



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:35 PM GMT

PDB ID : 4FFG
Title : Crystal Structure of Levan Fructotransferase from *Arthrobacter ureafaciens* in complex with DFA-IV
Authors : Park, J.; Rhee, S.
Deposited on : 2012-06-01
Resolution : 2.30 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
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

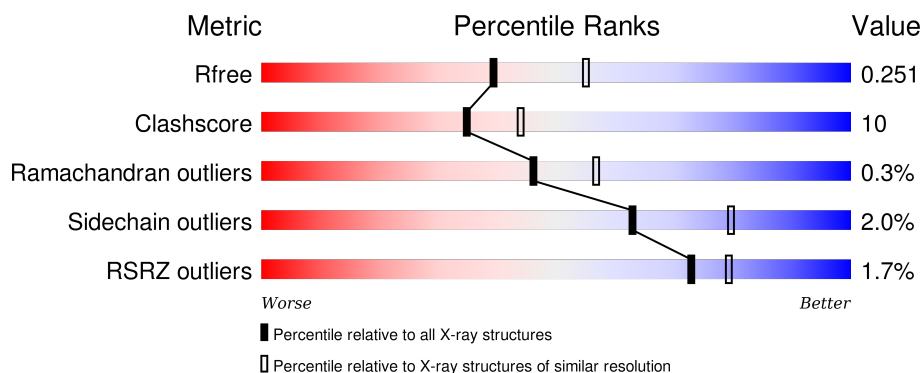
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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}	91344	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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. 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	492	<div> <div>2%</div> <div>79% 17% ..</div> </div>
1	B	492	<div> <div>2%</div> <div>78% 18% ..</div> </div>
1	C	492	<div> <div>%</div> <div>77% 20% ..</div> </div>
1	D	492	<div> <div>%</div> <div>81% 16% ..</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
2	LBS	C	601	-	-	-	X
2	LBS	D	601	-	-	-	X
3	0U8	B	602	-	-	-	X
3	0U8	D	602	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 15976 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 Levan fructotransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	480	Total	C	N	O	S	0	0	0
			3739	2375	645	711	8			
1	B	480	Total	C	N	O	S	0	0	0
			3739	2375	645	711	8			
1	C	479	Total	C	N	O	S	0	0	0
			3734	2372	644	710	8			
1	D	480	Total	C	N	O	S	0	0	0
			3739	2375	645	711	8			

There are 48 discrepancies between the modelled and reference sequences:

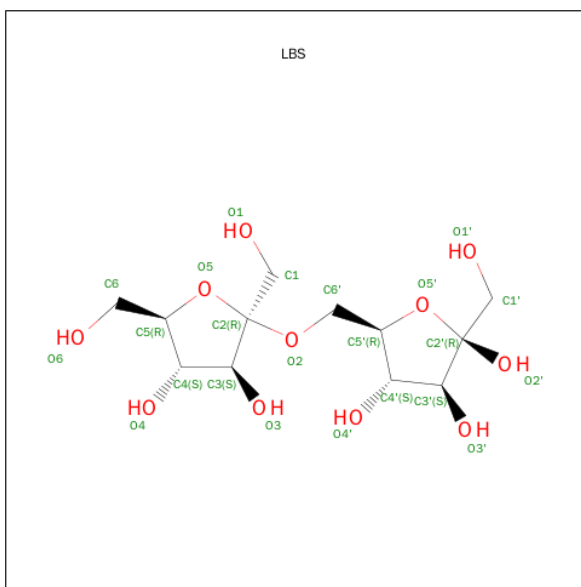
Chain	Residue	Modelled	Actual	Comment	Reference
A	40	MET	-	EXPRESSION TAG	UNP Q9KJD0
A	115	ASP	GLY	CONFLICT	UNP Q9KJD0
A	522	LEU	-	EXPRESSION TAG	UNP Q9KJD0
A	523	GLU	-	EXPRESSION TAG	UNP Q9KJD0
A	524	HIS	-	EXPRESSION TAG	UNP Q9KJD0
A	525	HIS	-	EXPRESSION TAG	UNP Q9KJD0
A	526	HIS	-	EXPRESSION TAG	UNP Q9KJD0
A	527	HIS	-	EXPRESSION TAG	UNP Q9KJD0
A	528	HIS	-	EXPRESSION TAG	UNP Q9KJD0
A	529	HIS	-	EXPRESSION TAG	UNP Q9KJD0
A	530	HIS	-	EXPRESSION TAG	UNP Q9KJD0
A	531	HIS	-	EXPRESSION TAG	UNP Q9KJD0
B	40	MET	-	EXPRESSION TAG	UNP Q9KJD0
B	115	ASP	GLY	CONFLICT	UNP Q9KJD0
B	522	LEU	-	EXPRESSION TAG	UNP Q9KJD0
B	523	GLU	-	EXPRESSION TAG	UNP Q9KJD0
B	524	HIS	-	EXPRESSION TAG	UNP Q9KJD0
B	525	HIS	-	EXPRESSION TAG	UNP Q9KJD0
B	526	HIS	-	EXPRESSION TAG	UNP Q9KJD0
B	527	HIS	-	EXPRESSION TAG	UNP Q9KJD0
B	528	HIS	-	EXPRESSION TAG	UNP Q9KJD0

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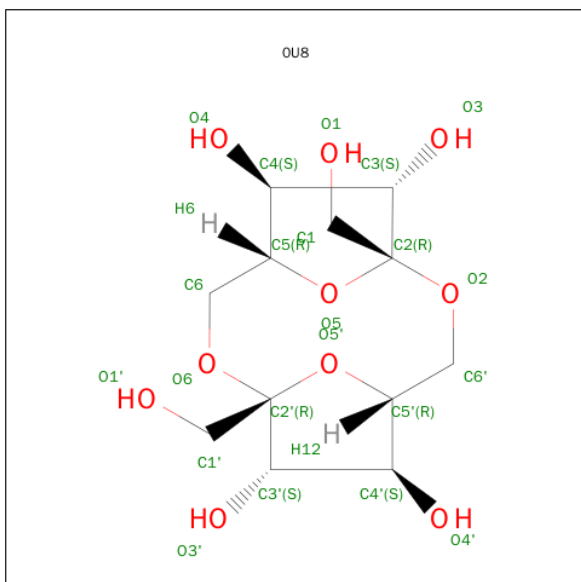
Chain	Residue	Modelled	Actual	Comment	Reference
B	529	HIS	-	EXPRESSION TAG	UNP Q9KJD0
B	530	HIS	-	EXPRESSION TAG	UNP Q9KJD0
B	531	HIS	-	EXPRESSION TAG	UNP Q9KJD0
C	40	MET	-	EXPRESSION TAG	UNP Q9KJD0
C	115	ASP	GLY	CONFLICT	UNP Q9KJD0
C	522	LEU	-	EXPRESSION TAG	UNP Q9KJD0
C	523	GLU	-	EXPRESSION TAG	UNP Q9KJD0
C	524	HIS	-	EXPRESSION TAG	UNP Q9KJD0
C	525	HIS	-	EXPRESSION TAG	UNP Q9KJD0
C	526	HIS	-	EXPRESSION TAG	UNP Q9KJD0
C	527	HIS	-	EXPRESSION TAG	UNP Q9KJD0
C	528	HIS	-	EXPRESSION TAG	UNP Q9KJD0
C	529	HIS	-	EXPRESSION TAG	UNP Q9KJD0
C	530	HIS	-	EXPRESSION TAG	UNP Q9KJD0
C	531	HIS	-	EXPRESSION TAG	UNP Q9KJD0
D	40	MET	-	EXPRESSION TAG	UNP Q9KJD0
D	115	ASP	GLY	CONFLICT	UNP Q9KJD0
D	522	LEU	-	EXPRESSION TAG	UNP Q9KJD0
D	523	GLU	-	EXPRESSION TAG	UNP Q9KJD0
D	524	HIS	-	EXPRESSION TAG	UNP Q9KJD0
D	525	HIS	-	EXPRESSION TAG	UNP Q9KJD0
D	526	HIS	-	EXPRESSION TAG	UNP Q9KJD0
D	527	HIS	-	EXPRESSION TAG	UNP Q9KJD0
D	528	HIS	-	EXPRESSION TAG	UNP Q9KJD0
D	529	HIS	-	EXPRESSION TAG	UNP Q9KJD0
D	530	HIS	-	EXPRESSION TAG	UNP Q9KJD0
D	531	HIS	-	EXPRESSION TAG	UNP Q9KJD0

