



Full wwPDB X-ray Structure Validation Report i

Feb 26, 2014 – 02:51 PM GMT

PDB ID : 2VXM
Title : SCREENING A LIMITED STRUCTURE-BASED LIBRARY IDENTIFIES
UDP-GALNAC-SPECIFIC MUTANTS OF ALPHA-1,3 GALACTOSYLTRANSFERASE
Authors : Tumbale, P.; Jamaluddin, H.; Thiagarajan, N.; Acharya, K.R.; Brew, K.
Deposited on : 2008-07-07
Resolution : 2.82 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

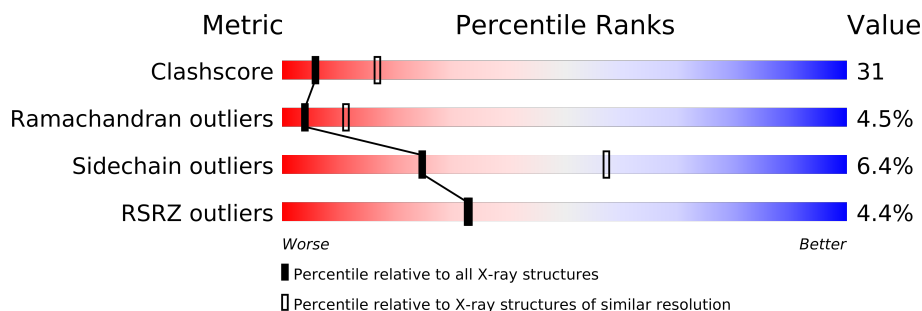
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.82 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	79885	2478 (2.84-2.80)
Ramachandran outliers	78287	2429 (2.84-2.80)
Sidechain outliers	78261	2431 (2.84-2.80)
RSRZ outliers	66119	1966 (2.84-2.80)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	273	
1	B	273	
1	C	273	
1	D	273	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	GOL	B	1340	X	-
3	GOL	C	1340	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8653 atoms, of which 0 are hydrogen and 0 are deuterium.

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 N-ACETYLLACTOSAMINIDEALPHA-1,3-GALACTOSYL TRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	268	Total	C	N	O	S	0	0	0
			2211	1450	360	389	12			
1	B	252	Total	C	N	O	S	0	0	1
			2079	1360	341	368	10			
1	C	255	Total	C	N	O	S	0	0	1
			2101	1373	344	373	11			
1	D	260	Total	C	N	O	S	0	0	1
			2141	1402	351	377	11			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	280	ARG	HIS	ENGINEERED MUTATION	UNP P14769
B	280	ARG	HIS	ENGINEERED MUTATION	UNP P14769
C	280	ARG	HIS	ENGINEERED MUTATION	UNP P14769
D	280	ARG	HIS	ENGINEERED MUTATION	UNP P14769

- Molecule 2 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: C₆H₁₄O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	C	O	0	0
			8	6	2		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is water.

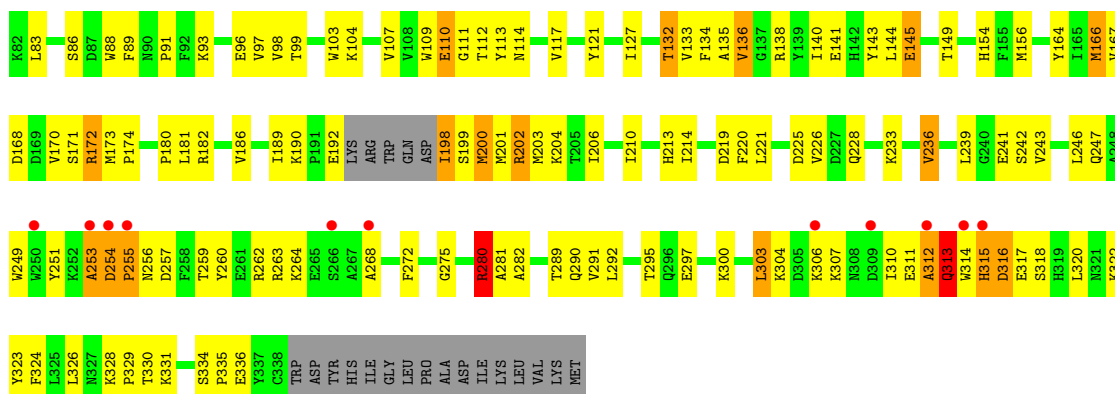
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	33	Total 33	O 33	0	0
4	B	26	Total 26	O 26	0	0
4	C	17	Total 17	O 17	0	0
4	D	25	Total 25	O 25	0	0

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● Molecule 1: N-ACETYLLACTOSAMINIDEALPHA-1,3-GALACTOSYLTRANSFERAS

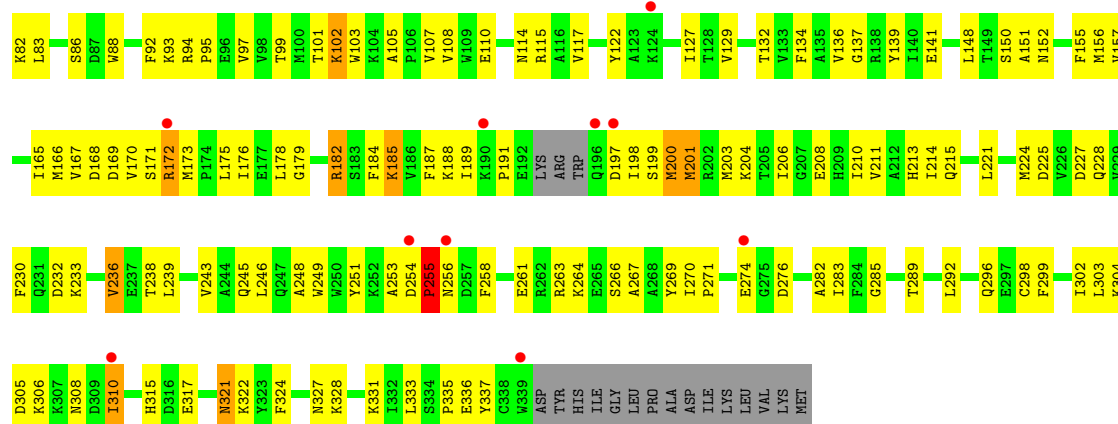
L320	L321	L322	L323	L324	L325	L326	L327	L328	L329	L330	L331	L332	L333	L334	L335	L336	L337	L338	L339	L340	L341	L342	L343	L344	L345	L346	L347	L348	L349	L350	L351	L352	L353	L354																																																																																																																																																																																																																																																																																																																																																																																																											
W250	W251	K252	A253	D254	P255	N256	D257	F258	T259	V260	E261	R262	R263	P264	E265	S266	A267	A268	W269	T270	G271	G272	E273	E274	G275		V276	A277	A278	A279	T280	T281	T282	T283	Q284	Q285	Q286	Q287	Q288	Q289	Q290	Q291	L292	N293	L294	T295	Q296	E297	C298	F299	K300	G301	L302	L303	K304	D305	K306	K307	N308	D309	L310	E311	A312	Q313	W314	H315	D316		W317	W318	W319	W320	W321	W322	W323	W324	W325	W326	W327	W328	W329	W330	W331	W332	W333	W334	W335	W336	W337	W338	W339	W340	W341	W342	W343	W344	W345	W346	W347	W348	W349	W350	W351	W352	W353	W354	W355	W356	W357	W358	W359	W360	W361	W362	W363	W364	W365	W366	W367	W368	W369	W370	W371	W372	W373	W374	W375	W376	W377	W378	W379	W380	W381	W382	W383	W384	W385	W386	W387	W388	W389	W390	W391	W392	W393	W394	W395	W396	W397	W398	W399	W400	W401	W402	W403	W404	W405	W406	W407	W408	W409	W410	W411	W412	W413	W414	W415	W416	W417	W418	W419	W420	W421	W422	W423	W424	W425	W426	W427	W428	W429	W430	W431	W432	W433	W434	W435	W436	W437	W438	W439	W440	W441	W442	W443	W444	W445	W446	W447	W448	W449	W450	W451	W452	W453	W454	W455	W456	W457	W458	W459	W460	W461	W462	W463	W464	W465	W466	W467	W468	W469	W470	W471	W472	W473	W474	W475	W476	W477	W478	W479	W480	W481	W482	W483	W484	W485	W486	W487	W488	W489	W490	W491	W492	W493	W494	W495	W496	W497	W498	W499	W500	W501	W502	W503	W504	W505	W506	W507	W508	W509	W510	W511	W512	W513	W514	W515	W516	W517	W518	W519	W520	W521	W522	W523	W524	W525	W526	W527	W528	W529	W530	W531	W532	W533	W534	W535	W536	W537	W538	W539	W540	W541	W542	W543	W544	W545	W546	W547	W548	W549	W550	W551	W552	W553	W554	W555	W556	W557	W558	W559	W560	W561	W562	W563	W564	W565	W566	W567	W568	W569	W570	W571	W572	W573	W574	W575	W576	W577	W578	W579	W580	W581	W582	W583	W584	W585	W586	W587	W588	W589	W590	W591	W592	W593	W594	W595	W596	W597	W598	W599	W600	W601	W602	W603	W604	W605	W606	W607	W608	W609	W610	W611	W612	W613	W614	W615	W616	W617	W618	W619	W620	W621	W622	W623	W624	W625	W626	W627	W628	W629	W630	W631	W632	W633	W634	W635	W636	W637	W638	W639	W640	W641	W642	W643	W644	W645	W646	W647	W648	W649	W650	W651	W652	W653	W654	W655	W656	W657	W658	W659	W660	W661	W662	W663	W664	W665	W666	W667	W668	W669	W670	W671	W672	W673	W674	W675	W676	W677

