



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 03:36 AM UTC

PDB ID : 3L7J / pdb_00003l7j
Title : Structure of the Wall Teichoic Acid Polymerase TagF, H444N variant
Authors : Strynadka, N.C.J.; Lovering, A.L.
Deposited on : 2009-12-28
Resolution : 2.81 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
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

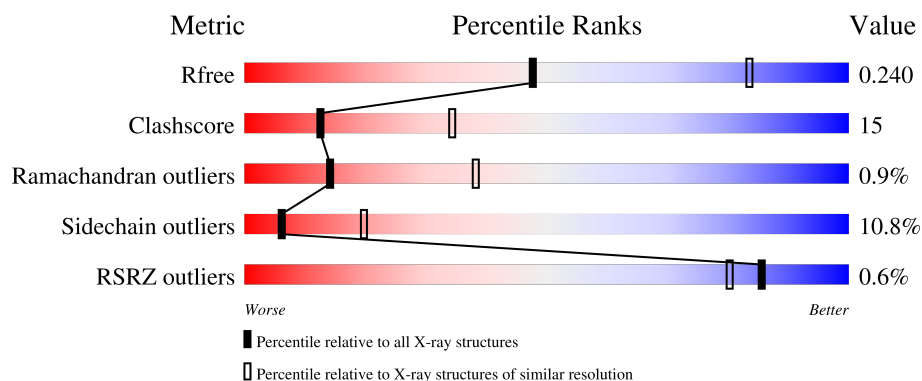
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.81 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	4591 (2.84-2.80)
Clashscore	190562	5010 (2.84-2.80)
Ramachandran outliers	187476	4916 (2.84-2.80)
Sidechain outliers	187428	4918 (2.84-2.80)
RSRZ outliers	180081	4594 (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 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	
1	B	729	
1	C	729	
1	D	729	

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	SO4	B	730	-	-	X	-
3	CL	B	732	-	-	X	-
3	CL	B	736	-	-	X	-
3	CL	C	733	-	-	X	-
3	CL	D	731	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13970 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	412	Total	C	N	O	S	0	0	0
			3477	2233	581	652	11			
1	C	411	Total	C	N	O	S	0	0	0
			3467	2227	578	651	11			
1	D	411	Total	C	N	O	S	0	0	0
			3472	2230	580	651	11			

There are 36 discrepancies between the modelled and reference sequences:

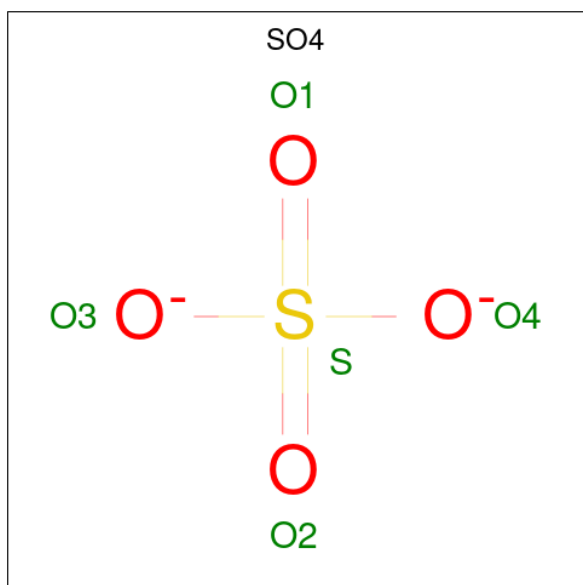
Chain	Residue	Modelled	Actual	Comment	Reference
A	444	ASN	HIS	engineered mutation	UNP Q5HLM5
A	722	LEU	-	expression tag	UNP Q5HLM5
A	723	GLU	-	expression tag	UNP Q5HLM5
A	724	HIS	-	expression tag	UNP Q5HLM5
A	725	HIS	-	expression tag	UNP Q5HLM5
A	726	HIS	-	expression tag	UNP Q5HLM5
A	727	HIS	-	expression 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	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		