- Molecule 2 is 6-O-BETA-D-FRUCTOFURANOSYL-BETA-D-FRUCTOFURANOSE (three-letter code: LBS) (formula: C₁₂H₂₂O₁₁).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			23	12	11		
2	B	1	Total	C	O	0	0
			23	12	11		
2	C	1	Total	C	O	0	0
			23	12	11		
2	D	1	Total	C	O	0	0
			23	12	11		

- Molecule 3 is (1R,4R,5S,6S,7R,10R,11S,12S)-1,7-BIS(HYDROXYMETHYL)-2,8,13,14-TETRAOXATRICYCLO[8.2.1.1 4,7]TETRADECANE-5,6,11,12-TETROL (three-letter code: 0U8) (formula: C₁₂H₂₀O₁₀).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			22	12	10		
3	B	1	Total	C	O	0	0
			22	12	10		
3	C	1	Total	C	O	0	0
			22	12	10		
3	D	1	Total	C	O	0	0
			22	12	10		

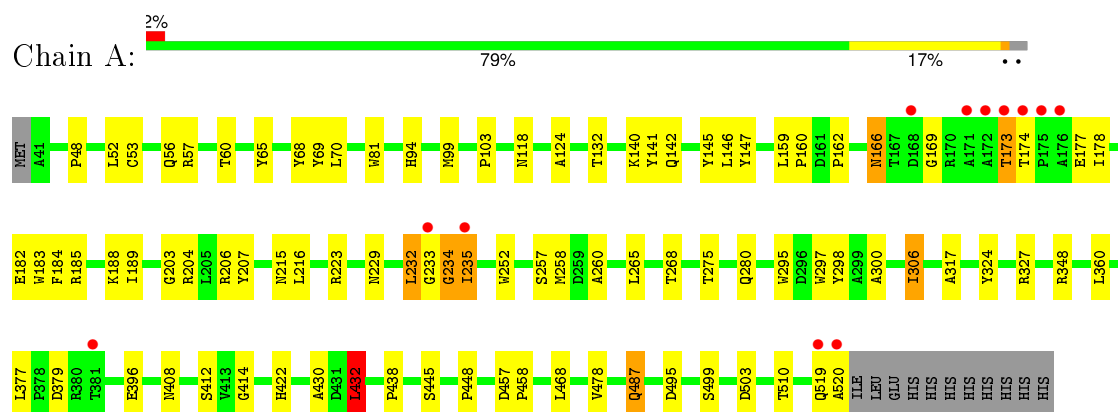
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	193	Total	O	0	0
			193	193		
4	B	184	Total	O	0	0
			184	184		
4	C	240	Total	O	0	0
			240	240		
4	D	228	Total	O	0	0
			228	228		