Chain B:



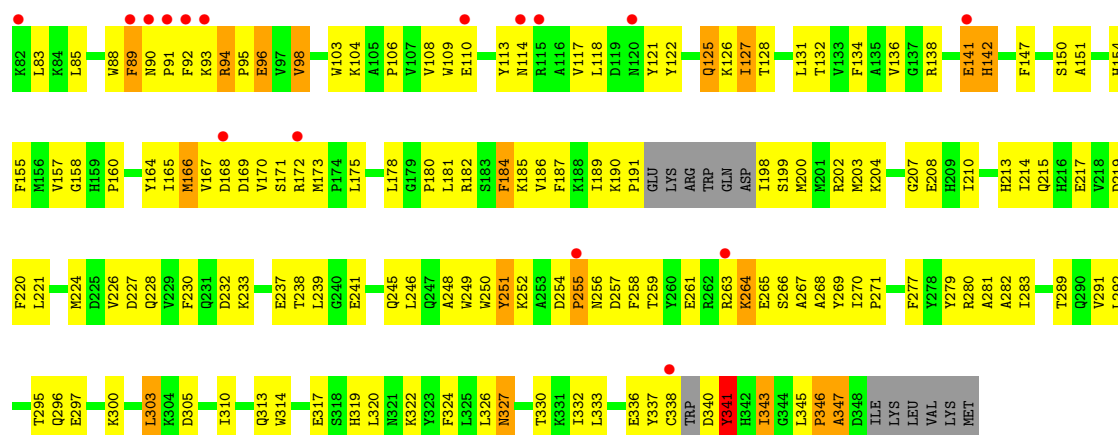
● Molecule 1: N-ACETYLLACTOSAMINIDEALPHA-1,3-GALACTOSYLTRANSFERASE

Chain C:



• Molecule 1: N-ACETYLLACTOSAMINIDEALPHA-1,3-GALACTOSYLTRANSFERASE

Chain D:



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	130.72Å 65.30Å 163.69Å 90.00° 105.40° 90.00°	Depositor
Resolution (Å)	32.93 – 2.82 38.33 – 2.82	Depositor EDS
% Data completeness (in resolution range)	80.0 (32.93-2.82) 80.0 (38.33-2.82)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.01 (at 2.81Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.219 , 0.290 0.221 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	34.3	Xtriage
Anisotropy	0.204	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.42 , 38.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 27676 reflections	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	8653	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.30% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

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

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	0.42	0/2276	0.67	0/3079
1	B	0.52	3/2140 (0.1%)	0.79	4/2896 (0.1%)
1	C	0.43	0/2162	0.66	0/2926
1	D	0.42	0/2204	0.63	0/2983
All	All	0.45	3/8782 (0.0%)	0.69	4/11884 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	280	ARG	C-O	-8.39	1.07	1.23
1	B	280	ARG	CZ-NH2	-8.13	1.22	1.33
1	B	280	ARG	CZ-NH1	-7.61	1.23	1.33

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	280	ARG	NE-CZ-NH1	15.47	128.04	120.30
1	B	280	ARG	NH1-CZ-NH2	-11.28	107.00	119.40
1	B	280	ARG	NE-CZ-NH2	9.19	124.90	120.30
1	B	280	ARG	CG-CD-NE	6.81	126.11	111.80

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit,

and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2211	0	2183	143	0
1	B	2079	0	2042	139	0
1	C	2101	0	2062	130	0
1	D	2141	0	2106	125	0
2	B	8	0	14	1	0
3	B	6	0	4	0	0
3	C	6	0	4	0	0
4	A	33	0	0	0	0
4	B	26	0	0	4	0
4	C	17	0	0	0	0
4	D	25	0	0	0	0
All	All	8653	0	8415	529	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 31.

All (529) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:259:THR:HB	1:B:314:TRP:CE2	1.61	1.35
1:A:249:TRP:C	1:A:250:TRP:HD1	1.46	1.18
1:B:259:THR:O	1:B:314:TRP:CD1	2.02	1.13
1:B:313:GLN:HG3	1:B:314:TRP:N	1.55	1.10
1:B:259:THR:HB	1:B:314:TRP:NE1	1.68	1.08
1:A:345:LEU:H	1:A:346:PRO:HD3	1.16	1.06
1:B:259:THR:HB	1:B:314:TRP:CZ2	1.94	1.02
1:B:200:MET:HG3	1:B:316:ASP:OD1	1.61	1.01
1:B:263:ARG:NH2	1:B:312:ALA:O	1.94	1.00
1:A:249:TRP:C	1:A:250:TRP:CD1	2.34	1.00
1:B:259:THR:CB	1:B:314:TRP:CE2	2.45	1.00
1:B:259:THR:CB	1:B:314:TRP:CZ2	2.46	0.99
1:B:259:THR:HG21	1:B:314:TRP:CZ2	2.00	0.95
1:C:198:ILE:HG13	1:C:200:MET:HG2	1.48	0.94
1:A:200:MET:HB3	1:A:302:ILE:HD13	1.51	0.93
1:B:259:THR:CG2	1:B:314:TRP:CZ2	2.51	0.92
1:C:200:MET:HG3	1:C:302:ILE:HD13	1.51	0.92
1:D:265:GLU:HB2	1:D:310:ILE:HD12	1.51	0.91
1:B:198:ILE:CD1	1:B:199:SER:H	1.84	0.91
1:B:145:GLU:O	1:B:149:THR:HG23	1.72	0.90
1:C:148:LEU:HD21	1:C:165:ILE:HD11	1.55	0.89

