



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 11:46 AM UTC

PDB ID : 3L7L / pdb_00003L7L
Title : Structure of the Wall Teichoic Acid Polymerase TagF, H444N + CDPG (30 minute soak)
Authors : Lovering, A.L.; Strynadka, N.C.J.
Deposited on : 2009-12-28
Resolution : 2.95 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

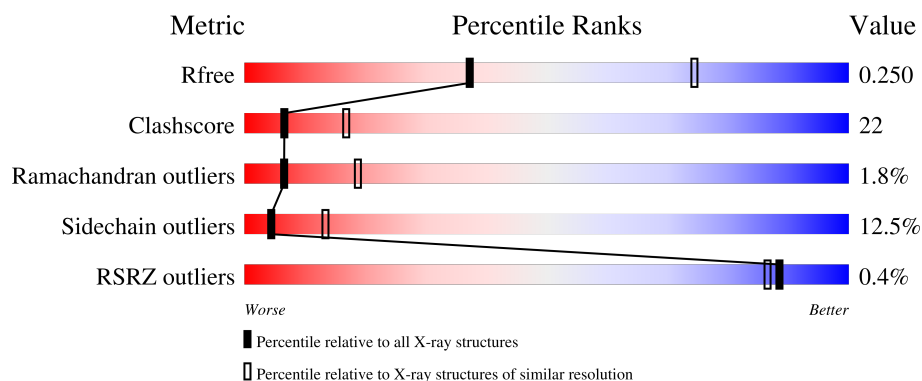
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.95 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1130 (2.98-2.94)
Clashscore	190562	1157 (2.98-2.94)
Ramachandran outliers	187476	1101 (2.98-2.94)
Sidechain outliers	187428	1101 (2.98-2.94)
RSRZ outliers	180081	1130 (2.98-2.94)

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

Mol	Chain	Length	Quality of chain
1	A	729	30% 23% • 44%
1	B	729	31% 20% 5% 44%
1	C	729	32% 21% • 44%
1	D	729	29% 21% • 45%

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	CL	B	734	-	-	X	-
3	CL	B	735	-	-	X	-
3	CL	D	732	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 13868 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 Teichoic acid biosynthesis protein F.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	410	Total	C	N	O	S	0	0	0
			3462	2224	577	650	11			
1	B	411	Total	C	N	O	S	0	0	0
			3467	2227	578	651	11			
1	C	411	Total	C	N	O	S	0	0	0
			3467	2227	578	651	11			
1	D	401	Total	C	N	O	S	0	0	0
			3383	2169	568	635	11			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	444	ASN	HIS	engineered mutation	UNP Q5HLM5
A	722	LEU	-	expression tag	UNP Q5HLM5
A	723	GLU	-	expression tag	UNP Q5HLM5
A	724	HIS	-	expression tag	UNP Q5HLM5
A	725	HIS	-	expression tag	UNP Q5HLM5
A	726	HIS	-	expression tag	UNP Q5HLM5
A	727	HIS	-	expression tag	UNP Q5HLM5
A	728	HIS	-	expression tag	UNP Q5HLM5
A	729	HIS	-	expression tag	UNP Q5HLM5
B	444	ASN	HIS	engineered mutation	UNP Q5HLM5
B	722	LEU	-	expression tag	UNP Q5HLM5
B	723	GLU	-	expression tag	UNP Q5HLM5
B	724	HIS	-	expression tag	UNP Q5HLM5
B	725	HIS	-	expression tag	UNP Q5HLM5
B	726	HIS	-	expression tag	UNP Q5HLM5
B	727	HIS	-	expression tag	UNP Q5HLM5
B	728	HIS	-	expression tag	UNP Q5HLM5
B	729	HIS	-	expression tag	UNP Q5HLM5
C	444	ASN	HIS	engineered mutation	UNP Q5HLM5
C	722	LEU	-	expression tag	UNP Q5HLM5
C	723	GLU	-	expression tag	UNP Q5HLM5

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Chain	Residue	Modelled	Actual	Comment	Reference
C	724	HIS	-	expression tag	UNP Q5HLM5
C	725	HIS	-	expression tag	UNP Q5HLM5
C	726	HIS	-	expression tag	UNP Q5HLM5
C	727	HIS	-	expression tag	UNP Q5HLM5
C	728	HIS	-	expression tag	UNP Q5HLM5
C	729	HIS	-	expression tag	UNP Q5HLM5
D	444	ASN	HIS	engineered mutation	UNP Q5HLM5
D	722	LEU	-	expression tag	UNP Q5HLM5
D	723	GLU	-	expression tag	UNP Q5HLM5
D	724	HIS	-	expression tag	UNP Q5HLM5
D	725	HIS	-	expression tag	UNP Q5HLM5
D	726	HIS	-	expression tag	UNP Q5HLM5
D	727	HIS	-	expression tag	UNP Q5HLM5
D	728	HIS	-	expression tag	UNP Q5HLM5
D	729	HIS	-	expression tag	UNP Q5HLM5

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		

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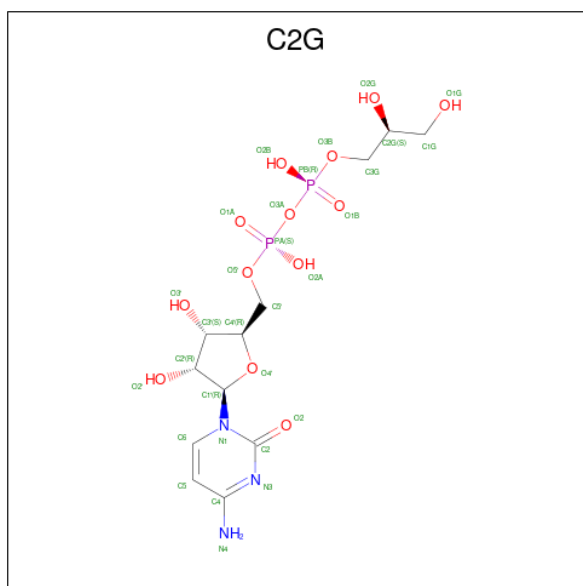
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	8	Total Cl 8 8	0	0
3	B	5	Total Cl 5 5	0	0
3	C	5	Total Cl 5 5	0	0
3	D	3	Total Cl 3 3	0	0

- Molecule 4 is [CYTIDINE-5'-PHOSPHATE] GLYCERYLPHOSPHORIC ACID ESTER (CCD ID: C2G) (formula: $\text{C}_{12}\text{H}_{21}\text{N}_3\text{O}_{13}\text{P}_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	D	1	Total	C	N	O	P	0	0
			30	12	3	13	2		

- Molecule 5 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $\text{C}_2\text{H}_6\text{O}_2$).



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

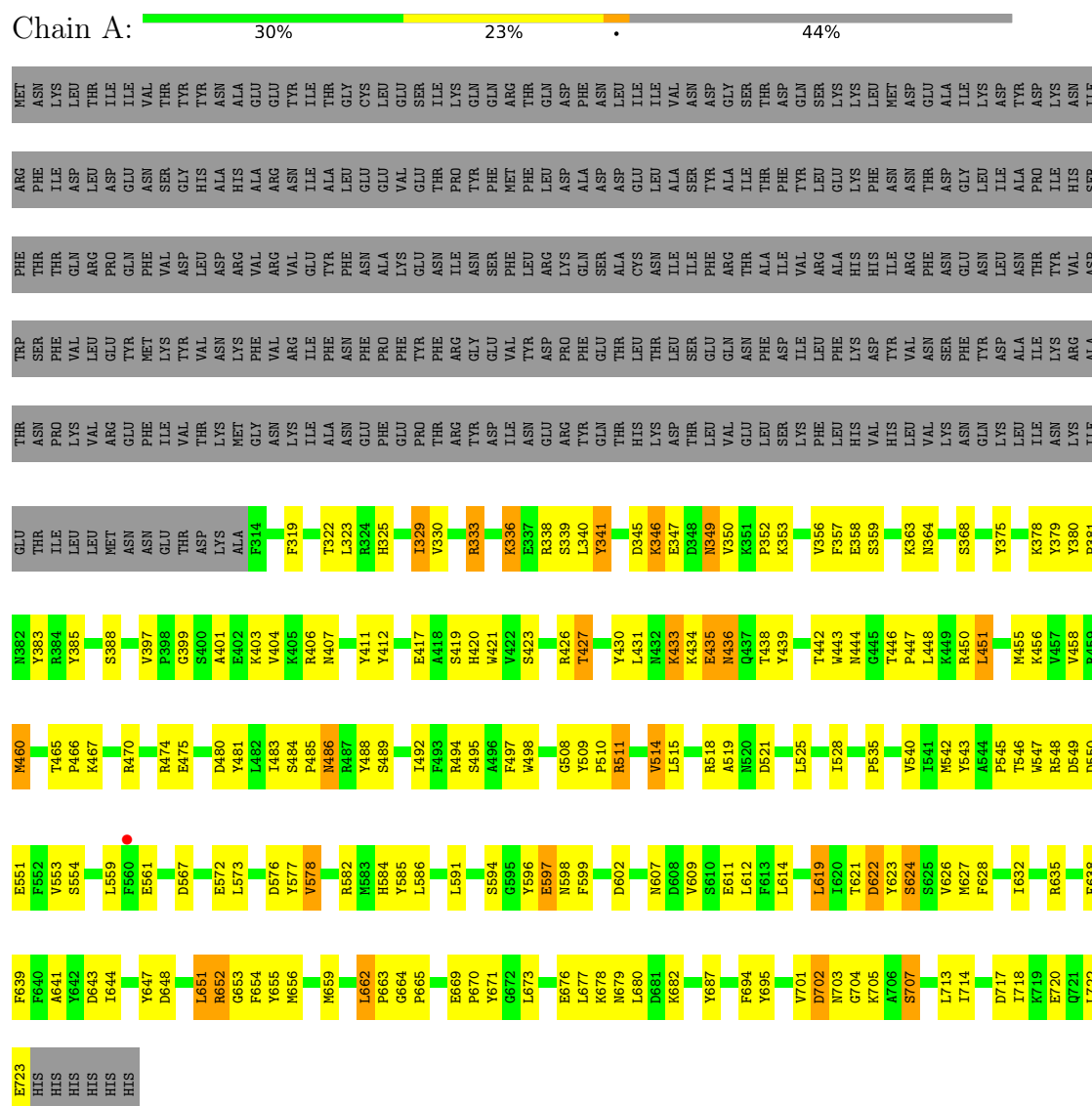
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	2	Total	O	0	0
			2	2		
6	D	2	Total	O	0	0
			2	2		

