



Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 03:40 am BST

PDB ID : 4MJM
Title : Crystal Structure of the Inosine 5'-monophosphate Dehydrogenase, with a Short Internal Deletion of CBS Domain from Bacillus anthracis str. Ames
Authors : Kim, Y.; Makowska-Grzyska, M.; Gu, M.; Anderson, W.F.; Joachimiak, A.; Center for Structural Genomics of Infectious Diseases (CSGID)
Deposited on : 2013-09-03
Resolution : 2.25 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

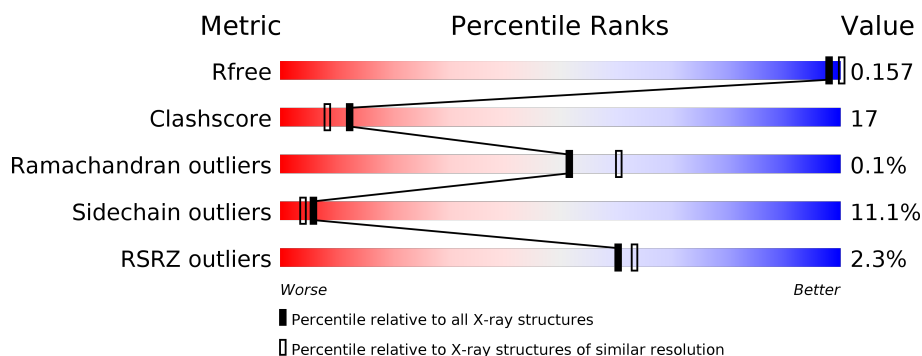
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1377 (2.26-2.26)
Clashscore	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (2.26-2.26)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	385	<div> <div>2%</div> <div> <div></div> <div>59%</div> <div>23%</div> <div>•</div> <div>15%</div> </div> </div>
1	B	385	<div> <div>%</div> <div> <div></div> <div>53%</div> <div>28%</div> <div>•</div> <div>15%</div> </div> </div>
1	C	385	<div> <div>3%</div> <div> <div></div> <div>52%</div> <div>29%</div> <div>•</div> <div>15%</div> </div> </div>
1	D	385	<div> <div>2%</div> <div> <div></div> <div>52%</div> <div>29%</div> <div>•</div> <div>15%</div> </div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10136 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 Inosine-5'-monophosphate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	328	Total	C	N	O	S	0	1	0
			2411	1514	421	463	13			
1	B	328	Total	C	N	O	S	0	0	0
			2408	1514	419	461	14			
1	C	329	Total	C	N	O	S	0	0	0
			2412	1517	419	462	14			
1	D	328	Total	C	N	O	S	0	0	0
			2409	1514	422	460	13			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	EXPRESSION TAG	UNP Q81W29
A	-1	ASN	-	EXPRESSION TAG	UNP Q81W29
A	0	ALA	-	EXPRESSION TAG	UNP Q81W29
A	95	GLY	-	LINKER	UNP Q81W29
B	-2	SER	-	EXPRESSION TAG	UNP Q81W29
B	-1	ASN	-	EXPRESSION TAG	UNP Q81W29
B	0	ALA	-	EXPRESSION TAG	UNP Q81W29
B	200	GLY	-	LINKER	UNP Q81W29
C	-2	SER	-	EXPRESSION TAG	UNP Q81W29
C	-1	ASN	-	EXPRESSION TAG	UNP Q81W29
C	0	ALA	-	EXPRESSION TAG	UNP Q81W29
C	95	GLY	-	LINKER	UNP Q81W29
D	-2	SER	-	EXPRESSION TAG	UNP Q81W29
D	-1	ASN	-	EXPRESSION TAG	UNP Q81W29
D	0	ALA	-	EXPRESSION TAG	UNP Q81W29
D	200	GLY	-	LINKER	UNP Q81W29

- Molecule 2 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).




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

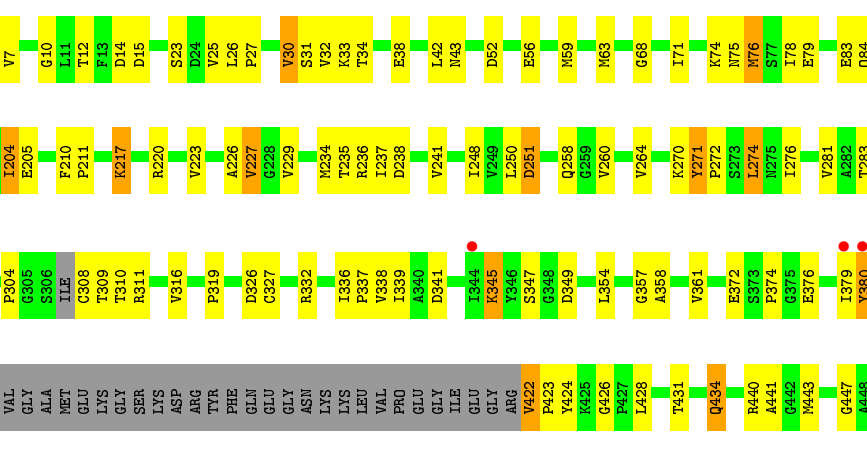
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	113	Total O 113 113	0	0
3	B	106	Total O 106 106	0	0
3	C	108	Total O 108 108	0	0
3	D	137	Total O 137 137	0	0

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

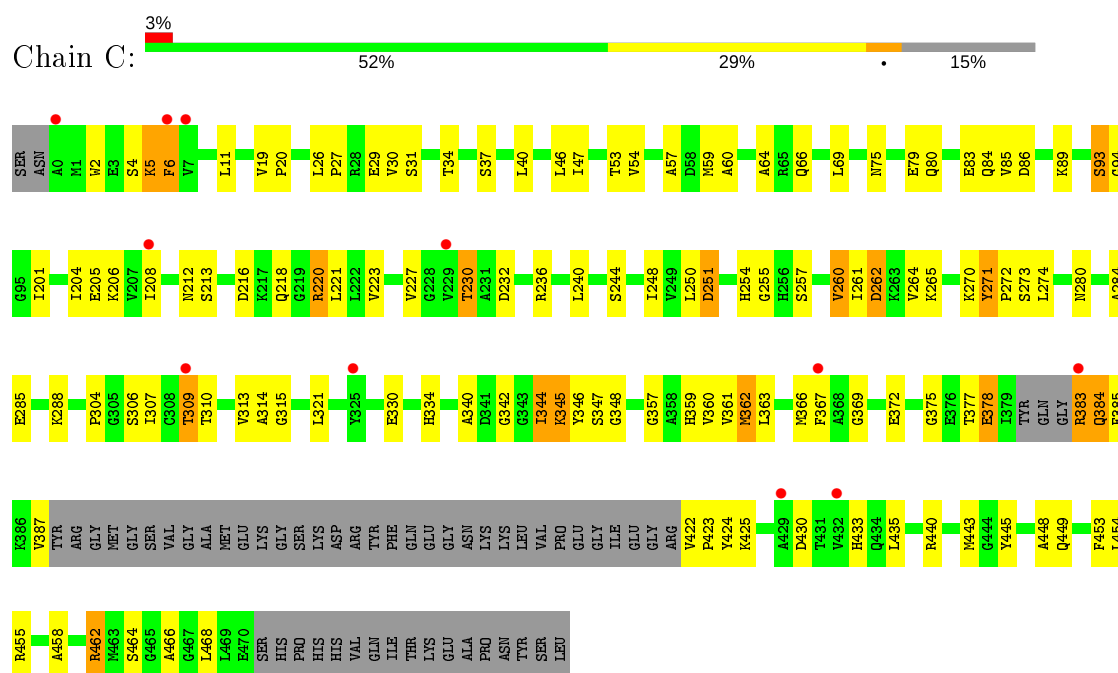
- [illegible]