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:252:LYS:O	1:A:253:ALA:O	1.89	0.89
1:A:345:LEU:H	1:A:346:PRO:CD	1.87	0.86
1:C:215:GLN:HE21	1:D:300:LYS:HE3	1.39	0.85
1:C:263:ARG:HH12	1:C:310:ILE:HG13	1.42	0.85
1:C:267:ALA:HB2	1:C:304:LYS:HE2	1.59	0.84
1:C:215:GLN:NE2	1:D:300:LYS:HE3	1.92	0.83
1:B:198:ILE:HD13	1:B:199:SER:H	1.43	0.83
1:A:250:TRP:N	1:A:250:TRP:CD1	2.43	0.82
1:C:305:ASP:HB3	1:C:310:ILE:O	1.79	0.82
1:B:313:GLN:CG	1:B:314:TRP:N	2.33	0.81
1:A:231:GLN:OE1	1:A:349:ILE:HB	1.80	0.81
1:A:251:TYR:O	1:A:252:LYS:HB2	1.80	0.80
1:A:120:ASN:HD21	1:A:124:LYS:NZ	1.80	0.80
1:B:268:ALA:HB1	1:B:318:SER:O	1.81	0.80
1:D:228:GLN:HB3	1:D:341:TYR:HE1	1.46	0.79
1:D:122:TYR:HB3	1:D:127:ILE:HD12	1.65	0.78
1:D:94:ARG:HA	1:D:94:ARG:HE	1.49	0.78
1:D:88:TRP:O	1:D:113:TYR:HA	1.83	0.78
1:A:345:LEU:N	1:A:346:PRO:HD3	1.95	0.78
1:A:210:ILE:HA	1:A:214:ILE:HB	1.65	0.76
1:D:131:LEU:HD21	1:D:147:PHE:HZ	1.49	0.76
1:A:292:LEU:O	1:A:296:GLN:HB2	1.86	0.76
1:A:157:VAL:HG21	1:A:233:LYS:HD2	1.67	0.75
1:A:279:TYR:N	1:A:321:ASN:HD21	1.84	0.75
1:B:313:GLN:O	1:B:315:HIS:ND1	2.19	0.75
1:D:305:ASP:HB3	1:D:310:ILE:O	1.85	0.75
1:C:204:LYS:O	1:C:208:GLU:HG3	1.86	0.75
1:B:259:THR:O	1:B:314:TRP:NE1	2.20	0.74
1:B:313:GLN:HG3	1:B:314:TRP:H	1.49	0.74
1:D:154:HIS:HB3	1:D:233:LYS:HA	1.70	0.74
1:A:132:THR:HG23	1:A:221:LEU:HD11	1.69	0.73
1:C:199:SER:C	1:C:201:MET:H	1.92	0.73
1:C:150:SER:HB2	1:C:230:PHE:HB2	1.68	0.73
1:C:167:VAL:O	1:C:189:ILE:HG12	1.88	0.73
1:B:202:ARG:O	1:B:206:ILE:HG13	1.88	0.72
1:D:94:ARG:HH22	1:D:96:GLU:HB2	1.54	0.72
1:B:314:TRP:CZ2	4:B:2023:HOH:O	2.41	0.72
1:C:303:LEU:HA	1:C:306:LYS:HB3	1.72	0.72
1:B:97:VAL:HA	1:B:249:TRP:CH2	2.25	0.72
1:C:269:TYR:OH	1:C:271:PRO:HB3	1.90	0.72
1:C:136:VAL:O	1:C:139:TYR:HB2	1.90	0.71
1:D:185:LYS:HE2	1:D:187:PHE:HZ	1.54	0.71

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:314:TRP:O	1:B:315:HIS:HB2	1.90	0.71
1:B:198:ILE:HG23	1:B:199:SER:N	2.05	0.70
1:D:265:GLU:HB2	1:D:310:ILE:CD1	2.20	0.70
1:D:283:ILE:HD11	1:D:338:CYS:SG	2.31	0.70
1:B:198:ILE:HG23	1:B:200:MET:H	1.56	0.70
1:B:313:GLN:CG	1:B:314:TRP:H	2.01	0.69
1:B:200:MET:CG	1:B:316:ASP:OD1	2.38	0.69
1:C:148:LEU:HD21	1:C:165:ILE:CD1	2.22	0.69
1:D:267:ALA:O	1:D:322:LYS:HE2	1.92	0.69
1:A:302:ILE:HG22	1:A:306:LYS:HE3	1.75	0.68
1:A:198:ILE:HG22	1:A:199:SER:N	2.08	0.68
1:D:83:LEU:HD22	1:D:121:TYR:CD2	2.29	0.68
1:C:292:LEU:O	1:C:296:GLN:HG2	1.93	0.68
1:D:204:LYS:HE2	1:D:208:GLU:OE2	1.94	0.68
1:B:98:VAL:HG23	1:B:249:TRP:NE1	2.09	0.67
1:A:101:THR:HG21	1:A:332:ILE:HD12	1.75	0.67
1:C:200:MET:HE2	1:C:302:ILE:HG23	1.77	0.67
1:A:120:ASN:HD21	1:A:124:LYS:HZ3	1.41	0.67
1:B:136:VAL:HG23	1:B:168:ASP:HB3	1.75	0.67
1:C:152:ASN:ND2	1:C:178:LEU:HA	2.10	0.67
1:C:156:MET:HE2	1:C:239:LEU:HD21	1.77	0.67
1:B:280:ARG:HE	1:B:282:ALA:HB3	1.58	0.66
1:A:270:ILE:HD11	1:A:322:LYS:HA	1.75	0.66
1:D:94:ARG:NH2	1:D:96:GLU:HB2	2.10	0.66
1:C:152:ASN:HD21	1:C:179:GLY:H	1.42	0.66
1:B:98:VAL:CG2	1:B:249:TRP:HE1	2.07	0.66
1:A:141:GLU:OE2	1:A:172:ARG:HB3	1.94	0.66
1:C:210:ILE:HA	1:C:214:ILE:HB	1.77	0.66
1:A:250:TRP:O	1:A:251:TYR:HB2	1.96	0.66
1:C:170:VAL:O	1:C:173:MET:HG2	1.96	0.66
1:C:114:ASN:CG	1:C:117:VAL:HG23	2.16	0.65
1:B:198:ILE:HG23	1:B:200:MET:N	2.11	0.65
1:C:267:ALA:CB	1:C:304:LYS:HE2	2.25	0.65
1:A:134:PHE:CD1	1:A:202:ARG:HD2	2.32	0.65
1:A:252:LYS:O	1:A:253:ALA:C	2.34	0.65
1:C:263:ARG:HH12	1:C:310:ILE:CG1	2.08	0.65
1:B:214:ILE:HG21	1:B:221:LEU:CD1	2.27	0.65
1:A:345:LEU:N	1:A:346:PRO:CD	2.55	0.64
1:A:200:MET:HB3	1:A:302:ILE:HG21	1.79	0.64
1:C:152:ASN:HD21	1:C:179:GLY:N	1.95	0.64
1:A:242:SER:HB3	1:A:330:THR:H	1.63	0.64
1:D:172:ARG:HG3	1:D:172:ARG:HH21	1.62	0.64