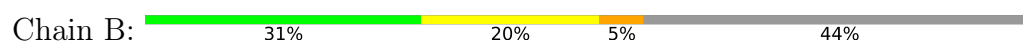
3 Residue-property plots

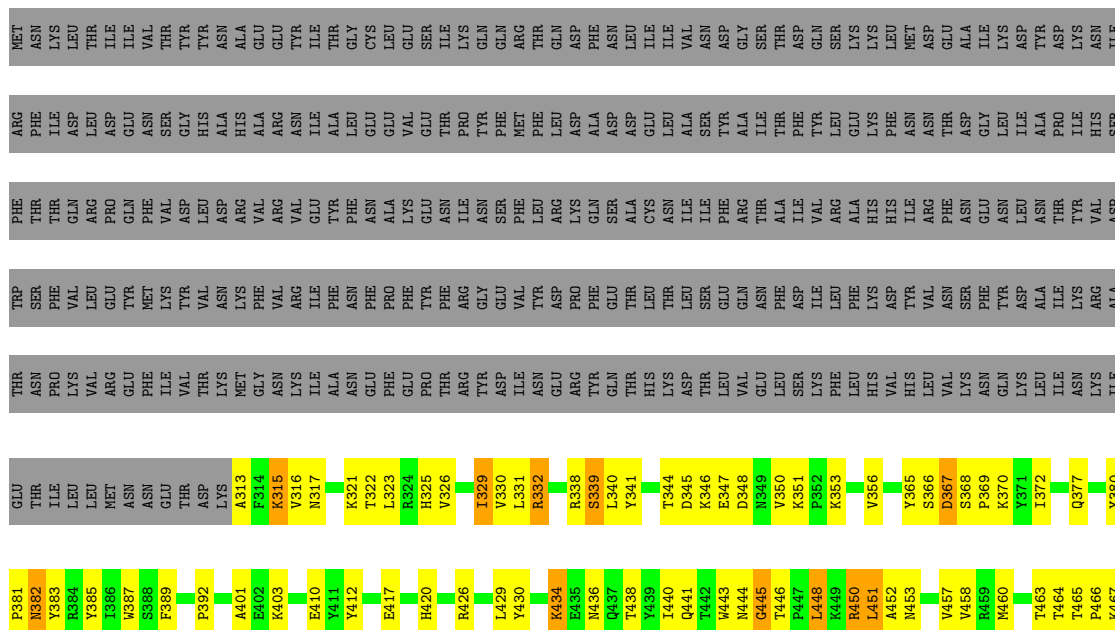
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: Teichoic acid biosynthesis protein F



• Molecule 1: Teichoic acid biosynthesis protein F





4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	222.88Å 222.88Å 100.75Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.01 – 2.95 20.01 – 2.95	Depositor EDS
% Data completeness (in resolution range)	98.7 (20.01-2.95) 98.3 (20.01-2.95)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.57 (at 2.93Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.193 , 0.254 0.186 , 0.250	Depositor DCC
R_{free} test set	2650 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	88.4	Xtriage
Anisotropy	0.014	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 44.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	13868	wwPDB-VP
Average B, all atoms (Å ²)	97.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.04% 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: C2G, CL, SO4, EDO

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.63	0/3551	0.99	16/4798 (0.3%)
1	B	0.64	1/3556 (0.0%)	0.99	9/4805 (0.2%)
1	C	0.56	0/3556	0.96	4/4805 (0.1%)
1	D	0.61	0/3469	0.95	8/4688 (0.2%)
All	All	0.61	1/14132 (0.0%)	0.97	37/19096 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	425	ALA	CA-CB	-5.12	1.47	1.53

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	484	SER	CA-C-N	9.17	128.91	119.64
1	B	484	SER	C-N-CA	9.17	128.91	119.64
1	B	460	MET	CA-C-N	8.14	130.01	119.84
1	B	460	MET	C-N-CA	8.14	130.01	119.84
1	C	448	LEU	N-CA-C	-7.01	104.60	113.43
1	D	366	SER	N-CA-C	6.49	118.08	108.60
1	A	664	GLY	CA-C-N	5.89	125.65	119.76
1	A	664	GLY	C-N-CA	5.89	125.65	119.76
1	B	390	LYS	N-CA-C	-5.63	104.77	111.69
1	B	540	VAL	N-CA-C	5.61	115.95	107.75
1	D	531	HIS	N-CA-C	-5.59	106.43	113.20
1	A	436	ASN	N-CA-C	5.56	118.06	111.33
1	B	382	ASN	N-CA-C	5.54	118.08	111.71
1	A	704	GLY	N-CA-C	-5.51	107.67	115.43
1	A	486	ASN	N-CA-C	5.43	115.54	107.88
1	A	702	ASP	N-CA-C	5.41	118.16	107.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	445	GLY	N-CA-C	5.40	118.33	111.37
1	B	366	SER	N-CA-C	5.36	114.91	107.73
1	A	448	LEU	N-CA-C	-5.35	106.69	113.43
1	A	624	SER	N-CA-C	5.33	117.49	109.23
1	A	397	VAL	N-CA-C	5.29	113.90	107.61
1	A	652	ARG	N-CA-C	-5.28	106.62	113.16
1	C	669	GLU	N-CA-C	-5.24	102.91	110.40
1	C	366	SER	N-CA-C	5.24	116.10	108.14
1	D	397	VAL	N-CA-C	5.21	113.81	107.61
1	B	498	TRP	CB-CA-C	-5.20	104.50	111.89
1	A	435	GLU	CA-C-N	5.20	127.50	120.38
1	A	435	GLU	C-N-CA	5.20	127.50	120.38
1	A	399	GLY	N-CA-C	5.15	119.58	112.52
1	D	351	LYS	CA-C-N	5.12	124.91	119.28
1	D	351	LYS	C-N-CA	5.12	124.91	119.28
1	A	427	THR	CA-C-N	5.12	125.05	119.78
1	A	427	THR	C-N-CA	5.12	125.05	119.78
1	A	423	SER	N-CA-C	5.09	116.03	108.60
1	D	534	LEU	CA-C-N	5.07	125.36	119.93
1	D	534	LEU	C-N-CA	5.07	125.36	119.93
1	D	356	VAL	N-CA-C	5.04	115.84	108.53

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	3462	0	3369	136	0
1	B	3467	0	3374	140	0
1	C	3467	0	3374	157	0
1	D	3383	0	3289	160	0
2	A	10	0	0	0	0
2	B	10	0	0	0	0
2	C	10	0	0	0	0
3	A	8	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	5	0	0	5	0
3	C	5	0	0	2	0
3	D	3	0	0	5	0
4	D	30	0	19	3	0
5	D	4	0	6	0	0
6	A	2	0	0	0	0
6	D	2	0	0	0	0
All	All	13868	0	13431	591	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 22.