- Chain B: 

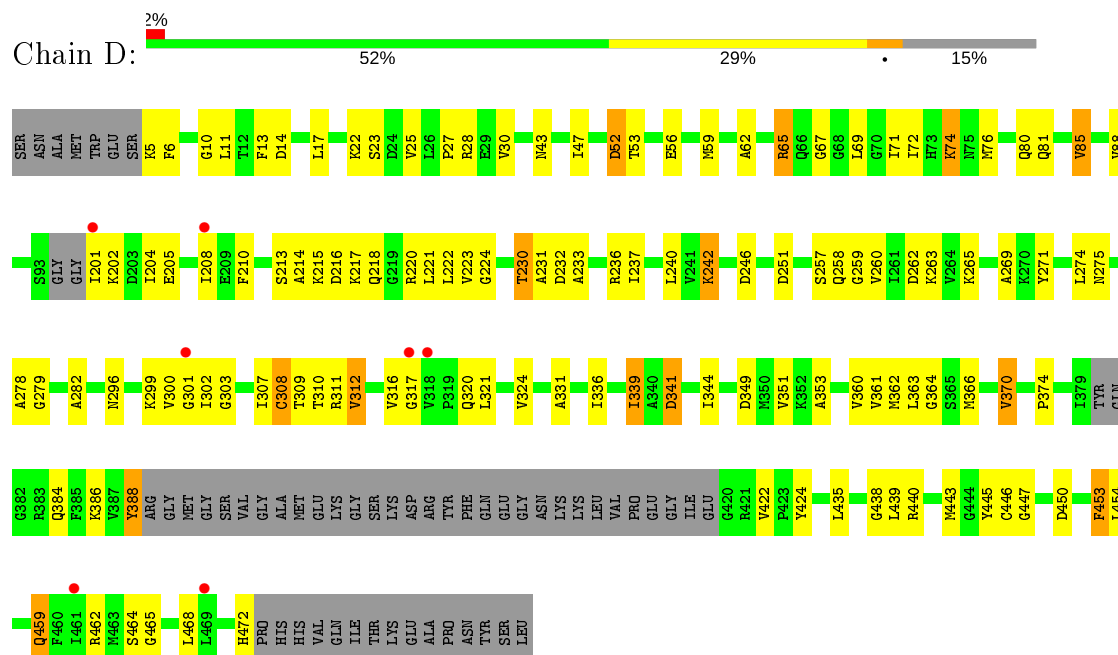


Category	Q459	S464	L468	L469	Q460	S461	L462	L463	Q464	S465	L466	L467	Q468	S469	L470	L471	Q472	S473	L474	L475	Q476	S477	L478	L479	Q480	S481	L482	L483	Q484	S485	L486	L487	Q488	S489	L490	L491	Q492	S493	L494	L495	Q496	S497	L498	L499	Q500	S501	L502	L503	Q504	S505	L506	L507	Q508	S509	L510	L511	Q512	S513	L514	L515	Q516	S517	L518	L519	Q520	S521	L522	L523	Q524	S525	L526	L527	Q528	S529	L530	L531	Q532	S533	L534	L535	Q536	S537	L538	L539	Q540	S541	L542	L543	Q544	S545	L546	L547	Q548	S549	L550	L551	Q552	S553	L554	L555	Q556	S557	L558	L559	Q560	S561	L562	L563	Q564	S565	L566	L567	Q568	S569	L570	L571	Q572	S573	L574	L575	Q576	S577	L578	L579	Q580	S581	L582	L583	Q584	S585	L586	L587	Q588	S589	L590	L591	Q592	S593	L594	L595	Q596	S597	L598	L599	Q600	S601	L602	L603	Q604	S605	L606	L607	Q608	S609	L610	L611	Q612	S613	L614	L615	Q616	S617	L618	L619	Q620	S621	L622	L623	Q624	S625	L626	L627	Q628	S629	L630	L631	Q632	S633	L634	L635	Q636	S637	L638	L639	Q640	S641	L642	L643	Q644	S645	L646	L647	Q648	S649	L650	L651	Q652	S653	L654	L655	Q656	S657	L658	L659	Q660	S661	L662	L663	Q664	S665	L666	L667	Q668	S669	L670	L671	Q672	S673	L674	L675	Q676	S677	L678	L679	Q680	S681	L682	L683	Q684	S685	L686	L687	Q688	S689	L690	L691	Q692	S693	L694	L695	Q696	S697	L698	L699	Q700	S701	L702	L703	Q704	S705	L706	L707	Q708	S709	L710	L711	Q712	S713	L714	L715	Q716	S717	L718	L719	Q720	S721	L722	L723	Q724	S725	L726	L727	Q728	S729	L730	L731	Q732	S733	L734	L735	Q736	S737	L738	L739	Q740	S741	L742	L743	Q744	S745	L746	L747	Q748	S749	L750	L751	Q752	S753	L754	L755	Q756	S757	L758	L759	Q760	S761	L762	L763	Q764	S765	L766	L767	Q768	S769	L770	L771	Q772	S773	L774	L775	Q776	S777	L778	L779	Q780	S781	L782	L783	Q784	S785	L786	L787	Q788	S789	L790	L791	Q792	S793	L794	L795	Q796	S797	L798	L799	Q800	S801	L802	L803	Q804	S805	L806	L807	Q808	S809	L810	L811	Q812	S813	L814	L815	Q816	S817	L818	L819	Q820	S821	L822	L823	Q824	S825	L826	L827	Q828	S829	L830	L831	Q832	S833	L834	L835	Q836	S837	L838	L839	Q840	S841	L842	L843	Q844	S845	L846	L847	Q848	S849	L850	L851	Q852	S853	L854	L855	Q856	S857	L858	L859	Q860	S861	L862	L863	Q864
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- 
- WORLD WIDE
PDB
PROTEIN DATA BANK



• Molecule 1: Inosine-5'-monophosphate dehydrogenase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	84.33Å 84.25Å 84.31Å 110.01° 109.22° 109.19°	Depositor
Resolution (Å)	48.83 – 2.25 48.83 – 2.25	Depositor EDS
% Data completeness (in resolution range)	94.1 (48.83-2.25) 94.0 (48.83-2.25)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.29 (at 2.24Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.206 , 0.232 0.160 , 0.157	Depositor DCC
R_{free} test set	3951 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	40.4	Xtriage
Anisotropy	0.135	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 69.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.22$	Xtriage

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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.