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:311:GLU:O	1:B:312:ALA:C	2.35	0.63
1:B:200:MET:C	1:B:202:ARG:H	2.00	0.63
1:A:115:ARG:HH22	1:A:233:LYS:CB	2.10	0.63
1:D:151:ALA:O	1:D:155:PHE:HB3	1.98	0.63
1:B:127:ILE:HA	1:B:219:ASP:OD2	1.99	0.63
1:B:259:THR:CG2	1:B:314:TRP:HZ2	2.07	0.63
1:C:115:ARG:HH22	1:C:233:LYS:CB	2.12	0.63
1:A:185:LYS:HE2	1:A:187:PHE:HZ	1.64	0.62
1:A:224:MET:HG2	1:A:283:ILE:HG12	1.80	0.62
1:C:132:THR:HG23	1:C:221:LEU:HD11	1.81	0.62
1:A:204:LYS:O	1:A:208:GLU:HG3	1.99	0.62
1:A:140:ILE:HD11	1:A:167:VAL:HB	1.81	0.62
1:A:98:VAL:HG13	1:A:249:TRP:CH2	2.33	0.62
1:D:220:PHE:CG	1:D:239:LEU:HD22	2.35	0.62
1:B:303:LEU:HD22	1:B:307:LYS:HE3	1.81	0.62
1:D:103:TRP:O	1:D:104:LYS:HB2	2.00	0.62
1:C:175:LEU:HD22	1:C:184:PHE:CE1	2.34	0.62
1:A:256:ASN:ND2	1:A:273:GLY:H	1.98	0.61
1:A:145:GLU:HB2	1:A:174:PRO:HG3	1.82	0.61
1:A:256:ASN:ND2	1:A:273:GLY:N	2.48	0.61
1:C:110:GLU:HG2	1:C:336:GLU:OE1	2.00	0.61
1:A:134:PHE:HB2	1:A:202:ARG:HH11	1.65	0.61
1:B:98:VAL:HG23	1:B:249:TRP:HE1	1.63	0.61
1:A:270:ILE:HD12	1:A:325:LEU:CD2	2.30	0.61
1:C:255:PRO:HA	1:C:258:PHE:CD1	2.35	0.61
1:D:94:ARG:CA	1:D:94:ARG:HE	2.14	0.60
1:B:132:THR:HG23	1:B:164:TYR:HB2	1.83	0.60
1:D:185:LYS:HE2	1:D:187:PHE:CZ	2.36	0.60
1:B:210:ILE:HA	1:B:214:ILE:HB	1.82	0.60
1:B:246:LEU:HB2	1:B:335:PRO:HG3	1.83	0.60
1:D:95:PRO:HG2	1:D:96:GLU:OE1	2.02	0.60
1:C:224:MET:HA	1:C:282:ALA:O	2.00	0.60
1:B:109:TRP:CH2	1:B:335:PRO:HD2	2.36	0.60
1:B:259:THR:HG21	1:B:314:TRP:HZ2	1.64	0.60
1:B:198:ILE:HD13	1:B:199:SER:N	2.15	0.60
1:B:214:ILE:HG21	1:B:221:LEU:HD12	1.84	0.60
1:A:298:CYS:O	1:A:302:ILE:HG13	2.02	0.60
1:D:90:ASN:OD1	1:D:93:LYS:HG3	2.01	0.60
1:B:103:TRP:CE3	1:B:328:LYS:HD2	2.37	0.59
1:C:83:LEU:HD21	1:C:88:TRP:HD1	1.67	0.59
1:C:198:ILE:HG12	1:C:200:MET:SD	2.42	0.59
1:A:96:GLU:OE2	1:A:96:GLU:N	2.34	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:182:ARG:HD2	1:A:182:ARG:N	2.18	0.59
1:C:198:ILE:CG1	1:C:200:MET:SD	2.91	0.59
1:D:157:VAL:HG21	1:D:233:LYS:HE3	1.84	0.58
1:A:281:ALA:HA	1:A:320:LEU:CD2	2.33	0.58
1:C:267:ALA:HB2	1:C:304:LYS:CE	2.31	0.58
1:A:256:ASN:HD21	1:A:273:GLY:N	2.01	0.58
1:D:270:ILE:HD11	1:D:322:LYS:HA	1.85	0.58
1:B:103:TRP:CD2	1:B:328:LYS:HD2	2.38	0.58
1:B:154:HIS:CE1	1:B:233:LYS:HZ2	2.22	0.58
1:A:84:LYS:HD2	1:A:87:ASP:OD2	2.02	0.58
1:A:343:ILE:N	1:A:343:ILE:HD13	2.19	0.58
1:C:129:VAL:HG21	1:C:156:MET:HE2	1.85	0.58
1:A:173:MET:HG3	1:A:173:MET:O	2.02	0.58
1:A:115:ARG:HH22	1:A:233:LYS:HB2	1.68	0.58
1:D:136:VAL:HG21	1:D:202:ARG:HH21	1.68	0.58
1:A:342:HIS:CD2	1:A:343:ILE:HG23	2.39	0.57
1:C:199:SER:C	1:C:201:MET:N	2.57	0.57
1:A:160:PRO:HA	1:A:181:LEU:HB3	1.85	0.57
1:B:334:SER:OG	1:B:336:GLU:HG3	2.04	0.57
1:D:238:THR:HG22	1:D:333:LEU:HD22	1.86	0.57
1:A:225:ASP:OD2	1:A:282:ALA:HA	2.04	0.57
1:C:99:THR:HA	1:C:107:VAL:HB	1.86	0.57
1:B:314:TRP:CE2	4:B:2023:HOH:O	2.57	0.57
1:C:215:GLN:HE21	1:D:300:LYS:CE	2.13	0.57
1:A:341:TYR:CE1	1:A:343:ILE:HD11	2.40	0.57
1:D:255:PRO:HA	1:D:258:PHE:CD1	2.40	0.57
1:C:266:SER:HB2	1:C:310:ILE:HD11	1.87	0.56
1:B:241:GLU:O	1:B:290:GLN:HG3	2.05	0.56
1:D:141:GLU:CD	1:D:141:GLU:H	2.09	0.56
1:B:255:PRO:HG3	1:B:275:GLY:O	2.06	0.56
1:B:289:THR:O	1:B:292:LEU:HB3	2.05	0.56
1:C:179:GLY:O	1:C:182:ARG:HB2	2.06	0.56
1:D:268:ALA:HB2	1:D:319:HIS:CE1	2.40	0.56
1:A:266:SER:HB2	1:A:310:ILE:HD11	1.87	0.56
1:B:198:ILE:HD12	1:B:199:SER:H	1.68	0.56
1:B:110:GLU:HA	1:B:113:TYR:HE2	1.71	0.56
1:D:109:TRP:HE3	1:D:336:GLU:OE1	1.89	0.56
1:A:132:THR:HG22	1:A:164:TYR:HB2	1.88	0.56
1:B:254:ASP:N	1:B:255:PRO:CD	2.68	0.56
1:C:214:ILE:HG21	1:C:221:LEU:HD22	1.86	0.56
1:C:169:ASP:HA	1:C:188:LYS:NZ	2.21	0.56
1:D:178:LEU:HD11	1:D:184:PHE:CD2	2.41	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:136:VAL:HG13	1:C:168:ASP:CG	2.26	0.55
1:D:346:PRO:O	1:D:347:ALA:HB2	2.06	0.55
1:B:323:TYR:CD1	1:B:323:TYR:C	2.80	0.55
1:A:109:TRP:CH2	1:A:335:PRO:HD2	2.42	0.55
1:C:198:ILE:HG13	1:C:200:MET:CG	2.28	0.55
1:D:291:VAL:O	1:D:295:THR:HG23	2.06	0.55
1:D:132:THR:HG23	1:D:221:LEU:HD11	1.89	0.55
1:D:170:VAL:O	1:D:170:VAL:HG12	2.07	0.55
1:D:125:GLN:HB3	1:D:127:ILE:CG2	2.37	0.54
1:A:101:THR:HG21	1:A:332:ILE:CD1	2.36	0.54
1:D:263:ARG:HH11	1:D:263:ARG:HB2	1.72	0.54
1:B:254:ASP:N	1:B:255:PRO:HD2	2.22	0.54
1:C:148:LEU:HB3	1:C:176:ILE:HD11	1.88	0.54
1:C:269:TYR:CE2	1:C:271:PRO:HD3	2.42	0.54
1:C:276:ASP:OD2	1:C:328:LYS:NZ	2.33	0.54
1:C:141:GLU:HB2	1:C:172:ARG:NH2	2.22	0.54
1:D:264:LYS:HA	1:D:269:TYR:CG	2.43	0.54
1:A:296:GLN:O	1:A:300:LYS:HG3	2.08	0.54
1:C:185:LYS:HE2	1:C:187:PHE:HZ	1.72	0.54
1:C:270:ILE:HD11	1:C:322:LYS:HA	1.88	0.54
1:B:138:ARG:NH1	1:B:138:ARG:O	2.39	0.54
1:D:128:THR:HG23	1:D:160:PRO:HB2	1.90	0.54
1:A:200:MET:CB	1:A:302:ILE:HD13	2.33	0.53
