



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 22, 2020 – 12:14 AM BST

PDB ID : 5O80
Title : Crystal Structure of R67A Mutant of alpha-L-arabinofuranosidase Ara51 from Clostridium thermocellum in complex with L-Arabinofuranose
Authors : Lafite, P.; Daniellou, R.
Deposited on : 2017-06-12
Resolution : 2.92 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	:	2.13.1
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)	:	2.13.1

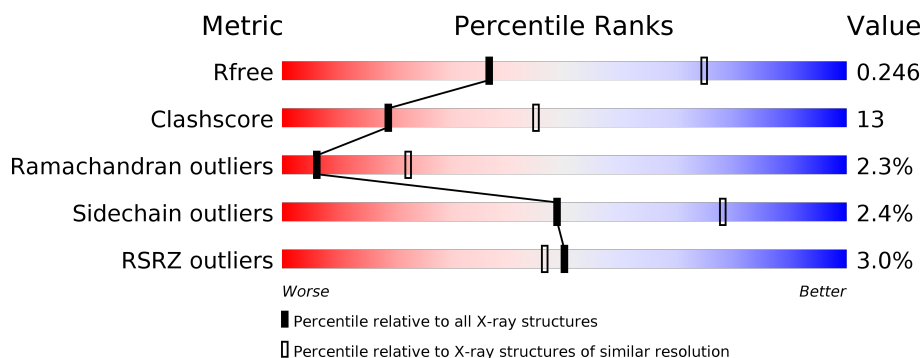
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.92 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	2307 (2.94-2.90)
Clashscore	141614	2531 (2.94-2.90)
Ramachandran outliers	138981	2462 (2.94-2.90)
Sidechain outliers	138945	2464 (2.94-2.90)
RSRZ outliers	127900	2248 (2.94-2.90)

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 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	501	<div> <div>2%</div> <div> <div></div> <div>72%</div> <div>25%</div> <div>..</div> </div> </div>
1	B	501	<div> <div>4%</div> <div> <div></div> <div>72%</div> <div>25%</div> <div>..</div> </div> </div>
1	C	501	<div> <div>2%</div> <div> <div></div> <div>71%</div> <div>26%</div> <div>..</div> </div> </div>
1	D	501	<div> <div>5%</div> <div> <div></div> <div>69%</div> <div>27%</div> <div>..</div> </div> </div>
1	E	501	<div> <div>%</div> <div> <div></div> <div>71%</div> <div>26%</div> <div>..</div> </div> </div>
1	F	501	<div> <div>4%</div> <div> <div></div> <div>72%</div> <div>26%</div> <div>..</div> </div> </div>

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
3	DIO	A	601	-	-	X	-
3	DIO	B	601	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 23944 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.

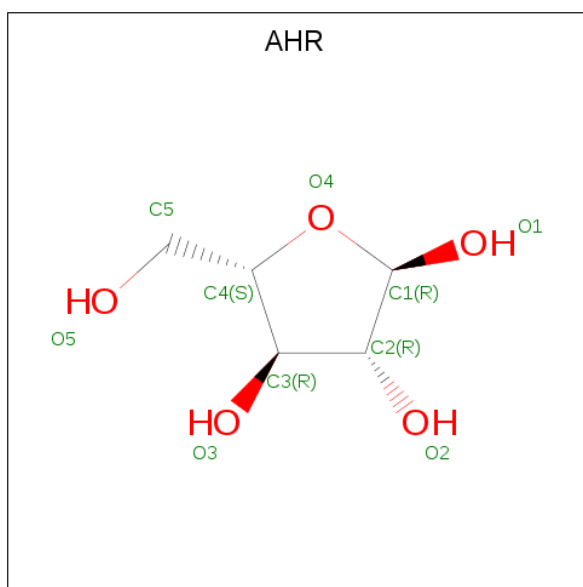
- Molecule 1 is a protein called Intracellular exo-alpha-(1->5)-L-arabinofuranosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	496	Total	C	N	O	S	0	1	0
			3978	2527	675	754	22			
1	B	496	Total	C	N	O	S	0	1	0
			3978	2527	674	755	22			
1	C	496	Total	C	N	O	S	0	1	0
			3962	2518	669	752	23			
1	D	496	Total	C	N	O	S	0	1	0
			3978	2527	674	755	22			
1	E	496	Total	C	N	O	S	0	0	0
			3963	2519	670	752	22			
1	F	496	Total	C	N	O	S	0	1	0
			3977	2527	674	754	22			

There are 6 discrepancies between the modelled and reference sequences:

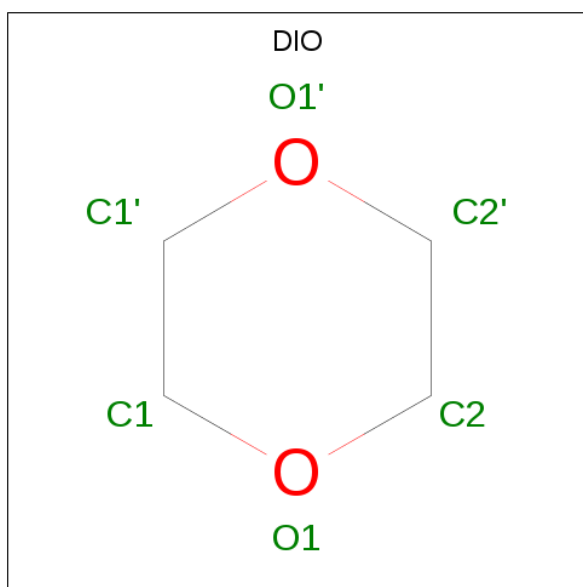
Chain	Residue	Modelled	Actual	Comment	Reference
A	67	ALA	ARG	engineered mutation	UNP A3DIH0
B	67	ALA	ARG	engineered mutation	UNP A3DIH0
C	67	ALA	ARG	engineered mutation	UNP A3DIH0
D	67	ALA	ARG	engineered mutation	UNP A3DIH0
E	67	ALA	ARG	engineered mutation	UNP A3DIH0
F	67	ALA	ARG	engineered mutation	UNP A3DIH0

- Molecule 2 is alpha-L-arabinofuranose (three-letter code: AHR) (formula: C₅H₁₀O₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			10	5	5		
2	B	1	Total	C	O	0	0
			10	5	5		
2	C	1	Total	C	O	0	0
			10	5	5		
2	D	1	Total	C	O	0	0
			10	5	5		
2	E	1	Total	C	O	0	0
			10	5	5		
2	F	1	Total	C	O	0	0
			10	5	5		

- Molecule 3 is 1,4-DIETHYLENE DIOXIDE (three-letter code: DIO) (formula: C₄H₈O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	4	2		
3	B	1	Total	C	O	0	0
			6	4	2		
3	C	1	Total	C	O	0	0
			6	4	2		
3	D	1	Total	C	O	0	0
			6	4	2		
3	E	1	Total	C	O	0	0
			6	4	2		
3	F	1	Total	C	O	0	0
			6	4	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	O	0	0
			1	1		
4	B	2	Total	O	0	0
			2	2		
4	C	2	Total	O	0	0
			2	2		
4	D	2	Total	O	0	0
			2	2		
4	E	3	Total	O	0	0
			3	3		
4	F	2	Total	O	0	0
			2	2		

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.

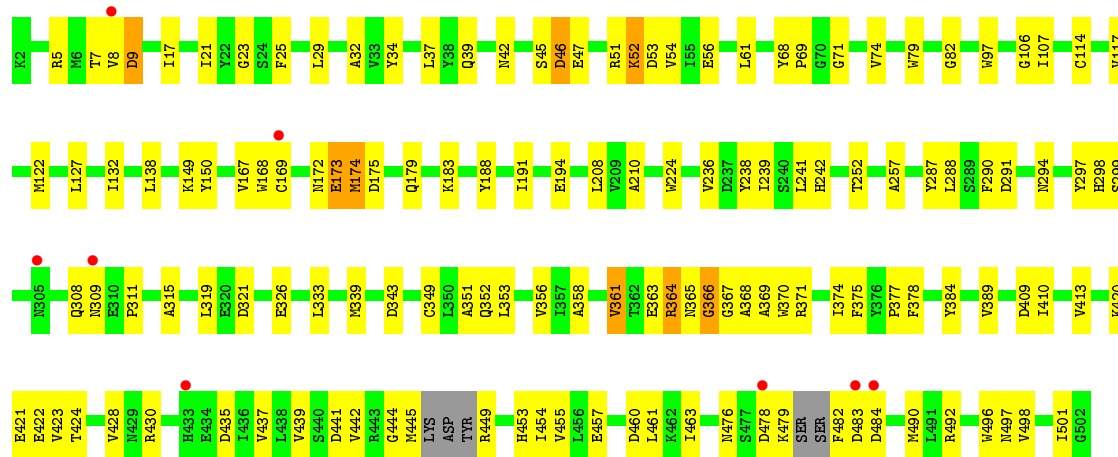
- Chain A:
-
- 29% 72% 25%

- Chain B:

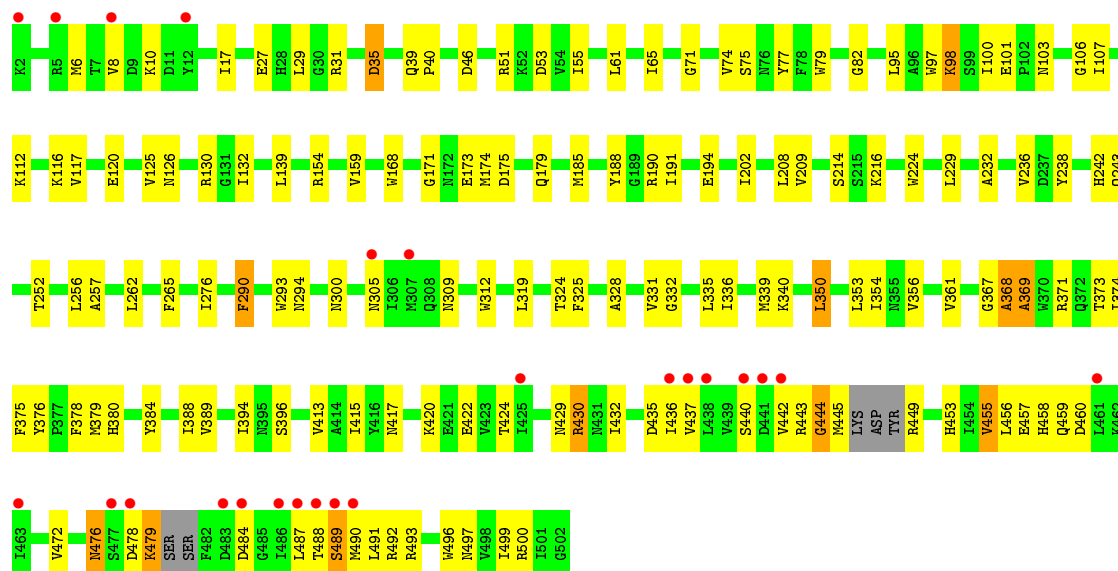
72% 25% 4%

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
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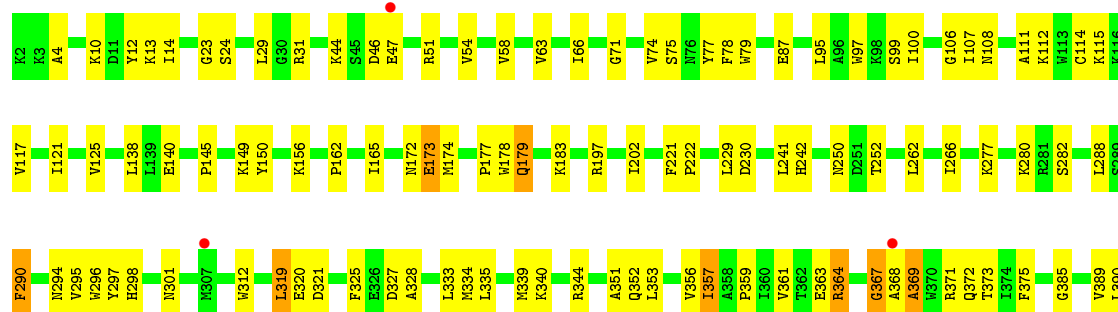
- Chain C:  29% 71% 26%

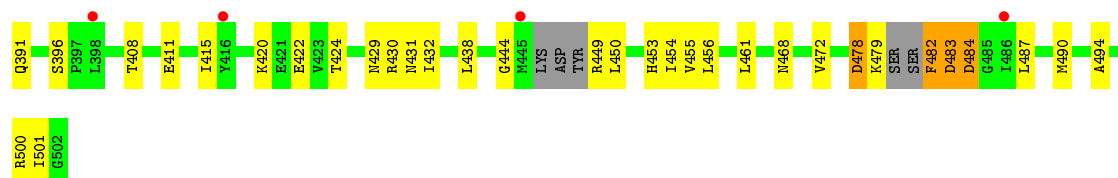


• Molecule 1: Intracellular exo- α -(1 \rightarrow 5)-L-arabinofuranosidase

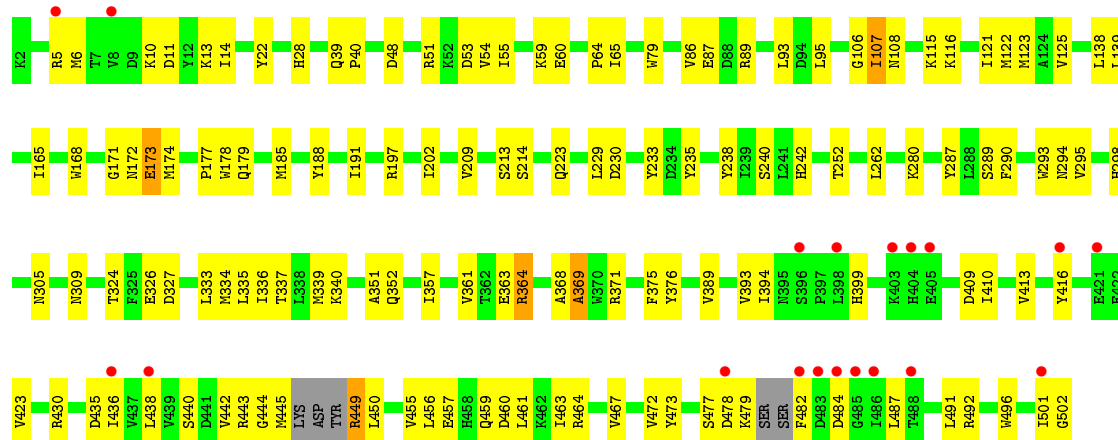


• Molecule 1: Intracellular exo- α -(1 \rightarrow 5)-L-arabinofuranosidase





- Molecule 1: Intracellular exo-alpha-(1->5)-L-arabinofuranosidase



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	173.74Å 173.74Å 271.11Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.76 – 2.92 48.76 – 2.91	Depositor EDS
% Data completeness (in resolution range)	99.8 (48.76-2.92) 99.9 (48.76-2.91)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.06 (at 2.91Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.179 , 0.246 0.179 , 0.246	Depositor DCC
R_{free} test set	4538 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	63.8	Xtriage
Anisotropy	0.088	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 49.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	23944	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.23% 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: AHR, DIO

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	0.55	0/4068	0.69	0/5509
1	B	0.49	0/4068	0.66	0/5509
1	C	0.54	0/4055	0.67	0/5494
1	D	0.49	0/4068	0.68	0/5509
1	E	0.48	0/4053	0.64	0/5490
1	F	0.50	0/4067	0.64	0/5508
All	All	0.51	0/24379	0.66	0/33019

There are no bond length outliers.

There are no bond angle outliers.

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	3978	0	3869	128	0
1	B	3978	0	3867	102	0
1	C	3962	0	3845	102	0
1	D	3978	0	3867	124	0
1	E	3963	0	3851	93	0
1	F	3977	0	3864	86	0
2	A	10	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	10	0	0	0	0
2	C	10	0	0	0	0
2	D	10	0	0	0	0
2	E	10	0	0	0	0
2	F	10	0	0	0	0
3	A	6	0	8	4	0
3	B	6	0	8	4	0
3	C	6	0	8	2	0
3	D	6	0	8	2	0
3	E	6	0	8	1	0
3	F	6	0	8	3	0
4	A	1	0	0	0	0
4	B	2	0	0	0	0
4	C	2	0	0	0	0
4	D	2	0	0	0	0
4	E	3	0	0	0	0
4	F	2	0	0	0	0
All	All	23944	0	23211	619	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 13.