All (591) 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:333:ARG:HG2	1:A:333:ARG:HH11	1.13	1.13
1:D:333:ARG:HH11	1:D:333:ARG:HG2	1.16	1.08
1:D:470:ARG:HG2	1:D:470:ARG:HH11	1.07	1.08
1:B:470:ARG:HG2	1:B:470:ARG:HH11	1.24	1.01
1:B:333:ARG:HH11	1:B:333:ARG:HG2	1.24	1.00
1:B:382:ASN:H	1:B:382:ASN:ND2	1.66	0.92
1:D:353:LYS:HG3	3:D:732:CL:CL	2.06	0.91
1:D:547:TRP:H	1:D:547:TRP:CD1	1.82	0.91
1:D:450:ARG:HA	1:D:655:TYR:CE2	2.06	0.90
1:C:367:ASP:HB2	1:C:511:ARG:HD3	1.54	0.89
1:C:383:TYR:CE2	1:C:718:ILE:HD11	2.08	0.88
1:B:458:VAL:HG13	1:B:460:MET:HE2	1.56	0.88
1:B:722:LEU:O	1:B:723:GLU:HG3	1.75	0.87
1:B:561:GLU:HB2	3:B:734:CL:CL	2.12	0.85
1:B:451:LEU:HD12	1:B:451:LEU:H	1.42	0.84
1:C:383:TYR:CZ	1:C:718:ILE:HD11	2.11	0.84
1:B:714:ILE:O	1:B:718:ILE:HG22	1.77	0.84
1:D:470:ARG:HG2	1:D:470:ARG:NH1	1.86	0.84
1:A:333:ARG:HH11	1:A:333:ARG:CG	1.92	0.82
1:B:413:GLN:O	1:B:417:GLU:HG3	1.79	0.82
1:C:648:ASP:HB2	1:C:651:LEU:HB3	1.62	0.81
1:D:585:TYR:CZ	1:D:586:LEU:HG	2.15	0.81
1:B:403:LYS:HE2	3:B:735:CL:CL	2.18	0.81
1:A:485:PRO:HG3	1:A:509:TYR:CE2	2.16	0.80
1:D:543:TYR:CZ	1:D:545:PRO:HG3	2.15	0.80
1:C:662:LEU:CD2	1:C:662:LEU:H	1.95	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:346:LYS:HE3	1:B:349:ASN:HD21	1.46	0.79
1:D:442:THR:HG22	1:D:483:ILE:HD12	1.62	0.79
1:A:333:ARG:HG2	1:A:333:ARG:NH1	1.91	0.79
1:D:447:PRO:HA	4:D:730:C2G:H1G2	1.65	0.79
1:A:648:ASP:HB2	1:A:651:LEU:HB2	1.65	0.78
1:B:333:ARG:HH11	1:B:333:ARG:CG	1.95	0.78
1:A:451:LEU:H	1:A:451:LEU:HD12	1.50	0.77
1:A:383:TYR:CZ	1:A:718:ILE:HD11	2.20	0.77
1:D:451:LEU:HD12	1:D:451:LEU:H	1.48	0.77
1:C:662:LEU:H	1:C:662:LEU:HD23	1.51	0.76
1:C:316:VAL:HG23	1:D:331:LEU:HD22	1.66	0.75
1:B:465:THR:HB	1:B:466:PRO:HD3	1.68	0.75
1:D:363:LYS:HE2	1:D:364:ASN:OD1	1.85	0.75
1:D:451:LEU:HA	1:D:455:MET:HE3	1.68	0.75
1:D:670:PRO:HD2	1:D:671:TYR:CD2	2.22	0.75
1:A:662:LEU:HD23	1:A:662:LEU:H	1.52	0.75
1:D:465:THR:HB	1:D:466:PRO:HD3	1.67	0.75
1:A:345:ASP:OD1	1:A:434:LYS:HE3	1.87	0.74
1:B:347:GLU:O	1:B:436:ASN:ND2	2.20	0.74
1:C:458:VAL:CG1	1:C:460:MET:HG2	2.17	0.74
1:C:470:ARG:HH11	1:C:470:ARG:HG2	1.51	0.74
1:A:338:ARG:HD2	1:A:430:TYR:CD1	2.23	0.73
1:D:434:LYS:HG3	1:D:437:GLN:OE1	1.88	0.73
1:C:485:PRO:HG3	1:C:509:TYR:CE2	2.25	0.72
1:B:372:ILE:HD13	1:B:710:ILE:HG21	1.72	0.71
1:A:542:MET:HE2	1:A:612:LEU:HB3	1.73	0.70
1:B:624:SER:OG	1:B:626:VAL:HG22	1.90	0.70
1:D:333:ARG:HH11	1:D:333:ARG:CG	1.98	0.70
1:D:697:ARG:HD3	1:D:698:PHE:CZ	2.27	0.70
1:B:663:PRO:HG3	1:B:694:PHE:CG	2.27	0.69
1:C:470:ARG:HH11	1:C:470:ARG:CG	2.05	0.69
1:A:486:ASN:HA	1:A:701:VAL:HG21	1.74	0.69
1:B:470:ARG:HG2	1:B:470:ARG:NH1	2.00	0.69
1:B:333:ARG:HG2	1:B:333:ARG:NH1	2.01	0.69
1:A:341:TYR:CD1	1:A:412:TYR:HB3	2.28	0.69
1:C:546:THR:HG23	1:C:624:SER:HB2	1.75	0.69
1:D:434:LYS:C	1:D:436:ASN:H	2.00	0.69
1:C:523:GLU:O	1:C:527:GLU:HG3	1.93	0.68
1:C:670:PRO:HD2	1:C:671:TYR:CD2	2.29	0.68
1:D:547:TRP:CD1	1:D:547:TRP:N	2.59	0.68
1:D:438:THR:HA	1:D:480:ASP:OD2	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:470:ARG:HD2	1:A:474:ARG:HH21	1.58	0.67
1:A:514:VAL:HG12	1:A:518:ARG:HG3	1.76	0.67
1:D:367:ASP:CG	1:D:368:SER:H	2.03	0.67
1:C:597:GLU:O	1:C:598:ASN:HB2	1.95	0.66
1:B:446:THR:O	1:B:625:SER:HB2	1.95	0.66
1:C:543:TYR:CZ	1:C:545:PRO:HG3	2.30	0.66
1:C:714:ILE:O	1:C:718:ILE:HG23	1.96	0.66
1:C:718:ILE:HG13	1:C:718:ILE:O	1.94	0.66
1:B:543:TYR:CZ	1:B:545:PRO:HG3	2.31	0.65
1:C:420:HIS:CD2	1:C:438:THR:HB	2.32	0.65
1:D:669:GLU:HG2	1:D:671:TYR:H	1.60	0.65
1:C:722:LEU:O	1:C:723:GLU:HG3	1.96	0.65
1:D:338:ARG:HD3	1:D:412:TYR:OH	1.97	0.65
1:D:365:TYR:CZ	1:D:370:LYS:HG3	2.32	0.64
1:C:460:MET:HE2	1:C:460:MET:N	2.12	0.64
1:D:714:ILE:O	1:D:718:ILE:HG23	1.98	0.64
1:B:563:LYS:H	1:B:563:LYS:HD2	1.62	0.64
1:D:480:ASP:O	1:D:503:ARG:HG2	1.98	0.64
1:D:542:MET:HE1	1:D:612:LEU:HB3	1.78	0.64
1:B:470:ARG:HH11	1:B:470:ARG:CG	2.05	0.64
1:D:597:GLU:O	1:D:598:ASN:HB2	1.96	0.64
1:D:485:PRO:HB2	1:D:486:ASN:ND2	2.13	0.64
1:B:679:ASN:HD22	1:B:682:LYS:HE3	1.63	0.64
1:C:662:LEU:CD2	1:C:662:LEU:N	2.61	0.64
1:C:347:GLU:HG3	1:C:436:ASN:HB2	1.79	0.63
1:D:619:LEU:HD23	1:D:620:ILE:N	2.13	0.63
1:A:426:ARG:HG2	1:A:475:GLU:HG2	1.79	0.63
1:B:619:LEU:HD21	1:B:621:THR:HB	1.81	0.63
1:B:703:ASN:HD22	1:B:705:LYS:H	1.45	0.63
1:B:548:ARG:HD3	1:B:643:ASP:OD2	1.99	0.63
1:A:648:ASP:OD2	1:A:651:LEU:HD12	1.99	0.63
1:B:329:ILE:HD12	1:B:336:LYS:HB2	1.81	0.63
1:B:380:TYR:N	1:B:381:PRO:HD3	2.14	0.63
1:B:648:ASP:HB2	1:B:651:LEU:HB3	1.81	0.63
1:A:470:ARG:HD2	1:A:474:ARG:NH2	2.14	0.62
1:D:317:ASN:ND2	1:D:320:ARG:HH21	1.97	0.62
1:D:325:HIS:CE1	1:D:329:ILE:CD1	2.81	0.62
1:B:352:PRO:O	1:B:718:ILE:HD12	1.99	0.62
1:B:513:ASP:HA	1:B:704:GLY:HA2	1.80	0.62
1:A:662:LEU:HB2	1:A:663:PRO:HD3	1.82	0.62
1:C:346:LYS:C	1:C:348:ASP:H	2.08	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:651:LEU:HD21	1:D:654:PHE:CD1	2.34	0.62
1:A:383:TYR:CE2	1:A:718:ILE:HD11	2.35	0.62
1:B:665:PRO:HB2	1:B:667:TYR:CE2	2.35	0.62
1:D:652:ARG:C	1:D:654:PHE:H	2.07	0.62
1:C:470:ARG:HG2	1:C:470:ARG:NH1	2.13	0.61
1:D:333:ARG:HG2	1:D:333:ARG:NH1	1.97	0.61
1:D:338:ARG:HD2	1:D:430:TYR:CD1	2.35	0.61
1:D:352:PRO:HD2	3:D:732:CL:CL	2.38	0.61
1:B:461:PRO:O	1:B:463:THR:HG22	1.99	0.61
1:C:448:LEU:HD13	1:C:627:MET:HE1	1.83	0.61
1:B:485:PRO:HB2	1:B:486:ASN:ND2	2.15	0.61
1:C:434:LYS:C	1:C:436:ASN:H	2.09	0.60
1:C:511:ARG:HH22	1:C:629:ASP:CG	2.09	0.60
1:A:662:LEU:H	1:A:662:LEU:CD2	2.13	0.60
1:B:382:ASN:H	1:B:382:ASN:HD22	1.44	0.60
1:D:451:LEU:HA	1:D:455:MET:CE	2.31	0.60
1:B:633:LEU:HB3	1:B:635:ARG:HD3	1.83	0.60
1:C:340:LEU:O	1:C:344:THR:HG23	2.02	0.60
1:A:679:ASN:ND2	1:A:682:LYS:HE3	2.17	0.59
1:C:322:THR:O	1:C:326:VAL:HG23	2.03	0.59
1:C:316:VAL:CG2	1:D:331:LEU:HD22	2.31	0.59
1:C:387:TRP:HB3	1:C:389:PHE:CE2	2.37	0.59
1:D:325:HIS:CE1	1:D:329:ILE:HD11	2.38	0.59
1:A:651:LEU:HD21	1:A:654:PHE:CD1	2.38	0.59
1:C:338:ARG:HD2	1:C:430:TYR:CD1	2.37	0.59
1:D:633:LEU:HB3	1:D:635:ARG:HD3	1.84	0.59
1:B:382:ASN:ND2	1:B:382:ASN:N	2.46	0.59
1:A:485:PRO:HG3	1:A:509:TYR:CZ	2.38	0.58
1:D:458:VAL:C	1:D:460:MET:H	2.10	0.58
1:D:331:LEU:HB2	1:D:333:ARG:HD3	1.85	0.58
1:A:627:MET:HE3	1:A:628:PHE:CZ	2.38	0.58
1:A:652:ARG:C	1:A:654:PHE:H	2.11	0.58
1:B:679:ASN:ND2	1:B:682:LYS:HB2	2.18	0.58
1:A:353:LYS:HB2	1:A:383:TYR:HD2	1.69	0.58
1:D:615:ILE:HD12	1:D:615:ILE:C	2.29	0.58
1:A:546:THR:HG21	1:A:623:TYR:O	2.04	0.58
1:A:662:LEU:CD2	1:A:662:LEU:N	2.66	0.58
1:D:434:LYS:HB2	1:D:436:ASN:HB3	1.85	0.58
1:C:458:VAL:HG13	1:C:460:MET:HG2	1.84	0.57
1:C:648:ASP:HB2	1:C:651:LEU:CB	2.31	0.57
1:A:325:HIS:CE1	1:A:340:LEU:HB2	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:543:TYR:CE2	1:C:545:PRO:HG3	2.39	0.57
1:A:443:TRP:CG	1:A:444:ASN:H	2.21	0.57
1:A:515:LEU:HD12	1:A:632:ILE:HD12	1.86	0.57
1:B:450:ARG:HA	1:B:655:TYR:CE2	2.38	0.57
1:D:451:LEU:HD12	1:D:451:LEU:N	2.18	0.57
1:B:540:VAL:HG22	1:B:578:VAL:HG12	1.86	0.57
1:B:491:GLU:OE2	1:B:491:GLU:HA	2.05	0.57
1:D:347:GLU:CG	1:D:436:ASN:HD22	2.17	0.57
1:D:546:THR:HG23	1:D:547:TRP:CD1	2.39	0.57
1:D:653:GLY:O	1:D:654:PHE:HD1	1.86	0.57
1:A:492:ILE:HD13	1:A:655:TYR:CD2	2.39	0.57
1:A:368:SER:OG	1:A:511:ARG:HG2	2.05	0.57
1:B:475:GLU:OE1	1:B:478:ARG:NH1	2.38	0.57
1:C:492:ILE:HD13	1:C:655:TYR:CD2	2.40	0.57
1:C:494:ARG:HA	1:C:499:MET:HB2	1.86	0.57
1:A:543:TYR:CZ	1:A:545:PRO:HG3	2.40	0.56
1:A:358:GLU:HB2	1:A:388:SER:HB3	1.88	0.56
1:B:345:ASP:OD1	1:B:434:LYS:HE3	2.05	0.56
1:B:563:LYS:H	1:B:563:LYS:CD	2.18	0.56
1:C:372:ILE:HD13	1:C:710:ILE:HG21	1.86	0.56
1:C:392:PRO:HD2	3:C:733:CL:CL	2.42	0.56
1:B:451:LEU:HD12	1:B:451:LEU:N	2.14	0.56
1:C:467:LYS:NZ	1:C:470:ARG:HH22	2.03	0.56
1:A:638:PHE:HE1	1:A:676:GLU:HG2	1.71	0.56
1:C:325:HIS:ND1	1:C:339:SER:HB2	2.20	0.56
1:C:367:ASP:HB2	1:C:511:ARG:CD	2.32	0.56
1:D:439:TYR:N	1:D:480:ASP:OD2	2.33	0.56
1:C:663:PRO:HG3	1:C:694:PHE:CG	2.40	0.56
1:A:353:LYS:HB2	1:A:383:TYR:CD2	2.40	0.56
1:C:382:ASN:H	1:C:382:ASN:ND2	2.01	0.56
1:C:640:PHE:CE2	1:C:642:TYR:HB3	2.41	0.56
1:C:657:ASN:O	1:C:661:ASP:OD1	2.24	0.56
1:A:450:ARG:HD2	1:A:653:GLY:HA2	1.87	0.55
1:A:548:ARG:NH2	1:A:622:ASP:OD1	2.33	0.55
1:A:722:LEU:O	1:A:723:GLU:HG3	2.07	0.55
1:D:464:THR:OG1	1:D:466:PRO:HD2	2.07	0.55
1:C:559:LEU:HD12	1:C:559:LEU:C	2.30	0.55
1:C:627:MET:HE3	1:C:628:PHE:CZ	2.42	0.55
1:A:510:PRO:HB3	1:A:707:SER:HB3	1.88	0.55
1:B:662:LEU:HB2	1:B:663:PRO:CD	2.37	0.55
1:D:564:ILE:HG12	1:D:569:LEU:HD11	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:387:TRP:HB3	1:B:389:PHE:CE2	2.42	0.54
1:D:434:LYS:C	1:D:436:ASN:N	2.65	0.54
1:A:662:LEU:HB2	1:A:663:PRO:CD	2.37	0.54
1:A:641:ALA:HB1	1:A:644:ILE:HB	1.89	0.54
1:A:651:LEU:HD23	1:A:651:LEU:O	2.08	0.54
1:B:364:ASN:HB3	1:B:366:SER:OG	2.08	0.54