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Property	Value	Source
Estimated twinning fraction	0.077 for -k,-l,h+k+l 0.077 for h+k+l,-h,-k 0.457 for -l,-h,h+k+l 0.457 for -k,h+k+l,-h 0.078 for h+k+l,-l,-h 0.078 for -l,h+k+l,-k 0.078 for -h-k-l,k,h 0.078 for l,k,-h-k-l 0.078 for l,h,k 0.078 for k,l,h 0.078 for k,-h-k-l,l 0.078 for -h-k-l,h,l 0.078 for h,-h-k-l,k 0.078 for h,l,-h-k-l 0.377 for l,-h-k-l,h 0.077 for -h,h+k+l,-l 0.458 for -h-k-l,l,k 0.377 for -h,-l,-k 0.377 for k,h,-h-k-l 0.078 for -h,-k,h+k+l 0.077 for -l,-k,-h 0.377 for h+k+l,-k,-l 0.079 for -k,-h,-l	Xtriage
Reported twinning fraction	0.500 for -h-k-l,l,k	Depositor
Outliers	0 of 79280 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	10136	wwPDB-VP
Average B, all atoms (\AA^2)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.16% of the height of the origin peak. No significant pseudotranslation is detected.*

5 Model quality

5.1 Standard geometry

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

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	0.27	1/2438 (0.0%)	0.46	1/3290 (0.0%)
1	B	0.26	1/2436 (0.0%)	0.47	1/3287 (0.0%)
1	C	0.26	1/2440 (0.0%)	0.46	1/3294 (0.0%)
1	D	0.27	0/2436	0.46	1/3286 (0.0%)
All	All	0.27	3/9750 (0.0%)	0.46	4/13157 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	211	PRO	N-CD	5.31	1.55	1.47
1	C	272	PRO	N-CD	5.29	1.55	1.47
1	B	272	PRO	N-CD	5.13	1.55	1.47

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	303	GLY	C-N-CD	5.99	140.99	128.40
1	B	271	TYR	C-N-CD	5.75	140.47	128.40
1	C	271	TYR	C-N-CD	5.51	139.97	128.40
1	A	210	PHE	C-N-CD	5.38	139.71	128.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	230	THR	Peptide

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	2411	0	2482	86	0
1	B	2408	0	2475	94	0
1	C	2412	0	2487	86	0
1	D	2409	0	2482	86	0
2	A	12	0	18	0	0
2	B	4	0	6	0	0
2	C	4	0	6	0	0
2	D	12	0	18	1	0
3	A	113	0	0	6	0
3	B	106	0	0	18	0
3	C	108	0	0	13	0
3	D	137	0	0	9	0
All	All	10136	0	9974	331	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 17.