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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		
2	C	1	Total	O	S	0	0
			5	4	1		
2	D	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	11	Total	Cl	0	0
			11	11		
3	B	8	Total	Cl	0	0
			8	8		
3	C	7	Total	Cl	0	0
			7	7		
3	D	6	Total	Cl	0	0
			6	6		

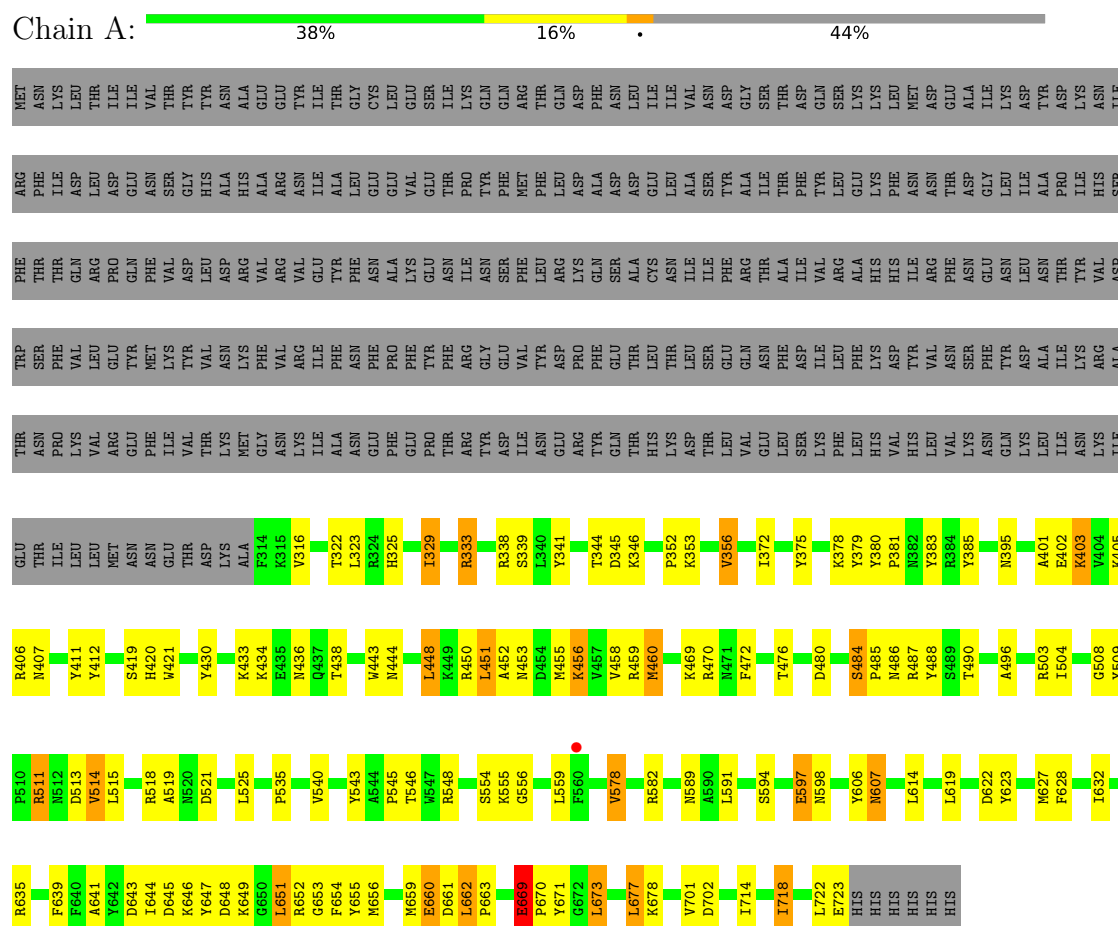
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	8	Total	O	0	0
			8	8		
4	B	5	Total	O	0	0
			5	5		
4	C	3	Total	O	0	0
			3	3		
4	D	4	Total	O	0	0
			4	4		