All (619) 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:240:SER:C	1:A:241:LEU:HD23	1.66	1.15
1:A:240:SER:C	1:A:241:LEU:CD2	2.16	1.14
1:D:256:LEU:O	1:D:430:ARG:NH2	1.83	1.11
1:A:240:SER:O	1:A:241:LEU:HD22	1.51	1.10
1:A:241:LEU:HD11	1:A:269:VAL:HG11	1.13	1.09
1:C:257:ALA:HA	1:C:430:ARG:HH21	1.00	1.08
1:A:223:GLN:NE2	1:B:279:LYS:HE2	1.73	1.03
1:A:241:LEU:N	1:A:241:LEU:HD23	1.77	0.99
1:A:173:GLU:O	1:A:179[B]:GLN:NE2	1.94	0.98
1:A:241:LEU:HD13	1:A:269:VAL:HG21	1.47	0.97
1:A:241:LEU:CD1	1:A:269:VAL:HG21	1.96	0.96
1:E:44:LYS:HD2	1:E:51:ARG:NH2	1.80	0.96
1:A:241:LEU:HD11	1:A:269:VAL:CG1	1.95	0.95
1:A:241:LEU:CD1	1:A:269:VAL:HG11	1.98	0.93
1:C:257:ALA:HA	1:C:430:ARG:NH2	1.83	0.93
1:B:363:GLU:HB2	1:B:367:GLY:HA3	1.52	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:331:VAL:O	1:D:335:LEU:HD22	1.72	0.89
1:A:241:LEU:N	1:A:241:LEU:CD2	2.35	0.89
1:B:478:ASP:HA	1:B:479:LYS:HG3	1.58	0.86
1:E:479:LYS:HE2	1:E:490:MET:HG2	1.59	0.85
1:E:385:GLY:HA2	1:E:415:ILE:HD11	1.59	0.84
1:E:478:ASP:HA	1:E:479:LYS:HB3	1.59	0.84
1:C:252:THR:HG21	1:C:461:LEU:HD13	1.58	0.84
1:E:44:LYS:HD2	1:E:51:ARG:HH21	1.43	0.84
1:A:240:SER:O	1:A:241:LEU:CD2	2.23	0.83
1:A:478:ASP:HA	1:A:479:LYS:HB3	1.61	0.82
1:A:240:SER:C	1:A:241:LEU:HD22	1.91	0.82
1:A:263:ASP:OD1	1:A:341:HIS:NE2	2.13	0.82
1:A:223:GLN:HE22	1:B:279:LYS:HE2	1.44	0.81
1:A:452:GLU:OE2	1:A:500:ARG:NH1	2.14	0.81
1:E:432:ILE:HG22	1:E:494:ALA:HB2	1.61	0.80
1:C:435:ASP:HB3	1:C:490:MET:HE3	1.62	0.79
1:D:380:HIS:HD2	1:D:496:TRP:HE1	1.29	0.79
1:E:75:SER:OG	1:E:179:GLN:OE1	1.98	0.79
1:C:363:GLU:O	1:C:364:ARG:CB	2.32	0.78
1:D:51:ARG:HH12	1:D:367:GLY:HA3	1.47	0.78
1:D:39:GLN:OE1	1:D:51:ARG:NH1	2.16	0.78
1:D:75:SER:OG	1:D:179:GLN:NE2	2.16	0.78
1:F:252:THR:HG21	1:F:461:LEU:HD13	1.65	0.78
1:F:14:ILE:HB	1:F:389:VAL:HG23	1.65	0.76
1:C:435:ASP:HB3	1:C:490:MET:CE	2.14	0.76
1:D:437:VAL:HG12	1:D:490:MET:HG2	1.68	0.76
1:F:242:HIS:CE1	3:F:601:DIO:H2'2	2.20	0.76
1:A:407:VAL:HG13	1:A:430:ARG:HH21	1.50	0.76
1:F:340:LYS:HG3	1:F:413:VAL:HG21	1.68	0.76
1:D:325:PHE:HE1	1:D:456:LEU:CD2	2.00	0.75
1:C:420:LYS:HB2	1:C:422:GLU:HG3	1.66	0.75
1:F:361:VAL:O	1:F:369:ALA:HA	1.87	0.75
1:D:340:LYS:HG2	1:D:413:VAL:HG11	1.67	0.75
1:A:172:ASN:OD1	3:A:601:DIO:H1'2	1.87	0.74
1:B:408:THR:HG23	1:B:430:ARG:HH21	1.53	0.74
1:E:325:PHE:HA	1:E:373:THR:HG21	1.67	0.73
1:D:432:ILE:H	1:D:432:ILE:HD12	1.54	0.73
1:C:257:ALA:CA	1:C:430:ARG:HH21	1.92	0.73
1:D:35:ASP:HA	1:D:39:GLN:HG2	1.71	0.72
1:E:252:THR:HG21	1:E:461:LEU:HD13	1.70	0.72
1:B:252:THR:HG21	1:B:461:LEU:HD13	1.69	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:172:ASN:O	1:B:174:MET:HG3	1.89	0.72
1:E:363:GLU:O	1:E:364:ARG:HB2	1.89	0.72
1:A:29:LEU:HD13	1:A:356:VAL:HG11	1.72	0.71
1:D:479:LYS:CD	1:D:489:SER:HA	2.20	0.71
1:A:128:GLY:HA2	1:A:174:MET:CE	2.21	0.71
1:D:252:THR:O	1:D:256:LEU:HD12	1.89	0.71
1:D:336:ILE:HA	1:D:339:MET:HE2	1.73	0.71
1:D:324:THR:O	1:D:373:THR:HG21	1.90	0.70
1:D:51:ARG:HH22	1:D:368:ALA:H	1.39	0.70
1:A:385:GLY:HA2	1:A:415:ILE:HD11	1.73	0.70
1:D:29:LEU:HD13	1:D:356:VAL:HG11	1.74	0.70
1:A:71:GLY:H	3:A:601:DIO:H1'2	1.56	0.70
1:A:128:GLY:HA2	1:A:174:MET:HE2	1.72	0.69
1:F:363:GLU:O	1:F:364:ARG:HB2	1.92	0.69
1:B:51:ARG:NH2	1:B:367:GLY:O	2.26	0.69
1:D:185:MET:HG2	1:D:224:TRP:HA	1.75	0.68
1:A:12:TYR:HH	1:B:12:TYR:HE2	1.39	0.68
1:E:100:ILE:HD11	1:E:312:TRP:HB3	1.76	0.67
1:F:399:HIS:ND1	1:F:409:ASP:OD1	2.24	0.67
1:D:376:TYR:HD1	1:D:379:MET:HE2	1.60	0.67
1:F:449:ARG:N	1:F:482:PHE:HE2	1.92	0.67
1:B:444:GLY:HA3	1:B:445:MET:HB3	1.76	0.67
1:C:361:VAL:HG21	1:C:370:TRP:CZ2	2.29	0.67
1:A:324:THR:HG23	1:A:462:LYS:HA	1.77	0.66
1:F:172:ASN:O	1:F:174:MET:HG3	1.96	0.66
1:D:35:ASP:HB2	1:D:39:GLN:HE21	1.59	0.66
1:D:444:GLY:HA3	1:D:445:MET:C	2.15	0.66
1:C:361:VAL:CG2	1:C:370:TRP:CE2	2.79	0.66
1:A:361:VAL:O	1:A:369:ALA:HA	1.95	0.66
1:E:31:ARG:NH1	1:E:320:GLU:OE2	2.26	0.66
1:A:172:ASN:OD1	3:A:601:DIO:C1'	2.44	0.65
1:F:337:THR:HA	1:F:340:LYS:HE3	1.79	0.65
1:D:305:ASN:OD1	1:D:305:ASN:N	2.29	0.65
1:F:449:ARG:NH2	1:F:502:GLY:HA2	2.11	0.65
1:A:240:SER:CA	1:A:241:LEU:HD23	2.27	0.65
1:D:168:TRP:HB2	1:D:208:LEU:HD23	1.78	0.64
1:D:331:VAL:HG12	1:D:335:LEU:HD21	1.77	0.64
1:F:444:GLY:HA3	1:F:445:MET:C	2.17	0.64
1:D:46:ASP:OD2	1:D:116:LYS:NZ	2.29	0.64
1:A:6:MET:HB3	1:A:394:ILE:HD13	1.78	0.64
1:E:361:VAL:O	1:E:369:ALA:HA	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:10:LYS:HA	1:E:390:LEU:HD22	1.80	0.63
1:F:48:ASP:OD2	1:F:116:LYS:NZ	2.31	0.63
1:E:77:TYR:CE2	1:E:79:TRP:HA	2.34	0.63
1:A:445:MET:HB3	1:A:449:ARG:NH1	2.14	0.63
1:D:456:LEU:C	1:D:456:LEU:HD23	2.18	0.63
1:B:53:ASP:OD1	1:B:53:ASP:N	2.32	0.62
1:D:173[B]:GLU:HG3	1:D:242:HIS:CE1	2.34	0.62
1:D:332:GLY:HA2	1:D:335:LEU:HD23	1.81	0.62
1:B:478:ASP:HA	1:B:479:LYS:CG	2.27	0.62
1:A:252:THR:OG1	1:A:326:GLU:OE1	2.18	0.62
1:D:331:VAL:O	1:D:335:LEU:CD2	2.45	0.62
1:A:451:LEU:HD11	1:A:502:GLY:HA3	1.81	0.62
1:C:5:ARG:HA	1:C:439:VAL:HG23	1.81	0.62
1:D:458:HIS:ND1	1:D:459:GLN:N	2.48	0.61
1:A:445:MET:HB3	1:A:449:ARG:HH12	1.64	0.61
1:C:172:ASN:ND2	1:C:179:GLN:OE1	2.33	0.61
1:C:478:ASP:HA	1:C:479:LYS:HB3	1.82	0.61
1:C:188:TYR:HA	1:C:191:ILE:HG22	1.82	0.61
1:A:241:LEU:CD1	1:A:269:VAL:CG2	2.77	0.61
1:F:106:GLY:O	1:F:108:ASN:N	2.34	0.61
1:C:34:TYR:HB2	1:C:315:ALA:HB2	1.83	0.61
1:B:328:ALA:HA	1:B:374:ILE:HG22	1.80	0.61
1:E:173:GLU:OE2	1:E:173:GLU:N	2.31	0.61
1:B:459:GLN:HG3	1:B:492:ARG:NH2	2.16	0.61
1:E:449:ARG:O	1:E:449:ARG:HG2	2.00	0.60
1:C:291:ASP:OD2	3:C:601:DIO:H2'1	2.01	0.60
1:D:242:HIS:CE1	3:D:601:DIO:H11	2.36	0.60
1:F:340:LYS:HG3	1:F:413:VAL:CG2	2.30	0.60
1:D:476:ASN:C	1:D:476:ASN:HD22	2.04	0.60
1:E:125:VAL:HG12	1:E:138:LEU:HD23	1.83	0.60
1:D:340:LYS:HG2	1:D:413:VAL:CG1	2.32	0.60
1:A:478:ASP:CA	1:A:479:LYS:HB3	2.32	0.60
1:B:172:ASN:ND2	3:B:601:DIO:H21	2.17	0.60
1:A:12:TYR:OH	1:B:12:TYR:HE2	1.85	0.60
1:B:51:ARG:O	1:B:54:VAL:HG22	2.02	0.60
1:D:455:VAL:HG13	1:D:457:GLU:HG2	1.83	0.60
1:F:298:HIS:HE1	1:F:327:ASP:OD2	1.85	0.60
1:F:305:ASN:O	1:F:309:ASN:HB2	2.02	0.59
1:B:482:PHE:HB2	1:B:487:LEU:HD12	1.84	0.59
1:A:340:LYS:NZ	1:A:411:GLU:OE1	2.35	0.59
1:A:10:LYS:HG3	1:A:416:TYR:HE2	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:440:SER:HB2	1:D:487:LEU:HB3	1.85	0.59
1:E:242:HIS:NE2	3:E:601:DIO:H2'2	2.18	0.59
1:F:209:VAL:HG13	1:F:238:TYR:HB2	1.84	0.59
1:D:257:ALA:HA	1:D:430:ARG:NH2	2.18	0.58
1:A:252:THR:HG21	1:A:461:LEU:HD13	1.83	0.58
1:C:483:ASP:OD1	1:C:484:ASP:N	2.35	0.58
1:D:479:LYS:HD3	1:D:489:SER:HA	1.85	0.58
1:C:51:ARG:HH12	1:C:367:GLY:HA2	1.68	0.58
1:C:23:GLY:O	1:C:349:CYS:HA	2.03	0.58
1:F:335:LEU:O	1:F:339:MET:HG2	2.04	0.58
1:D:458:HIS:CE1	1:D:460:ASP:H	2.22	0.58
1:E:277:LYS:NZ	1:E:282:SER:O	2.37	0.58
1:E:456:LEU:HD22	1:E:472:VAL:HG12	1.86	0.58
1:F:185:MET:SD	1:F:223:GLN:HG2	2.44	0.58
1:B:302:GLU:O	1:B:306:ILE:HG13	2.04	0.58
1:F:294:ASN:OD1	1:F:295:VAL:N	2.36	0.57