1:D:136:VAL:CG2	1:D:202:ARG:HH21	2.21	0.53
1:D:254:ASP:C	1:D:256:ASN:H	2.12	0.53
1:B:143:TYR:HB3	1:B:226:VAL:HG22	1.89	0.53
1:C:263:ARG:HH12	1:C:310:ILE:CD1	2.22	0.53
1:C:213:HIS:CE1	1:C:214:ILE:HG13	2.44	0.53
1:B:171:SER:O	1:B:172:ARG:HB2	2.08	0.53
1:A:249:TRP:CA	1:A:250:TRP:HD1	2.18	0.53
1:D:254:ASP:O	1:D:256:ASN:N	2.42	0.53
1:B:98:VAL:HG23	1:B:249:TRP:CE2	2.44	0.53
1:C:114:ASN:ND2	1:C:117:VAL:HG23	2.24	0.53
1:B:83:LEU:HD22	1:B:121:TYR:CE2	2.43	0.53
1:D:89:PHE:CE2	1:D:106:PRO:HB2	2.43	0.53
1:C:261:GLU:OE2	1:C:263:ARG:HB2	2.08	0.52
1:A:275:GLY:HA2	1:A:325:LEU:HD13	1.90	0.52
1:D:134:PHE:CZ	1:D:166:MET:HG2	2.44	0.52
1:C:215:GLN:NE2	1:D:300:LYS:CE	2.67	0.52
1:C:156:MET:HE1	1:C:236:VAL:HA	1.91	0.52
1:C:115:ARG:HH22	1:C:233:LYS:HB3	1.74	0.52
1:A:165:ILE:HG22	1:A:167:VAL:HG13	1.92	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:198:ILE:CG2	1:A:199:SER:N	2.73	0.52
1:C:264:LYS:HA	1:C:269:TYR:CD1	2.45	0.52
1:C:269:TYR:CZ	1:C:271:PRO:HB3	2.45	0.52
1:A:101:THR:HG23	1:A:105:ALA:O	2.10	0.52
1:C:245:GLN:OE1	1:C:283:ILE:HD12	2.10	0.52
1:A:88:TRP:O	1:A:114:ASN:N	2.42	0.52
1:A:241:GLU:HG2	1:A:290:GLN:HG3	1.91	0.52
1:C:215:GLN:OE1	1:D:296:GLN:NE2	2.43	0.52
1:D:122:TYR:HB3	1:D:127:ILE:CD1	2.39	0.52
1:C:156:MET:CE	1:C:239:LEU:HD21	2.39	0.52
1:D:228:GLN:HB3	1:D:341:TYR:CE1	2.36	0.51
1:D:125:GLN:HB3	1:D:127:ILE:HG23	1.91	0.51
1:A:270:ILE:HD12	1:A:325:LEU:HD22	1.92	0.51
1:A:236:VAL:HG12	1:A:239:LEU:HD11	1.92	0.51
1:B:322:LYS:HE2	1:B:326:LEU:HD11	1.92	0.51
1:D:241:GLU:HB2	1:D:330:THR:HG21	1.91	0.51
1:A:267:ALA:O	1:A:322:LYS:HE2	2.11	0.51
1:D:131:LEU:HD21	1:D:147:PHE:CZ	2.39	0.51
1:C:129:VAL:HG21	1:C:156:MET:CE	2.40	0.51
1:B:259:THR:HG21	1:B:314:TRP:CH2	2.44	0.51
1:C:238:THR:HG22	1:C:333:LEU:HD22	1.92	0.51
1:C:203:MET:HE3	1:C:298:CYS:HB2	1.91	0.51
1:A:270:ILE:HD12	1:A:325:LEU:HD23	1.91	0.51
1:C:83:LEU:O	1:C:83:LEU:HD23	2.10	0.51
1:A:227:ASP:OD2	1:A:352:VAL:HA	2.11	0.51
1:D:114:ASN:OD1	1:D:117:VAL:HG23	2.10	0.51
1:A:302:ILE:O	1:A:306:LYS:HG3	2.11	0.51
1:D:118:LEU:HD13	1:D:237:GLU:HA	1.93	0.51
1:C:255:PRO:O	1:C:258:PHE:HB2	2.11	0.51
1:B:256:ASN:OD1	1:B:272:PHE:HB3	2.10	0.51
1:A:253:ALA:O	1:A:255:PRO:HD3	2.11	0.50
1:A:339:TRP:HB3	1:A:349:ILE:HD12	1.93	0.50
1:A:343:ILE:H	1:A:343:ILE:HD13	1.76	0.50
1:B:303:LEU:O	1:B:306:LYS:N	2.43	0.50
1:C:94:ARG:N	1:C:95:PRO:HD3	2.27	0.50
1:A:98:VAL:HG22	1:A:249:TRP:CE2	2.47	0.50
1:A:251:TYR:O	1:A:252:LYS:CB	2.55	0.50
1:C:308:ASN:O	1:C:310:ILE:HG22	2.12	0.50
1:A:127:ILE:O	1:A:160:PRO:HD2	2.12	0.50
1:B:253:ALA:O	1:B:255:PRO:N	2.44	0.50
1:B:114:ASN:OD1	1:B:117:VAL:HG23	2.12	0.50
1:B:221:LEU:CD2	1:B:291:VAL:HG11	2.42	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:185:LYS:HE2	1:A:187:PHE:CZ	2.47	0.49
1:B:241:GLU:HB2	1:B:330:THR:HG21	1.93	0.49
1:D:268:ALA:HB2	1:D:319:HIS:ND1	2.27	0.49
1:D:164:TYR:CZ	1:D:214:ILE:HG12	2.47	0.49
1:C:141:GLU:HB2	1:C:172:ARG:HH22	1.77	0.49
1:D:259:THR:HB	1:D:314:TRP:HE1	1.77	0.49
1:D:289:THR:O	1:D:292:LEU:HB3	2.13	0.49
1:A:204:LYS:HD2	1:A:299:PHE:CZ	2.47	0.49
1:C:228:GLN:OE1	1:C:282:ALA:HB1	2.12	0.49
1:C:289:THR:HG21	1:D:297:GLU:OE2	2.11	0.49
1:A:347:ALA:O	1:A:348:ASP:HB2	2.13	0.49
1:B:133:VAL:O	1:B:133:VAL:HG13	2.11	0.49
1:A:189:ILE:O	1:A:189:ILE:HG13	2.11	0.49
1:B:98:VAL:CG2	1:B:249:TRP:NE1	2.70	0.49
1:D:281:ALA:HA	1:D:320:LEU:CD2	2.43	0.49
1:D:265:GLU:CB	1:D:310:ILE:HD12	2.35	0.49
1:A:279:TYR:H	1:A:321:ASN:HD21	1.54	0.49
1:C:254:ASP:O	1:C:256:ASN:N	2.46	0.49
1:D:85:LEU:HD13	1:D:85:LEU:C	2.33	0.49
1:B:254:ASP:O	1:B:256:ASN:N	2.45	0.49
1:D:250:TRP:O	1:D:251:TYR:C	2.51	0.49
1:B:88:TRP:CE3	1:B:89:PHE:HB2	2.48	0.49
1:B:281:ALA:HA	1:B:320:LEU:HD22	1.95	0.49
1:B:172:ARG:O	1:B:172:ARG:HG2	2.13	0.48
1:A:350:LYS:NZ	1:A:352:VAL:HB	2.27	0.48
1:A:352:VAL:O	1:A:352:VAL:HG13	2.12	0.48
1:B:253:ALA:O	1:B:254:ASP:OD1	2.32	0.48
1:D:343:ILE:HD12	1:D:343:ILE:C	2.34	0.48
1:C:198:ILE:HG23	1:C:201:MET:SD	2.53	0.48
1:A:102:LYS:C	1:A:104:LYS:H	2.16	0.48
1:A:249:TRP:CG	1:A:250:TRP:N	2.81	0.48
1:D:292:LEU:O	1:D:296:GLN:HG2	2.13	0.48
1:B:98:VAL:HG21	1:B:249:TRP:HE1	1.78	0.48
1:B:83:LEU:HD22	1:B:121:TYR:CD2	2.47	0.48
1:B:314:TRP:NE1	4:B:2023:HOH:O	2.47	0.48
1:A:261:GLU:OE1	1:A:263:ARG:HB2	2.13	0.48
1:B:313:GLN:HG2	1:B:314:TRP:CD1	2.48	0.48
1:D:127:ILE:HA	1:D:219:ASP:OD2	2.13	0.48
1:D:210:ILE:HA	1:D:214:ILE:HB	1.93	0.48
1:A:246:LEU:HG	1:A:332:ILE:CG2	2.44	0.48
1:B:144:LEU:HD23	1:B:174:PRO:HD2	1.96	0.48
1:B:97:VAL:HG12	1:B:249:TRP:CZ3	2.48	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:281:ALA:HA	1:A:320:LEU:HD23	1.95	0.48
1:D:89:PHE:HE2	1:D:106:PRO:HB2	1.79	0.48
1:D:164:TYR:CE2	1:D:214:ILE:HG12	2.49	0.48
1:B:281:ALA:HA	1:B:320:LEU:CD2	2.44	0.48