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

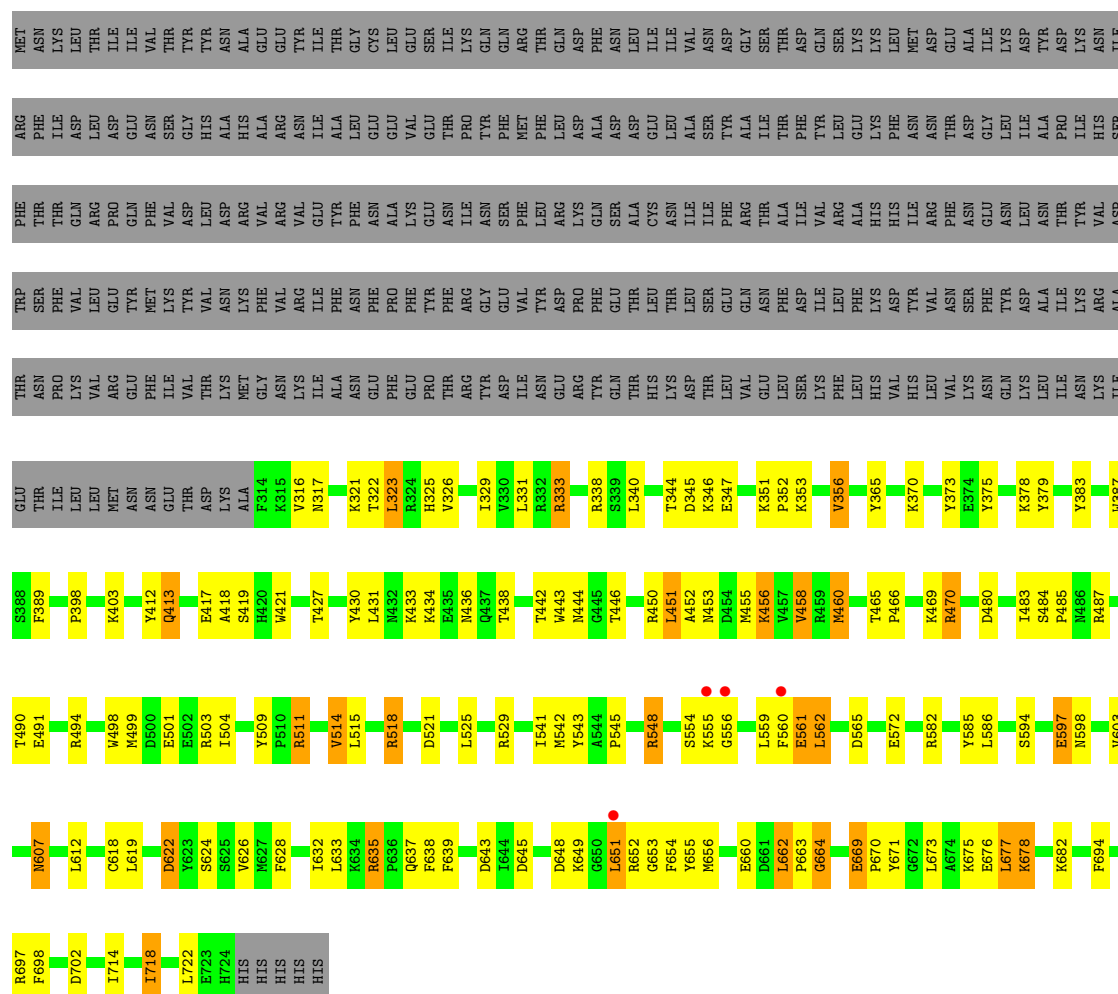
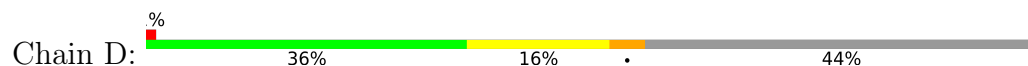


• Molecule 1: Teichoic acid biosynthesis protein F





- 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	223.60Å 223.60Å 100.57Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.80 – 2.81 19.80 – 2.81	Depositor EDS
% Data completeness (in resolution range)	97.9 (19.80-2.81) 97.5 (19.80-2.81)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.64 (at 2.79Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.197 , 0.246 0.192 , 0.240	Depositor DCC
R_{free} test set	3046 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	72.4	Xtriage
Anisotropy	0.048	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 25.5	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	13970	wwPDB-VP
Average B, all atoms (Å ²)	86.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.40% 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: SO4, CL

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	0.58	0/3551	0.95	8/4798 (0.2%)
1	B	0.59	0/3567	0.94	6/4820 (0.1%)
1	C	0.54	0/3556	0.93	8/4805 (0.2%)
1	D	0.56	0/3562	0.93	5/4813 (0.1%)
All	All	0.57	0/14236	0.94	27/19236 (0.1%)

There are no bond length outliers.