1:A:202:ILE:HG12	1:D:95:LEU:HD22	1.86	0.57
1:D:325:PHE:HE1	1:D:456:LEU:HD22	1.70	0.57
1:C:168:TRP:HB2	1:C:208:LEU:HD23	1.86	0.57
1:C:361:VAL:HG22	1:C:370:TRP:CE2	2.40	0.57
1:A:173:GLU:O	1:A:179[B]:GLN:HG2	2.05	0.57
1:A:324:THR:HG22	1:A:326:GLU:H	1.69	0.57
1:C:52:LYS:HD2	1:C:52:LYS:O	2.03	0.57
1:B:483:ASP:OD1	1:B:484:ASP:N	2.36	0.56
1:A:173:GLU:H	1:A:173:GLU:CD	2.07	0.56
1:A:444:GLY:HA2	1:A:445:MET:HB2	1.87	0.56
1:C:363:GLU:O	1:C:364:ARG:HB3	2.05	0.56
1:E:87:GLU:H	1:E:87:GLU:CD	2.09	0.56
1:C:454:ILE:HB	1:C:498:VAL:HG22	1.86	0.56
1:C:333:LEU:HG	1:C:428:VAL:HG21	1.87	0.56
1:E:58:VAL:HG22	1:E:353:LEU:HD11	1.88	0.56
1:F:455:VAL:HG12	1:F:457:GLU:HG2	1.87	0.56
1:B:197:ARG:HD3	1:E:177:PRO:O	2.06	0.56
1:C:361:VAL:HG21	1:C:370:TRP:CE2	2.41	0.56
1:A:127:LEU:O	1:A:174:MET:HE2	2.06	0.55
1:C:82:GLY:O	1:C:106:GLY:HA3	2.06	0.55
1:B:106:GLY:O	1:B:108:ASN:N	2.39	0.55
1:C:437:VAL:HG22	1:C:490:MET:SD	2.47	0.55
1:E:328:ALA:HB2	1:E:373:THR:HG22	1.89	0.55
1:F:409:ASP:O	1:F:410:ILE:HD12	2.07	0.55
1:D:479:LYS:HD2	1:D:489:SER:HA	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:442:VAL:O	1:F:444:GLY:N	2.40	0.55
1:F:39:GLN:OE1	1:F:51:ARG:NH1	2.40	0.55
1:C:17:ILE:HD12	1:C:21:ILE:HD11	1.89	0.55
1:A:128:GLY:CA	1:A:174:MET:CE	2.85	0.55
1:A:206:ILE:HD12	1:A:208:LEU:HD21	1.89	0.55
1:C:51:ARG:O	1:C:54:VAL:HG22	2.07	0.55
1:D:8:VAL:HG22	1:D:442:VAL:HA	1.89	0.55
1:D:188:TYR:HA	1:D:191:ILE:HG22	1.89	0.54
1:E:23:GLY:HA2	1:E:63:VAL:HG13	1.89	0.54
1:D:479:LYS:HB3	1:D:479:LYS:NZ	2.22	0.54
1:E:106:GLY:O	1:E:108:ASN:N	2.40	0.54
1:A:252:THR:O	1:A:256:LEU:HD12	2.07	0.54
1:B:333:LEU:O	1:B:337:THR:HG23	2.07	0.54
1:B:392:PRO:HG3	1:B:413:VAL:HG23	1.90	0.54
1:F:376:TYR:CE2	1:F:473:TYR:HA	2.42	0.54
1:A:10:LYS:HG3	1:A:416:TYR:CE2	2.42	0.54
1:C:363:GLU:O	1:C:364:ARG:HB2	2.07	0.54
1:B:175:ASP:OD1	1:B:214:SER:OG	2.23	0.54
1:B:17:ILE:HD13	1:B:385:GLY:O	2.08	0.54
1:C:308:GLN:O	1:C:309:ASN:ND2	2.41	0.54
1:A:83:VAL:HG13	1:A:107:ILE:HD13	1.89	0.54
1:B:336:ILE:HA	1:B:339:MET:HE2	1.90	0.54
1:B:437:VAL:HG23	1:B:490:MET:HB2	1.90	0.54
1:D:417:ASN:HD22	1:D:420:LYS:HE2	1.71	0.54
1:E:262:LEU:HD22	1:E:334:MET:HG2	1.90	0.54
1:A:429:ASN:HD21	1:A:436:ILE:HG13	1.72	0.53
1:C:479:LYS:HE3	1:C:490:MET:HG2	1.89	0.53
1:D:82:GLY:O	1:D:106:GLY:HA3	2.07	0.53
1:D:429:ASN:ND2	1:D:436:ILE:HG22	2.23	0.53
1:D:478:ASP:HB3	1:D:479:LYS:HG3	1.89	0.53
1:F:450:LEU:HD12	1:F:501:ILE:HG22	1.90	0.53
1:B:202:ILE:HG12	1:E:95:LEU:HD22	1.90	0.53
1:E:29:LEU:HD13	1:E:356:VAL:HG11	1.90	0.53
1:A:278:ALA:HB3	1:B:222:PRO:HG3	1.90	0.53
1:E:478:ASP:HB3	1:E:479:LYS:C	2.28	0.53
1:F:242:HIS:HE1	3:F:601:DIO:H2'2	1.73	0.53
1:A:112:LYS:HA	1:A:115:LYS:HG3	1.91	0.53
1:E:335:LEU:O	1:E:339:MET:HG2	2.08	0.53
1:C:210:ALA:HB2	1:C:236:VAL:HG11	1.91	0.53
1:B:487:LEU:HD13	1:B:501:ILE:HD11	1.90	0.53
1:B:361:VAL:O	1:B:369:ALA:HA	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:175:ASP:HB3	1:D:224:TRP:CZ3	2.44	0.52
1:E:298:HIS:HE1	1:E:327:ASP:OD2	1.93	0.52
1:E:408:THR:OG1	1:E:430:ARG:NH2	2.41	0.52
1:E:411:GLU:OE1	1:E:430:ARG:NH2	2.42	0.52
1:E:97:TRP:O	1:E:99:SER:OG	2.23	0.52
1:A:12:TYR:HE2	1:B:12:TYR:HD2	1.58	0.52
1:B:167:VAL:HG22	1:B:207:GLU:HB2	1.91	0.52
1:B:51:ARG:NH2	1:B:368:ALA:O	2.37	0.52
1:C:51:ARG:NH2	1:C:53:ASP:OD2	2.26	0.52
1:B:302:GLU:O	1:B:302:GLU:HG3	2.10	0.52
1:D:6:MET:SD	1:D:394:ILE:HD11	2.50	0.52
1:D:479:LYS:CB	1:D:479:LYS:NZ	2.73	0.52
1:B:473:TYR:CZ	1:B:475:LYS:HE3	2.44	0.52
1:C:127:LEU:O	1:C:183:LYS:HE2	2.10	0.52
1:A:241:LEU:HD11	1:A:269:VAL:CB	2.39	0.52
1:E:149:LYS:HG2	1:E:150:TYR:CD1	2.45	0.52
1:F:177:PRO:HD2	1:F:178:TRP:CZ3	2.45	0.52
1:A:141:TYR:O	1:A:154:ARG:HD3	2.10	0.52
1:A:172:ASN:OD1	3:A:601:DIO:O1'	2.28	0.52
1:D:61:LEU:HD22	1:D:378:PHE:HD2	1.74	0.52
1:E:71:GLY:O	1:E:74:VAL:HG12	2.10	0.52
1:A:250:ASN:OD1	1:A:462:LYS:NZ	2.28	0.51
1:D:242:HIS:HE1	3:D:601:DIO:H11	1.76	0.51
1:A:61:LEU:HD22	1:A:378:PHE:HD1	1.74	0.51
1:D:100:ILE:HD12	1:D:312:TRP:HB3	1.92	0.51
1:D:55:ILE:HG23	1:D:117:VAL:HG12	1.91	0.51
1:E:424:THR:HG23	1:E:500:ARG:HG2	1.92	0.51
1:B:29:LEU:HD13	1:B:356:VAL:HG11	1.92	0.51
1:B:439:VAL:HG12	1:B:488:THR:HG23	1.93	0.51
1:B:28:HIS:NE2	1:B:68:TYR:OH	2.33	0.51
1:C:444:GLY:HA3	1:C:445:MET:HB3	1.93	0.51
1:F:79:TRP:CG	1:F:138:LEU:HD13	2.44	0.51
1:E:450:LEU:HB2	1:E:482:PHE:HB2	1.93	0.51
1:F:438:LEU:HB2	1:F:491:LEU:HD11	1.92	0.51
1:F:479:LYS:HZ1	1:F:482:PHE:N	2.08	0.51
1:A:324:THR:HG22	1:A:326:GLU:N	2.25	0.51
1:E:328:ALA:CB	1:E:373:THR:HG22	2.40	0.51
1:A:492:ARG:HG2	1:A:493:ARG:O	2.11	0.51
1:F:121:ILE:HG21	1:F:123:MET:HE1	1.93	0.51
1:C:7:THR:HG22	1:C:441:ASP:HB3	1.93	0.51
1:E:449:ARG:N	1:E:482:PHE:CE2	2.79	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:436:ILE:HD12	1:D:437:VAL:H	1.76	0.51
1:D:107:ILE:H	1:D:107:ILE:HD12	1.76	0.50
1:D:17:ILE:HG13	1:D:389:VAL:HG23	1.92	0.50
1:E:262:LEU:O	1:E:266:ILE:HG13	2.10	0.50
1:A:478:ASP:HB3	1:A:479:LYS:C	2.31	0.50
1:E:422:GLU:HA	1:E:501:ILE:O	2.12	0.50
1:E:296:TRP:CZ2	1:E:319:LEU:HD21	2.46	0.50
1:D:361:VAL:O	1:D:369:ALA:HA	2.11	0.50
1:F:87:GLU:H	1:F:87:GLU:CD	2.12	0.50
1:D:139:LEU:HD23	1:D:202:ILE:HB	1.94	0.50
1:E:51:ARG:O	1:E:54:VAL:HG22	2.12	0.49
1:F:6:MET:HB2	1:F:394:ILE:HD12	1.93	0.49
1:B:376:TYR:CE2	1:B:474:PRO:HD3	2.47	0.49
1:C:39:GLN:HG3	1:C:51:ARG:HG2	1.93	0.49
1:D:492:ARG:HG3	1:D:493:ARG:N	2.27	0.49
1:D:77:TYR:CE2	1:D:79:TRP:HA	2.47	0.49
1:A:15:ALA:HB2	1:A:343:ASP:HB3	1.94	0.49
1:C:361:VAL:CG2	1:C:370:TRP:NE1	2.75	0.49
1:B:174:MET:HE1	1:B:188:TYR:CE1	2.47	0.49
1:C:241:LEU:O	1:C:242:HIS:HD2	1.95	0.49
1:B:139:LEU:HD23	1:B:202:ILE:HB	1.92	0.49
1:C:53:ASP:N	1:C:53:ASP:OD1	2.44	0.49
1:F:393:VAL:C	1:F:394:ILE:HD13	2.32	0.49
1:F:6:MET:O	1:F:440:SER:HA	2.13	0.49
1:F:449:ARG:N	1:F:482:PHE:CE2	2.77	0.49
1:A:12:TYR:HE2	1:B:12:TYR:CD2	2.29	0.49
1:B:70:GLY:O	3:B:601:DIO:H2'2	2.12	0.49
1:C:29:LEU:HG	1:C:97:TRP:CE2	2.48	0.49
1:F:371:ARG:HG2	1:F:375:PHE:CG	2.47	0.49
1:A:107:ILE:H	1:A:107:ILE:HD12	1.78	0.49
1:C:435:ASP:HB3	1:C:490:MET:HE1	1.93	0.49
1:E:389:VAL:HA	1:E:415:ILE:HG22	1.95	0.49
1:C:132:ILE:HD11	1:C:194:GLU:HB3	1.95	0.49
1:C:455:VAL:HG11	1:C:457:GLU:OE1	2.12	0.49
1:A:453:HIS:CD2	1:A:455:VAL:HG23	2.48	0.48
1:C:29:LEU:HD13	1:C:356:VAL:HG11	1.95	0.48
1:D:29:LEU:HD21	1:D:319:LEU:HD13	1.95	0.48
1:D:331:VAL:HG12	1:D:335:LEU:CD2	2.41	0.48
1:E:145:PRO:HA	1:E:162:PRO:HG3	1.96	0.48
1:A:442:VAL:O	1:A:444:GLY:N	2.47	0.48
1:B:383:LYS:HD3	1:B:384:TYR:CE1	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:298:HIS:HB2	1:C:321:ASP:CG	2.34	0.48
1:C:169[B]:CYS:SG	3:C:601:DIO:H22	2.53	0.48
1:C:175:ASP:HB3	1:C:224:TRP:CZ3	2.47	0.48
1:E:241:LEU:O	1:E:242:HIS:HD2	1.97	0.48
1:E:298:HIS:HB2	1:E:321:ASP:CG	2.33	0.48
1:D:125:VAL:O	1:D:171:GLY:HA2	2.14	0.48
1:E:450:LEU:C	1:E:450:LEU:HD23	2.34	0.48
1:E:483:ASP:OD1	1:E:484:ASP:N	2.46	0.48
1:F:376:TYR:HB3	1:F:456:LEU:HD11	1.96	0.48