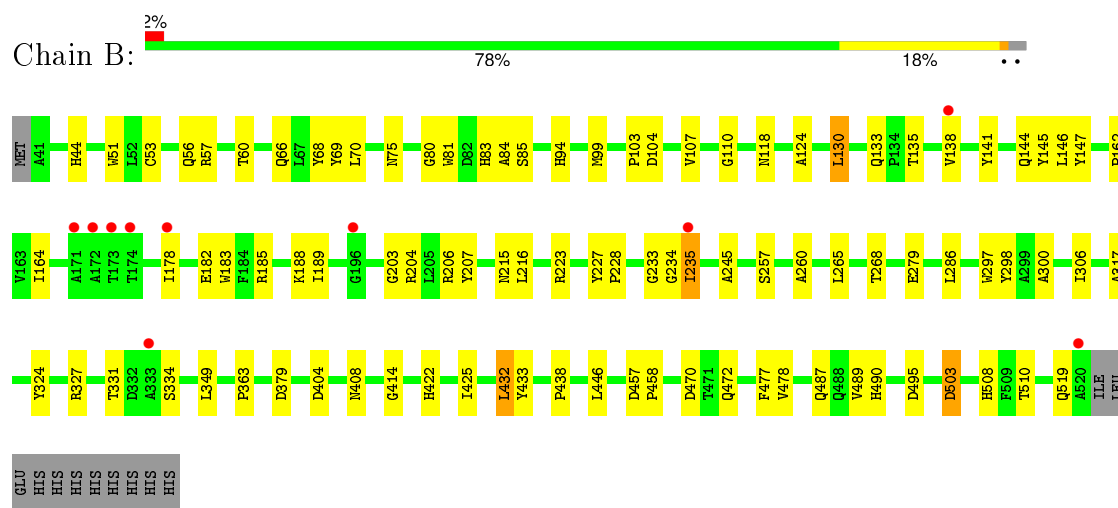
3 Residue-property plots

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

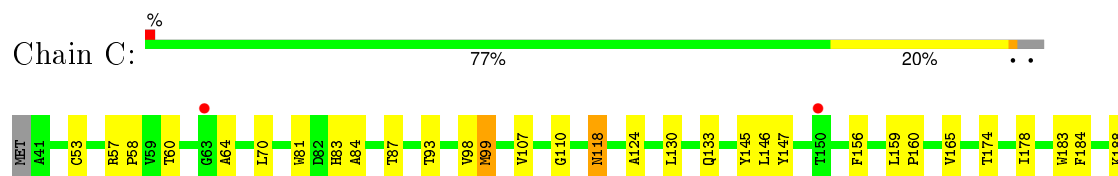
• Molecule 1: Levan fructotransferase

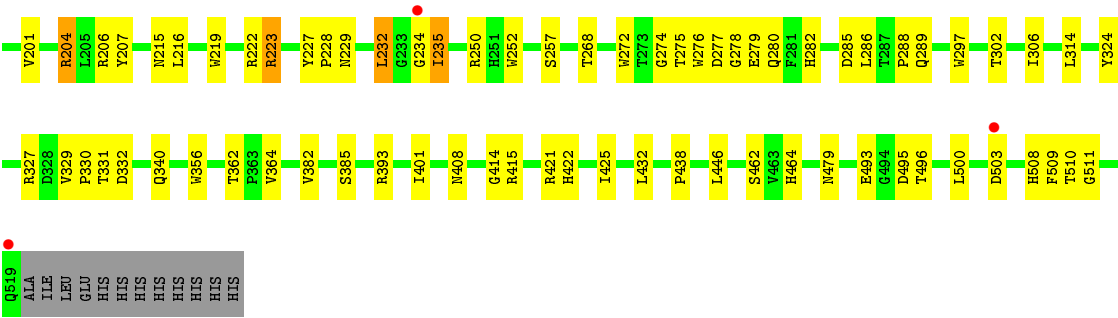


• Molecule 1: Levan fructotransferase

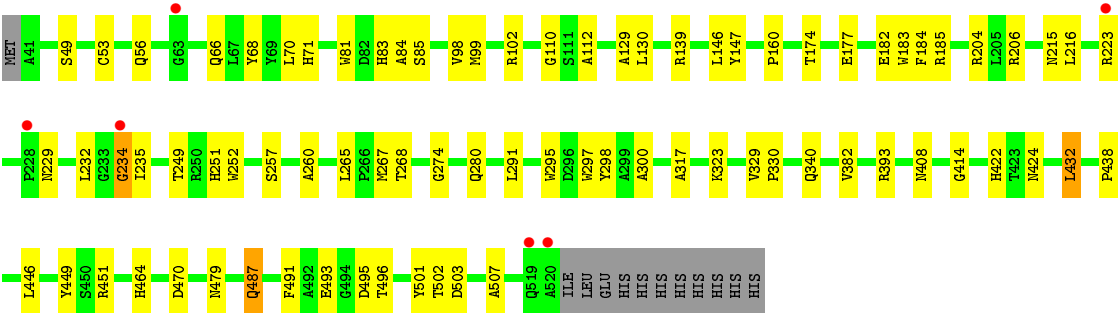
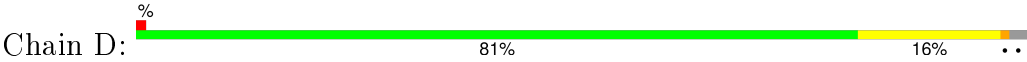


• Molecule 1: Levan fructotransferase





● Molecule 1: Levan fructotransferase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	81.86Å 161.91Å 263.06Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.30 50.04 – 2.30	Depositor EDS
% Data completeness (in resolution range)	87.8 (50.00-2.30) 96.9 (50.04-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.72 (at 2.29Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.205 , 0.240 0.218 , 0.251	Depositor DCC
R_{free} test set	15040 reflections (10.00%)	DCC
Wilson B-factor (Å ²)	26.1	Xtriage
Anisotropy	0.757	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 37.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 154962 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	15976	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.43% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: LBS, 0U8

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	0.31	0/3863	0.65	3/5312 (0.1%)
1	B	0.33	0/3863	0.65	2/5312 (0.0%)
1	C	0.33	0/3858	0.64	1/5305 (0.0%)
1	D	0.33	0/3863	0.65	2/5312 (0.0%)
All	All	0.32	0/15447	0.64	8/21241 (0.0%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	432	LEU	CA-CB-CG	-7.53	97.97	115.30
1	C	432	LEU	N-CA-C	-6.60	93.18	111.00
1	A	432	LEU	N-CA-C	-6.20	94.25	111.00
1	D	432	LEU	N-CA-C	-6.05	94.66	111.00
1	A	234	GLY	N-CA-C	5.89	127.83	113.10
1	B	432	LEU	N-CA-C	-5.78	95.40	111.00
1	D	234	GLY	N-CA-C	5.55	126.98	113.10
1	B	234	GLY	N-CA-C	5.41	126.61	113.10

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	3739	0	3489	69	0
1	B	3739	0	3489	66	0
1	C	3734	0	3484	82	0
1	D	3739	0	3489	61	0
2	A	23	0	22	1	0
2	B	23	0	22	0	0
2	C	23	0	22	3	0
2	D	23	0	22	3	0
3	A	22	0	19	1	0
3	B	22	0	19	6	0
3	C	22	0	19	3	0
3	D	22	0	19	1	0
4	A	193	0	0	2	0
4	B	184	0	0	3	0
4	C	240	0	0	6	0
4	D	228	0	0	4	0
All	All	15976	0	14115	288	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 10.