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	448	LEU	N-CA-C	-7.34	103.41	113.18
1	D	664	GLY	CA-C-N	7.17	126.93	119.76
1	D	664	GLY	C-N-CA	7.17	126.93	119.76
1	A	669	GLU	CA-C-N	6.34	125.76	118.85
1	A	669	GLU	C-N-CA	6.34	125.76	118.85
1	B	366	SER	N-CA-C	6.15	116.55	107.88
1	C	704	GLY	N-CA-C	-5.98	107.06	115.32
1	B	460	MET	CA-C-N	5.84	127.14	119.84
1	B	460	MET	C-N-CA	5.84	127.14	119.84
1	A	484	SER	CA-C-N	5.78	125.48	119.64
1	A	484	SER	C-N-CA	5.78	125.48	119.64
1	C	534	LEU	CA-C-N	5.65	125.67	119.90
1	C	534	LEU	C-N-CA	5.65	125.67	119.90
1	B	704	GLY	N-CA-C	-5.63	107.47	115.30
1	A	372	ILE	N-CA-C	-5.61	104.90	110.62
1	B	448	LEU	N-CA-C	-5.55	105.55	112.93
1	D	427	THR	CA-C-N	5.53	125.45	119.76
1	D	427	THR	C-N-CA	5.53	125.45	119.76
1	C	427	THR	CA-C-N	5.50	125.42	119.76
1	C	427	THR	C-N-CA	5.50	125.42	119.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	448	LEU	N-CA-C	-5.44	106.57	113.43
1	C	397	VAL	N-CA-C	5.39	113.87	107.73
1	B	538	LYS	N-CA-C	5.35	117.69	109.07
1	A	701	VAL	N-CA-C	-5.31	108.32	113.53
1	D	452	ALA	CB-CA-C	-5.18	110.58	116.54
1	C	435	GLU	N-CA-C	-5.14	107.08	113.19
1	A	486	ASN	N-CA-C	5.12	115.93	108.14

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	93	0
1	B	3477	0	3381	112	0
1	C	3467	0	3374	111	0
1	D	3472	0	3376	105	0
2	A	15	0	0	0	0
2	B	5	0	0	2	0
2	C	15	0	0	0	0
2	D	5	0	0	0	0
3	A	11	0	0	1	0
3	B	8	0	0	6	0
3	C	7	0	0	2	0
3	D	6	0	0	4	0
4	A	8	0	0	1	0
4	B	5	0	0	0	0
4	C	3	0	0	0	0
4	D	4	0	0	0	0
All	All	13970	0	13500	419	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 15.