1:C:315:LYS:H	1:C:315:LYS:HD3	1.72	0.54
1:C:671:TYR:O	1:C:675:LYS:HG2	2.06	0.54
1:C:682:LYS:NZ	1:C:682:LYS:HB2	2.23	0.54
1:A:443:TRP:CD1	1:A:444:ASN:H	2.25	0.54
1:B:345:ASP:CG	1:B:434:LYS:HE3	2.32	0.54
1:A:553:VAL:O	1:A:554:SER:HB2	2.08	0.54
1:C:350:VAL:CG2	1:C:436:ASN:HD22	2.21	0.54
1:C:420:HIS:HD2	1:C:438:THR:HB	1.71	0.54
1:C:467:LYS:NZ	1:C:470:ARG:NH2	2.56	0.54
1:C:572:GLU:O	1:C:678:LYS:HE3	2.08	0.54
1:D:483:ILE:HD11	1:D:710:ILE:HD11	1.90	0.54
1:A:519:ALA:HA	1:A:614:LEU:HD22	1.90	0.53
1:D:347:GLU:HG2	1:D:436:ASN:ND2	2.24	0.53
1:D:367:ASP:CG	1:D:368:SER:N	2.65	0.53
1:D:514:VAL:C	1:D:516:VAL:H	2.16	0.53
1:A:679:ASN:HD22	1:A:682:LYS:HE3	1.72	0.53
1:C:465:THR:HB	1:C:466:PRO:HD3	1.89	0.53
1:A:624:SER:OG	1:A:626:VAL:HG22	2.09	0.53
1:B:461:PRO:O	1:B:463:THR:N	2.41	0.53
1:D:697:ARG:HD3	1:D:698:PHE:CE2	2.44	0.53
1:C:443:TRP:CG	1:C:444:ASN:H	2.26	0.53
1:A:350:VAL:HA	1:A:417:GLU:O	2.09	0.53
1:B:488:TYR:OH	1:B:655:TYR:HB2	2.09	0.53
1:B:663:PRO:HG3	1:B:694:PHE:CD2	2.44	0.53
1:C:450:ARG:NH1	1:C:652:ARG:O	2.41	0.53
1:D:412:TYR:O	1:D:413:GLN:C	2.52	0.53
1:D:639:PHE:CZ	1:D:663:PRO:HD2	2.44	0.53
1:C:441:GLN:HG2	1:C:479:TRP:CE2	2.44	0.53
3:A:735:CL:CL	1:C:313:ALA:HB2	2.46	0.53
1:C:581:LEU:C	1:C:603:VAL:HG12	2.34	0.53
1:D:375:TYR:C	1:D:375:TYR:CD2	2.87	0.53
1:A:380:TYR:N	1:A:381:PRO:HD3	2.24	0.52
1:C:347:GLU:HA	1:C:434:LYS:HD3	1.89	0.52
1:C:445:GLY:HA2	1:C:509:TYR:CE2	2.44	0.52
1:A:347:GLU:O	1:A:436:ASN:ND2	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:485:PRO:HD2	1:D:489:SER:CB	2.39	0.52
1:A:572:GLU:O	1:A:573:LEU:HD23	2.10	0.52
1:C:701:VAL:HG12	1:C:701:VAL:O	2.09	0.52
1:B:350:VAL:HA	1:B:417:GLU:O	2.10	0.52
1:C:350:VAL:HG21	1:C:436:ASN:ND2	2.24	0.52
1:C:581:LEU:O	1:C:603:VAL:HG12	2.10	0.52
1:C:665:PRO:HG3	1:C:687:TYR:CE1	2.44	0.52
1:C:380:TYR:CE1	1:C:715:HIS:ND1	2.77	0.52
1:B:379:TYR:C	1:B:381:PRO:HD3	2.35	0.52
1:B:461:PRO:C	1:B:463:THR:H	2.18	0.52
1:D:548:ARG:NH2	1:D:622:ASP:OD1	2.42	0.52
1:B:458:VAL:C	1:B:460:MET:H	2.18	0.52
1:C:559:LEU:C	1:C:559:LEU:CD1	2.83	0.51
1:D:443:TRP:CG	1:D:444:ASN:H	2.29	0.51
1:A:438:THR:HA	1:A:480:ASP:OD2	2.11	0.51
1:A:561:GLU:HA	3:A:738:CL:CL	2.48	0.51
1:B:456:LYS:HA	1:B:456:LYS:HE2	1.92	0.51
1:A:547:TRP:CG	1:A:548:ARG:N	2.78	0.51
1:B:560:PHE:O	1:B:561:GLU:C	2.53	0.51
1:D:413:GLN:O	1:D:417:GLU:HG3	2.10	0.51
1:D:458:VAL:HG12	1:D:460:MET:HB2	1.92	0.51
1:A:540:VAL:HG22	1:A:578:VAL:HG12	1.92	0.51
1:C:639:PHE:CZ	1:C:663:PRO:HD2	2.45	0.51
1:D:347:GLU:HG2	1:D:436:ASN:HD22	1.75	0.51
1:C:341:TYR:O	1:C:345:ASP:HB2	2.11	0.51
1:A:670:PRO:HG2	1:A:671:TYR:CE2	2.46	0.51
1:C:559:LEU:HD13	1:C:560:PHE:C	2.35	0.51
1:A:345:ASP:OD1	1:A:434:LYS:CE	2.58	0.50
1:A:467:LYS:HG3	1:A:470:ARG:NH2	2.26	0.50
1:C:367:ASP:CG	1:C:368:SER:H	2.18	0.50
1:D:542:MET:HE1	1:D:612:LEU:HD13	1.93	0.50
1:B:325:HIS:CE1	1:B:329:ILE:HD13	2.45	0.50
1:D:458:VAL:HG12	1:D:458:VAL:O	2.11	0.50
1:C:588:SER:C	1:C:590:ALA:H	2.18	0.50
1:D:340:LEU:O	1:D:344:THR:HG23	2.11	0.50
1:B:511:ARG:HH22	1:B:629:ASP:CG	2.19	0.50
1:C:453:ASN:HB2	1:C:496:ALA:O	2.11	0.50
1:C:545:PRO:HG2	1:C:583:MET:HE1	1.92	0.50
1:D:325:HIS:CE1	1:D:329:ILE:HD13	2.46	0.50
1:D:317:ASN:O	1:D:321:LYS:HG3	2.11	0.50
1:C:367:ASP:CB	1:C:511:ARG:HD3	2.34	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:665:PRO:HG3	1:A:687:TYR:CE1	2.47	0.50
1:C:683:VAL:O	1:C:687:TYR:HB2	2.11	0.50
1:D:581:LEU:O	1:D:603:VAL:HG12	2.12	0.49
1:B:675:LYS:O	1:B:678:LYS:HB2	2.12	0.49
1:D:467:LYS:HE3	1:D:470:ARG:HH22	1.77	0.49
1:A:485:PRO:HA	1:A:508:GLY:HA2	1.93	0.49
1:B:695:TYR:C	1:B:695:TYR:CD2	2.90	0.49
1:D:446:THR:O	1:D:625:SER:HB2	2.13	0.49
1:D:637:GLN:O	1:D:664:GLY:HA3	2.12	0.49
1:D:585:TYR:CE2	1:D:586:LEU:HG	2.46	0.49
1:A:497:PHE:O	1:A:498:TRP:C	2.55	0.49
1:D:662:LEU:HB2	1:D:663:PRO:HD3	1.95	0.49
1:D:460:MET:N	1:D:460:MET:HE2	2.27	0.49
1:D:470:ARG:HH11	1:D:470:ARG:CG	1.99	0.49
1:C:467:LYS:CE	1:C:470:ARG:HH22	2.26	0.49
1:A:325:HIS:CE1	1:A:329:ILE:HD13	2.48	0.49
1:B:487:ARG:HB2	1:B:487:ARG:HH11	1.78	0.49
1:C:662:LEU:H	1:C:662:LEU:HD22	1.77	0.49
1:B:404:VAL:HG12	1:B:410:GLU:HB3	1.94	0.48
1:C:329:ILE:HG22	1:C:330:VAL:N	2.29	0.48
1:C:669:GLU:HG2	1:C:671:TYR:H	1.78	0.48
1:D:487:ARG:HD3	1:D:506:GLU:OE2	2.14	0.48
1:B:542:MET:HE1	1:B:613:PHE:HD1	1.79	0.48
1:C:350:VAL:HG21	1:C:436:ASN:HD22	1.78	0.48
1:A:378:LYS:HD3	1:A:379:TYR:CE2	2.48	0.48
1:D:485:PRO:HG3	1:D:509:TYR:CE2	2.49	0.48
1:A:420:HIS:CD2	1:A:714:ILE:HG12	2.48	0.48
1:D:565:ASP:OD1	1:D:671:TYR:OH	2.26	0.48
1:B:669:GLU:HG2	1:B:671:TYR:H	1.78	0.48
1:A:572:GLU:C	1:A:573:LEU:HD23	2.38	0.48
1:A:576:ASP:HB2	1:A:577:TYR:CD2	2.49	0.48
1:B:603:VAL:O	1:B:603:VAL:HG13	2.14	0.48
1:D:450:ARG:HA	1:D:655:TYR:HE2	1.73	0.48
1:A:621:THR:O	1:A:639:PHE:HA	2.13	0.48
1:D:541:ILE:HD13	1:D:677:LEU:HD21	1.95	0.48
1:A:521:ASP:O	1:A:525:LEU:HG	2.13	0.48
1:B:525:LEU:O	1:B:529:ARG:HG3	2.14	0.48
1:B:438:THR:HA	1:B:480:ASP:OD2	2.13	0.47
1:B:443:TRP:CG	1:B:444:ASN:H	2.32	0.47
1:D:669:GLU:OE2	1:D:672:GLY:N	2.47	0.47
1:D:673:LEU:O	1:D:677:LEU:HB2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:338:ARG:HD2	1:B:430:TYR:HB2	1.97	0.47
1:B:445:GLY:HA2	1:B:509:TYR:CE2	2.49	0.47
1:C:350:VAL:CG2	1:C:436:ASN:ND2	2.78	0.47
1:C:493:PHE:O	1:C:494:ARG:C	2.57	0.47
1:C:542:MET:HB3	1:C:619:LEU:HD23	1.96	0.47
1:C:559:LEU:HD12	1:C:559:LEU:O	2.14	0.47
1:D:355:ILE:CD1	1:D:376:MET:HE1	2.44	0.47
1:B:619:LEU:HD23	1:B:619:LEU:C	2.40	0.47
1:A:363:LYS:HE3	1:A:364:ASN:ND2	2.29	0.47
1:B:451:LEU:HD13	1:B:496:ALA:HB1	1.96	0.47
1:C:521:ASP:HB3	1:C:524:TYR:HB3	1.97	0.47
1:A:547:TRP:CD1	1:A:548:ARG:N	2.82	0.47
1:D:351:LYS:HB3	3:D:732:CL:CL	2.52	0.47
1:D:357:PHE:CE1	1:D:373:TYR:HB2	2.50	0.47
1:A:319:PHE:HE1	1:D:330:VAL:HG21	1.80	0.47
1:B:355:ILE:HG22	1:B:357:PHE:CE2	2.49	0.47
1:C:353:LYS:HG2	3:C:732:CL:CL	2.51	0.47
1:D:353:LYS:CG	3:D:732:CL:CL	2.91	0.47
1:D:546:THR:CG2	1:D:547:TRP:N	2.77	0.47
1:D:639:PHE:CE2	1:D:663:PRO:HD2	2.50	0.47
1:B:333:ARG:CG	1:B:333:ARG:NH1	2.64	0.47
1:B:411:TYR:CE1	1:B:415:TYR:HE2	2.33	0.47
1:D:619:LEU:HB2	1:D:630:TYR:CE2	2.50	0.47
1:A:509:TYR:HB3	1:A:511:ARG:HG3	1.96	0.47
1:A:662:LEU:HD23	1:A:662:LEU:N	2.21	0.47
1:A:701:VAL:HG12	1:A:701:VAL:O	2.14	0.47
1:D:411:TYR:CE1	1:D:415:TYR:HE2	2.33	0.47
1:A:329:ILE:HG22	1:A:330:VAL:N	2.30	0.47
1:A:665:PRO:HG3	1:A:687:TYR:CZ	2.50	0.47
1:C:444:ASN:O	1:C:511:ARG:NH1	2.43	0.47
1:D:442:THR:O	1:D:509:TYR:HE1	1.98	0.47
1:A:378:LYS:HD3	1:A:379:TYR:HE2	1.80	0.46
1:B:434:LYS:C	1:B:436:ASN:N	2.74	0.46
1:B:670:PRO:HD2	1:B:671:TYR:CD2	2.49	0.46
1:A:663:PRO:HG3	1:A:694:PHE:CG	2.50	0.46
1:B:325:HIS:CE1	1:B:340:LEU:HB2	2.49	0.46
1:B:542:MET:HE1	1:B:613:PHE:CD1	2.50	0.46
1:C:548:ARG:HD3	1:C:643:ASP:OD2	2.15	0.46
1:C:621:THR:OG1	1:C:622:ASP:N	2.48	0.46
1:D:652:ARG:C	1:D:654:PHE:N	2.74	0.46
1:A:385:TYR:O	1:A:401:ALA:HA	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:509:TYR:HB3	1:B:511:ARG:HG2	1.95	0.46
1:C:446:THR:HB	1:C:628:PHE:CD2	2.50	0.46
1:A:427:THR:HG23	1:A:439:TYR:OH	2.16	0.46
1:B:396:VAL:HA	3:B:735:CL:CL	2.52	0.46
1:B:443:TRP:CD1	1:B:444:ASN:H	2.33	0.46
1:D:452:ALA:HB2	1:D:497:PHE:CE2	2.51	0.46
1:A:559:LEU:HD12	1:A:559:LEU:O	2.16	0.46
1:C:510:PRO:HA	1:C:706:ALA:HB3	1.98	0.46
1:D:562:LEU:HD23	1:D:562:LEU:HA	1.74	0.46
1:A:481:TYR:CE2	1:A:713:LEU:HD21	2.51	0.46
1:A:652:ARG:C	1:A:654:PHE:N	2.73	0.46
1:C:321:LYS:O	1:C:322:THR:C	2.57	0.46
1:D:608:ASP:OD2	1:D:610:SER:HB2	2.15	0.46
1:A:639:PHE:CD2	1:A:639:PHE:N	2.84	0.46
1:B:648:ASP:HB2	1:B:651:LEU:CB	2.45	0.46
1:C:385:TYR:O	1:C:401:ALA:HA	2.15	0.46
1:D:410:GLU:OE1	1:D:410:GLU:N	2.37	0.46
1:C:365:TYR:CE2	1:C:370:LYS:HD2	2.50	0.45
1:C:410:GLU:CD	1:C:410:GLU:H	2.24	0.45
1:C:429:LEU:HD23	1:C:429:LEU:HA	1.51	0.45
1:A:338:ARG:HD3	1:A:412:TYR:OH	2.17	0.45
1:A:543:TYR:CE2	1:A:545:PRO:HG3	2.52	0.45
1:B:403:LYS:CE	3:B:735:CL:CL	2.98	0.45
1:C:367:ASP:CG	1:C:368:SER:N	2.75	0.45
1:C:528:ILE:HD11	1:C:611:GLU:HG2	1.98	0.45
1:A:549:ASP:C	1:A:551:GLU:H	2.25	0.45
1:C:562:LEU:H	1:C:562:LEU:HG	1.55	0.45
1:D:395:ASN:O	1:D:403:LYS:HE2	2.16	0.45
1:A:549:ASP:O	1:A:551:GLU:N	2.49	0.45
1:B:485:PRO:HD2	1:B:489:SER:HB2	1.98	0.45
1:C:620:ILE:HD13	1:C:673:LEU:HD11	1.99	0.45
1:D:705:LYS:O	1:D:708:GLN:HB3	2.17	0.45
1:A:548:ARG:HD3	1:A:643:ASP:OD2	2.16	0.45
1:B:467:LYS:O	1:B:467:LYS:HG3	2.16	0.45
1:C:441:GLN:HG2	1:C:479:TRP:CZ2	2.52	0.45
1:C:485:PRO:HD2	1:C:489:SER:HB2	1.99	0.45
1:C:657:ASN:ND2	1:C:660:GLU:HB2	2.32	0.45
1:D:387:TRP:HB3	1:D:389:PHE:CE2	2.52	0.45
1:A:559:LEU:HD12	1:A:559:LEU:C	2.42	0.45
1:B:329:ILE:CG2	1:B:330:VAL:N	2.78	0.45
1:B:434:LYS:C	1:B:436:ASN:H	2.25	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:442:THR:HG22	1:B:483:ILE:HD12	1.99	0.45
1:B:487:ARG:HA	1:B:487:ARG:HD3	1.78	0.45
