-C4-C5-O4
3	A	601	CBH	C21-C22-C23-O25
4	A	701	CIT	C3-C4-C5-O3
4	A	701	CIT	O1-C1-C2-C3
4	B	702	CIT	C3-C4-C5-O3
4	A	701	CIT	O2-C1-C2-C3

There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	602	CBH	5	0
3	A	601	CBH	3	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	348/406 (85%)	-0.05	8 (2%) 61 63	16, 42, 74, 88	0
1	B	340/406 (83%)	-0.02	4 (1%) 76 78	17, 44, 67, 83	0
All	All	688/812 (84%)	-0.03	12 (1%) 69 70	16, 43, 71, 88	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	330	SER	4.8
1	A	329	GLY	4.7
1	B	129	LEU	3.1
1	A	332	GLY	3.0
1	A	331	TRP	2.8
1	B	131	ALA	2.5
1	B	77	TYR	2.5
1	A	131	ALA	2.3
1	A	342	TRP	2.2
1	B	149	MET	2.2
1	A	80	GLU	2.1
1	A	133	SER	2.1

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	CIT	B	702	13/13	0.76	0.11	31,36,38,40	13
3	CBH	B	602	15/15	0.79	0.12	35,37,48,49	15
4	CIT	A	701	13/13	0.84	0.09	22,29,35,35	13
2	ZN	B	502	1/1	0.84	0.07	30,30,30,30	1
3	CBH	A	601	15/15	0.89	0.08	32,35,36,38	0
2	ZN	A	501	1/1	0.94	0.06	24,24,24,24	0

6.5 Other polymers [i](#)

There are no such residues in this entry.