All (419) 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	1.02	1.19
1:D:470:ARG:HG2	1:D:470:ARG:HH11	1.04	1.10
1:C:333:ARG:HG2	1:C:333:ARG:HH11	1.28	0.99
1:B:333:ARG:HH11	1:B:333:ARG:HG2	1.28	0.98
1:C:470:ARG:HH11	1:C:470:ARG:HG2	1.27	0.97
1:B:470:ARG:HG2	1:B:470:ARG:HH11	1.25	0.97
1:D:333:ARG:HH11	1:D:333:ARG:HG2	1.35	0.91
1:A:470:ARG:HG2	1:A:470:ARG:HH11	1.35	0.91
1:D:470:ARG:HG2	1:D:470:ARG:NH1	1.85	0.89
1:A:333:ARG:HG2	1:A:333:ARG:NH1	1.84	0.86
1:A:333:ARG:HH11	1:A:333:ARG:CG	1.87	0.84
1:A:648:ASP:HB2	1:A:651:LEU:HB2	1.64	0.80
1:B:663:PRO:HG3	1:B:694:PHE:CG	2.17	0.79
1:B:413:GLN:O	1:B:417:GLU:HG3	1.83	0.79
1:C:648:ASP:HB2	1:C:651:LEU:HB2	1.63	0.79
1:B:548:ARG:HD3	1:B:643:ASP:OD2	1.83	0.78
1:C:333:ARG:HH11	1:C:333:ARG:CG	1.95	0.78
1:C:383:TYR:CE2	1:C:718:ILE:HD11	2.20	0.77
1:A:383:TYR:CE2	1:A:718:ILE:HD11	2.20	0.77
1:A:485:PRO:HG3	1:A:509:TYR:CE2	2.20	0.75
1:C:662:LEU:HD23	1:C:662:LEU:H	1.51	0.75
1:B:561:GLU:HB2	3:B:734:CL:CL	2.24	0.74
1:A:662:LEU:HB2	1:A:663:PRO:HD3	1.68	0.74
1:B:470:ARG:HH11	1:B:470:ARG:CG	2.00	0.74
1:C:545:PRO:HG2	1:C:583:MET:HE1	1.69	0.73
1:C:383:TYR:CZ	1:C:718:ILE:HD11	2.24	0.73
1:A:353:LYS:HG2	3:A:733:CL:CL	2.26	0.73
1:A:514:VAL:HG12	1:A:518:ARG:HG3	1.69	0.72
1:C:543:TYR:CZ	1:C:545:PRO:HG3	2.24	0.72
1:D:639:PHE:CZ	1:D:663:PRO:HD2	2.25	0.72
1:D:572:GLU:OE1	1:D:678:LYS:HE3	1.90	0.72
1:C:470:ARG:HG2	1:C:470:ARG:NH1	2.03	0.71
1:C:662:LEU:H	1:C:662:LEU:CD2	2.03	0.71
1:C:372:ILE:HD13	1:C:710:ILE:HG21	1.72	0.71
1:A:338:ARG:HD2	1:A:430:TYR:CD1	2.25	0.70
1:D:485:PRO:HG3	1:D:509:TYR:CE2	2.27	0.70
1:D:648:ASP:HB2	1:D:651:LEU:HB2	1.72	0.70
1:A:714:ILE:O	1:A:718:ILE:HG23	1.92	0.69
1:B:467:LYS:HE3	1:B:470:ARG:NH2	2.07	0.69
1:C:620:ILE:HD11	1:C:677:LEU:HD21	1.73	0.69
1:B:511:ARG:HH22	1:B:629:ASP:CG	2.02	0.68
1:B:542:MET:HE2	1:B:612:LEU:HB3	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:548:ARG:NH2	1:D:622:ASP:OD1	2.23	0.68
1:C:548:ARG:HD3	1:C:643:ASP:OD2	1.94	0.68
1:D:548:ARG:HH22	1:D:622:ASP:CG	2.01	0.67
1:D:333:ARG:HG2	1:D:333:ARG:NH1	2.08	0.67
1:C:467:LYS:HE3	1:C:470:ARG:HH22	1.60	0.67
1:D:543:TYR:CZ	1:D:545:PRO:HG3	2.29	0.67
1:A:325:HIS:CE1	1:A:329:ILE:HD13	2.30	0.67