1:C:368:SER:HB2	1:C:369:PRO:HD3	1.99	0.45
1:C:569:LEU:N	1:C:569:LEU:HD23	2.31	0.45
1:C:612:LEU:HD23	1:C:612:LEU:HA	1.77	0.45
1:B:431:LEU:HA	1:B:431:LEU:HD23	1.63	0.45
1:B:719:LYS:O	1:B:720:GLU:C	2.59	0.45
1:C:380:TYR:C	1:C:382:ASN:H	2.25	0.45
1:D:343:LEU:HA	1:D:343:LEU:HD23	1.78	0.45
1:A:722:LEU:C	1:A:723:GLU:HG3	2.42	0.44
1:B:396:VAL:O	1:B:396:VAL:HG12	2.18	0.44
1:B:652:ARG:C	1:B:654:PHE:H	2.24	0.44
1:C:440:ILE:HD12	1:C:714:ILE:HD11	1.99	0.44
1:C:470:ARG:HH11	1:C:470:ARG:CB	2.30	0.44
1:B:684:GLN:O	1:B:688:GLN:HB2	2.16	0.44
1:C:377:GLN:O	1:C:381:PRO:HG3	2.16	0.44
1:C:450:ARG:HA	1:C:655:TYR:CZ	2.53	0.44
1:C:546:THR:CG2	1:C:624:SER:HB2	2.47	0.44
1:D:548:ARG:HH22	1:D:622:ASP:CG	2.24	0.44
1:D:458:VAL:C	1:D:460:MET:N	2.76	0.44
1:A:375:TYR:CD2	1:A:375:TYR:C	2.95	0.44
1:A:443:TRP:CG	1:A:444:ASN:N	2.85	0.44
1:D:446:THR:HA	1:D:447:PRO:HD3	1.88	0.44
1:D:483:ILE:HD11	1:D:710:ILE:CD1	2.47	0.44
1:A:421:TRP:CZ3	1:A:433:LYS:HG3	2.53	0.44
1:A:585:TYR:CD1	1:A:585:TYR:C	2.96	0.44
1:A:703:ASN:HB3	1:A:705:LYS:HB2	1.98	0.44
1:B:531:HIS:HD2	1:B:531:HIS:O	2.01	0.44
1:C:347:GLU:O	1:C:436:ASN:ND2	2.51	0.44
1:C:639:PHE:HZ	1:C:663:PRO:HD2	1.82	0.44
1:D:359:SER:HB3	1:D:369:PRO:HG2	2.00	0.44
1:D:651:LEU:HD23	1:D:651:LEU:O	2.18	0.44
1:A:420:HIS:HA	1:A:438:THR:O	2.17	0.44
1:A:451:LEU:HD12	1:A:451:LEU:N	2.16	0.44
1:A:638:PHE:CE1	1:A:676:GLU:HG2	2.52	0.44
1:C:316:VAL:HG13	1:C:317:ASN:N	2.33	0.44
1:C:552:PHE:O	1:C:553:VAL:HG13	2.18	0.44
1:B:722:LEU:C	1:B:723:GLU:HG3	2.41	0.44
1:D:458:VAL:CG1	1:D:460:MET:HB2	2.48	0.44
1:D:615:ILE:HD12	1:D:615:ILE:O	2.17	0.44
1:A:542:MET:CE	1:A:612:LEU:HB3	2.45	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:376:MET:HE2	1:B:376:MET:HB3	1.73	0.43
1:C:464:THR:HG23	1:C:467:LYS:H	1.83	0.43
1:C:661:ASP:OD1	1:C:661:ASP:N	2.50	0.43
1:A:624:SER:CB	1:A:626:VAL:HG22	2.48	0.43
1:C:695:TYR:CD2	1:C:695:TYR:C	2.96	0.43
1:D:383:TYR:CE2	1:D:718:ILE:HD11	2.52	0.43
1:D:710:ILE:O	1:D:711:GLY:C	2.62	0.43
1:A:444:ASN:O	1:A:511:ARG:NH1	2.50	0.43
1:A:458:VAL:O	1:A:458:VAL:HG12	2.18	0.43
1:A:458:VAL:C	1:A:460:MET:HE2	2.44	0.43
1:B:411:TYR:CE1	1:B:415:TYR:CE2	3.05	0.43
1:C:637:GLN:O	1:C:664:GLY:HA3	2.18	0.43
1:D:578:VAL:HG23	1:D:599:PHE:HA	2.00	0.43
1:A:458:VAL:HB	1:A:465:THR:OG1	2.18	0.43
1:D:445:GLY:HA2	1:D:509:TYR:CE2	2.53	0.43
1:C:426:ARG:H	1:C:426:ARG:HG3	1.65	0.43
1:C:470:ARG:HH11	1:C:470:ARG:HB3	1.82	0.43
1:C:488:TYR:OH	1:C:655:TYR:HB2	2.19	0.43
1:D:662:LEU:HB2	1:D:663:PRO:CD	2.48	0.43
1:A:357:PHE:CD2	1:A:357:PHE:N	2.87	0.43
1:A:451:LEU:HA	1:A:455:MET:HE3	2.01	0.43
1:B:329:ILE:HG22	1:B:330:VAL:N	2.34	0.43
1:B:347:GLU:HG2	1:B:436:ASN:ND2	2.34	0.43
1:B:554:SER:C	1:B:556:GLY:H	2.26	0.43
1:C:367:ASP:O	1:C:368:SER:C	2.61	0.43
1:D:351:LYS:HA	1:D:352:PRO:HD3	1.85	0.43
1:D:441:GLN:O	1:D:482:LEU:HA	2.18	0.43
1:A:528:ILE:HD13	1:A:611:GLU:HG2	2.01	0.43
1:B:642:TYR:CD1	1:B:642:TYR:N	2.87	0.43
1:C:469:LYS:O	1:C:470:ARG:C	2.61	0.43
1:C:670:PRO:HD2	1:C:671:TYR:CE2	2.53	0.43
1:D:356:VAL:HG22	1:D:418:ALA:CB	2.48	0.43
1:B:526:ASP:O	1:B:527:GLU:C	2.61	0.43
1:C:380:TYR:CE1	1:C:715:HIS:CE1	3.06	0.43
1:C:451:LEU:H	1:C:451:LEU:HD12	1.83	0.43
1:A:597:GLU:O	1:A:598:ASN:HB2	2.18	0.43
1:D:317:ASN:ND2	1:D:320:ARG:NH2	2.65	0.43
1:D:364:ASN:HD22	1:D:366:SER:HB3	1.84	0.43
1:D:373:TYR:CZ	1:D:377:GLN:HG3	2.54	0.43
1:D:641:ALA:O	1:D:668:THR:HG22	2.18	0.43
1:A:485:PRO:HD2	1:A:489:SER:HB2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:457:VAL:HG11	1:B:459:ARG:NH2	2.34	0.42
1:B:597:GLU:O	1:B:598:ASN:HB2	2.19	0.42
1:C:718:ILE:O	1:C:722:LEU:HD22	2.18	0.42
1:D:318:GLN:HG2	3:D:731:CL:CL	2.55	0.42
1:D:452:ALA:HB2	1:D:497:PHE:HE2	1.82	0.42
1:A:596:TYR:O	1:A:597:GLU:C	2.62	0.42
1:B:662:LEU:HB2	1:B:663:PRO:HD3	2.01	0.42
1:B:713:LEU:HD12	1:B:713:LEU:O	2.19	0.42
1:D:404:VAL:O	1:D:404:VAL:HG23	2.18	0.42
1:D:626:VAL:HG12	4:D:730:C2G:HC2	2.00	0.42
4:D:730:C2G:O5'	4:D:730:C2G:HC6	2.19	0.42
1:A:450:ARG:HA	1:A:655:TYR:CZ	2.55	0.42
1:B:317:ASN:O	1:B:321:LYS:HG3	2.18	0.42
1:B:366:SER:HA	1:B:370:LYS:HD2	2.01	0.42
1:D:513:ASP:HA	1:D:704:GLY:HA2	2.00	0.42
1:A:333:ARG:CG	1:A:333:ARG:NH1	2.61	0.42
1:C:485:PRO:HG3	1:C:509:TYR:CZ	2.53	0.42
1:C:367:ASP:O	1:C:370:LYS:N	2.51	0.42
1:C:521:ASP:O	1:C:524:TYR:HB3	2.20	0.42
1:D:368:SER:O	1:D:372:ILE:HG13	2.19	0.42
1:D:408:SER:O	1:D:411:TYR:HB3	2.19	0.42
1:D:470:ARG:NH1	1:D:471:ASN:OD1	2.52	0.42
1:D:682:LYS:HE3	1:D:682:LYS:HB2	1.53	0.42
1:B:458:VAL:O	1:B:458:VAL:HG12	2.20	0.42
1:B:673:LEU:HD22	1:B:677:LEU:HD22	2.02	0.42
1:C:443:TRP:CD1	1:C:444:ASN:H	2.37	0.42
1:D:358:GLU:OE1	1:D:388:SER:HB3	2.20	0.42
1:B:509:TYR:C	1:B:511:ARG:N	2.77	0.42
1:B:531:HIS:O	1:B:531:HIS:CD2	2.72	0.42
1:A:578:VAL:HG22	1:A:599:PHE:O	2.19	0.42
1:B:446:THR:HA	1:B:447:PRO:HD3	1.76	0.42
1:B:455:MET:O	1:B:456:LYS:HE2	2.19	0.42
1:D:653:GLY:C	1:D:654:PHE:HD1	2.28	0.42
1:D:670:PRO:HD2	1:D:671:TYR:CE2	2.55	0.42
1:A:329:ILE:HD12	1:A:336:LYS:HB2	2.01	0.42
1:A:446:THR:HA	1:A:447:PRO:HD3	1.91	0.42
1:B:499:MET:HE3	1:B:499:MET:HB3	1.77	0.42
1:D:387:TRP:O	1:D:404:VAL:HG22	2.20	0.42
1:A:352:PRO:HA	1:A:419:SER:HB3	2.02	0.41
1:A:442:THR:HG22	1:A:483:ILE:HD12	2.02	0.41
1:A:484:SER:HA	1:A:485:PRO:HD3	1.79	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:697:ARG:HD3	1:B:698:PHE:CE2	2.55	0.41
1:C:434:LYS:HZ2	1:C:434:LYS:HG3	1.76	0.41
1:C:458:VAL:HG13	1:C:460:MET:HE3	2.02	0.41
1:C:580:LEU:HA	1:C:580:LEU:HD23	1.79	0.41
1:D:492:ILE:HD13	1:D:655:TYR:CG	2.55	0.41
1:A:346:LYS:HG3	1:A:349:ASN:HD21	1.85	0.41
1:A:431:LEU:HA	1:A:431:LEU:HD23	1.83	0.41
1:A:465:THR:N	1:A:466:PRO:CD	2.83	0.41
1:D:450:ARG:HA	1:D:655:TYR:CZ	2.54	0.41
1:B:338:ARG:HD2	1:B:430:TYR:CG	2.56	0.41
1:B:484:SER:HA	1:B:485:PRO:HD3	1.52	0.41
1:C:526:ASP:O	1:C:530:THR:HG23	2.20	0.41
1:A:584:HIS:HE1	1:A:586:LEU:HG	1.86	0.41
1:B:382:ASN:HD22	1:B:382:ASN:N	2.13	0.41
1:B:418:ALA:O	1:B:437:GLN:HG2	2.19	0.41
1:B:484:SER:O	1:B:506:GLU:HA	2.20	0.41
1:C:488:TYR:O	1:C:492:ILE:HG13	2.20	0.41
1:D:472:PHE:O	1:D:476:THR:HG23	2.21	0.41
1:A:406:ARG:O	1:A:407:ASN:HB2	2.21	0.41
1:A:542:MET:O	1:A:619:LEU:HD23	2.21	0.41
1:B:380:TYR:N	1:B:381:PRO:CD	2.83	0.41
1:B:528:ILE:HG22	1:B:615:ILE:HD13	2.03	0.41
1:C:509:TYR:HA	1:C:510:PRO:HD3	1.93	0.41
1:C:542:MET:CE	1:C:612:LEU:HB3	2.49	0.41
1:D:484:SER:HA	1:D:485:PRO:HD3	1.90	0.41
1:B:638:PHE:CD1	1:B:665:PRO:HG2	2.56	0.41
1:C:341:TYR:CD1	1:C:412:TYR:HB3	2.56	0.41
1:C:346:LYS:C	1:C:348:ASP:N	2.73	0.41
1:C:353:LYS:HA	1:C:718:ILE:HD12	2.02	0.41
1:C:380:TYR:N	1:C:381:PRO:HD3	2.35	0.41
1:A:325:HIS:HE1	1:A:340:LEU:HB2	1.82	0.41
1:B:675:LYS:HA	1:B:675:LYS:HD3	1.83	0.41
1:C:351:LYS:HD2	1:C:417:GLU:OE1	2.20	0.41
1:D:341:TYR:O	1:D:345:ASP:HB2	2.21	0.41
1:D:379:TYR:C	1:D:381:PRO:HD3	2.46	0.41
1:D:586:LEU:HA	1:D:586:LEU:HD23	1.52	0.41
1:D:712:ASP:O	1:D:713:LEU:C	2.63	0.41
1:A:485:PRO:HD2	1:A:489:SER:CB	2.51	0.41
1:A:549:ASP:C	1:A:551:GLU:N	2.79	0.41
1:B:316:VAL:O	1:B:320:ARG:HG3	2.21	0.41
1:B:532:LEU:O	1:B:533:ASN:C	2.64	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:380:TYR:CE1	1:C:715:HIS:CG	3.09	0.41
1:C:434:LYS:C	1:C:436:ASN:N	2.75	0.41
1:C:577:TYR:OH	1:C:680:LEU:HG	2.21	0.41
1:D:446:THR:OG1	1:D:485:PRO:HG2	2.20	0.41
1:D:645:ASP:C	1:D:647:TYR:H	2.28	0.41
1:A:406:ARG:HA	1:A:411:TYR:CD1	2.56	0.41
1:B:670:PRO:HD2	1:B:671:TYR:CE2	2.55	0.41
1:C:710:ILE:O	1:C:711:GLY:C	2.64	0.41
1:D:485:PRO:HD2	1:D:489:SER:HB2	2.03	0.41
1:B:485:PRO:HG3	1:B:509:TYR:CZ	2.56	0.40
1:B:638:PHE:HE1	1:B:676:GLU:HG2	1.85	0.40
1:D:464:THR:O	1:D:465:THR:C	2.62	0.40
1:D:572:GLU:OE1	1:D:572:GLU:HA	2.21	0.40
1:A:509:TYR:HA	1:A:510:PRO:HD3	1.91	0.40
1:D:451:LEU:HD13	1:D:496:ALA:HB1	2.03	0.40
1:A:695:TYR:CD2	1:A:695:TYR:C	2.99	0.40
1:B:380:TYR:CE1	1:B:715:HIS:CG	3.10	0.40
1:D:638:PHE:CE2	1:D:677:LEU:CD1	3.04	0.40
1:B:323:LEU:HD12	1:B:323:LEU:HA	1.83	0.40
1:B:460:MET:HA	1:B:461:PRO:HD3	1.76	0.40
1:B:549:ASP:O	1:B:550:ASP:C	2.65	0.40
1:B:561:GLU:CB	3:B:734:CL:CL	2.97	0.40
1:C:331:LEU:O	1:C:332:ARG:C	2.64	0.40
1:D:376:MET:HE2	1:D:376:MET:HB3	1.98	0.40
1:D:515:LEU:HD23	1:D:515:LEU:HA	1.74	0.40
1:D:651:LEU:HG	1:D:653:GLY:H	1.87	0.40
1:A:602:ASP:C	1:A:602:ASP:OD1	2.64	0.40
1:A:639:PHE:CZ	1:A:663:PRO:HD2	2.57	0.40
1:C:316:VAL:CG1	1:C:317:ASN:N	2.84	0.40
1:C:656:MET:HE2	1:C:656:MET:HB2	1.84	0.40
1:C:658:TYR:C	1:C:660:GLU:H	2.30	0.40
1:D:665:PRO:HG3	1:D:687:TYR:OH	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	408/729 (56%)	376 (92%)	28 (7%)	4 (1%)	12	32
1	B	409/729 (56%)	362 (88%)	38 (9%)	9 (2%)	5	15
1	C	409/729 (56%)	356 (87%)	46 (11%)	7 (2%)	7	20
1	D	397/729 (54%)	346 (87%)	42 (11%)	9 (2%)	5	14
All	All	1623/2916 (56%)	1440 (89%)	154 (10%)	29 (2%)	6	19