All (288) 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)
3:C:602:0U8:H11	3:C:602:0U8:H19	1.34	1.07
3:C:602:0U8:H11	3:C:602:0U8:C4	1.91	0.99
1:A:57:ARG:HD2	1:A:188:LYS:HE3	1.56	0.86
1:D:329:VAL:HG13	1:D:330:PRO:HD2	1.58	0.86
1:D:206:ARG:HH11	1:D:234:GLY:HA3	1.44	0.82
1:B:57:ARG:HD2	1:B:188:LYS:HE2	1.61	0.80
1:C:329:VAL:HG13	1:C:330:PRO:HD2	1.65	0.79
1:C:206:ARG:HD3	1:C:234:GLY:HA2	1.66	0.77
1:D:464:HIS:H	1:D:479:ASN:ND2	1.83	0.76
1:B:327:ARG:HH22	1:B:490:HIS:HE1	1.36	0.73
1:B:53:CYS:HB3	1:B:70:LEU:HB2	1.70	0.73
1:C:503:ASP:OD2	3:C:602:0U8:H7	1.88	0.72
1:D:223:ARG:HD2	1:D:280:GLN:CD	2.10	0.72
1:B:331:THR:HA	1:B:334:SER:HB3	1.70	0.72
1:C:234:GLY:O	1:C:235:ILE:HG12	1.89	0.71
1:A:81:TRP:HB2	1:A:99:MET:HB2	1.73	0.71
2:C:601:LBS:H3	2:C:601:LBS:H8	1.72	0.70
1:C:229:ASN:HB3	1:C:232:LEU:HD22	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:57:ARG:HH12	1:C:188:LYS:NZ	1.91	0.69
1:C:206:ARG:HH11	1:C:234:GLY:CA	2.07	0.68
1:C:414:GLY:O	1:C:495:ASP:HB3	1.92	0.68
1:A:142:GLN:HE22	1:A:185:ARG:HH11	1.41	0.67
1:D:464:HIS:H	1:D:479:ASN:HD21	1.42	0.67
1:C:53:CYS:HB3	1:C:70:LEU:HB2	1.77	0.67
1:A:53:CYS:HB3	1:A:70:LEU:HB2	1.78	0.66
1:B:145:TYR:CZ	1:B:162:PRO:HG3	2.30	0.66
1:B:146:LEU:HD23	1:B:147:TYR:N	2.11	0.65
1:A:432:LEU:HD22	1:A:478:VAL:CG2	2.28	0.64
1:D:53:CYS:HB3	1:D:70:LEU:HB2	1.78	0.64
1:C:464:HIS:H	1:C:479:ASN:ND2	1.95	0.63
2:D:601:LBS:H8	2:D:601:LBS:C6	2.29	0.63
1:A:206:ARG:NE	1:A:233:GLY:HA2	2.14	0.63
1:A:229:ASN:O	1:A:232:LEU:HB2	1.99	0.62
1:B:408:ASN:HB3	1:B:503:ASP:HB2	1.82	0.62
1:D:267:MET:CE	1:D:323:LYS:HD3	2.30	0.62
1:C:285:ASP:HB3	4:C:754:HOH:O	1.98	0.61
1:D:249:THR:OG1	1:D:251:HIS:HE1	1.83	0.61
1:C:422:HIS:O	1:C:438:PRO:HB2	2.01	0.61
1:D:229:ASN:O	1:D:232:LEU:HB2	1.99	0.60
1:D:329:VAL:CG1	1:D:330:PRO:HD2	2.30	0.60
1:A:174:THR:HG23	1:A:177:GLU:OE1	2.01	0.60
1:A:324:TYR:O	1:A:327:ARG:HG2	2.02	0.60
1:B:203:GLY:HA2	1:B:235:ILE:HG22	1.82	0.60
1:A:223:ARG:HB2	1:A:280:GLN:HB3	1.84	0.59
1:B:324:TYR:O	1:B:327:ARG:HG2	2.02	0.59
1:D:66:GLN:HE22	1:D:85:SER:HB3	1.68	0.59
1:B:327:ARG:HH22	1:B:490:HIS:CE1	2.20	0.59
1:A:229:ASN:ND2	1:A:232:LEU:HD13	2.18	0.58
1:A:422:HIS:O	1:A:438:PRO:HB2	2.03	0.58
1:B:206:ARG:NE	1:B:233:GLY:HA2	2.18	0.58
1:A:306:ILE:HD13	1:A:306:ILE:O	2.04	0.58
1:C:64:ALA:HB2	1:C:87:THR:HG22	1.85	0.58
1:A:203:GLY:HA2	1:A:235:ILE:HG22	1.85	0.58
1:C:329:VAL:HG13	1:C:330:PRO:CD	2.33	0.58
1:D:329:VAL:HG13	1:D:330:PRO:CD	2.33	0.57
3:B:602:OU8:H19	3:B:602:OU8:H11	1.86	0.57
1:D:267:MET:HE1	1:D:323:LYS:HD3	1.86	0.57
1:D:184:PHE:HD1	1:D:204:ARG:HD3	1.69	0.57
1:A:204:ARG:HD3	1:A:207:TYR:CE1	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:329:VAL:HG12	1:C:331:THR:H	1.69	0.57
1:A:146:LEU:C	1:A:146:LEU:HD23	2.25	0.57
1:D:206:ARG:HH11	1:D:234:GLY:CA	2.14	0.56
1:D:215:ASN:O	1:D:216:LEU:HB2	2.06	0.56
1:D:422:HIS:O	1:D:438:PRO:HB2	2.05	0.55
1:D:257:SER:HA	1:D:268:THR:O	2.06	0.55
1:B:145:TYR:CE1	1:B:162:PRO:HG3	2.41	0.55
1:B:51:TRP:HB2	1:B:75:ASN:HD22	1.72	0.55
1:A:188:LYS:HE2	1:A:189:ILE:O	2.06	0.55
1:C:204:ARG:HH21	2:C:601:LBS:H15	1.71	0.55
1:D:323:LYS:HG2	1:D:449:TYR:CZ	2.42	0.55
1:B:44:HIS:HD2	1:B:470:ASP:OD2	1.88	0.55
1:C:83:HIS:CD2	1:C:84:ALA:N	2.75	0.55
1:A:432:LEU:HD22	1:A:478:VAL:HG21	1.87	0.54
2:D:601:LBS:H3	2:D:601:LBS:H8	1.89	0.54
1:B:130:LEU:HB2	1:B:189:ILE:HD11	1.89	0.54
1:B:327:ARG:NH2	1:B:490:HIS:HE1	2.03	0.54
1:D:206:ARG:NH1	1:D:234:GLY:HA3	2.19	0.54
1:C:215:ASN:O	1:C:216:LEU:HB2	2.07	0.54
1:C:229:ASN:O	1:C:232:LEU:HB2	2.07	0.54
3:B:602:OU8:H11	3:B:602:OU8:C4	2.35	0.53
1:D:251:HIS:HD2	4:D:749:HOH:O	1.91	0.53
1:A:166:ASN:HD22	1:A:166:ASN:C	2.11	0.53
1:C:183:TRP:O	1:C:204:ARG:HD2	2.09	0.53
1:A:145:TYR:CE1	1:A:162:PRO:HD3	2.43	0.53
1:C:510:THR:HG22	1:C:511:GLY:N	2.23	0.53
3:B:602:OU8:O3	3:B:602:OU8:H11	2.09	0.53
1:B:215:ASN:O	1:B:216:LEU:HB2	2.10	0.52
1:C:393:ARG:HD3	1:C:496:THR:HG22	1.91	0.52
1:B:508:HIS:HB2	4:B:861:HOH:O	2.08	0.52
1:C:57:ARG:HH12	1:C:188:LYS:HZ1	1.56	0.52
1:A:60:THR:HG22	1:A:65:TYR:HD1	1.73	0.52
1:D:393:ARG:HD3	1:D:496:THR:HG22	1.92	0.52
1:C:324:TYR:O	1:C:327:ARG:HG2	2.10	0.52
1:A:142:GLN:NE2	1:A:184:PHE:H	2.08	0.51
1:B:519:GLN:N	1:B:519:GLN:OE1	2.41	0.51
1:B:118:ASN:HB2	1:B:124:ALA:HA	1.92	0.51