1:B:403:LYS:HE2	3:B:736:CL:CL	2.32	0.66
1:C:673:LEU:HD22	1:C:677:LEU:HD22	1.76	0.66
1:D:325:HIS:CE1	1:D:329:ILE:HD11	2.30	0.66
1:C:444:ASN:O	1:C:511:ARG:NH1	2.28	0.66
1:B:383:TYR:CE2	1:B:718:ILE:HD11	2.31	0.66
1:D:451:LEU:HD12	1:D:451:LEU:H	1.60	0.66
1:A:470:ARG:HG2	1:A:470:ARG:NH1	2.07	0.65
1:A:508:GLY:HA3	1:A:702:ASP:OD1	1.95	0.65
1:B:333:ARG:HH11	1:B:333:ARG:CG	2.08	0.65
1:C:487:ARG:HH11	1:C:487:ARG:HB2	1.61	0.65
1:B:470:ARG:HG2	1:B:470:ARG:NH1	2.03	0.65
1:C:465:THR:HB	1:C:466:PRO:HD3	1.77	0.65
1:B:456:LYS:HA	1:B:456:LYS:HE2	1.78	0.64
1:B:538:LYS:HE2	1:B:575:ASP:O	1.97	0.64
1:C:333:ARG:HG2	1:C:333:ARG:NH1	2.02	0.64
1:C:714:ILE:O	1:C:718:ILE:HG23	1.98	0.63
1:B:542:MET:CE	1:B:612:LEU:HB3	2.29	0.63
1:C:569:LEU:HD22	1:C:573:LEU:HD12	1.80	0.63
1:B:372:ILE:HD13	1:B:710:ILE:HG21	1.79	0.63
1:A:383:TYR:CZ	1:A:718:ILE:HD11	2.33	0.62
1:B:434:LYS:C	1:B:436:ASN:H	2.07	0.62
1:C:633:LEU:HB3	1:C:635:ARG:HD3	1.82	0.62
1:C:434:LYS:C	1:C:436:ASN:H	2.07	0.62
1:D:353:LYS:HG2	3:D:731:CL:CL	2.37	0.61
1:D:413:GLN:O	1:D:417:GLU:HG3	2.00	0.61
1:D:338:ARG:HD2	1:D:430:TYR:CD1	2.35	0.61
1:D:662:LEU:HB2	1:D:663:PRO:HD3	1.82	0.61
1:A:662:LEU:HD23	1:A:662:LEU:H	1.64	0.61
1:A:673:LEU:HD22	1:A:677:LEU:HD22	1.83	0.61
1:B:353:LYS:HG2	3:B:732:CL:CL	2.38	0.61
1:C:487:ARG:HB2	1:C:487:ARG:NH1	2.16	0.60
1:C:665:PRO:HG3	1:C:687:TYR:CZ	2.35	0.60
1:B:451:LEU:HD12	1:B:451:LEU:H	1.64	0.60
1:D:317:ASN:O	1:D:321:LYS:HG3	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:325:HIS:CE1	1:B:329:ILE:HD13	2.37	0.60
1:B:652:ARG:C	1:B:654:PHE:H	2.08	0.60
1:B:662:LEU:H	1:B:662:LEU:HD23	1.67	0.60
1:C:511:ARG:HH22	1:C:629:ASP:CG	2.10	0.60
1:D:470:ARG:HH11	1:D:470:ARG:CG	1.95	0.59
1:B:548:ARG:HH22	1:B:622:ASP:CG	2.08	0.59
1:B:559:LEU:HD23	1:B:587:ILE:HG23	1.84	0.59
1:D:347:GLU:HG3	1:D:436:ASN:HB2	1.82	0.59
1:C:701:VAL:HG12	1:C:701:VAL:O	2.02	0.59
1:D:438:THR:HA	1:D:480:ASP:OD2	2.02	0.59
1:D:670:PRO:HD2	1:D:671:TYR:CD2	2.38	0.59
1:D:554:SER:O	1:D:555:LYS:HB2	2.02	0.59
1:A:338:ARG:HD3	1:A:412:TYR:OH	2.03	0.59
1:B:480:ASP:O	1:B:503:ARG:HG2	2.03	0.59
1:A:443:TRP:CG	1:A:444:ASN:H	2.21	0.58
1:D:465:THR:HB	1:D:466:PRO:HD3	1.84	0.58
1:A:451:LEU:HA	1:A:455:MET:HE3	1.85	0.58