1:C:248:ALA:HB2	1:C:335:PRO:HB3	1.96	0.48
1:D:190:LYS:HG3	1:D:190:LYS:O	2.14	0.48
1:D:269:TYR:CE2	1:D:271:PRO:HG3	2.49	0.47
1:B:200:MET:C	1:B:202:ARG:N	2.67	0.47
1:C:315:HIS:ND1	1:C:315:HIS:N	2.62	0.47
1:B:220:PHE:CE1	1:B:239:LEU:HD13	2.50	0.47
1:D:280:ARG:HA	1:D:317:GLU:OE2	2.14	0.47
1:A:120:ASN:C	1:A:120:ASN:HD22	2.16	0.47
1:B:263:ARG:NH1	1:B:310:ILE:HG13	2.30	0.47
1:B:98:VAL:HG23	1:B:249:TRP:CZ2	2.50	0.47
1:C:168:ASP:HB2	1:C:191:PRO:HG3	1.96	0.47
1:C:115:ARG:HH22	1:C:233:LYS:HB2	1.80	0.47
1:A:305:ASP:O	1:A:310:ILE:O	2.33	0.47
1:B:236:VAL:HG12	1:B:239:LEU:HD11	1.96	0.47
1:A:110:GLU:HG2	1:A:345:LEU:CD2	2.45	0.47
1:A:110:GLU:HG2	1:A:345:LEU:HD23	1.96	0.47
1:D:280:ARG:HG2	1:D:282:ALA:H	1.79	0.47
1:A:249:TRP:O	1:A:250:TRP:HD1	1.92	0.47
1:A:279:TYR:H	1:A:321:ASN:ND2	2.13	0.47
1:C:82:LYS:HG2	1:C:83:LEU:N	2.29	0.47
1:B:314:TRP:HB2	1:B:318:SER:OG	2.14	0.47
1:D:167:VAL:O	1:D:189:ILE:HG12	2.15	0.47
1:B:93:LYS:HD2	1:B:111:GLY:O	2.14	0.47
1:A:259:THR:HB	1:A:314:TRP:HE1	1.78	0.47
1:D:93:LYS:O	1:D:95:PRO:HD3	2.15	0.46
1:C:134:PHE:CZ	1:C:166:MET:HG2	2.50	0.46
1:C:132:THR:HB	1:C:166:MET:HE1	1.97	0.46
1:C:245:GLN:NE2	1:C:337:TYR:HB2	2.29	0.46
1:C:317:GLU:O	1:C:321:ASN:HB2	2.15	0.46
1:A:157:VAL:CG2	1:A:233:LYS:HD2	2.42	0.46
1:D:213:HIS:O	1:D:217:GLU:HG3	2.15	0.46
1:C:198:ILE:HD12	1:C:198:ILE:HA	1.78	0.46
1:C:206:ILE:O	1:C:210:ILE:HG13	2.15	0.46
1:D:168:ASP:HB2	1:D:191:PRO:HD3	1.97	0.46
1:B:311:GLU:OE2	1:B:311:GLU:HA	2.16	0.46
1:B:198:ILE:CD1	1:B:199:SER:N	2.67	0.46
1:C:261:GLU:O	1:C:269:TYR:HA	2.15	0.46
1:D:138:ARG:HA	1:D:141:GLU:OE2	2.14	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:170:VAL:O	1:B:172:ARG:N	2.45	0.46
1:C:185:LYS:HG2	1:C:187:PHE:CE1	2.50	0.46
1:A:279:TYR:O	1:A:321:ASN:ND2	2.48	0.46
1:B:228:GLN:NE2	1:B:280:ARG:NH2	2.64	0.46
1:A:310:ILE:HG12	1:A:311:GLU:N	2.31	0.46
1:A:228:GLN:HG2	1:A:350:LYS:HG2	1.98	0.46
1:C:148:LEU:HB3	1:C:176:ILE:CD1	2.45	0.46
1:C:152:ASN:HD21	1:C:178:LEU:HA	1.77	0.46
1:C:94:ARG:O	1:C:97:VAL:HG22	2.15	0.46
1:A:103:TRP:CE2	1:A:328:LYS:HB3	2.51	0.46
1:A:169:ASP:OD1	1:A:172:ARG:HG3	2.16	0.46
1:A:264:LYS:HA	1:A:269:TYR:CD1	2.51	0.46
1:C:136:VAL:HG12	1:C:137:GLY:N	2.30	0.46
1:A:88:TRP:HA	1:A:114:ASN:HB3	1.98	0.46
1:B:89:PHE:CE1	1:B:112:THR:HB	2.51	0.46
1:A:313:GLN:NE2	1:A:314:TRP:NE1	2.64	0.46
1:A:254:ASP:O	1:A:257:ASP:OD2	2.33	0.45
1:C:178:LEU:HD11	1:C:184:PHE:CD2	2.51	0.45
1:B:213:HIS:CE1	1:B:214:ILE:HG13	2.52	0.45
1:B:281:ALA:HB2	1:B:317:GLU:HG2	1.98	0.45
1:C:122:TYR:HB3	1:C:127:ILE:HG12	1.98	0.45
1:D:263:ARG:NH1	1:D:263:ARG:HB2	2.31	0.45
1:A:236:VAL:HA	1:A:239:LEU:HG	1.98	0.45
1:B:262:ARG:HB3	4:B:2018:HOH:O	2.16	0.45
1:A:138:ARG:N	1:A:138:ARG:HD3	2.31	0.45
1:C:83:LEU:HD21	1:C:88:TRP:CD1	2.48	0.45
1:A:109:TRP:CD2	1:A:334:SER:HB2	2.52	0.45
1:D:108:VAL:HG13	1:D:113:TYR:CD2	2.52	0.45
1:A:201:MET:HG3	1:A:201:MET:O	2.16	0.45
1:C:224:MET:HG2	1:C:283:ILE:HG23	1.97	0.45
1:A:96:GLU:HG2	1:A:97:VAL:HG13	1.98	0.45
1:B:251:TYR:CD1	2:B:1339:MPD:H32	2.52	0.45
1:B:315:HIS:O	1:B:318:SER:HB2	2.17	0.45
1:C:271:PRO:HG2	1:C:274:GLU:CD	2.36	0.45
1:C:225:ASP:O	1:C:228:GLN:HG2	2.16	0.45
1:C:243:VAL:N	1:C:285:GLY:O	2.43	0.45
1:C:225:ASP:OD2	1:C:282:ALA:HA	2.17	0.45
1:D:170:VAL:HG13	1:D:186:VAL:HG11	1.99	0.45
1:C:178:LEU:HD21	1:C:184:PHE:CE2	2.52	0.45
1:A:134:PHE:CG	1:A:202:ARG:HD2	2.51	0.45
1:C:151:ALA:O	1:C:155:PHE:HB3	2.17	0.45
1:C:211:VAL:HG11	1:D:207:GLY:C	2.37	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:92:PHE:CE1	1:C:93:LYS:HG3	2.52	0.45
1:C:204:LYS:HE3	1:C:299:PHE:CE1	2.51	0.44
1:D:224:MET:HG2	1:D:283:ILE:HG12	1.99	0.44
1:B:320:LEU:HG	1:B:324:PHE:CE1	2.53	0.44
1:C:108:VAL:HG21	1:C:331:LYS:HD2	1.99	0.44
1:B:135:ALA:HB3	1:B:167:VAL:HG12	1.99	0.44
1:D:281:ALA:HB2	1:D:317:GLU:HA	1.98	0.44
1:B:281:ALA:CB	1:B:317:GLU:HG2	2.47	0.44
1:C:298:CYS:O	1:C:302:ILE:HG13	2.18	0.44
1:A:115:ARG:HH22	1:A:233:LYS:HB3	1.80	0.44
1:B:334:SER:C	1:B:336:GLU:H	2.21	0.44
1:A:266:SER:HB2	1:A:310:ILE:CD1	2.46	0.44
1:D:228:GLN:CB	1:D:341:TYR:HE1	2.24	0.44
1:B:280:ARG:NE	1:B:282:ALA:HB3	2.30	0.44
1:A:143:TYR:OH	1:A:353:LYS:HA	2.18	0.44
1:D:261:GLU:HG2	1:D:266:SER:OG	2.16	0.44
1:C:169:ASP:HA	1:C:188:LYS:HZ2	1.82	0.44
1:A:294:ILE:HG12	1:A:323:TYR:CE1	2.52	0.44
1:B:190:LYS:HB3	1:B:190:LYS:HE2	1.90	0.44
1:D:172:ARG:HG3	1:D:172:ARG:NH2	2.31	0.44
1:B:134:PHE:O	1:B:226:VAL:HB	2.18	0.44
1:B:268:ALA:HA	1:B:322:LYS:HG2	1.99	0.44
1:C:303:LEU:HA	1:C:306:LYS:CB	2.45	0.44
1:A:198:ILE:O	1:A:201:MET:N	2.49	0.44
1:C:175:LEU:HA	1:C:175:LEU:HD23	1.89	0.44
1:C:132:THR:HB	1:C:166:MET:CE	2.48	0.44
1:D:165:ILE:HG22	1:D:167:VAL:HG13	1.99	0.44
1:C:94:ARG:HB3	1:C:97:VAL:CG2	2.48	0.43
1:C:324:PHE:HA	1:C:327:ASN:O	2.18	0.43