1:A:432:LEU:HD22	1:A:478:VAL:HG22	1.91	0.51
1:B:178:ILE:O	1:B:182:GLU:HG3	2.10	0.51
1:D:252:TRP:HB2	1:D:274:GLY:O	2.09	0.51
1:A:408:ASN:HB3	1:A:503:ASP:HB2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:57:ARG:NH1	1:C:188:LYS:HE2	2.26	0.51
1:D:56:GLN:HB2	1:D:68:TYR:HB2	1.92	0.51
1:C:252:TRP:HB2	1:C:274:GLY:O	2.11	0.51
1:C:329:VAL:O	1:C:332:ASP:HB2	2.11	0.51
1:B:257:SER:HB3	1:B:298:TYR:CE1	2.46	0.50
1:B:69:TYR:OH	1:B:94:HIS:HD2	1.94	0.50
2:C:601:LBS:C6	2:C:601:LBS:H8	2.41	0.50
1:D:257:SER:HB3	1:D:298:TYR:CE2	2.47	0.50
1:C:146:LEU:HD23	1:C:146:LEU:C	2.32	0.50
1:D:146:LEU:HD23	1:D:146:LEU:C	2.32	0.50
1:D:295:TRP:H	1:D:487:GLN:HG3	1.77	0.50
1:D:66:GLN:NE2	1:D:85:SER:HB3	2.26	0.50
1:D:139:ARG:HG2	1:D:182:GLU:HG2	1.94	0.50
1:B:363:PRO:HG3	1:B:477:PHE:CE2	2.46	0.50
1:C:81:TRP:HB2	1:C:99:MET:HB2	1.93	0.50
1:A:257:SER:HB3	1:A:298:TYR:CE1	2.47	0.49
1:B:404:ASP:HB3	4:B:850:HOH:O	2.12	0.49
1:A:379:ASP:HB3	1:A:510:THR:HG22	1.93	0.49
1:C:234:GLY:O	1:C:235:ILE:CG1	2.60	0.49
1:A:295:TRP:HD1	1:A:487:GLN:HG2	1.77	0.49
1:C:57:ARG:NH1	1:C:188:LYS:NZ	2.58	0.49
1:A:178:ILE:O	1:A:182:GLU:HG3	2.12	0.49
1:D:174:THR:OG1	1:D:177:GLU:HG3	2.13	0.49
1:A:207:TYR:CE2	2:A:601:LBS:H3	2.47	0.49
1:C:393:ARG:CD	1:C:496:THR:HG22	2.42	0.49
1:C:464:HIS:H	1:C:479:ASN:HD21	1.58	0.49
1:B:118:ASN:HB2	1:B:124:ALA:CA	2.42	0.49
1:B:138:VAL:HB	1:B:141:TYR:CD2	2.48	0.49
1:C:510:THR:CG2	1:C:511:GLY:N	2.75	0.48
1:A:48:PRO:HD3	1:A:94:HIS:CD2	2.48	0.48
1:C:276:TRP:NE1	1:C:278:GLY:HA2	2.28	0.48
1:B:146:LEU:HD23	1:B:146:LEU:C	2.34	0.48
1:B:260:ALA:CB	1:B:265:LEU:HB2	2.43	0.48
1:C:408:ASN:HB3	1:C:503:ASP:HB2	1.94	0.48
1:B:432:LEU:HD13	1:B:478:VAL:HG21	1.95	0.48
1:A:146:LEU:HD23	1:A:147:TYR:N	2.29	0.48
1:C:165:VAL:HG22	4:C:886:HOH:O	2.13	0.48
1:B:81:TRP:HB2	1:B:99:MET:HB2	1.95	0.48
1:A:396:GLU:HG3	1:A:468:LEU:HD12	1.96	0.48
1:C:204:ARG:HB2	1:C:207:TYR:O	2.13	0.47
1:A:140:LYS:HG3	1:A:141:TYR:CD1	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:260:ALA:CB	1:A:265:LEU:HB2	2.45	0.47
1:D:329:VAL:CG1	1:D:330:PRO:CD	2.92	0.47
1:D:267:MET:HE3	1:D:323:LYS:HD3	1.96	0.47
1:D:300:ALA:HB2	1:D:317:ALA:HB2	1.96	0.47
1:C:206:ARG:HD3	1:C:234:GLY:CA	2.41	0.47
1:B:183:TRP:HA	1:B:185:ARG:NH1	2.30	0.47
1:C:252:TRP:HB2	1:C:275:THR:HA	1.97	0.47
1:B:83:HIS:CD2	1:B:84:ALA:N	2.82	0.47
1:D:204:ARG:O	1:D:234:GLY:O	2.33	0.47
1:C:206:ARG:H	1:C:234:GLY:HA2	1.80	0.47
1:D:408:ASN:HB3	1:D:503:ASP:HB2	1.97	0.47
1:B:433:TYR:CZ	3:B:602:OU8:H2	2.50	0.47
1:C:493:GLU:HG2	1:D:493:GLU:HG2	1.95	0.47
1:C:206:ARG:NH1	1:C:234:GLY:CA	2.78	0.47
1:A:118:ASN:HB2	1:A:124:ALA:HA	1.97	0.47
1:A:300:ALA:HB2	1:A:317:ALA:HB2	1.97	0.46
1:C:206:ARG:NH1	1:C:234:GLY:N	2.63	0.46
1:B:257:SER:HA	1:B:268:THR:O	2.15	0.46
1:D:81:TRP:HB2	1:D:99:MET:HB2	1.97	0.46
1:B:300:ALA:HB2	1:B:317:ALA:HB2	1.98	0.46
1:B:60:THR:HG21	1:B:306:ILE:HD13	1.97	0.46
1:C:133:GLN:HB2	1:C:145:TYR:CD2	2.51	0.46
1:D:102:ARG:HD3	4:D:780:HOH:O	2.16	0.46
1:D:414:GLY:O	1:D:495:ASP:HB3	2.16	0.46
1:C:234:GLY:O	1:C:235:ILE:CB	2.63	0.46
1:A:252:TRP:HB2	1:A:275:THR:HA	1.98	0.46
1:A:118:ASN:HB2	1:A:124:ALA:CA	2.45	0.46
1:B:432:LEU:HD13	1:B:478:VAL:CG2	2.46	0.46
1:B:433:TYR:CE2	3:B:602:OU8:H2	2.50	0.46
1:C:160:PRO:HG2	4:C:772:HOH:O	2.16	0.46
1:A:174:THR:O	1:A:178:ILE:HG12	2.15	0.46
1:B:425:ILE:HD12	1:B:425:ILE:N	2.31	0.46
1:B:472:GLN:OE1	1:B:490:HIS:HD2	1.99	0.45
1:B:470:ASP:HB3	4:B:708:HOH:O	2.15	0.45
1:C:302:THR:HA	1:C:314:LEU:O	2.16	0.45
1:A:203:GLY:CA	1:A:235:ILE:HG22	2.47	0.45
1:A:166:ASN:ND2	1:A:169:GLY:H	2.14	0.45
1:A:56:GLN:HB2	1:A:68:TYR:HB2	1.98	0.45
1:A:215:ASN:O	1:A:216:LEU:HB2	2.16	0.45
1:A:60:THR:HG22	1:A:65:TYR:CD1	2.52	0.45
1:D:260:ALA:HB1	1:D:265:LEU:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:80:GLY:HA2	1:B:107:VAL:HB	1.99	0.45
1:C:228:PRO:CG	1:C:286:LEU:HD13	2.47	0.45
1:A:183:TRP:CD1	1:A:204:ARG:HA	2.52	0.45
1:C:118:ASN:HB2	1:C:124:ALA:CA	2.47	0.45
1:B:422:HIS:O	1:B:438:PRO:HB2	2.17	0.45
1:B:457:ASP:HA	1:B:458:PRO:HD3	1.89	0.45
1:C:60:THR:HG21	1:C:306:ILE:HD13	1.99	0.45
1:D:183:TRP:HA	1:D:185:ARG:NH1	2.32	0.44
1:A:173:THR:HG23	1:A:177:GLU:OE1	2.16	0.44
1:C:98:VAL:HG13	1:C:156:PHE:CD2	2.52	0.44