1:F:60:GLU:OE1	1:F:371:ARG:NH2	2.46	0.48
1:B:203:ASP:O	1:B:206:ILE:HG12	2.13	0.48
1:D:457:GLU:OE2	1:D:492:ARG:HB3	2.14	0.48
1:F:467:VAL:HG22	1:F:467:VAL:O	2.13	0.48
1:A:371:ARG:HD3	1:A:375:PHE:CD1	2.49	0.48
1:D:214:SER:O	1:D:242:HIS:HB2	2.14	0.48
1:E:241:LEU:HD11	1:E:288:LEU:HG	1.96	0.48
1:A:239:ILE:HG23	1:A:241:LEU:HD21	1.95	0.47
1:C:241:LEU:HD11	1:C:288:LEU:HG	1.95	0.47
1:C:371:ARG:HD3	1:C:375:PHE:CD1	2.49	0.47
1:E:4:ALA:O	1:E:438:LEU:HD12	2.14	0.47
1:A:239:ILE:HG23	1:A:239:ILE:O	2.14	0.47
1:D:256:LEU:O	1:D:430:ARG:CZ	2.58	0.47
1:A:483:ASP:CG	1:A:484:ASP:N	2.67	0.47
1:B:408:THR:HG23	1:B:430:ARG:NH2	2.27	0.47
1:D:35:ASP:CB	1:D:39:GLN:HE21	2.27	0.47
1:D:491:LEU:HD22	1:D:497:ASN:CG	2.34	0.47
1:F:333:LEU:HD22	1:F:430:ARG:HH11	1.78	0.47
1:B:34:TYR:HB2	1:B:315:ALA:HB2	1.96	0.47
1:C:122:MET:HG3	1:C:167:VAL:HG23	1.96	0.47
1:A:449:ARG:N	1:A:482:PHE:CD2	2.83	0.47
1:B:376:TYR:CZ	1:B:474:PRO:HD3	2.49	0.47
1:C:51:ARG:HH12	1:C:367:GLY:CA	2.27	0.47
1:D:112:LYS:HB2	1:D:112:LYS:HE3	1.60	0.47
1:E:420:LYS:O	1:E:422:GLU:HG3	2.14	0.47
1:F:336:ILE:HG22	1:F:340:LYS:HE2	1.96	0.47
1:C:8:VAL:HG22	1:C:442:VAL:HA	1.97	0.47
1:A:243:GLN:O	1:A:293:TRP:HA	2.15	0.47
1:B:351:ALA:HA	1:B:352:GLN:HA	1.60	0.47
1:C:333:LEU:HD11	1:C:430:ARG:HG2	1.96	0.47
1:C:8:VAL:O	1:C:9:ASP:HB2	2.15	0.47
1:E:172:ASN:O	1:E:174:MET:HE2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:410:ILE:HD13	1:F:436:ILE:HD12	1.97	0.47
1:F:460:ASP:HB3	1:F:463:ILE:HB	1.96	0.47
1:C:17:ILE:HG12	1:C:389:VAL:HG23	1.97	0.47
1:E:487:LEU:HD13	1:E:501:ILE:HD11	1.97	0.47
1:B:230:ASP:OD2	1:B:279:LYS:HE3	2.15	0.47
1:B:51:ARG:NH1	1:B:53:ASP:OD2	2.35	0.47
1:E:24:SER:O	1:E:66:ILE:HA	2.16	0.46
1:F:293:TRP:O	1:F:294:ASN:HB2	2.14	0.46
1:B:51:ARG:NH1	1:B:53:ASP:OD1	2.48	0.46
1:A:460:ASP:HB3	1:A:463:ILE:HB	1.96	0.46
1:A:61:LEU:HD23	1:A:61:LEU:HA	1.77	0.46
1:D:336:ILE:O	1:D:340:LYS:HG3	2.15	0.46
1:F:197:ARG:NH1	1:F:235:TYR:OH	2.48	0.46
1:F:22:TYR:O	1:F:64:PRO:HD2	2.16	0.46
1:F:86:VAL:HA	1:F:89:ARG:HG3	1.97	0.46
1:E:140:GLU:HG3	1:F:93:LEU:HD11	1.97	0.46
1:A:363:GLU:O	1:A:364:ARG:HB2	2.16	0.46
1:C:173:GLU:H	1:C:173:GLU:CD	2.19	0.46
1:A:224:TRP:O	1:A:228:VAL:HG23	2.15	0.46
1:B:459:GLN:HG3	1:B:492:ARG:HH22	1.81	0.46
1:D:458:HIS:ND1	1:D:460:ASP:N	2.54	0.46
1:F:123:MET:HE2	1:F:165:ILE:HD13	1.98	0.46
1:F:55:ILE:O	1:F:59:LYS:HG3	2.16	0.46
1:D:262:LEU:HD11	1:D:290:PHE:CE2	2.51	0.46
1:D:442:VAL:O	1:D:444:GLY:N	2.44	0.46
1:D:380:HIS:CD2	1:D:496:TRP:HE1	2.20	0.46
1:E:371:ARG:HD3	1:E:375:PHE:CD1	2.51	0.46
1:F:53:ASP:N	1:F:53:ASP:OD1	2.49	0.46
1:D:154:ARG:HD2	1:D:159:VAL:O	2.16	0.46
1:D:27:GLU:HG2	1:D:29:LEU:HB2	1.97	0.46
1:C:384:TYR:HB3	1:C:424:THR:HG21	1.98	0.46
1:D:243:GLN:O	1:D:293:TRP:HA	2.16	0.46
1:D:417:ASN:ND2	1:D:420:LYS:HE2	2.31	0.46
1:A:324:THR:CG2	1:A:462:LYS:HA	2.46	0.45
1:E:351:ALA:HA	1:E:352:GLN:HA	1.56	0.45
1:A:29:LEU:HD23	1:A:30:GLY:N	2.31	0.45
1:B:174:MET:CE	1:B:188:TYR:CD1	2.99	0.45
1:B:90:PRO:O	1:B:103:ASN:ND2	2.46	0.45
1:A:209:VAL:HG13	1:A:238:TYR:HB2	1.98	0.45
1:A:371:ARG:HD3	1:A:375:PHE:CE1	2.51	0.45
1:C:453:HIS:O	1:C:453:HIS:ND1	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:114:CYS:HA	1:C:117:VAL:HG22	1.99	0.45
1:C:299:SER:OG	1:C:321:ASP:OD1	2.30	0.45
1:E:51:ARG:NH1	1:E:367:GLY:O	2.50	0.45
1:B:343:ASP:OD1	1:B:343:ASP:N	2.50	0.45
1:C:29:LEU:HD21	1:C:319:LEU:HD13	1.97	0.45
1:F:336:ILE:HG23	1:F:413:VAL:HG23	1.98	0.45
1:A:373:THR:HG22	1:A:472:VAL:HB	1.99	0.45
1:C:449:ARG:N	1:C:482:PHE:HE2	2.13	0.45
1:D:132:ILE:HD11	1:D:194:GLU:HB3	1.98	0.45
1:D:216:LYS:HB3	1:D:265:PHE:CE1	2.52	0.45
1:F:188:TYR:HA	1:F:191:ILE:HG22	1.99	0.45
1:B:461:LEU:HD21	1:B:494:ALA:HB1	1.99	0.45
1:B:492:ARG:HG3	1:B:493:ARG:N	2.30	0.45
1:B:425:ILE:HG23	1:B:499:ILE:HB	1.99	0.45
1:C:68:TYR:CD1	1:C:69:PRO:HA	2.52	0.45
1:D:53:ASP:N	1:D:53:ASP:OD1	2.50	0.45
1:B:174:MET:HE3	1:B:188:TYR:CD1	2.52	0.45
1:B:294:ASN:ND2	1:B:357:ILE:O	2.50	0.45
1:E:51:ARG:HB2	1:E:54:VAL:HG22	1.98	0.45
1:A:58:VAL:CG2	1:A:117:VAL:HB	2.47	0.44
1:B:172:ASN:O	1:B:173[A]:GLU:C	2.55	0.44
1:B:383:LYS:HD3	1:B:384:TYR:CZ	2.52	0.44
1:C:498:VAL:O	1:C:498:VAL:HG23	2.16	0.44
1:E:359:PRO:HA	1:E:372:GLN:HB2	1.99	0.44
1:F:351:ALA:HA	1:F:352:GLN:HA	1.63	0.44
1:A:53:ASP:N	1:A:53:ASP:OD1	2.47	0.44
1:B:24:SER:OG	1:B:25:PHE:N	2.49	0.44
1:F:238:TYR:HA	1:F:287:TYR:O	2.17	0.44
1:C:423:VAL:HG12	1:C:423:VAL:O	2.17	0.44
1:F:455:VAL:HG21	1:F:478:ASP:OD2	2.18	0.44
1:F:242:HIS:NE2	3:F:601:DIO:H2'2	2.31	0.44
1:A:4:ALA:O	1:A:438:LEU:HA	2.18	0.44
1:A:51:ARG:HB2	1:A:54:VAL:HG12	2.00	0.44
1:C:42:ASN:HB3	1:C:45:SER:OG	2.16	0.44
1:D:65:ILE:HA	1:D:120:GLU:O	2.18	0.44
1:D:35:ASP:HB2	1:D:39:GLN:NE2	2.31	0.44
1:E:344:ARG:HD2	1:E:344:ARG:HA	1.72	0.44
1:B:162:PRO:HG2	1:B:164:ASN:OD1	2.17	0.44
1:B:477:SER:O	1:B:478:ASP:HB2	2.17	0.44
1:D:293:TRP:O	1:D:294:ASN:HB2	2.17	0.44
1:D:71:GLY:O	1:D:74:VAL:HG12	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:368:ALA:O	1:F:369:ALA:HB3	2.18	0.44
1:F:60:GLU:CD	1:F:371:ARG:HH21	2.21	0.44
1:E:368:ALA:O	1:E:369:ALA:HB3	2.17	0.44
1:E:371:ARG:HD3	1:E:375:PHE:CE1	2.52	0.44
1:F:262:LEU:HD22	1:F:334:MET:HG2	2.00	0.44
1:F:65:ILE:HD11	1:F:122:MET:HB2	2.00	0.44
1:A:416:TYR:CE1	1:A:418:GLU:HA	2.52	0.44
1:A:432:ILE:HG22	1:A:494:ALA:HB2	1.99	0.44
1:D:328:ALA:HB2	1:D:373:THR:HG23	2.00	0.44
1:F:139:LEU:HA	1:F:168:TRP:CH2	2.53	0.44
1:A:32:ALA:HB2	1:A:356:VAL:HG23	2.00	0.43
1:A:449:ARG:N	1:A:482:PHE:HD2	2.16	0.43
1:B:127:LEU:HD23	1:B:127:LEU:HA	1.85	0.43
1:A:12:TYR:CZ	1:B:12:TYR:HE2	2.36	0.43
1:D:456:LEU:C	1:D:456:LEU:CD2	2.86	0.43
1:A:351:ALA:HA	1:A:352:GLN:HA	1.67	0.43
1:A:407:VAL:CG1	1:A:430:ARG:HH21	2.25	0.43
1:C:353:LEU:O	1:C:358:ALA:HB1	2.18	0.43
1:C:32:ALA:O	1:C:37:LEU:HD23	2.17	0.43
1:A:363:GLU:HB2	1:A:367:GLY:HA2	2.00	0.43
1:B:303:ASP:O	1:B:307:MET:HG2	2.18	0.43
1:D:126:ASN:ND2	1:D:130:ARG:HG3	2.34	0.43
1:F:107:ILE:CD1	1:F:138:LEU:HD11	2.48	0.43
1:A:257:ALA:CB	1:A:404:HIS:HD2	2.32	0.43
1:C:52:LYS:NZ	1:C:56:GLU:OE1	2.47	0.43
1:E:230:ASP:O	1:E:280:LYS:HE3	2.18	0.43
1:F:459:GLN:CD	1:F:459:GLN:H	2.22	0.43
1:A:461:LEU:HA	1:A:461:LEU:HD23	1.86	0.43
1:B:55:ILE:HG22	1:B:59:LYS:HE2	2.00	0.43
1:E:356:VAL:O	1:E:357:ILE:C	2.56	0.43
1:B:188:TYR:HA	1:B:191:ILE:HG22	2.01	0.43
1:D:190:ARG:HD2	1:D:190:ARG:HA	1.77	0.43
1:D:388:ILE:O	1:D:415:ILE:HA	2.19	0.43
1:D:453:HIS:ND1	1:D:499:ILE:HG12	2.34	0.43
1:F:125:VAL:O	1:F:171:GLY:HA2	2.19	0.43
1:A:55:ILE:HG23	1:A:117:VAL:HG12	2.00	0.43
1:B:95:LEU:CD2	1:F:202:ILE:HG12	2.49	0.43
1:C:460:ASP:O	1:C:463:ILE:HG22	2.19	0.43
1:C:478:ASP:HA	1:C:479:LYS:CB	2.49	0.43
1:D:174:MET:HA	1:D:179:GLN:HG2	2.01	0.43
1:F:230:ASP:O	1:F:280:LYS:NZ	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:214:SER:O	1:F:242:HIS:HB2	2.18	0.43
1:A:72:ASN:ND2	1:A:179[A]:GLN:OE1	2.51	0.43
1:A:257:ALA:HB2	1:A:407:VAL:HG11	2.00	0.43