All (331) 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:B:281:VAL:HG21	1:B:287:THR:HG23	1.48	0.94
1:B:455:ARG:HD3	3:B:704:HOH:O	1.77	0.83
1:D:76:MET:HB2	1:D:80:GLN:HG3	1.62	0.81
1:A:387:VAL:O	1:A:388:TYR:HB2	1.84	0.76
1:A:470:GLU:OE2	1:B:12:THR:HG21	1.86	0.75
1:D:47:ILE:HG12	1:D:69:LEU:HB3	1.69	0.74
1:D:65:ARG:HD2	1:D:210:PHE:CG	2.23	0.73
1:D:344:ILE:HG23	1:D:349:ASP:HB2	1.71	0.73
1:A:24:ASP:N	1:A:24:ASP:OD1	2.23	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:89:LYS:HE2	3:C:662:HOH:O	1.91	0.71
1:D:468:LEU:HB3	3:D:686:HOH:O	1.90	0.71
1:C:89:LYS:NZ	1:C:216:ASP:OD2	2.23	0.71
1:A:376:GLU:HG2	1:A:387:VAL:HG13	1.72	0.71
1:C:248:ILE:HG12	1:C:274:LEU:HD21	1.74	0.70
1:D:344:ILE:HD13	1:D:361:VAL:HG13	1.74	0.69
1:D:370:VAL:O	1:D:386:LYS:NZ	2.26	0.69
1:A:205:GLU:O	1:A:209:GLU:N	2.21	0.69
1:D:344:ILE:HD13	1:D:361:VAL:CG1	2.23	0.69
1:B:74:LYS:NZ	1:B:251:ASP:O	2.26	0.68
1:B:14:ASP:OD2	1:B:345:LYS:HE3	1.92	0.68
1:A:459:GLN:NE2	3:A:647:HOH:O	2.26	0.68
1:B:327:CYS:SG	3:B:647:HOH:O	2.51	0.68
1:C:443:MET:HB2	1:C:448:ALA:HB3	1.76	0.68
1:D:230:THR:OG1	1:D:231:ALA:N	2.28	0.67
1:D:43:ASN:HB2	1:D:67:GLY:HA3	1.77	0.67
1:D:65:ARG:HD2	1:D:210:PHE:CD1	2.30	0.67
1:A:230:THR:O	1:A:263:LYS:NZ	2.22	0.66
1:D:6:PHE:H	2:D:502:EDO:H21	1.60	0.66
1:A:366:MET:O	1:A:425:LYS:NZ	2.28	0.66
1:D:71:ILE:HD13	1:D:224:GLY:HA3	1.78	0.66
1:B:455:ARG:NH1	3:B:691:HOH:O	2.28	0.66
1:B:14:ASP:OD2	1:B:345:LYS:CE	2.44	0.66
1:C:304:PRO:HB2	1:C:342:GLY:HA3	1.76	0.66
1:D:216:ASP:OD2	1:D:220:ARG:HB2	1.96	0.65
1:A:18:LEU:HB2	1:B:316:VAL:HG12	1.79	0.65
1:B:87:LYS:NZ	3:B:678:HOH:O	2.28	0.65
1:D:472:HIS:NE2	3:D:697:HOH:O	2.30	0.65
1:A:258:GLN:NE2	3:A:648:HOH:O	2.29	0.65
1:D:72:ILE:HG13	1:D:85:VAL:HG22	1.79	0.65
1:D:301:GLY:HA3	1:D:341:ASP:OD2	1.97	0.65
1:C:5:LYS:HG2	1:C:6:PHE:N	2.12	0.65
1:B:379:ILE:HG12	1:B:384:GLN:HG2	1.77	0.64
1:B:379:ILE:HG12	1:B:384:GLN:CG	2.27	0.64
1:A:387:VAL:HG11	3:A:675:HOH:O	1.97	0.64
1:C:29:GLU:O	1:C:449:GLN:NE2	2.31	0.64
1:B:241:VAL:HG12	1:B:274:LEU:HD13	1.79	0.63
1:D:440:ARG:NH1	3:D:709:HOH:O	2.30	0.63
1:D:56:GLU:HB2	1:D:374:PRO:HG3	1.81	0.62
1:B:38:GLU:OE1	1:B:217:LYS:NZ	2.33	0.62
1:C:86:ASP:HA	1:C:89:LYS:HB2	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:80:GLN:NE2	3:C:619:HOH:O	2.33	0.62
1:D:282:ALA:HB3	1:D:302:ILE:HD12	1.82	0.62
1:D:311:ARG:HG2	1:D:317:GLY:HA3	1.82	0.62
1:A:74:LYS:NZ	1:A:251:ASP:OD1	2.32	0.62
1:B:229:VAL:HG12	1:B:229:VAL:O	1.99	0.62
1:D:386:LYS:N	1:D:422:VAL:O	2.33	0.61
1:D:263:LYS:NZ	3:D:644:HOH:O	2.33	0.61
1:C:270:LYS:HG3	1:C:271:TYR:CD2	2.35	0.61
1:A:470:GLU:OE1	1:B:14:ASP:HB2	1.99	0.61
1:C:462:ARG:NH1	3:C:672:HOH:O	2.24	0.60
1:A:33:LYS:NZ	3:A:604:HOH:O	2.26	0.60
1:C:26:LEU:HD21	1:D:257:SER:HB2	1.82	0.60
1:A:305:GLY:O	1:D:472:HIS:ND1	2.35	0.60
1:C:310:THR:HB	1:C:314:ALA:HB3	1.84	0.60
1:D:308:CYS:SG	1:D:311:ARG:NH2	2.75	0.59
1:A:12:THR:OG1	1:A:15:ASP:OD1	2.20	0.59
1:B:300:VAL:N	1:B:339:ILE:O	2.30	0.59
1:C:89:LYS:HD2	1:C:220:ARG:HG2	1.84	0.59
1:A:34:THR:HG23	1:A:42:LEU:HB2	1.84	0.59
1:B:300:VAL:O	1:B:341:ASP:N	2.28	0.59
1:A:29:GLU:O	1:A:449:GLN:NE2	2.35	0.59
1:D:282:ALA:CB	1:D:302:ILE:HD12	2.33	0.59
1:C:357:GLY:HA2	1:C:455:ARG:HD3	1.85	0.59
1:B:310:THR:N	3:B:667:HOH:O	2.29	0.58
1:D:13:PHE:CE2	1:D:344:ILE:HG13	2.39	0.58
1:D:275:ASN:HA	1:D:296:ASN:HD21	1.69	0.57
1:C:47:ILE:HG12	1:C:69:LEU:HB3	1.86	0.57
1:B:281:VAL:CG2	1:B:287:THR:HG23	2.27	0.57
1:A:94:GLY:N	1:A:203[B]:ASP:OD1	2.26	0.57
1:C:466:ALA:HB2	1:D:465:GLY:HA2	1.87	0.57
1:A:8:LYS:O	1:D:462:ARG:N	2.38	0.57
1:A:225:ALA:HB2	1:A:245:VAL:HG21	1.87	0.57
1:A:32:VAL:H	1:A:33:LYS:HE2	1.70	0.57