All (29) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	651	LEU
1	C	367	ASP
1	D	367	ASP
1	A	647	TYR
1	B	462	GLY
1	C	647	TYR
1	C	648	ASP
1	D	332	ARG
1	D	521	ASP
1	D	655	TYR
1	A	550	ASP
1	B	345	ASP
1	B	461	PRO
1	B	561	GLU
1	B	649	LYS
1	D	515	LEU
1	C	565	ASP
1	D	458	VAL
1	B	443	TRP
1	B	459	ARG
1	B	565	ASP
1	C	535	PRO
1	C	614	LEU
1	D	443	TRP
1	C	452	ALA
1	B	603	VAL
1	D	545	PRO
1	D	603	VAL

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Mol	Chain	Res	Type
1	A	535	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	379/675 (56%)	333 (88%)	46 (12%)	5	14
1	B	379/675 (56%)	326 (86%)	53 (14%)	3	10
1	C	379/675 (56%)	334 (88%)	45 (12%)	5	15
1	D	370/675 (55%)	325 (88%)	45 (12%)	5	14
All	All	1507/2700 (56%)	1318 (88%)	189 (12%)	4	13

All (189) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	322	THR
1	A	323	LEU
1	A	329	ILE
1	A	333	ARG
1	A	336	LYS
1	A	339	SER
1	A	341	TYR
1	A	346	LYS
1	A	349	ASN
1	A	356	VAL
1	A	359	SER
1	A	403	LYS
1	A	404	VAL
1	A	433	LYS
1	A	435	GLU
1	A	451	LEU
1	A	456	LYS
1	A	460	MET
1	A	488	TYR
1	A	494	ARG