1:A:305:ASN:O	1:A:309:ASN:HB2	2.18	0.43
1:C:238:TYR:HA	1:C:287:TYR:O	2.19	0.43
1:D:479:LYS:HB3	1:D:479:LYS:HZ2	1.84	0.43
1:E:114:CYS:HA	1:E:117:VAL:HG22	2.01	0.43
1:E:202:ILE:HG12	1:F:95:LEU:HD22	2.00	0.43
1:A:241:LEU:CD1	1:A:269:VAL:CB	2.97	0.43
1:B:177:PRO:HD2	1:B:178:TRP:CZ3	2.54	0.43
1:B:456:LEU:HD12	1:B:456:LEU:HA	1.72	0.43
1:C:339:MET:HE3	1:C:413:VAL:HG11	2.00	0.43
1:C:374:ILE:O	1:C:377:PRO:HD2	2.18	0.43
1:C:478:ASP:HB3	1:C:479:LYS:C	2.39	0.43
1:E:333:LEU:HD21	1:E:430:ARG:HD3	2.01	0.43
1:E:456:LEU:HD23	1:E:456:LEU:HA	1.94	0.43
1:A:456:LEU:HB2	1:A:496:TRP:HD1	1.83	0.43
1:B:31:ARG:NE	1:B:320:GLU:OE2	2.41	0.43
1:C:39:GLN:HG3	1:C:51:ARG:CG	2.49	0.43
1:E:112:LYS:HE2	1:E:112:LYS:HB2	1.74	0.43
1:F:440:SER:HB2	1:F:487:LEU:HB3	1.99	0.43
1:A:27:GLU:HG3	1:A:70:GLY:HA2	2.01	0.42
1:B:2:LYS:HB3	1:B:2:LYS:HE2	1.73	0.42
1:F:123:MET:HE2	1:F:123:MET:HB2	1.76	0.42
1:B:172:ASN:HD22	3:B:601:DIO:H21	1.84	0.42
1:D:479:LYS:HD3	1:D:489:SER:OG	2.18	0.42
1:F:463:ILE:HD12	1:F:464:ARG:H	1.84	0.42
1:B:32:ALA:HB2	1:B:356:VAL:HG23	2.01	0.42
1:B:342:ALA:O	1:B:346:LYS:HE2	2.18	0.42
1:C:25:PHE:O	1:C:352:GLN:HB3	2.19	0.42
1:C:343:ASP:N	1:C:343:ASP:OD1	2.50	0.42
1:C:422:GLU:HA	1:C:501:ILE:O	2.19	0.42
1:D:229:LEU:HA	1:D:229:LEU:HD23	1.92	0.42
1:D:442:VAL:HG23	1:D:442:VAL:O	2.19	0.42
1:E:221:PHE:HA	1:E:222:PRO:HA	1.76	0.42
1:E:429:ASN:OD1	1:E:431:ASN:N	2.50	0.42
1:F:324:THR:OG1	1:F:326:GLU:HG2	2.19	0.42
1:A:126:ASN:ND2	1:A:130:ARG:HG3	2.34	0.42
1:C:149:LYS:HD3	1:C:150:TYR:CE2	2.55	0.42
1:C:52:LYS:HZ2	1:C:56:GLU:HG2	1.84	0.42
1:C:52:LYS:NZ	1:C:56:GLU:HG2	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:246:GLY:HA2	1:B:297:TYR:CD1	2.55	0.42
1:B:478:ASP:HA	1:B:479:LYS:CB	2.50	0.42
1:C:351:ALA:HA	1:C:352:GLN:HA	1.59	0.42
1:C:61:LEU:HD22	1:C:378:PHE:HD1	1.84	0.42
1:D:232:ALA:O	1:D:236:VAL:HG22	2.19	0.42
1:D:257:ALA:CA	1:D:430:ARG:NH2	2.82	0.42
1:E:177:PRO:HD2	1:E:178:TRP:CZ3	2.54	0.42
1:F:376:TYR:CB	1:F:456:LEU:HD11	2.49	0.42
1:C:428:VAL:HG12	1:C:496:TRP:HA	2.01	0.42
1:B:442:VAL:O	1:B:444:GLY:N	2.53	0.42
1:B:61:LEU:HD22	1:B:378:PHE:HD2	1.85	0.42
1:D:453:HIS:CE1	1:D:499:ILE:HG12	2.55	0.42
1:A:58:VAL:HG23	1:A:117:VAL:HB	2.02	0.42
1:A:376:TYR:CD2	1:A:473:TYR:HA	2.54	0.42
1:B:123:MET:HE2	1:B:165:ILE:HD13	2.01	0.42
1:D:185:MET:HE2	1:D:185:MET:HB2	1.77	0.42
1:D:209:VAL:HG13	1:D:238:TYR:HB2	2.00	0.42
1:D:276:ILE:HA	1:D:276:ILE:HD13	1.89	0.42
1:D:476:ASN:C	1:D:476:ASN:ND2	2.72	0.42
1:A:453:HIS:HD2	1:A:455:VAL:HG23	1.83	0.42
1:B:408:THR:CG2	1:B:430:ARG:HH21	2.28	0.42
1:C:79:TRP:CD2	1:C:138:LEU:HD13	2.55	0.42
1:D:432:ILE:CD1	1:D:432:ILE:H	2.24	0.42
1:D:487:LEU:HD21	1:D:499:ILE:HG21	2.01	0.42
1:E:156:LYS:O	1:E:156:LYS:HG2	2.20	0.42
1:E:478:ASP:HA	1:E:479:LYS:CB	2.36	0.42
1:A:203:ASP:OD1	1:A:205:SER:OG	2.33	0.42
1:A:444:GLY:HA2	1:A:445:MET:CB	2.48	0.42
1:B:38:TYR:CE1	1:B:40:PRO:HG3	2.54	0.42
1:C:46:ASP:HB2	1:C:47:GLU:H	1.68	0.42
1:B:95:LEU:HB2	1:B:180:VAL:HG21	2.02	0.41
1:B:376:TYR:CE2	1:B:473:TYR:HA	2.55	0.41
1:B:10:LYS:HA	1:B:390:LEU:HD22	2.02	0.41
1:D:479:LYS:HE2	1:D:488:THR:O	2.20	0.41
1:E:363:GLU:HB2	1:E:367:GLY:HA3	2.02	0.41
1:F:456:LEU:HD22	1:F:472:VAL:HG13	2.02	0.41
1:D:216:LYS:HB2	1:D:216:LYS:HE3	1.60	0.41
1:E:14:ILE:HG13	1:E:391:GLN:HA	2.01	0.41
1:A:420:LYS:O	1:A:422:GLU:HG3	2.20	0.41
1:B:238:TYR:HA	1:B:287:TYR:O	2.20	0.41
1:C:210:ALA:O	1:C:239:ILE:HD12	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:241:LEU:C	1:C:242:HIS:HD2	2.24	0.41
1:C:252:THR:HG23	1:C:326:GLU:OE1	2.20	0.41
1:D:436:ILE:HD12	1:D:437:VAL:N	2.35	0.41
1:D:97:TRP:O	1:D:98:LYS:C	2.59	0.41
1:A:451:LEU:HD12	1:A:451:LEU:N	2.35	0.41
1:A:12:TYR:CE2	1:B:12:TYR:CD2	3.08	0.41
1:B:297:TYR:CZ	1:B:298:HIS:CE1	3.08	0.41
1:B:77:TYR:CE2	1:B:79:TRP:HA	2.55	0.41
1:C:174:MET:HE2	1:C:174:MET:HB2	1.81	0.41
1:D:31:ARG:HD2	1:D:35:ASP:OD1	2.20	0.41
1:B:31:ARG:HD2	1:B:35:ASP:OD2	2.21	0.41
1:D:293:TRP:CH2	1:D:350:LEU:HD12	2.55	0.41
1:D:371:ARG:HD3	1:D:375:PHE:CD1	2.55	0.41
1:F:173[A]:GLU:HG2	1:F:242:HIS:CE1	2.55	0.41
1:A:297:TYR:CZ	1:A:298:HIS:CE1	3.09	0.41
1:F:229:LEU:O	1:F:233:TYR:HB2	2.19	0.41
1:A:294:ASN:OD1	1:A:295:VAL:N	2.49	0.41
1:A:385:GLY:CA	1:A:415:ILE:HD11	2.48	0.41
1:B:172:ASN:HD22	3:B:601:DIO:H12	1.86	0.41
1:D:35:ASP:CA	1:D:39:GLN:HE21	2.34	0.41
1:E:111:ALA:HA	1:E:121:ILE:HD11	2.02	0.41
1:E:454:ILE:HG22	1:E:455:VAL:H	1.85	0.41
1:F:423:VAL:HG22	1:F:501:ILE:HG12	2.01	0.41
1:A:276:ILE:HD13	1:A:276:ILE:HA	1.89	0.41
1:A:23:GLY:O	1:A:349:CYS:HA	2.21	0.41
1:A:368:ALA:O	1:A:369:ALA:HB3	2.20	0.41
1:C:319:LEU:HB2	1:C:356:VAL:HG13	2.03	0.41
1:C:364:ARG:O	1:C:366:GLY:N	2.54	0.41
1:D:100:ILE:CD1	1:D:312:TRP:HB3	2.50	0.41
1:A:324:THR:CG2	1:A:326:GLU:HG2	2.49	0.41
1:A:482:PHE:HA	1:A:486:ILE:O	2.21	0.41
1:F:363:GLU:O	1:F:364:ARG:CB	2.65	0.41
1:A:376:TYR:CE2	1:A:473:TYR:HA	2.55	0.41
1:B:139:LEU:HD12	1:B:168:TRP:CZ2	2.55	0.41
1:C:409:ASP:O	1:C:410:ILE:HD13	2.21	0.41
1:D:325:PHE:CE1	1:D:456:LEU:CD2	2.90	0.41
1:D:456:LEU:HD21	1:D:472:VAL:HG13	2.02	0.41
1:E:121:ILE:HB	1:E:165:ILE:HD13	2.01	0.41
1:E:229:LEU:HD23	1:E:229:LEU:HA	1.89	0.41
1:E:294:ASN:OD1	1:E:295:VAL:N	2.50	0.41
1:B:173[B]:GLU:OE2	1:B:214:SER:HA	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:309:ASN:C	1:C:311:PRO:HD3	2.41	0.41
1:C:39:GLN:HE21	1:C:51:ARG:HG3	1.86	0.41
1:D:101:GLU:HG3	1:D:103:ASN:ND2	2.36	0.41
1:D:422:GLU:OE1	1:D:500:ARG:NH2	2.31	0.41
1:E:262:LEU:HD11	1:E:290:PHE:CZ	2.56	0.41
1:F:240:SER:HA	1:F:289:SER:O	2.21	0.41
1:A:173:GLU:N	1:A:173:GLU:CD	2.69	0.40
1:A:333:LEU:HG	1:A:428:VAL:HG11	2.03	0.40
1:B:307:MET:O	1:B:307:MET:HG3	2.21	0.40
1:B:483:ASP:CG	1:B:484:ASP:N	2.74	0.40
1:D:353:LEU:O	1:D:354:ILE:HD13	2.21	0.40
1:F:51:ARG:O	1:F:54:VAL:HG22	2.21	0.40
1:A:216:LYS:HB3	1:A:265:PHE:CE1	2.56	0.40
1:A:72:ASN:HD22	1:A:179[A]:GLN:CD	2.24	0.40
1:B:456:LEU:HB2	1:B:496:TRP:HD1	1.87	0.40
1:E:13:LYS:HB2	1:E:13:LYS:HE2	1.81	0.40
1:E:174:MET:HB3	1:E:183:LYS:H	1.86	0.40
1:F:10:LYS:O	1:F:13:LYS:HD3	2.20	0.40
1:E:197:ARG:HD3	1:F:177:PRO:O	2.21	0.40
1:C:239:ILE:HA	1:C:239:ILE:HD12	1.85	0.40
1:D:328:ALA:HA	1:D:374:ILE:HG22	2.04	0.40
1:D:384:TYR:HB2	1:D:424:THR:HG21	2.03	0.40
1:E:340:LYS:HB3	1:E:340:LYS:HE2	1.95	0.40
1:E:78:PHE:CD1	1:E:78:PHE:N	2.89	0.40
1:C:455:VAL:HG22	1:C:497:ASN:HD22	1.86	0.40
1:C:71:GLY:O	1:C:74:VAL:HG12	2.22	0.40
1:E:453:HIS:CD2	1:E:453:HIS:C	2.95	0.40
1:A:307:MET:HG3	1:A:307:MET:O	2.21	0.40
1:D:389:VAL:HG22	1:D:415:ILE:HD11	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	491/501 (98%)	447 (91%)	36 (7%)	8 (2%)	9	31
1	B	491/501 (98%)	436 (89%)	42 (9%)	13 (3%)	5	19
1	C	491/501 (98%)	438 (89%)	40 (8%)	13 (3%)	5	19
1	D	491/501 (98%)	427 (87%)	55 (11%)	9 (2%)	8	28
1	E	490/501 (98%)	438 (89%)	39 (8%)	13 (3%)	5	18
1	F	491/501 (98%)	441 (90%)	38 (8%)	12 (2%)	6	21
All	All	2945/3006 (98%)	2627 (89%)	250 (8%)	68 (2%)	6	22