1:B:297:VAL:HG22	1:B:337:PRO:HG2	1.87	0.57
1:B:43:ASN:ND2	3:B:635:HOH:O	2.38	0.56
1:A:469:LEU:N	1:A:469:LEU:HD23	2.20	0.56
1:C:254:HIS:HB3	1:C:257:SER:HB3	1.87	0.56
1:A:92:GLU:HA	1:A:203[A]:ASP:OD2	2.05	0.56
1:A:261:ILE:HG23	1:A:293:ALA:HB2	1.87	0.56
1:B:33:LYS:HG2	1:B:43:ASN:HA	1.88	0.56
1:C:218:GLN:HB2	1:C:220:ARG:HE	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:339:ILE:HD11	1:D:362:MET:HB2	1.87	0.56
1:C:11:LEU:HD21	1:C:462:ARG:HD3	1.87	0.56
1:C:369:GLY:HA3	1:C:425:LYS:HG3	1.87	0.56
1:A:78:ILE:HG23	1:A:236:ARG:HA	1.87	0.56
1:B:10:GLY:HA3	1:B:319:PRO:HG2	1.88	0.56
1:C:310:THR:O	1:C:315:GLY:N	2.39	0.55
1:B:311:ARG:NH1	3:B:637:HOH:O	2.36	0.55
1:C:223:VAL:N	3:C:662:HOH:O	2.32	0.55
1:C:27:PRO:O	1:C:440:ARG:NH1	2.38	0.55
1:C:340:ALA:HB3	1:C:361:VAL:HG12	1.87	0.55
1:D:237:ILE:HA	1:D:240:LEU:HD12	1.89	0.55
1:C:94:GLY:HA3	1:C:220:ARG:HD3	1.87	0.55
1:D:74:LYS:O	1:D:236:ARG:NH2	2.40	0.55
1:A:279:GLY:HA3	1:A:299:LYS:HB2	1.89	0.55
1:A:460:PHE:H	1:B:5:LYS:HB2	1.71	0.55
1:A:52:ASP:HA	1:A:73:HIS:CD2	2.42	0.55
1:B:386:LYS:HB3	1:B:422:VAL:HG13	1.89	0.55
1:A:313:VAL:HG12	1:D:438:GLY:HA3	1.89	0.55
1:A:227:VAL:HG21	1:A:237:ILE:HG12	1.87	0.54
1:B:291:ILE:HD13	1:B:336:ILE:HG13	1.89	0.54
1:B:347:SER:HB2	1:C:313:VAL:HA	1.89	0.54
1:D:331:ALA:O	1:D:336:ILE:N	2.37	0.54
1:C:223:VAL:HG12	3:C:662:HOH:O	2.07	0.54
1:C:232:ASP:N	1:C:232:ASP:OD1	2.33	0.54
1:D:27:PRO:HA	1:D:30:VAL:HG22	1.89	0.54
1:B:304:PRO:HD2	3:B:667:HOH:O	2.07	0.54
1:A:308:CYS:SG	1:A:309:THR:N	2.81	0.54
1:A:37:SER:HA	3:A:680:HOH:O	2.07	0.54
1:C:66:GLN:NE2	3:C:635:HOH:O	2.37	0.54
1:A:254:HIS:CG	1:A:257:SER:HB2	2.43	0.53
1:D:233:ALA:HB3	1:D:263:LYS:HE2	1.90	0.53
1:A:462:ARG:NH2	1:B:6:PHE:O	2.40	0.53
1:B:345:LYS:HB2	1:B:349:ASP:OD2	2.08	0.53
1:C:458:ALA:O	1:D:5:LYS:NZ	2.30	0.53
1:D:301:GLY:HA2	1:D:320:GLN:HE22	1.73	0.53
1:C:227:VAL:HA	1:C:236:ARG:HH12	1.74	0.53
1:C:213:SER:N	3:C:674:HOH:O	2.42	0.53
1:A:466:ALA:HA	1:A:469:LEU:HG	1.90	0.53
1:B:52:ASP:OD1	1:B:52:ASP:N	2.42	0.52
1:C:11:LEU:HB3	1:C:321:LEU:HD23	1.91	0.52
1:B:204:ILE:HD12	1:B:205:GLU:H	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:SER:N	1:A:203[B]:ASP:OD1	2.42	0.52
1:D:279:GLY:HA3	1:D:299:LYS:HB3	1.91	0.52
1:A:88:VAL:HG11	1:A:223:VAL:HB	1.92	0.51
1:B:25:VAL:HB	1:B:447:GLY:HA2	1.92	0.51
1:A:223:VAL:HG13	1:A:245:VAL:HG23	1.91	0.51
1:C:344:ILE:HD13	1:C:344:ILE:H	1.75	0.51
1:C:27:PRO:HB3	1:C:440:ARG:HB3	1.92	0.51
1:A:201:ILE:HA	1:A:204:ILE:HG12	1.93	0.51
1:C:47:ILE:HG13	1:C:360:VAL:HG21	1.92	0.51
1:B:56:GLU:HG3	1:B:374:PRO:HG3	1.93	0.51
1:A:89:LYS:HD3	1:A:223:VAL:HG12	1.92	0.50
1:C:372:GLU:OE2	1:C:372:GLU:N	2.44	0.50
1:C:204:ILE:O	1:C:208:ILE:N	2.44	0.50
1:C:440:ARG:NH2	3:C:641:HOH:O	2.42	0.50
1:A:36:LEU:HB2	1:A:40:LEU:HB3	1.94	0.50
1:C:220:ARG:NH1	1:C:244:SER:OG	2.39	0.50
1:C:359:HIS:HA	1:C:455:ARG:HH11	1.75	0.50
1:C:375:GLY:HA2	1:C:387:VAL:HG12	1.94	0.50
1:B:298:VAL:HB	1:B:338:VAL:HG12	1.93	0.50
1:C:362:MET:C	1:C:363:LEU:HD12	2.31	0.50
1:D:28:ARG:NH1	3:D:636:HOH:O	2.44	0.50
1:C:280:ASN:ND2	3:C:637:HOH:O	2.32	0.50
1:B:424:TYR:CZ	1:B:426:GLY:HA2	2.47	0.50
1:B:304:PRO:HG3	1:B:308:CYS:O	2.11	0.50
1:A:95:GLY:O	1:A:204:ILE:HD11	2.12	0.49
1:B:354:LEU:HB3	3:B:691:HOH:O	2.11	0.49
1:B:89:LYS:HD3	1:B:223:VAL:HG12	1.92	0.49
1:D:88:VAL:HG12	1:D:221:LEU:HB2	1.95	0.49
1:B:27:PRO:HG3	1:B:441:ALA:HA	1.94	0.49
1:A:32:VAL:N	1:A:33:LYS:HE2	2.26	0.49
1:A:65:ARG:HD3	1:A:210:PHE:CE2	2.48	0.49
1:D:81:GLN:OE1	1:D:236:ARG:NH2	2.40	0.49
1:B:31:SER:N	1:B:449:GLN:O	2.33	0.49
1:D:443:MET:HG2	1:D:454:LEU:HD22	1.94	0.49
1:A:249:VAL:HG22	1:A:277:ILE:HB	1.95	0.49
1:C:454:LEU:O	1:C:458:ALA:HB2	2.13	0.49