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Mol	Chain	Res	Type
1	A	495	SER
1	A	511	ARG
1	A	514	VAL
1	A	567	ASP
1	A	578	VAL
1	A	582	ARG
1	A	591	LEU
1	A	594	SER
1	A	597	GLU
1	A	607	ASN
1	A	609	VAL
1	A	619	LEU
1	A	622	ASP
1	A	635	ARG
1	A	656	MET
1	A	659	MET
1	A	662	LEU
1	A	669	GLU
1	A	673	LEU
1	A	677	LEU
1	A	678	LYS
1	A	680	LEU
1	A	702	ASP
1	A	707	SER
1	A	717	ASP
1	A	720	GLU
1	B	316	VAL
1	B	323	LEU
1	B	329	ILE
1	B	333	ARG
1	B	339	SER
1	B	343	LEU
1	B	356	VAL
1	B	367	ASP
1	B	382	ASN
1	B	396	VAL
1	B	402	GLU
1	B	403	LYS
1	B	404	VAL
1	B	433	LYS
1	B	449	LYS
1	B	450	ARG

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Mol	Chain	Res	Type
1	B	451	LEU
1	B	456	LYS
1	B	470	ARG
1	B	477	SER
1	B	487	ARG
1	B	491	GLU
1	B	514	VAL
1	B	533	ASN
1	B	548	ARG
1	B	549	ASP
1	B	559	LEU
1	B	563	LYS
1	B	571	LYS
1	B	578	VAL
1	B	579	ILE
1	B	582	ARG
1	B	589	ASN
1	B	597	GLU
1	B	603	VAL
1	B	607	ASN
1	B	609	VAL
1	B	622	ASP
1	B	635	ARG
1	B	645	ASP
1	B	647	TYR
1	B	651	LEU
1	B	661	ASP
1	B	662	LEU
1	B	668	THR
1	B	673	LEU
1	B	677	LEU
1	B	678	LYS
1	B	702	ASP
1	B	703	ASN
1	B	717	ASP
1	B	718	ILE
1	B	722	LEU
1	C	315	LYS
1	C	323	LEU
1	C	329	ILE
1	C	332	ARG
1	C	339	SER

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Mol	Chain	Res	Type
1	C	356	VAL
1	C	382	ASN
1	C	403	LYS
1	C	434	LYS
1	C	450	ARG
1	C	451	LEU
1	C	457	VAL
1	C	463	THR
1	C	470	ARG
1	C	487	ARG
1	C	491	GLU
1	C	500	ASP
1	C	536	SER
1	C	559	LEU
1	C	569	LEU
1	C	578	VAL
1	C	589	ASN
1	C	591	LEU
1	C	597	GLU
1	C	603	VAL
1	C	609	VAL
1	C	619	LEU
1	C	622	ASP
1	C	623	TYR
1	C	635	ARG
1	C	648	ASP
1	C	656	MET
1	C	660	GLU
1	C	661	ASP
1	C	662	LEU
1	C	669	GLU
1	C	673	LEU
1	C	677	LEU
1	C	682	LYS
1	C	683	VAL
1	C	707	SER
1	C	714	ILE
1	C	718	ILE
1	C	720	GLU
1	C	722	LEU
1	D	315	LYS
1	D	316	VAL

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Mol	Chain	Res	Type
1	D	317	ASN
1	D	323	LEU
1	D	333	ARG
1	D	334	LYS
1	D	337	GLU
1	D	353	LYS
1	D	356	VAL
1	D	367	ASP
1	D	388	SER
1	D	402	GLU
1	D	403	LYS
1	D	433	LYS
1	D	450	ARG
1	D	451	LEU
1	D	456	LYS
1	D	460	MET
1	D	470	ARG
1	D	487	ARG
1	D	489	SER
1	D	490	THR
1	D	500	ASP
1	D	511	ARG
1	D	514	VAL
1	D	518	ARG
1	D	546	THR
1	D	547	TRP
1	D	548	ARG
1	D	576	ASP
1	D	579	ILE
1	D	583	MET
1	D	609	VAL
1	D	622	ASP
1	D	626	VAL
1	D	635	ARG
1	D	645	ASP
1	D	647	TYR
1	D	660	GLU
1	D	662	LEU
1	D	669	GLU
1	D	673	LEU
1	D	678	LYS
1	D	702	ASP

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Mol	Chain	Res	Type
1	D	718	ILE

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

Mol	Chain	Res	Type
1	A	325	HIS
1	A	349	ASN
1	A	436	ASN
1	A	679	ASN
1	A	708	GLN
1	B	318	GLN
1	B	325	HIS
1	B	349	ASN
1	B	382	ASN
1	B	407	ASN
1	B	531	HIS
1	B	584	HIS
1	B	679	ASN
1	B	686	GLN
1	B	703	ASN
1	B	721	GLN
1	C	349	ASN
1	C	382	ASN
1	C	391	ASN
1	C	420	HIS
1	C	436	ASN
1	C	657	ASN
1	C	684	GLN
1	C	686	GLN
1	D	317	ASN
1	D	349	ASN
1	D	413	GLN
1	D	436	ASN
1	D	688	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 29 ligands modelled in this entry, 21 are monoatomic - leaving 8 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	SO4	B	731	-	4,4,4	0.26	0	6,6,6	0.21	0
2	SO4	C	731	-	4,4,4	0.21	0	6,6,6	0.24	0
4	C2G	D	730	-	31,31,31	3.88	14 (45%)	42,46,46	1.10	4 (9%)
2	SO4	C	730	-	4,4,4	0.25	0	6,6,6	0.20	0
2	SO4	A	731	-	4,4,4	0.25	0	6,6,6	0.10	0
2	SO4	A	730	-	4,4,4	0.22	0	6,6,6	0.20	0
5	EDO	D	734	-	3,3,3	0.63	0	2,2,2	0.09	0
2	SO4	B	730	-	4,4,4	0.25	0	6,6,6	0.23	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	C2G	D	730	-	-	13/24/40/40	0/2/2/2
5	EDO	D	734	-	-	1/1/1/1	-

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	730	C2G	O2-C2	8.93	1.40	1.23
4	D	730	C2G	C4-N3	7.31	1.48	1.34
4	D	730	C2G	C6-C5	7.00	1.51	1.35
4	D	730	C2G	C2-N1	6.97	1.54	1.40
4	D	730	C2G	C2-N3	6.89	1.50	1.36
4	D	730	C2G	PB-O3A	6.01	1.66	1.59
4	D	730	C2G	PA-O3A	5.82	1.65	1.59
4	D	730	C2G	C4-N4	4.79	1.45	1.33
4	D	730	C2G	PB-O1B	4.40	1.66	1.50
4	D	730	C2G	PA-O1A	4.35	1.65	1.50
4	D	730	C2G	C6-N1	3.96	1.47	1.38
4	D	730	C2G	C5-C4	3.54	1.51	1.42
4	D	730	C2G	O4'-C1'	2.71	1.48	1.42
4	D	730	C2G	PA-O5'	2.07	1.67	1.59

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	730	C2G	C1'-N1-C2	2.75	124.52	118.44
4	D	730	C2G	O2-C2-N3	-2.51	118.38	122.33
4	D	730	C2G	N4-C4-N3	2.29	122.00	117.91
4	D	730	C2G	C3'-C2'-C1'	2.27	105.76	101.46

There are no chirality outliers.