1:A:641:ALA:HB1	1:A:644:ILE:HB	1.84	0.58
1:D:453:ASN:HB2	1:D:498:TRP:CZ2	2.38	0.58
1:D:582:ARG:HD3	3:D:733:CL:CL	2.40	0.58
1:A:378:LYS:HD3	1:A:379:TYR:CE2	2.39	0.58
1:A:546:THR:HG21	1:A:623:TYR:O	2.04	0.58
1:C:347:GLU:O	1:C:436:ASN:ND2	2.37	0.58
1:B:546:THR:HG21	1:B:623:TYR:O	2.04	0.58
1:C:554:SER:C	1:C:556:GLY:H	2.11	0.58
1:D:714:ILE:O	1:D:718:ILE:HG23	2.04	0.58
1:D:585:TYR:CZ	1:D:586:LEU:HG	2.38	0.57
1:C:665:PRO:HG3	1:C:687:TYR:CE1	2.39	0.57
1:A:513:ASP:HB2	4:A:748:HOH:O	2.04	0.57
1:A:662:LEU:HB2	1:A:663:PRO:CD	2.35	0.57
1:B:624:SER:OG	1:B:626:VAL:HG22	2.03	0.57
1:B:648:ASP:HB2	1:B:651:LEU:HB2	1.84	0.57
1:A:420:HIS:CD2	1:A:438:THR:HB	2.40	0.57
1:A:548:ARG:HD3	1:A:643:ASP:OD2	2.05	0.57
1:B:338:ARG:HD2	1:B:430:TYR:CD1	2.40	0.56
1:C:387:TRP:HB3	1:C:389:PHE:CE2	2.41	0.56
1:B:347:GLU:O	1:B:436:ASN:ND2	2.39	0.56
1:B:443:TRP:CD1	1:B:444:ASN:H	2.24	0.56
1:C:559:LEU:HD23	1:C:587:ILE:HG23	1.88	0.56
1:B:675:LYS:O	1:B:678:LYS:HB2	2.06	0.56
1:B:368:SER:HB3	1:B:510:PRO:HD2	1.89	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:627:MET:HE3	1:C:628:PHE:CZ	2.41	0.55
1:D:325:HIS:CE1	1:D:340:LEU:HB2	2.42	0.55
1:B:625:SER:N	2:B:730:SO4:O2	2.39	0.55
1:C:662:LEU:CD2	1:C:662:LEU:N	2.68	0.55
1:C:652:ARG:C	1:C:654:PHE:H	2.15	0.54
1:B:632:ILE:HG12	1:B:699:CYS:HB3	1.89	0.54
1:A:325:HIS:CE1	1:A:329:ILE:CD1	2.90	0.54
1:A:451:LEU:H	1:A:451:LEU:HD12	1.72	0.54
1:C:340:LEU:O	1:C:344:THR:HG23	2.08	0.54
1:D:597:GLU:O	1:D:598:ASN:HB2	2.07	0.54
1:B:548:ARG:NH2	1:B:622:ASP:OD1	2.30	0.54
1:A:443:TRP:CD1	1:A:444:ASN:H	2.25	0.54
1:B:638:PHE:HE1	1:B:676:GLU:HG2	1.73	0.53
1:A:405:LYS:O	1:A:411:TYR:HB2	2.08	0.53
1:A:548:ARG:NH2	1:A:622:ASP:OD1	2.35	0.53
1:C:582:ARG:NH2	1:C:606:TYR:O	2.42	0.53
1:C:485:PRO:HD2	1:C:489:SER:HB2	1.90	0.53
1:D:652:ARG:C	1:D:654:PHE:H	2.16	0.53
1:A:485:PRO:HG3	1:A:509:TYR:CZ	2.45	0.52
1:C:485:PRO:HG3	1:C:509:TYR:CE2	2.44	0.52
1:D:383:TYR:CE2	1:D:718:ILE:HD11	2.44	0.52
1:B:475:GLU:OE1	1:B:478:ARG:NH1	2.41	0.52
1:C:443:TRP:CG	1:C:444:ASN:H	2.27	0.52
1:B:543:TYR:CZ	1:B:545:PRO:HG3	2.45	0.52
1:D:514:VAL:HG12	1:D:518:ARG:HG3	1.92	0.52
1:B:716:LYS:O	1:B:720:GLU:HG3	2.09	0.52
1:C:418:ALA:O	1:C:437:GLN:HG2	2.09	0.52