1:D:271:TYR:HB3	1:D:274:LEU:HB2	1.95	0.49
1:A:305:GLY:H	1:A:311:ARG:CZ	2.26	0.48
1:B:86:ASP:HA	1:B:89:LYS:HB2	1.94	0.48
1:C:93:SER:HB3	1:C:220:ARG:HG3	1.94	0.48
1:C:348:GLY:HA3	1:D:312:VAL:HA	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:460:PHE:HD2	1:B:5:LYS:HD2	1.78	0.48
1:C:270:LYS:HA	3:C:708:HOH:O	2.13	0.48
1:B:379:ILE:HG12	1:B:384:GLN:HG3	1.96	0.48
1:B:451:LEU:HD22	3:B:691:HOH:O	2.12	0.48
1:D:76:MET:SD	1:D:81:GLN:HA	2.54	0.48
1:B:30:VAL:O	1:B:440:ARG:NH1	2.45	0.48
1:A:256:HIS:ND1	1:D:22:LYS:HA	2.29	0.47
1:A:15:ASP:OD1	1:A:15:ASP:N	2.48	0.47
1:B:251:ASP:N	1:B:251:ASP:OD2	2.47	0.47
1:A:387:VAL:HG22	1:A:388:TYR:N	2.28	0.47
1:A:305:GLY:HA3	1:A:311:ARG:HD2	1.95	0.47
1:A:203[B]:ASP:OD2	1:A:203[B]:ASP:N	2.45	0.47
1:C:251:ASP:OD2	1:C:280:ASN:ND2	2.48	0.47
1:B:361:VAL:HA	3:B:631:HOH:O	2.14	0.47
1:A:443:MET:HG2	1:A:454:LEU:HD13	1.96	0.47
1:B:84:GLN:O	1:B:88:VAL:HG23	2.15	0.47
1:D:446:CYS:SG	3:D:616:HOH:O	2.25	0.47
1:A:306:SER:HA	1:D:472:HIS:HA	1.96	0.46
1:B:42:LEU:HD13	1:B:68:GLY:HA2	1.96	0.46
1:B:380:TYR:C	1:B:380:TYR:CD2	2.89	0.46
1:B:358:ALA:O	1:B:455:ARG:NH1	2.49	0.46
1:A:248:ILE:HD11	1:A:276:ILE:HG12	1.98	0.46
1:C:304:PRO:CG	1:C:307:ILE:HG22	2.45	0.46
1:C:37:SER:HB3	1:C:40:LEU:HB2	1.97	0.46
1:D:344:ILE:HD13	1:D:361:VAL:HG11	1.96	0.46
1:A:255:GLY:HA2	1:A:280:ASN:O	2.15	0.46
1:D:25:VAL:HG22	1:D:447:GLY:HA2	1.97	0.46
1:A:84:GLN:N	1:A:84:GLN:HE21	2.13	0.46
1:B:63:MET:SD	1:B:428:LEU:HD21	2.56	0.46
1:B:71:ILE:HG22	3:B:617:HOH:O	2.16	0.46
1:D:265:LYS:HE2	1:D:269:ALA:HB2	1.98	0.46
1:A:387:VAL:CG2	1:A:388:TYR:N	2.78	0.46
1:C:54:VAL:HG13	1:C:367:PHE:HB2	1.98	0.46
1:C:378:GLU:HG3	1:C:383:ARG:O	2.15	0.46
1:A:240:LEU:HB3	1:A:245:VAL:HG11	1.97	0.46
1:A:71:ILE:HD13	1:A:224:GLY:HA3	1.97	0.46
1:B:210:PHE:HA	1:B:211:PRO:HD3	1.68	0.46
1:C:378:GLU:O	1:C:384:GLN:NE2	2.48	0.46
1:B:220:ARG:NH1	3:B:611:HOH:O	2.49	0.45
1:C:250:LEU:HD12	1:C:264:VAL:HG22	1.98	0.45
1:C:284:ALA:HB1	1:C:330:GLU:HB2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:46:LEU:CD2	1:C:363:LEU:HD13	2.46	0.45
1:D:214:ALA:HB1	1:D:222:LEU:HD12	1.99	0.45
1:B:78:ILE:HG12	1:B:236:ARG:HG3	1.98	0.45
1:C:359:HIS:HA	1:C:455:ARG:NH1	2.31	0.45
1:D:217:LYS:HG2	1:D:217:LYS:H	1.56	0.45
1:D:53:THR:HB	1:D:388:TYR:CD1	2.51	0.45
1:D:74:LYS:HG3	3:D:609:HOH:O	2.15	0.45
1:C:220:ARG:HH12	1:C:244:SER:CB	2.30	0.45
1:D:10:GLY:O	3:D:687:HOH:O	2.21	0.45
1:D:205:GLU:HA	1:D:208:ILE:HB	1.98	0.45
1:D:366:MET:CE	1:D:435:LEU:HD11	2.47	0.45
1:C:37:SER:HB3	1:C:40:LEU:H	1.81	0.45
1:A:84:GLN:O	1:A:88:VAL:HG23	2.17	0.44
1:C:255:GLY:HA3	1:C:280:ASN:H	1.82	0.44
1:D:213:SER:OG	1:D:215:LYS:HE3	2.17	0.44
1:B:14:ASP:OD2	1:B:345:LYS:HE2	2.18	0.44
1:C:347:SER:HB3	1:C:435:LEU:HD13	2.00	0.44
1:B:250:LEU:HD12	1:B:264:VAL:HG22	2.00	0.44
1:B:33:LYS:HB3	3:B:679:HOH:O	2.17	0.44
1:C:31:SER:N	1:C:449:GLN:O	2.36	0.44
1:D:13:PHE:HE2	1:D:344:ILE:HG13	1.81	0.44
1:D:351:VAL:HG22	1:D:439:LEU:HA	1.98	0.44
1:D:47:ILE:HG13	1:D:360:VAL:HG21	1.98	0.44
1:B:270:LYS:HE2	1:B:271:TYR:CD2	2.52	0.44
1:A:93:SER:OG	1:A:203[B]:ASP:OD2	2.30	0.44
1:D:13:PHE:CE1	1:D:353:ALA:HB2	2.53	0.44
1:B:380:TYR:CE2	1:B:381:GLN:HG2	2.53	0.44
1:B:443:MET:SD	3:B:616:HOH:O	2.61	0.44
1:D:52:ASP:OD2	1:D:52:ASP:N	2.49	0.44
1:D:384:GLN:HB2	1:D:424:TYR:HB2	2.00	0.43
1:A:213:SER:O	1:A:215:LYS:NZ	2.51	0.43
1:A:383:ARG:HB3	1:A:385:PHE:CE2	2.53	0.43
1:C:345:LYS:HG3	1:C:346:TYR:CD2	2.53	0.43
1:B:75:ASN:ND2	3:B:610:HOH:O	2.43	0.43
1:D:459:GLN:HE21	1:D:459:GLN:HB3	1.57	0.43
1:A:236:ARG:O	1:A:240:LEU:HG	2.18	0.43
1:B:283:THR:HG22	1:B:285:GLU:H	1.83	0.43
1:B:12:THR:HG23	1:B:14:ASP:H	1.84	0.43
1:B:86:ASP:O	1:B:90:ARG:HG2	2.19	0.43