All (14) torsion outliers are listed below:

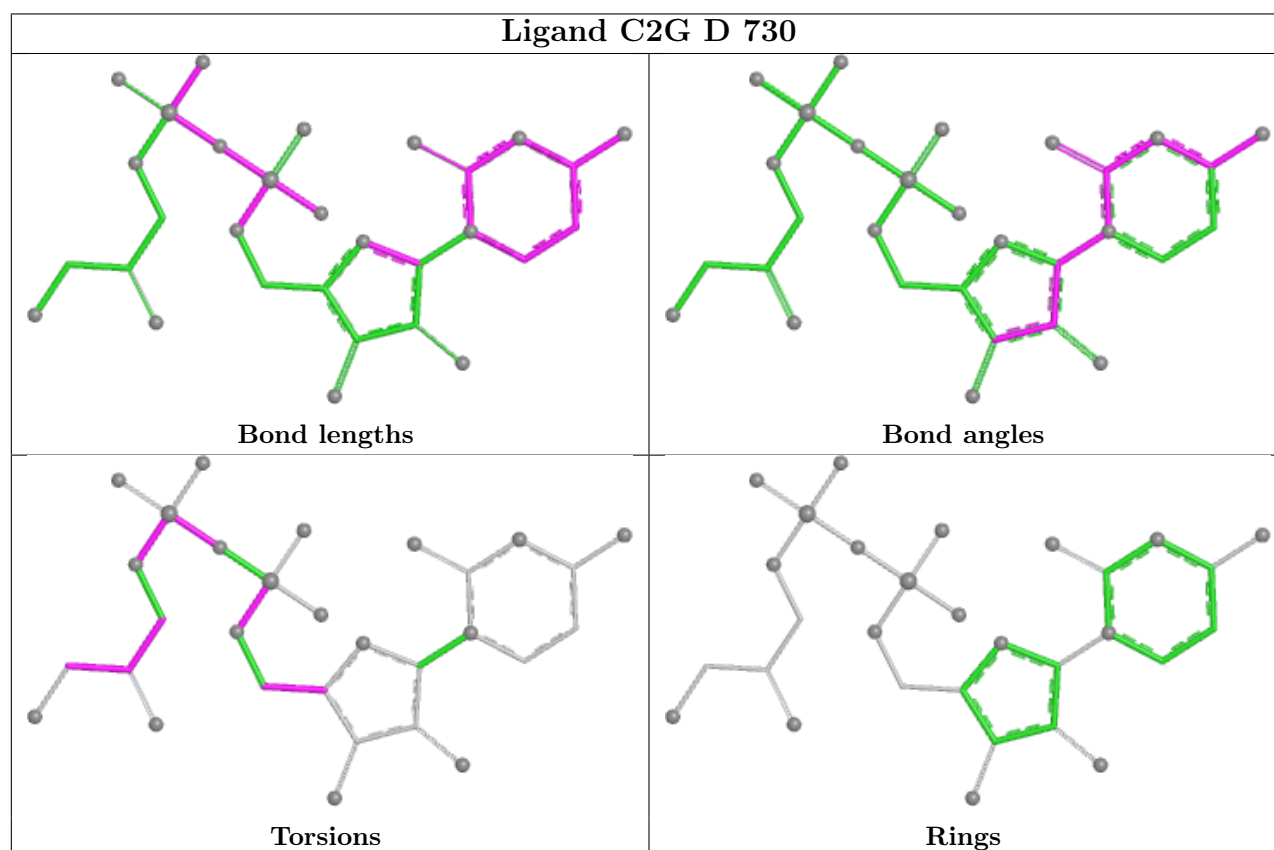
Mol	Chain	Res	Type	Atoms
4	D	730	C2G	C5'-O5'-PA-O1A
4	D	730	C2G	C5'-O5'-PA-O2A
4	D	730	C2G	C3G-O3B-PB-O3A
4	D	730	C2G	C3G-O3B-PB-O2B
4	D	730	C2G	O2G-C2G-C3G-O3B
4	D	730	C2G	C1G-C2G-C3G-O3B
5	D	734	EDO	O1-C1-C2-O2
4	D	730	C2G	O1G-C1G-C2G-O2G
4	D	730	C2G	O4'-C4'-C5'-O5'
4	D	730	C2G	C3'-C4'-C5'-O5'
4	D	730	C2G	C5'-O5'-PA-O3A
4	D	730	C2G	C3G-O3B-PB-O1B
4	D	730	C2G	PA-O3A-PB-O1B
4	D	730	C2G	PA-O3A-PB-O3B

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	730	C2G	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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 [i](#)

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2	OWAB(Å ²)	Q < 0.9
1	A	410/729 (56%)	-0.58	1 (0%) 91 90	61, 83, 149, 220	0
1	B	411/729 (56%)	-0.56	2 (0%) 87 83	64, 85, 159, 242	0
1	C	411/729 (56%)	-0.51	1 (0%) 91 90	69, 94, 166, 263	0
1	D	401/729 (55%)	-0.51	2 (0%) 87 83	66, 92, 151, 279	0
All	All	1633/2916 (56%)	-0.54	6 (0%) 88 86	61, 88, 156, 279	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	560	PHE	3.0
1	D	587	ILE	2.4
1	A	560	PHE	2.4
1	D	651	LEU	2.1
1	B	559	LEU	2.1
1	C	669	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 oligosaccharides in this entry.

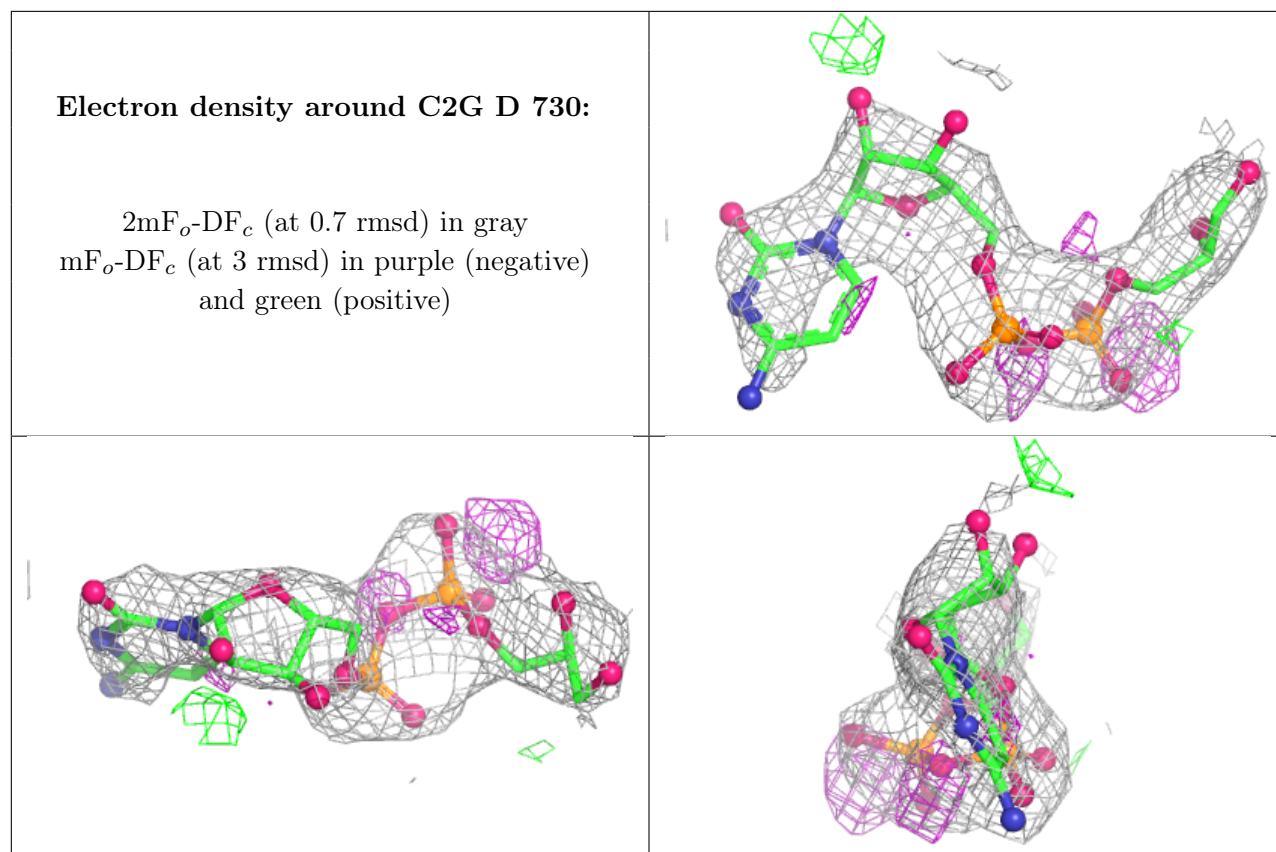
6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	SO4	B	731	5/5	0.57	0.12	171,171,171,171	0
2	SO4	A	731	5/5	0.74	0.12	166,166,166,166	0
3	CL	B	734	1/1	0.81	0.09	111,111,111,111	0
3	CL	C	735	1/1	0.81	0.12	118,118,118,118	0
3	CL	C	734	1/1	0.85	0.10	106,106,106,106	0
3	CL	A	732	1/1	0.87	0.06	114,114,114,114	0
5	EDO	D	734	4/4	0.87	0.10	90,90,90,90	0
3	CL	D	733	1/1	0.88	0.06	92,92,92,92	0
4	C2G	D	730	30/30	0.89	0.11	122,122,123,123	0
3	CL	A	737	1/1	0.89	0.07	108,108,108,108	0
3	CL	A	733	1/1	0.90	0.09	130,130,130,130	0
2	SO4	C	731	5/5	0.90	0.08	124,125,127,128	0
3	CL	A	739	1/1	0.90	0.12	88,88,88,88	0
3	CL	D	732	1/1	0.91	0.06	101,101,101,101	0
3	CL	B	735	1/1	0.91	0.09	127,127,127,127	0
3	CL	A	736	1/1	0.91	0.08	106,106,106,106	0
2	SO4	C	730	5/5	0.91	0.07	129,129,131,132	0
3	CL	C	733	1/1	0.92	0.04	102,102,102,102	0
3	CL	B	733	1/1	0.93	0.08	121,121,121,121	0
2	SO4	A	730	5/5	0.93	0.09	103,104,105,107	0
2	SO4	B	730	5/5	0.93	0.07	90,90,91,94	0
3	CL	C	736	1/1	0.93	0.06	106,106,106,106	0
3	CL	B	732	1/1	0.94	0.12	100,100,100,100	0
3	CL	A	734	1/1	0.95	0.07	96,96,96,96	0
3	CL	B	736	1/1	0.95	0.06	83,83,83,83	0
3	CL	A	735	1/1	0.96	0.09	94,94,94,94	0
3	CL	C	732	1/1	0.96	0.04	107,107,107,107	0
3	CL	A	738	1/1	0.97	0.06	97,97,97,97	0
3	CL	D	731	1/1	0.99	0.12	68,68,68,68	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



6.5 Other polymers [i](#)

There are no such residues in this entry.