All (68) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	173	GLU
1	A	364	ARG
1	A	444	GLY
1	A	484	ASP
1	B	250	ASN
1	B	368	ALA
1	B	443	ARG
1	C	364	ARG
1	C	365	ASN
1	C	368	ALA
1	C	421	GLU
1	D	484	ASP
1	E	107	ILE
1	E	364	ARG
1	F	40	PRO
1	F	364	ARG
1	A	367	GLY
1	A	369	ALA
1	B	164	ASN
1	B	367	GLY
1	B	369	ALA
1	C	9	ASP
1	C	173	GLU
1	D	35	ASP
1	D	98	LYS
1	D	368	ALA
1	E	46	ASP
1	E	250	ASN
1	E	357	ILE
1	E	367	GLY

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Mol	Chain	Res	Type
1	F	28	HIS
1	F	173[A]	GLU
1	F	173[B]	GLU
1	F	443	ARG
1	A	443	ARG
1	B	252	THR
1	B	364	ARG
1	B	441	ASP
1	B	478	ASP
1	C	46	ASP
1	C	297	TYR
1	C	476	ASN
1	E	297	TYR
1	E	369	ALA
1	B	309	ASN
1	B	363	GLU
1	C	294	ASN
1	C	369	ALA
1	D	10	LYS
1	D	369	ALA
1	D	443	ARG
1	E	173	GLU
1	E	483	ASP
1	E	484	ASP
1	F	11	ASP
1	F	107	ILE
1	F	477	SER
1	F	484	ASP
1	A	483	ASP
1	B	107	ILE
1	E	478	ASP
1	F	369	ALA
1	C	366	GLY
1	E	444	GLY
1	F	357	ILE
1	C	107	ILE
1	D	444	GLY
1	D	40	PRO