1:D:300:VAL:HG11	1:D:324:VAL:HA	2.00	0.43
1:B:12:THR:HG22	1:B:15:ASP:OD2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:296:ASN:ND2	1:B:297:VAL:HG23	2.34	0.43
1:A:256:HIS:O	1:D:23:SER:HB3	2.19	0.43
1:A:470:GLU:CD	1:B:12:THR:HG21	2.39	0.43
1:C:262:ASP:O	1:C:265:LYS:HG2	2.18	0.43
1:A:298:VAL:O	1:A:339:ILE:N	2.49	0.43
1:C:59:MET:HA	1:C:372:GLU:HB3	2.01	0.43
1:C:422:VAL:HA	1:C:423:PRO:HD3	1.89	0.43
1:D:307:ILE:HG13	1:D:307:ILE:O	2.18	0.43
1:B:32:VAL:HA	3:B:616:HOH:O	2.19	0.42
1:B:34:THR:HG23	1:B:42:LEU:HB2	2.01	0.42
1:A:232:ASP:OD2	3:A:616:HOH:O	2.22	0.42
1:B:270:LYS:CG	1:B:271:TYR:N	2.82	0.42
1:C:309:THR:N	3:C:649:HOH:O	2.52	0.42
1:C:57:ALA:N	1:C:84:GLN:OE1	2.52	0.42
1:B:299:LYS:HA	1:B:339:ILE:HB	2.00	0.42
1:B:383:ARG:H	1:B:383:ARG:HD2	1.84	0.42
1:B:422:VAL:HA	1:B:423:PRO:HD3	1.89	0.42
1:C:85:VAL:HG21	1:C:240:LEU:HD22	2.01	0.42
1:D:62:ALA:HA	1:D:65:ARG:HG3	2.01	0.42
1:B:248:ILE:HD11	1:B:276:ILE:HG23	2.00	0.42
1:C:19:VAL:HA	1:C:20:PRO:HD3	1.92	0.42
1:C:257:SER:O	1:C:261:ILE:HG13	2.19	0.42
1:D:278:ALA:O	1:D:299:LYS:N	2.37	0.42
1:A:218:GLN:HE21	1:A:218:GLN:HB3	1.65	0.42
1:B:383:ARG:H	1:B:383:ARG:CD	2.32	0.42
1:A:376:GLU:OE1	1:A:388:TYR:HB2	2.20	0.42
1:C:46:LEU:HD21	1:C:363:LEU:HD13	2.01	0.42
1:B:287:THR:HG21	1:B:327:CYS:HB3	2.01	0.42
1:C:464:SER:OG	3:C:663:HOH:O	2.22	0.42
1:B:380:TYR:O	1:B:380:TYR:CD2	2.73	0.41
1:C:288:LYS:NZ	1:C:334:HIS:HE1	2.18	0.41
1:D:259:GLY:HA2	1:D:262:ASP:HB2	2.00	0.41
1:D:223:VAL:HG23	1:D:246:ASP:H	1.85	0.41
1:B:23:SER:OG	1:B:25:VAL:O	2.36	0.41
1:B:76:MET:O	1:B:236:ARG:NH1	2.50	0.41
1:C:60:ALA:HB1	1:C:223:VAL:HG23	2.01	0.41
1:A:311:ARG:HD3	1:D:17:LEU:HD21	2.01	0.41
1:D:204:ILE:N	3:D:601:HOH:O	2.53	0.41
1:C:430:ASP:HA	1:C:433:HIS:CE1	2.54	0.41
1:A:204:ILE:O	1:A:207:VAL:HB	2.21	0.41
1:B:79:GLU:O	1:B:83:GLU:N	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:448:ALA:HA	1:C:453:PHE:HD2	1.86	0.41
1:A:215:LYS:HE2	1:A:215:LYS:HB2	1.88	0.41
1:A:290:LEU:HD23	1:A:290:LEU:HA	1.91	0.41
1:A:316:VAL:HG21	1:D:445:TYR:HB2	2.01	0.41
1:A:206:LYS:HD3	1:A:206:LYS:HA	1.78	0.41
1:C:304:PRO:HG2	1:C:307:ILE:HG22	2.03	0.41
1:A:261:ILE:HG22	1:A:265:LYS:HE3	2.03	0.41
1:A:280:ASN:C	1:A:280:ASN:HD22	2.24	0.41
1:A:84:GLN:NE2	1:A:84:GLN:CA	2.84	0.41
1:B:59:MET:HA	1:B:372:GLU:HB3	2.01	0.41
1:B:434:GLN:HB3	1:B:434:GLN:HE21	1.75	0.41
1:D:344:ILE:HG23	1:D:349:ASP:CB	2.47	0.41
1:B:74:LYS:HB3	1:B:226:ALA:O	2.21	0.41
1:D:341:ASP:CG	1:D:341:ASP:O	2.59	0.41
1:D:339:ILE:HB	1:D:360:VAL:HG13	2.03	0.41
1:A:84:GLN:NE2	1:A:84:GLN:HA	2.36	0.41
1:C:257:SER:O	1:C:260:VAL:HG12	2.21	0.41
1:D:11:LEU:O	1:D:321:LEU:HB3	2.21	0.41
1:B:227:VAL:HG21	1:B:237:ILE:HG12	2.03	0.41
1:B:332:ARG:HH12	1:C:2:TRP:HE1	1.67	0.41
1:C:27:PRO:O	1:C:30:VAL:HG22	2.21	0.41
1:C:64:ALA:HB1	1:C:221:LEU:HB2	2.03	0.41
1:A:92:GLU:HG3	1:A:203[A]:ASP:HB3	2.01	0.40
1:B:464:SER:O	1:B:468:LEU:HG	2.21	0.40
1:C:89:LYS:NZ	1:C:220:ARG:HB3	2.35	0.40
1:C:75:ASN:HA	3:C:704:HOH:O	2.20	0.40
1:D:450:ASP:OD2	1:D:453:PHE:N	2.43	0.40
1:A:300:VAL:N	1:A:339:ILE:O	2.52	0.40
1:A:263:LYS:O	1:A:267:VAL:HG23	2.22	0.40
1:B:237:ILE:HG23	1:B:248:ILE:HG21	2.04	0.40
1:B:299:LYS:NZ	3:B:676:HOH:O	2.54	0.40
1:D:242:LYS:NZ	1:D:242:LYS:HA	2.36	0.40
1:A:305:GLY:H	1:A:311:ARG:NE	2.18	0.40
1:B:357:GLY:HA2	1:B:455:ARG:HG2	2.04	0.40
1:D:22:LYS:O	1:D:447:GLY:HA3	2.21	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	323/385 (84%)	299 (93%)	24 (7%)	0	100	100
1	B	320/385 (83%)	292 (91%)	28 (9%)	0	100	100
1	C	323/385 (84%)	298 (92%)	25 (8%)	0	100	100
1	D	320/385 (83%)	296 (92%)	23 (7%)	1 (0%)	41	46
All	All	1286/1540 (84%)	1185 (92%)	100 (8%)	1 (0%)	51	60