1:D:424:ASN:HB3	1:D:501:TYR:OH	2.17	0.44
1:A:234:GLY:HA2	4:A:866:HOH:O	2.17	0.44
1:A:295:TRP:H	1:A:487:GLN:HG3	1.82	0.44
1:B:203:GLY:CA	1:B:235:ILE:HG22	2.46	0.44
1:A:257:SER:HA	1:A:268:THR:O	2.16	0.44
1:C:206:ARG:HH11	1:C:234:GLY:HA2	1.83	0.44
1:C:83:HIS:HD2	1:C:84:ALA:N	2.13	0.44
1:A:260:ALA:HB1	1:A:265:LEU:HB2	1.99	0.44
1:C:425:ILE:HD12	1:C:425:ILE:N	2.33	0.44
1:A:377:LEU:N	1:A:377:LEU:HD12	2.33	0.44
1:B:228:PRO:HD3	1:B:286:LEU:HD13	2.00	0.44
1:D:451:ARG:HE	3:D:602:OU8:H3	1.82	0.44
1:B:433:TYR:CE1	3:B:602:OU8:H15	2.52	0.44
1:C:216:LEU:HA	1:C:219:TRP:CZ2	2.53	0.44
1:B:183:TRP:CD1	1:B:204:ARG:HA	2.53	0.44
3:A:602:OU8:H10	3:A:602:OU8:O1	2.18	0.44
1:C:146:LEU:HD23	1:C:147:TYR:N	2.34	0.43
1:C:401:ILE:O	1:C:462:SER:HA	2.17	0.43
1:C:188:LYS:HB3	1:C:201:VAL:CG1	2.49	0.43
1:A:142:GLN:HE21	1:A:184:PHE:H	1.66	0.43
1:B:110:GLY:HA3	1:B:130:LEU:O	2.18	0.43
1:A:445:SER:HA	4:A:836:HOH:O	2.17	0.43
1:D:206:ARG:HA	1:D:234:GLY:HA2	1.99	0.43
1:D:260:ALA:CB	1:D:265:LEU:HB2	2.49	0.43
1:B:107:VAL:HA	1:B:133:GLN:HG2	2.00	0.43
1:C:362:THR:HG22	4:C:897:HOH:O	2.18	0.43
1:C:250:ARG:HH11	1:C:250:ARG:HG2	1.83	0.43
1:D:112:ALA:HB2	1:D:129:ALA:HB2	2.00	0.43
1:A:306:ILE:C	1:A:306:ILE:HD13	2.38	0.43
1:D:110:GLY:HA3	1:D:130:LEU:O	2.17	0.43
1:B:66:GLN:OE1	1:B:85:SER:HB3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:412:SER:HB2	1:A:499:SER:OG	2.19	0.43
1:A:229:ASN:HB3	1:A:232:LEU:HD22	2.01	0.43
1:C:415:ARG:HA	1:C:421:ARG:O	2.19	0.43
1:A:414:GLY:O	1:A:495:ASP:HB3	2.19	0.43
1:B:207:TYR:O	1:B:235:ILE:HG21	2.19	0.42
1:D:414:GLY:HA3	1:D:491:PHE:CE1	2.54	0.42
1:D:502:THR:HG21	1:D:507:ALA:HB3	2.01	0.42
1:B:414:GLY:O	1:B:495:ASP:HB3	2.19	0.42
1:C:110:GLY:HA3	1:C:130:LEU:O	2.19	0.42
1:B:472:GLN:HA	1:B:489:VAL:O	2.19	0.42
1:C:272:TRP:CE2	1:C:288:PRO:HB3	2.54	0.42
1:D:146:LEU:HD23	1:D:147:TYR:N	2.34	0.42
1:C:277:ASP:OD1	1:C:282:HIS:HE1	2.02	0.42
1:A:295:TRP:CD1	1:A:487:GLN:HG2	2.54	0.42
1:A:430:ALA:HB2	1:A:458:PRO:HG3	2.01	0.42
1:C:222:ARG:HA	1:C:222:ARG:HD3	1.86	0.42
1:B:144:GLN:HB2	1:B:164:ILE:HB	2.02	0.42
1:D:160:PRO:HG2	4:D:835:HOH:O	2.20	0.42
1:B:135:THR:HB	1:B:141:TYR:HB3	2.02	0.42
2:D:601:LBS:H8	2:D:601:LBS:C5	2.49	0.42
1:C:118:ASN:HB2	1:C:124:ALA:HA	2.01	0.42
1:B:223:ARG:HG2	1:B:223:ARG:NH1	2.35	0.42
1:D:470:ASP:HB3	4:D:777:HOH:O	2.20	0.42
1:C:159:LEU:HD12	1:C:160:PRO:HD2	2.02	0.41
1:C:227:TYR:HA	1:C:228:PRO:HD3	1.85	0.41
1:C:508:HIS:HB2	4:C:868:HOH:O	2.20	0.41
1:C:500:LEU:HD13	1:C:509:PHE:CG	2.54	0.41
1:B:327:ARG:NH2	1:B:446:LEU:HD21	2.35	0.41
1:C:184:PHE:HD1	1:C:204:ARG:HD3	1.85	0.41
1:A:203:GLY:HA2	1:A:235:ILE:CG2	2.50	0.41
1:C:159:LEU:HA	1:C:160:PRO:HD2	1.82	0.41
1:B:223:ARG:HG2	1:B:223:ARG:HH11	1.85	0.41
1:D:206:ARG:NH1	1:D:234:GLY:N	2.69	0.41
1:C:107:VAL:HA	1:C:133:GLN:HG2	2.02	0.41
1:B:379:ASP:HB3	1:B:510:THR:HG22	2.01	0.41
1:D:83:HIS:CD2	1:D:84:ALA:N	2.89	0.41
1:A:159:LEU:HA	1:A:160:PRO:HD2	1.85	0.41
1:B:432:LEU:HD13	1:B:478:VAL:HG11	2.02	0.41
1:A:457:ASP:HA	1:A:458:PRO:HD3	1.95	0.41
1:B:56:GLN:HB2	1:B:68:TYR:HB2	2.03	0.41
1:A:519:GLN:O	1:A:520:ALA:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:385:SER:HA	1:C:500:LEU:O	2.21	0.41
1:C:57:ARG:HA	1:C:58:PRO:HD3	1.89	0.41
1:D:223:ARG:HD2	1:D:280:GLN:CG	2.50	0.41
1:A:132:THR:HG21	1:A:185:ARG:HB3	2.03	0.41
1:B:227:TYR:CE2	1:B:235:ILE:HD11	2.56	0.41
1:A:140:LYS:O	1:A:169:GLY:HA3	2.21	0.41
1:D:291:LEU:HA	1:D:291:LEU:HD12	1.92	0.41
1:B:245:ALA:HB2	1:B:349:LEU:HD23	2.03	0.41
1:D:432:LEU:HA	1:D:432:LEU:HD22	1.96	0.41
1:C:223:ARG:HB2	1:C:280:GLN:HB3	2.03	0.41
1:C:84:ALA:HA	1:C:93:THR:O	2.20	0.41
1:C:174:THR:O	1:C:178:ILE:HG13	2.21	0.40
1:D:99:MET:HG2	1:D:147:TYR:CD1	2.56	0.40
1:A:379:ASP:CG	1:A:510:THR:HG22	2.42	0.40
1:C:257:SER:HA	1:C:268:THR:O	2.21	0.40
1:A:52:LEU:HD12	1:A:69:TYR:CD1	2.56	0.40
1:B:260:ALA:HB3	1:B:265:LEU:HB2	2.03	0.40
1:C:364:VAL:HG22	4:C:871:HOH:O	2.21	0.40
1:D:49:SER:O	1:D:71:HIS:HE1	2.05	0.40
1:A:348:ARG:NH2	1:A:360:LEU:HD13	2.36	0.40
1:C:289:GLN:NE2	1:C:356:TRP:HZ3	2.19	0.40
1:D:183:TRP:O	1:D:204:ARG:HD2	2.21	0.40
1:D:295:TRP:HD1	1:D:487:GLN:HG2	1.86	0.40
1:A:69:TYR:OH	1:A:94:HIS:HD2	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	478/492 (97%)	449 (94%)	27 (6%)	2 (0%)	39 48