1:C:246:LEU:HD13	1:C:251:TYR:HD2	1.83	0.43
1:A:204:LYS:HB2	1:A:299:PHE:CD1	2.53	0.43
1:D:98:VAL:CG2	1:D:252:LYS:NZ	2.81	0.43
1:B:201:MET:HG3	1:B:201:MET:O	2.19	0.43
1:C:227:ASP:O	1:C:227:ASP:CG	2.55	0.43
1:C:201:MET:O	1:C:204:LYS:HB3	2.18	0.43
1:D:261:GLU:OE1	1:D:313:GLN:N	2.50	0.43
1:A:154:HIS:CE1	1:A:233:LYS:HZ2	2.36	0.43
1:C:102:LYS:H	1:C:102:LYS:HG3	1.55	0.43
1:A:101:THR:O	1:A:104:LYS:N	2.51	0.43
1:B:303:LEU:O	1:B:304:LYS:C	2.57	0.43
1:D:198:ILE:HG22	1:D:199:SER:N	2.32	0.43
1:B:190:LYS:HE3	1:B:192:GLU:OE1	2.17	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:99:THR:HA	1:B:107:VAL:HB	1.99	0.43
1:C:198:ILE:O	1:C:198:ILE:HG23	2.19	0.43
1:D:337:TYR:O	1:D:338:CYS:HB2	2.18	0.43
1:D:110:GLU:N	1:D:336:GLU:OE2	2.44	0.43
1:A:293:ASN:ND2	1:A:323:TYR:OH	2.51	0.43
1:D:169:ASP:OD2	1:D:171:SER:OG	2.37	0.43
1:B:297:GLU:CD	1:B:300:LYS:HD2	2.38	0.43
1:D:200:MET:HE1	1:D:303:LEU:HD23	1.99	0.43
1:A:308:ASN:O	1:A:309:ASP:HB3	2.18	0.43
1:B:180:PRO:O	1:B:181:LEU:HB2	2.19	0.43
1:A:101:THR:CG2	1:A:332:ILE:HD12	2.45	0.43
1:A:256:ASN:HD21	1:A:273:GLY:CA	2.32	0.43
1:A:190:LYS:O	1:A:192:GLU:N	2.47	0.43
1:C:213:HIS:ND1	1:C:214:ILE:N	2.67	0.43
1:D:173:MET:CE	1:D:175:LEU:HD23	2.49	0.43
1:A:128:THR:HG23	1:A:160:PRO:HB2	2.01	0.43
1:C:200:MET:HE2	1:C:302:ILE:CG2	2.47	0.42
1:C:201:MET:HG2	1:C:201:MET:H	1.57	0.42
1:C:199:SER:HA	1:C:201:MET:HG2	2.00	0.42
1:C:102:LYS:CB	1:C:102:LYS:NZ	2.82	0.42
1:B:247:GLN:O	1:B:247:GLN:HG2	2.19	0.42
1:D:157:VAL:HG12	1:D:158:GLY:N	2.34	0.42
1:B:132:THR:CG2	1:B:166:MET:HE1	2.49	0.42
1:C:103:TRP:CE2	1:C:328:LYS:HB3	2.55	0.42
1:B:103:TRP:O	1:B:104:LYS:HB2	2.19	0.42
1:A:225:ASP:HB2	1:A:228:GLN:NE2	2.34	0.42
1:C:236:VAL:HA	1:C:239:LEU:HG	2.02	0.42
1:B:233:LYS:HD3	1:B:233:LYS:HA	1.78	0.42
1:B:253:ALA:C	1:B:255:PRO:N	2.73	0.42
1:B:297:GLU:OE2	1:B:300:LYS:HD2	2.19	0.42
1:D:246:LEU:HG	1:D:332:ILE:CG2	2.50	0.42
1:D:94:ARG:HA	1:D:94:ARG:NE	2.27	0.42
1:A:173:MET:SD	1:A:186:VAL:HG11	2.59	0.42
1:B:156:MET:HE1	1:B:236:VAL:HA	2.00	0.42
1:D:226:VAL:O	1:D:228:GLN:N	2.53	0.42
1:D:91:PRO:HG2	1:D:92:PHE:H	1.85	0.42
1:D:269:TYR:CZ	1:D:271:PRO:HG3	2.55	0.42
1:B:91:PRO:HD3	1:C:249:TRP:CZ2	2.54	0.42
1:B:243:VAL:HA	1:B:331:LYS:O	2.19	0.42
1:B:167:VAL:C	1:B:189:ILE:HG12	2.40	0.42
1:B:246:LEU:HD12	1:B:335:PRO:HD3	2.02	0.42
1:D:138:ARG:HD3	1:D:141:GLU:OE2	2.20	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:246:LEU:CD2	1:D:277:PHE:HB3	2.50	0.42
1:B:204:LYS:HE2	1:B:204:LYS:HB3	1.85	0.42
1:B:312:ALA:O	1:B:313:GLN:CB	2.68	0.41
1:A:336:GLU:O	1:A:347:ALA:HB3	2.20	0.41
1:D:248:ALA:O	1:D:250:TRP:N	2.53	0.41
1:A:98:VAL:HG22	1:A:249:TRP:CD2	2.55	0.41
1:A:115:ARG:NH2	1:A:233:LYS:HB3	2.35	0.41
1:A:350:LYS:HD3	1:A:352:VAL:HB	2.01	0.41
1:A:118:LEU:HD13	1:A:237:GLU:HA	2.01	0.41
1:A:350:LYS:CD	1:A:352:VAL:HB	2.51	0.41
1:D:266:SER:N	1:D:310:ILE:HD13	2.35	0.41
1:D:136:VAL:CG1	1:D:191:PRO:HB3	2.50	0.41
1:B:220:PHE:CD1	1:B:239:LEU:HD13	2.55	0.41
1:B:254:ASP:C	1:B:256:ASN:H	2.23	0.41
1:D:263:ARG:HH11	1:D:263:ARG:CB	2.32	0.41
1:D:210:ILE:O	1:D:215:GLN:HG2	2.21	0.41
1:D:324:PHE:HA	1:D:327:ASN:O	2.20	0.41
1:A:353:LYS:HA	1:A:353:LYS:HD3	1.88	0.41
1:A:304:LYS:HB3	1:A:304:LYS:HE3	1.96	0.41
1:A:225:ASP:HB2	1:A:228:GLN:HE21	1.85	0.41
1:D:254:ASP:HB2	1:D:257:ASP:OD2	2.19	0.41
1:D:180:PRO:O	1:D:181:LEU:HB2	2.21	0.41
1:A:336:GLU:O	1:A:346:PRO:O	2.38	0.41
1:D:150:SER:HB2	1:D:230:PHE:HB2	2.03	0.41
1:A:347:ALA:O	1:A:348:ASP:CB	2.68	0.41
1:A:303:LEU:HA	1:A:306:LYS:HD2	2.03	0.41
1:A:181:LEU:C	1:A:182:ARG:HD2	2.42	0.41
1:D:166:MET:HB3	1:D:189:ILE:HD13	2.02	0.41
1:D:251:TYR:CG	1:D:252:LYS:N	2.87	0.41
1:C:101:THR:OG1	1:C:105:ALA:HB3	2.21	0.41
1:B:242:SER:OG	1:B:329:PRO:HA	2.20	0.41
1:D:252:LYS:HD2	1:D:252:LYS:HA	1.85	0.41
1:D:199:SER:O	1:D:203:MET:HG2	2.20	0.41
1:D:131:LEU:C	1:D:131:LEU:HD23	2.42	0.40
1:B:203:MET:HB3	1:B:295:THR:O	2.21	0.40
1:A:206:ILE:O	1:A:210:ILE:HG13	2.22	0.40
1:B:221:LEU:HD22	1:B:291:VAL:HG11	2.03	0.40
1:C:185:LYS:HE2	1:C:187:PHE:CZ	2.52	0.40
1:B:138:ARG:HH11	1:B:138:ARG:C	2.21	0.40
1:B:173:MET:HG3	1:B:186:VAL:HG11	2.02	0.40
1:B:141:GLU:O	1:B:141:GLU:HG3	2.20	0.40
1:D:305:ASP:CB	1:D:310:ILE:HG23	2.51	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:245:GLN:O	1:D:279:TYR:HB3	2.21	0.40
1:D:125:GLN:O	1:D:126:LYS:HB2	2.21	0.40
1:A:254:ASP:O	1:A:256:ASN:N	2.55	0.40
1:B:241:GLU:HB2	1:B:330:THR:CG2	2.50	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	264/273 (97%)	217 (82%)	33 (12%)	14 (5%)	3	8
1	B	248/273 (91%)	204 (82%)	33 (13%)	11 (4%)	4	11
1	C	251/273 (92%)	219 (87%)	24 (10%)	8 (3%)	6	20
1	D	254/273 (93%)	212 (84%)	29 (11%)	13 (5%)	3	9
All	All	1017/1092 (93%)	852 (84%)	119 (12%)	46 (4%)	4	11