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	364	GLY

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	253/299 (85%)	233 (92%)	20 (8%)	12	10
1	B	252/299 (84%)	222 (88%)	30 (12%)	5	3
1	C	253/299 (85%)	219 (87%)	34 (13%)	4	2
1	D	253/299 (85%)	225 (89%)	28 (11%)	6	4
All	All	1011/1196 (84%)	899 (89%)	112 (11%)	6	4

All (112) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	ASP
1	A	24	ASP
1	A	31	SER
1	A	33	LYS
1	A	74	LYS
1	A	80	GLN
1	A	83	GLU
1	A	87	LYS
1	A	216	ASP
1	A	218	GLN
1	A	230	THR
1	A	250	LEU
1	A	258	GLN
1	A	280	ASN
1	A	346	TYR
1	A	370	VAL
1	A	376	GLU
1	A	453	PHE
1	A	469	LEU
1	A	470	GLU
1	B	7	VAL
1	B	26	LEU
1	B	30	VAL
1	B	76	MET
1	B	93	SER
1	B	204	ILE
1	B	217	LYS
1	B	227	VAL
1	B	234	MET
1	B	235	THR
1	B	238	ASP
1	B	251	ASP
1	B	258	GLN
1	B	260	VAL
1	B	274	LEU
1	B	287	THR
1	B	309	THR
1	B	326	ASP
1	B	345	LYS
1	B	376	GLU
1	B	380	TYR
1	B	383	ARG
1	B	384	GLN

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Mol	Chain	Res	Type
1	B	422	VAL
1	B	431	THR
1	B	434	GLN
1	B	449	GLN
1	B	455	ARG
1	B	456	GLU
1	B	459	GLN
1	C	4	SER
1	C	5	LYS
1	C	6	PHE
1	C	34	THR
1	C	53	THR
1	C	79	GLU
1	C	83	GLU
1	C	93	SER
1	C	201	ILE
1	C	205	GLU
1	C	206	LYS
1	C	212	ASN
1	C	220	ARG
1	C	230	THR
1	C	251	ASP
1	C	260	VAL
1	C	262	ASP
1	C	273	SER
1	C	285	GLU
1	C	306	SER
1	C	309	THR
1	C	344	ILE
1	C	345	LYS
1	C	362	MET
1	C	366	MET
1	C	377	THR
1	C	378	GLU
1	C	383	ARG
1	C	384	GLN
1	C	385	PHE
1	C	424	TYR
1	C	445	TYR
1	C	462	ARG
1	C	468	LEU
1	D	14	ASP

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Mol	Chain	Res	Type
1	D	52	ASP
1	D	59	MET
1	D	65	ARG
1	D	74	LYS
1	D	85	VAL
1	D	201	ILE
1	D	202	LYS
1	D	218	GLN
1	D	230	THR
1	D	232	ASP
1	D	242	LYS
1	D	251	ASP
1	D	258	GLN
1	D	260	VAL
1	D	308	CYS
1	D	309	THR
1	D	310	THR
1	D	312	VAL
1	D	316	VAL
1	D	339	ILE
1	D	341	ASP
1	D	363	LEU
1	D	370	VAL
1	D	388	TYR
1	D	453	PHE
1	D	459	GLN
1	D	464	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	80	GLN
1	A	84	GLN
1	A	258	GLN
1	A	384	GLN
1	A	449	GLN
1	B	75	ASN
1	B	80	GLN
1	B	218	GLN
1	B	254	HIS
1	B	275	ASN
1	B	384	GLN

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Mol	Chain	Res	Type
1	B	457	ASN
1	C	66	GLN
1	C	81	GLN
1	C	212	ASN
1	C	256	HIS
1	C	334	HIS
1	C	384	GLN
1	C	433	HIS
1	C	449	GLN
1	D	80	GLN
1	D	320	GLN
1	D	384	GLN
1	D	457	ASN
1	D	459	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

8 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	EDO	C	501	-	3,3,3	0.26	0	2,2,2	0.62	0
2	EDO	B	501	-	3,3,3	0.45	0	2,2,2	0.34	0
2	EDO	A	503	-	3,3,3	0.45	0	2,2,2	0.09	0
2	EDO	A	502	-	3,3,3	0.33	0	2,2,2	0.46	0
2	EDO	D	501	-	3,3,3	0.36	0	2,2,2	0.77	0
2	EDO	D	502	-	3,3,3	0.36	0	2,2,2	0.27	0
2	EDO	A	501	-	3,3,3	0.42	0	2,2,2	0.98	0
2	EDO	D	503	-	3,3,3	0.31	0	2,2,2	0.23	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
2	EDO	C	501	-	-	1/1/1/1	-
2	EDO	B	501	-	-	1/1/1/1	-
2	EDO	A	503	-	-	1/1/1/1	-
2	EDO	A	502	-	-	0/1/1/1	-
2	EDO	D	501	-	-	1/1/1/1	-
2	EDO	D	502	-	-	0/1/1/1	-
2	EDO	A	501	-	-	0/1/1/1	-
2	EDO	D	503	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	503	EDO	O1-C1-C2-O2
2	D	501	EDO	O1-C1-C2-O2
2	C	501	EDO	O1-C1-C2-O2
2	B	501	EDO	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	502	EDO	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 ⓘ

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	328/385 (85%)	-0.10	9 (2%) 54 57	24, 41, 77, 128	0
1	B	328/385 (85%)	-0.13	3 (0%) 84 85	24, 43, 79, 143	0
1	C	329/385 (85%)	0.02	11 (3%) 46 48	29, 49, 91, 141	0
1	D	328/385 (85%)	-0.09	7 (2%) 63 66	27, 45, 82, 161	0
All	All	1313/1540 (85%)	-0.08	30 (2%) 60 63	24, 45, 84, 161	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	201	ILE	7.0
1	A	293	ALA	5.1
1	C	309	THR	5.1
1	B	379	ILE	4.9
1	C	7	VAL	4.9
1	A	388	TYR	4.6
1	A	255	GLY	4.3
1	C	432	VAL	4.0
1	D	461	ILE	3.8
1	A	25	VAL	3.4
1	D	318	VAL	3.4
1	C	6	PHE	3.3
1	C	383	ARG	3.1
1	A	243	ALA	2.9
1	D	469	LEU	2.8
1	A	256	HIS	2.5
1	C	325	TYR	2.5
1	D	317	GLY	2.5
1	B	344	ILE	2.5
1	A	251	ASP	2.3
1	C	367	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	470	GLU	2.3
1	D	301	GLY	2.2
1	C	0	ALA	2.2
1	C	429	ALA	2.2
1	C	208	ILE	2.2
1	B	380	TYR	2.1
1	C	229	VAL	2.1
1	A	26	LEU	2.0
1	D	208	ILE	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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(Å ²)	Q<0.9
2	EDO	B	501	4/4	0.83	0.17	82,83,87,89	0
2	EDO	D	501	4/4	0.90	0.15	39,45,47,49	0
2	EDO	A	502	4/4	0.91	0.12	57,60,63,65	0
2	EDO	A	503	4/4	0.93	0.12	44,47,48,52	0
2	EDO	C	501	4/4	0.96	0.09	41,42,43,45	0
2	EDO	D	502	4/4	0.96	0.09	35,36,41,42	0
2	EDO	D	503	4/4	0.96	0.12	38,39,40,40	0
2	EDO	A	501	4/4	0.98	0.11	40,41,43,46	0

6.5 Other polymers [i](#)

There are no such residues in this entry.