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	478/492 (97%)	452 (95%)	24 (5%)	2 (0%)	39	48
1	C	477/492 (97%)	452 (95%)	24 (5%)	1 (0%)	52	64
1	D	478/492 (97%)	450 (94%)	27 (6%)	1 (0%)	52	64
All	All	1911/1968 (97%)	1803 (94%)	102 (5%)	6 (0%)	46	57

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	235	ILE
1	B	235	ILE
1	C	235	ILE
1	D	235	ILE
1	A	103	PRO
1	B	103	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	381/393 (97%)	372 (98%)	9 (2%)	57	74
1	B	381/393 (97%)	375 (98%)	6 (2%)	70	84
1	C	381/393 (97%)	371 (97%)	10 (3%)	54	71
1	D	381/393 (97%)	375 (98%)	6 (2%)	70	84
All	All	1524/1572 (97%)	1493 (98%)	31 (2%)	63	79

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

Mol	Chain	Res	Type
1	A	166	ASN
1	A	173	THR
1	A	232	LEU
1	A	258	MET
1	A	297	TRP

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Mol	Chain	Res	Type
1	A	306	ILE
1	A	432	LEU
1	A	448	PRO
1	A	487	GLN
1	B	104	ASP
1	B	130	LEU
1	B	279	GLU
1	B	297	TRP
1	B	487	GLN
1	B	503	ASP
1	C	99	MET
1	C	118	ASN
1	C	204	ARG
1	C	223	ARG
1	C	232	LEU
1	C	279	GLU
1	C	297	TRP
1	C	340	GLN
1	C	382	VAL
1	C	446	LEU
1	D	98	VAL
1	D	297	TRP
1	D	340	GLN
1	D	382	VAL
1	D	446	LEU
1	D	487	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	94	HIS
1	A	133	GLN
1	A	142	GLN
1	A	144	GLN
1	A	166	ASN
1	A	229	ASN
1	A	280	GLN
1	B	44	HIS
1	B	75	ASN
1	B	94	HIS
1	B	369	ASN
1	B	490	HIS

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Mol	Chain	Res	Type
1	C	94	HIS
1	C	118	ASN
1	C	282	HIS
1	C	289	GLN
1	C	341	ASN
1	C	479	ASN
1	D	66	GLN
1	D	71	HIS
1	D	144	GLN
1	D	251	HIS
1	D	280	GLN
1	D	289	GLN
1	D	341	ASN
1	D	391	ASN
1	D	422	HIS
1	D	479	ASN
1	D	519	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

8 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	LBS	A	601	-	23,24,24	1.28	2 (8%)	28,37,37	1.54	4 (14%)
3	0U8	A	602	-	24,24,24	1.93	5 (20%)	36,38,38	1.85	10 (27%)
2	LBS	B	601	-	23,24,24	1.23	1 (4%)	28,37,37	1.42	2 (7%)
3	0U8	B	602	-	24,24,24	1.82	6 (25%)	36,38,38	1.85	9 (25%)
2	LBS	C	601	-	23,24,24	1.21	0	28,37,37	1.48	3 (10%)
3	0U8	C	602	-	24,24,24	2.09	6 (25%)	36,38,38	1.96	11 (30%)
2	LBS	D	601	-	23,24,24	1.20	2 (8%)	28,37,37	1.64	5 (17%)
3	0U8	D	602	-	24,24,24	1.96	5 (20%)	36,38,38	2.38	11 (30%)

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	LBS	A	601	-	-	0/14/52/52	0/2/2/2
3	0U8	A	602	-	-	0/18/56/56	0/0/3/3
2	LBS	B	601	-	-	0/14/52/52	0/2/2/2
3	0U8	B	602	-	-	0/18/56/56	0/0/3/3
2	LBS	C	601	-	-	0/14/52/52	0/2/2/2
3	0U8	C	602	-	-	0/18/56/56	0/0/3/3
2	LBS	D	601	-	-	0/14/52/52	0/2/2/2
3	0U8	D	602	-	-	0/18/56/56	0/0/3/3

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	602	0U8	O4'-C4'	-3.00	1.35	1.43
3	D	602	0U8	O3-C3	-2.95	1.36	1.42
3	A	602	0U8	O3-C3	-2.89	1.36	1.42
3	B	602	0U8	O3-C3	-2.88	1.36	1.42
3	C	602	0U8	O3-C3	-2.67	1.37	1.42
3	B	602	0U8	O4'-C4'	-2.51	1.37	1.43
3	D	602	0U8	O4'-C4'	-2.49	1.37	1.43
3	A	602	0U8	O4'-C4'	-2.26	1.37	1.43
2	B	601	LBS	O3'-C3'	-2.23	1.38	1.42
3	C	602	0U8	O5'-C5'	-2.17	1.38	1.43
2	A	601	LBS	O3'-C3'	-2.15	1.38	1.42
2	D	601	LBS	O3-C3	-2.14	1.38	1.42
2	A	601	LBS	O3-C3	-2.14	1.38	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	602	0U8	O5'-C5'	-2.01	1.39	1.43
2	D	601	LBS	O3'-C3'	-2.01	1.38	1.42
3	A	602	0U8	O5-C5	2.10	1.48	1.43
3	B	602	0U8	O5-C5	2.53	1.49	1.43
3	D	602	0U8	O5-C5	2.68	1.49	1.43
3	C	602	0U8	O5-C5	2.68	1.49	1.43
3	D	602	0U8	O5'-C2'	2.72	1.49	1.42
3	C	602	0U8	O5'-C2'	2.86	1.49	1.42
3	B	602	0U8	O5'-C2'	2.94	1.49	1.42
3	A	602	0U8	O5'-C2'	3.11	1.50	1.42
3	B	602	0U8	O6-C2'	5.62	1.49	1.41
3	D	602	0U8	O6-C2'	6.31	1.50	1.41
3	A	602	0U8	O6-C2'	6.38	1.50	1.41
3	C	602	0U8	O6-C2'	7.22	1.51	1.41