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	429/439 (98%)	416 (97%)	13 (3%)	41	73
1	B	429/439 (98%)	416 (97%)	13 (3%)	41	73
1	C	427/439 (97%)	422 (99%)	5 (1%)	71	90
1	D	429/439 (98%)	417 (97%)	12 (3%)	43	75
1	E	427/439 (97%)	417 (98%)	10 (2%)	50	79
1	F	428/439 (98%)	418 (98%)	10 (2%)	50	79
All	All	2569/2634 (98%)	2506 (98%)	63 (2%)	49	77

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	TYR
1	A	46	ASP
1	A	241	LEU
1	A	242	HIS
1	A	256	LEU
1	A	280	LYS
1	A	290	PHE
1	A	396	SER
1	A	402	SER
1	A	416	TYR
1	A	449	ARG
1	A	482	PHE
1	A	484	ASP
1	B	13	LYS
1	B	122	MET
1	B	173[A]	GLU
1	B	173[B]	GLU
1	B	179	GLN
1	B	242	HIS
1	B	290	PHE
1	B	396	SER
1	B	445	MET

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Mol	Chain	Res	Type
1	B	466	SER
1	B	478	ASP
1	B	479	LYS
1	B	497	ASN
1	C	52	LYS
1	C	174	MET
1	C	290	PHE
1	C	361	VAL
1	C	492	ARG
1	D	290	PHE
1	D	300	ASN
1	D	309	ASN
1	D	350	LEU
1	D	396	SER
1	D	430	ARG
1	D	435	ASP
1	D	449	ARG
1	D	455	VAL
1	D	476	ASN
1	D	479	LYS
1	D	489	SER
1	E	12	TYR
1	E	47	GLU
1	E	115	LYS
1	E	179	GLN
1	E	290	PHE
1	E	301	ASN
1	E	319	LEU
1	E	396	SER
1	E	468	ASN
1	E	482	PHE
1	F	5	ARG
1	F	115	LYS
1	F	179	GLN
1	F	213	SER
1	F	290	PHE
1	F	416	TYR
1	F	435	ASP
1	F	449	ARG
1	F	492	ARG
1	F	496	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	ASN
1	A	223	GLN
1	A	497	ASN
1	B	172	ASN
1	B	459	GLN
1	C	39	GLN
1	C	172	ASN
1	C	179	GLN
1	C	242	HIS
1	C	309	ASN
1	C	497	ASN
1	D	72	ASN
1	D	172	ASN
1	D	179	GLN
1	D	242	HIS
1	D	380	HIS
1	D	417	ASN
1	D	453	HIS
1	D	476	ASN
1	E	242	HIS
1	E	250	ASN
1	F	242	HIS

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

12 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	$\# Z > 2$
3	DIO	E	601	-	6,6,6	0.54	0	6,6,6	0.72	0
3	DIO	D	601	-	6,6,6	0.54	0	6,6,6	0.61	0
3	DIO	A	601	-	6,6,6	0.52	0	6,6,6	0.36	0
3	DIO	B	601	-	6,6,6	0.44	0	6,6,6	0.57	0
2	AHR	A	600	-	10,10,10	1.66	2 (20%)	13,14,14	1.11	1 (7%)
2	AHR	B	600	-	10,10,10	1.95	2 (20%)	13,14,14	1.60	3 (23%)
2	AHR	C	600	-	10,10,10	1.71	2 (20%)	13,14,14	1.74	3 (23%)
3	DIO	F	601	-	6,6,6	0.48	0	6,6,6	0.71	0
2	AHR	E	600	-	10,10,10	1.94	4 (40%)	13,14,14	1.60	3 (23%)
2	AHR	D	600	-	10,10,10	1.63	2 (20%)	13,14,14	1.35	1 (7%)
3	DIO	C	601	-	6,6,6	0.41	0	6,6,6	0.40	0
2	AHR	F	600	-	10,10,10	1.64	3 (30%)	13,14,14	1.39	2 (15%)

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	DIO	E	601	-	-	-	0/1/1/1
3	DIO	D	601	-	-	-	0/1/1/1
3	DIO	A	601	-	-	-	0/1/1/1
3	DIO	F	601	-	-	-	0/1/1/1
3	DIO	B	601	-	-	-	0/1/1/1
2	AHR	A	600	-	-	0/2/18/18	0/1/1/1
2	AHR	C	600	-	-	0/2/18/18	0/1/1/1
2	AHR	B	600	-	-	2/2/18/18	0/1/1/1
2	AHR	E	600	-	-	1/2/18/18	0/1/1/1
2	AHR	D	600	-	-	0/2/18/18	0/1/1/1
3	DIO	C	601	-	-	-	0/1/1/1
2	AHR	F	600	-	-	0/2/18/18	0/1/1/1

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	600	AHR	C2-C3	-3.70	1.43	1.53
2	B	600	AHR	C1-C2	-3.69	1.48	1.52
2	A	600	AHR	C2-C3	-3.62	1.43	1.53
2	C	600	AHR	C2-C3	-3.56	1.43	1.53
2	E	600	AHR	C2-C3	-3.37	1.44	1.53
2	E	600	AHR	C1-C2	-3.25	1.48	1.52
2	D	600	AHR	C2-C3	-3.11	1.44	1.53
2	F	600	AHR	C2-C3	-3.01	1.45	1.53
2	F	600	AHR	C1-C2	-2.54	1.49	1.52
2	D	600	AHR	C1-C2	-2.37	1.50	1.52
2	E	600	AHR	C3-C4	-2.33	1.47	1.53
2	F	600	AHR	C3-C4	-2.16	1.47	1.53
2	A	600	AHR	C1-C2	-2.16	1.50	1.52
2	E	600	AHR	O4-C1	2.09	1.45	1.43
2	C	600	AHR	C3-C4	-2.07	1.47	1.53

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	600	AHR	C1-C2-C3	4.28	107.66	102.30
2	C	600	AHR	C5-C4-C3	-4.10	105.20	115.09
2	E	600	AHR	C1-C2-C3	3.84	107.10	102.30
2	F	600	AHR	C1-C2-C3	3.52	106.70	102.30
2	B	600	AHR	C1-C2-C3	3.39	106.54	102.30
2	B	600	AHR	C5-C4-C3	-3.22	107.32	115.09
2	B	600	AHR	C2-C3-C4	2.69	107.86	102.64
2	F	600	AHR	O4-C4-C5	2.68	115.01	109.21
2	C	600	AHR	C1-C2-C3	2.65	105.62	102.30
2	A	600	AHR	C1-C2-C3	2.44	105.35	102.30
2	C	600	AHR	C2-C3-C4	2.36	107.22	102.64
2	E	600	AHR	C5-C4-C3	-2.24	109.69	115.09
2	E	600	AHR	O4-C4-C5	2.22	114.01	109.21

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	600	AHR	O4-C4-C5-O5
2	B	600	AHR	C3-C4-C5-O5
2	E	600	AHR	O4-C4-C5-O5

There are no ring outliers.

6 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	601	DIO	1	0
3	D	601	DIO	2	0
3	A	601	DIO	4	0
3	B	601	DIO	4	0
3	F	601	DIO	3	0
3	C	601	DIO	2	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	496/501 (99%)	-0.11	12 (2%) 59 57	31, 51, 83, 116	0
1	B	496/501 (99%)	0.05	18 (3%) 42 39	31, 54, 89, 117	0
1	C	496/501 (99%)	0.01	8 (1%) 72 71	32, 54, 96, 120	0
1	D	496/501 (99%)	0.06	24 (4%) 30 27	34, 56, 100, 130	0
1	E	496/501 (99%)	0.01	7 (1%) 75 76	29, 56, 99, 125	0
1	F	496/501 (99%)	-0.10	19 (3%) 40 37	31, 53, 92, 118	0
All	All	2976/3006 (99%)	-0.01	88 (2%) 50 46	29, 54, 94, 130	0

All (88) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	169[A]	CYS	4.8
1	F	501	ILE	4.3
1	E	368	ALA	4.2
1	A	483	ASP	4.0
1	A	484	ASP	3.7
1	D	488	THR	3.7
1	D	478	ASP	3.6
1	F	404	HIS	3.6
1	D	437	VAL	3.5
1	D	440	SER	3.5
1	B	440	SER	3.4
1	C	8	VAL	3.4
1	D	8	VAL	3.4
1	A	486	ILE	3.3
1	D	436	ILE	3.3
1	B	436	ILE	3.2
1	A	501	ILE	3.1
1	D	483	ASP	3.1
1	F	398	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	435	ASP	3.0
1	F	483	ASP	3.0
1	B	488	THR	3.0
1	B	499	ILE	3.0
1	F	485	GLY	2.9
1	A	485	GLY	2.9
1	F	486	ILE	2.9
1	D	441	ASP	2.9
1	F	478	ASP	2.9
1	B	439	VAL	2.8
1	C	305	ASN	2.8
1	F	436	ILE	2.8
1	B	487	LEU	2.8
1	F	438	LEU	2.8
1	D	442	VAL	2.8
1	B	484	ASP	2.7
1	F	396	SER	2.7
1	D	461	LEU	2.7
1	D	486	ILE	2.7
1	F	8	VAL	2.6
1	F	5	ARG	2.6
1	C	484	ASP	2.6
1	E	307	MET	2.6
1	D	489	SER	2.6
1	F	405	GLU	2.6
1	F	488	THR	2.5
1	B	437	VAL	2.5
1	B	478	ASP	2.5
1	C	309	ASN	2.5
1	D	484	ASP	2.5
1	B	482	PHE	2.5
1	F	482	PHE	2.5
1	C	433	HIS	2.5
1	B	485	GLY	2.4
1	D	425	ILE	2.4
1	B	486	ILE	2.4
1	C	478	ASP	2.4
1	E	445	MET	2.4
1	D	305	ASN	2.4
1	B	491	LEU	2.4
1	B	451	LEU	2.4
1	B	434	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	F	484	ASP	2.4
1	E	486	ILE	2.4
1	F	403	LYS	2.4
1	A	482	PHE	2.3
1	D	438	LEU	2.3
1	A	421	GLU	2.2
1	F	416	TYR	2.2
1	D	477	SER	2.2
1	D	5	ARG	2.2
1	D	487	LEU	2.2
1	D	463	ILE	2.2
1	D	490	MET	2.2
1	E	398	LEU	2.1
1	A	5	ARG	2.1
1	E	416	TYR	2.1
1	A	398	LEU	2.1
1	E	47	GLU	2.1
1	B	483	ASP	2.1
1	C	483	ASP	2.1
1	D	12	TYR	2.1
1	D	2	LYS	2.1
1	A	431	ASN	2.1
1	B	309	ASN	2.1
1	D	307	MET	2.0
1	A	445	MET	2.0
1	A	433	HIS	2.0
1	F	421	GLU	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 monosaccharides 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
3	DIO	D	601	6/6	0.85	0.32	67,71,71,74	0
3	DIO	C	601	6/6	0.85	0.32	71,74,75,87	0
3	DIO	B	601	6/6	0.87	0.27	67,69,71,75	0
2	AHR	C	600	10/10	0.89	0.28	49,54,63,66	0
2	AHR	D	600	10/10	0.90	0.24	47,56,61,66	0
3	DIO	E	601	6/6	0.90	0.24	64,67,69,73	0
3	DIO	A	601	6/6	0.91	0.25	65,67,74,77	0
3	DIO	F	601	6/6	0.91	0.29	64,70,74,76	0
2	AHR	A	600	10/10	0.92	0.20	38,49,58,59	0
2	AHR	E	600	10/10	0.92	0.20	43,56,61,62	0
2	AHR	B	600	10/10	0.95	0.20	46,57,67,70	0
2	AHR	F	600	10/10	0.96	0.21	46,54,61,62	0

6.5 Other polymers [i](#)

There are no such residues in this entry.