All (46) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	171	SER
1	A	251	TYR
1	A	253	ALA
1	A	338	CYS
1	A	341	TYR
1	A	345	LEU
1	A	348	ASP
1	A	352	VAL
1	B	172	ARG
1	B	254	ASP
1	B	255	PRO
1	B	260	TYR
1	B	312	ALA
1	B	313	GLN

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Mol	Chain	Res	Type
1	C	253	ALA
1	C	255	PRO
1	D	142	HIS
1	D	251	TYR
1	B	140	ILE
1	C	86	SER
1	C	185	LYS
1	C	197	ASP
1	D	255	PRO
1	D	264	LYS
1	D	326	LEU
1	D	346	PRO
1	A	312	ALA
1	A	315	HIS
1	B	253	ALA
1	C	171	SER
1	C	172	ARG
1	D	227	ASP
1	D	249	TRP
1	D	341	TYR
1	D	347	ALA
1	A	342	HIS
1	B	200	MET
1	B	264	LYS
1	B	315	HIS
1	A	255	PRO
1	A	346	PRO
1	D	327	ASN
1	A	213	HIS
1	D	343	ILE
1	C	236	VAL
1	D	98	VAL

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	237/244 (97%)	219 (92%)	18 (8%)	19 46

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	223/244 (91%)	206 (92%)	17 (8%)	19	46
1	C	226/244 (93%)	217 (96%)	9 (4%)	42	78
1	D	230/244 (94%)	215 (94%)	15 (6%)	24	56
All	All	916/976 (94%)	857 (94%)	59 (6%)	25	57

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

Mol	Chain	Res	Type
1	A	98	VAL
1	A	120	ASN
1	A	157	VAL
1	A	173	MET
1	A	182	ARG
1	A	198	ILE
1	A	201	MET
1	A	232	ASP
1	A	234	PHE
1	A	250	TRP
1	A	296	GLN
1	A	304	LYS
1	A	309	ASP
1	A	316	ASP
1	A	321	ASN
1	A	343	ILE
1	A	346	PRO
1	A	354	MET
1	B	86	SER
1	B	96	GLU
1	B	110	GLU
1	B	132	THR
1	B	136	VAL
1	B	145	GLU
1	B	166	MET
1	B	182	ARG
1	B	198	ILE
1	B	202	ARG
1	B	225	ASP
1	B	236	VAL
1	B	257	ASP
1	B	280	ARG
1	B	303	LEU

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Mol	Chain	Res	Type
1	B	313	GLN
1	B	316	ASP
1	C	102	LYS
1	C	157	VAL
1	C	182	ARG
1	C	200	MET
1	C	201	MET
1	C	232	ASP
1	C	255	PRO
1	C	310	ILE
1	C	321	ASN
1	D	89	PHE
1	D	94	ARG
1	D	96	GLU
1	D	125	GLN
1	D	127	ILE
1	D	141	GLU
1	D	142	HIS
1	D	166	MET
1	D	182	ARG
1	D	184	PHE
1	D	232	ASP
1	D	303	LEU
1	D	340	ASP
1	D	341	TYR
1	D	345	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	120	ASN
1	A	142	HIS
1	A	228	GLN
1	A	256	ASN
1	A	293	ASN
1	A	296	GLN
1	A	308	ASN
1	A	321	ASN
1	A	327	ASN
1	B	120	ASN
1	C	90	ASN
1	C	152	ASN

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Mol	Chain	Res	Type
1	C	215	GLN
1	C	231	GLN
1	C	293	ASN
1	C	296	GLN
1	C	313	GLN
1	D	125	GLN
1	D	154	HIS
1	D	215	GLN
1	D	216	HIS
1	D	231	GLN
1	D	296	GLN
1	D	313	GLN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

3 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	MPD	B	1339	-	7,7,7	0.56	0	10,10,10	0.35	0
3	GOL	B	1340	-	5,5,5	4.44	5 (100%)	5,5,5	5.73	3 (60%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GOL	C	1340	-	5,5,5	4.54	5 (100%)	5,5,5	5.74	3 (60%)

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	MPD	B	1339	-	-	0/5/5/5	0/0/0/0
3	GOL	B	1340	-	-	0/4/4/4	0/0/0/0
3	GOL	C	1340	-	-	0/4/4/4	0/0/0/0

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1340	GOL	C3-C2	-7.56	1.21	1.52
3	B	1340	GOL	C3-C2	-7.47	1.21	1.52
3	C	1340	GOL	O1-C1	4.41	1.61	1.42
3	B	1340	GOL	O1-C1	4.31	1.61	1.42
3	B	1340	GOL	O3-C3	3.30	1.56	1.42
3	C	1340	GOL	O3-C3	3.26	1.56	1.42
3	C	1340	GOL	C1-C2	-2.91	1.40	1.52
3	B	1340	GOL	C1-C2	-2.81	1.40	1.52
3	C	1340	GOL	O2-C2	-2.72	1.35	1.43
3	B	1340	GOL	O2-C2	-2.36	1.36	1.43

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1340	GOL	O3-C3-C2	10.36	160.27	109.71
3	B	1340	GOL	O3-C3-C2	10.35	160.20	109.71
3	B	1340	GOL	O2-C2-C3	6.73	138.89	108.22
3	C	1340	GOL	O2-C2-C3	6.72	138.82	108.22
3	C	1340	GOL	O1-C1-C2	3.35	126.06	109.71
3	B	1340	GOL	O1-C1-C2	3.28	125.73	109.71

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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	268/273 (98%)	-0.08	9 (3%) 43 44	15, 22, 53, 73	3 (1%)
1	B	252/273 (92%)	-0.06	11 (4%) 33 33	15, 24, 50, 58	3 (1%)
1	C	255/273 (93%)	0.16	10 (3%) 37 37	15, 29, 54, 59	2 (0%)
1	D	260/273 (95%)	0.10	16 (6%) 20 19	15, 28, 58, 69	4 (1%)
All	All	1035/1092 (94%)	0.03	46 (4%) 33 33	15, 26, 54, 73	12 (1%)

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	314	TRP	6.3
1	A	342	HIS	4.8
1	C	197	ASP	3.5
1	A	250	TRP	3.5
1	B	306	LYS	3.4
1	C	196	GLN	3.3
1	A	341	TYR	3.1
1	C	274	GLU	3.1
1	C	310	ILE	3.1
1	D	141	GLU	3.0
1	C	172	ARG	3.0
1	B	254	ASP	2.8
1	D	114	ASN	2.8
1	A	257	ASP	2.7
1	D	92	PHE	2.7
1	D	82	LYS	2.7
1	D	255	PRO	2.7
1	A	198	ILE	2.7
1	B	250	TRP	2.6
1	D	172	ARG	2.6
1	B	312	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	268	ALA	2.4
1	B	309	ASP	2.4
1	D	91	PRO	2.4
1	C	256	ASN	2.4
1	D	110	GLU	2.4
1	D	90	ASN	2.3
1	A	306	LYS	2.3
1	D	120	ASN	2.2
1	C	254	ASP	2.2
1	A	200	MET	2.2
1	A	309	ASP	2.2
1	B	255	PRO	2.2
1	D	89	PHE	2.2
1	D	263	ARG	2.2
1	D	338	CYS	2.2
1	C	124	LYS	2.1
1	C	339	TRP	2.1
1	A	312	ALA	2.1
1	D	93	LYS	2.1
1	B	266	SER	2.1
1	D	115	ARG	2.1
1	B	253	ALA	2.0
1	D	168	ASP	2.0
1	B	315	HIS	2.0
1	C	190	LYS	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	MPD	B	1339	8/8	0.27	1.12	42,43,45,45	0
3	GOL	B	1340	6/6	0.19	0.74	30,33,34,35	0
3	GOL	C	1340	6/6	0.16	-1.50	53,55,55,55	0

6.5 Other polymers ⓘ

There are no such residues in this entry.