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	602	0U8	C1'-C2'-C3'	-5.53	95.82	114.49
3	D	602	0U8	O6-C2'-C1'	-5.51	92.39	109.67
3	C	602	0U8	C1'-C2'-C3'	-5.18	97.01	114.49
3	A	602	0U8	C1'-C2'-C3'	-4.99	97.65	114.49
3	B	602	0U8	C1'-C2'-C3'	-4.45	99.48	114.49
3	B	602	0U8	O6-C2'-C1'	-4.40	95.85	109.67
3	D	602	0U8	C6-O6-C2'	-3.92	108.74	116.08
3	A	602	0U8	O6-C2'-C1'	-3.60	98.38	109.67
3	A	602	0U8	C2'-C3'-C4'	-3.24	93.85	102.00
3	C	602	0U8	O6-C2'-C1'	-3.02	100.19	109.67
3	D	602	0U8	C2'-C3'-C4'	-2.91	94.69	102.00
3	D	602	0U8	C2'-O5'-C5'	-2.50	101.21	108.44
3	C	602	0U8	C6'-O2-C2	-2.46	111.47	116.08
3	C	602	0U8	C2'-O5'-C5'	-2.44	101.38	108.44
3	C	602	0U8	C2'-C3'-C4'	-2.40	95.96	102.00
3	B	602	0U8	C2'-O5'-C5'	-2.40	101.49	108.44
3	B	602	0U8	C1-C2-C3	-2.03	107.65	114.49
3	A	602	0U8	O5'-C2'-C3'	2.00	110.14	105.58
3	A	602	0U8	O4'-C4'-C5'	2.05	117.21	111.05
2	D	601	LBS	O6-C6-C5	2.06	118.12	111.33
3	D	602	0U8	O5'-C2'-C3'	2.06	110.26	105.58
2	D	601	LBS	O5'-C5'-C6'	2.06	114.18	109.49
2	A	601	LBS	O6-C6-C5	2.09	118.25	111.33
3	A	602	0U8	O5-C5-C6	2.13	114.33	109.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	601	LBS	O1-C1-C2	2.18	118.88	111.91
3	D	602	0U8	O1-C1-C2	2.28	119.20	111.91
3	B	602	0U8	O5'-C2'-C3'	2.29	110.79	105.58
2	A	601	LBS	O5'-C5'-C6'	2.30	114.73	109.49
3	A	602	0U8	O6-C6-C5	2.39	113.30	107.77
2	C	601	LBS	C6'-O2-C2	2.42	120.63	116.08
3	A	602	0U8	O1'-C1'-C2'	2.43	119.68	111.91
3	C	602	0U8	O2-C6'-C5'	2.54	113.64	107.77
3	B	602	0U8	O2-C2-C3	2.71	117.87	108.05
3	D	602	0U8	O2-C6'-C5'	2.75	114.13	107.77
3	C	602	0U8	O1'-C1'-C2'	2.86	121.07	111.91
2	B	601	LBS	O1'-C1'-C2'	2.91	117.05	111.39
3	C	602	0U8	O5-C5-C6	2.97	116.25	109.49
2	C	601	LBS	O2-C6'-C5'	3.00	114.70	107.77
3	C	602	0U8	O5'-C2'-C1'	3.19	116.67	107.98
3	A	602	0U8	O5'-C2'-C1'	3.21	116.72	107.98
3	B	602	0U8	O5'-C2'-C1'	3.22	116.73	107.98
3	B	602	0U8	O1'-C1'-C2'	3.31	122.49	111.91
3	D	602	0U8	O5-C5-C6	3.40	117.24	109.49
3	C	602	0U8	O6-C6-C5	3.58	116.05	107.77
2	A	601	LBS	O1'-C1'-C2'	3.69	118.57	111.39
3	B	602	0U8	O6-C2'-C3'	3.96	122.40	108.05
2	D	601	LBS	O1'-C1'-C2'	4.00	119.17	111.39
3	C	602	0U8	O6-C2'-C3'	4.06	122.75	108.05
3	A	602	0U8	O6-C2'-C3'	4.25	123.43	108.05
2	B	601	LBS	O2-C6'-C5'	4.76	118.78	107.77
2	C	601	LBS	O1'-C1'-C2'	5.20	121.50	111.39
2	A	601	LBS	O2-C6'-C5'	5.24	119.89	107.77
2	D	601	LBS	O2-C6'-C5'	5.30	120.02	107.77
3	D	602	0U8	O6-C2'-C3'	5.31	127.26	108.05
3	D	602	0U8	O5'-C2'-C1'	5.60	123.21	107.98

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	LBS	1	0
3	A	602	0U8	1	0
3	B	602	0U8	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	601	LBS	3	0
3	C	602	0U8	3	0
2	D	601	LBS	3	0
3	D	602	0U8	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	480/492 (97%)	-0.02	12 (2%) 61 70	12, 27, 42, 64	0
1	B	480/492 (97%)	0.00	10 (2%) 67 74	14, 27, 40, 65	0
1	C	479/492 (97%)	-0.07	5 (1%) 84 88	13, 24, 37, 55	0
1	D	480/492 (97%)	-0.11	6 (1%) 79 84	14, 23, 35, 59	0
All	All	1919/1968 (97%)	-0.05	33 (1%) 73 79	12, 25, 38, 65	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	520	ALA	6.7
1	D	520	ALA	5.1
1	A	173	THR	5.0
1	C	234	GLY	4.7
1	B	174	THR	4.7
1	B	173	THR	4.4
1	B	172	ALA	3.9
1	A	520	ALA	3.8
1	A	174	THR	3.5
1	D	234	GLY	3.0
1	A	175	PRO	2.9
1	A	176	ALA	2.9
1	D	519	GLN	2.7
1	C	519	GLN	2.7
1	B	171	ALA	2.6
1	C	503	ASP	2.4
1	D	228	PRO	2.4
1	A	171	ALA	2.4
1	D	223	ARG	2.4
1	D	63	GLY	2.4
1	C	150	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	381	THR	2.3
1	B	138	VAL	2.3
1	B	178	ILE	2.3
1	B	333	ALA	2.2
1	B	196	GLY	2.2
1	A	172	ALA	2.2
1	A	235	ILE	2.1
1	C	63	GLY	2.1
1	A	233	GLY	2.1
1	A	168	ASP	2.1
1	B	235	ILE	2.1
1	A	519	GLN	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	0U8	D	602	22/22	0.68	0.28	4.52	31,40,51,53	0
2	LBS	C	601	23/23	0.90	0.18	3.93	27,29,33,36	0
2	LBS	D	601	23/23	0.82	0.30	2.88	57,60,64,64	0
3	0U8	B	602	22/22	0.79	0.20	2.80	22,34,46,49	0
3	0U8	C	602	22/22	0.79	0.24	1.46	23,34,46,50	0
3	0U8	A	602	22/22	0.86	0.16	1.25	23,33,42,43	0
2	LBS	B	601	23/23	0.94	0.18	0.77	37,39,40,40	0
2	LBS	A	601	23/23	0.89	0.19	0.61	41,43,45,46	0

6.5 Other polymers [i](#)

There are no such residues in this entry.