1:D:352:PRO:HD2	3:D:731:CL:CL	2.47	0.52
1:C:453:ASN:HA	1:C:469:LYS:HD3	1.92	0.52
1:B:559:LEU:CD2	1:B:587:ILE:HG23	2.40	0.52
1:C:663:PRO:HG3	1:C:694:PHE:CG	2.45	0.52
1:B:434:LYS:C	1:B:436:ASN:N	2.67	0.52
1:D:442:THR:HG22	1:D:483:ILE:HD12	1.92	0.52
1:B:325:HIS:NE2	1:B:329:ILE:HD13	2.24	0.52
1:A:648:ASP:HB2	1:A:651:LEU:CB	2.37	0.51
1:C:718:ILE:HG13	1:C:718:ILE:O	2.10	0.51
1:D:662:LEU:HB2	1:D:663:PRO:CD	2.40	0.51
1:C:445:GLY:HA2	1:C:509:TYR:CE2	2.45	0.51
1:A:395:ASN:O	1:A:403:LYS:HE2	2.11	0.51
1:B:387:TRP:HB3	1:B:389:PHE:CE2	2.44	0.51
1:B:443:TRP:CG	1:B:444:ASN:H	2.29	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:316:VAL:HG13	1:C:317:ASN:N	2.25	0.51
1:D:338:ARG:HD3	1:D:412:TYR:OH	2.10	0.51
1:A:662:LEU:H	1:A:662:LEU:CD2	2.24	0.51
1:B:513:ASP:HA	1:B:704:GLY:HA2	1.92	0.51
1:B:354:THR:C	1:B:355:ILE:HG13	2.35	0.51
1:D:352:PRO:HA	1:D:419:SER:HB3	1.92	0.51
1:D:697:ARG:HD3	1:D:698:PHE:CZ	2.45	0.51
1:C:637:GLN:O	1:C:664:GLY:HA3	2.10	0.51
1:D:434:LYS:C	1:D:436:ASN:H	2.19	0.51
1:D:638:PHE:HE1	1:D:676:GLU:HG2	1.76	0.51
1:A:521:ASP:O	1:A:525:LEU:HG	2.10	0.51
1:B:467:LYS:HE3	1:B:470:ARG:HH22	1.76	0.51
1:B:329:ILE:HG22	1:B:330:VAL:N	2.26	0.50
1:D:639:PHE:CE2	1:D:663:PRO:HD2	2.46	0.50
1:D:451:LEU:HD12	1:D:451:LEU:N	2.23	0.50
1:A:341:TYR:CD1	1:A:412:TYR:HB3	2.46	0.50
1:A:543:TYR:CZ	1:A:545:PRO:HG3	2.46	0.50
1:D:669:GLU:HG2	1:D:671:TYR:H	1.76	0.50
1:C:344:THR:O	1:C:346:LYS:HG3	2.12	0.50
1:C:467:LYS:CE	1:C:470:ARG:HH22	2.25	0.50
1:A:718:ILE:O	1:A:722:LEU:HD13	2.11	0.50
1:C:322:THR:O	1:C:326:VAL:HG23	2.12	0.50
1:C:507:ILE:HG13	1:C:508:GLY:O	2.12	0.50
1:D:560:PHE:O	1:D:561:GLU:C	2.54	0.50
1:C:639:PHE:CZ	1:C:663:PRO:HD2	2.46	0.50
1:A:456:LYS:HE2	1:A:456:LYS:HA	1.93	0.50
1:B:627:MET:HE3	1:B:628:PHE:CZ	2.46	0.50
1:D:451:LEU:HA	1:D:455:MET:HE3	1.93	0.50
1:D:456:LYS:HE2	1:D:456:LYS:HA	1.94	0.50
1:A:652:ARG:C	1:A:654:PHE:H	2.19	0.49
1:B:687:TYR:O	1:B:688:GLN:C	2.54	0.49
1:C:450:ARG:HA	1:C:655:TYR:CE2	2.47	0.49
1:C:347:GLU:HA	1:C:434:LYS:HD3	1.95	0.49
1:C:341:TYR:O	1:C:345:ASP:HB2	2.12	0.49
1:D:322:THR:O	1:D:326:VAL:HG23	2.12	0.49
1:B:554:SER:C	1:B:556:GLY:H	2.20	0.49
1:C:442:THR:O	1:C:509:TYR:HE1	1.96	0.49
1:A:420:HIS:CE1	1:A:718:ILE:HG22	2.48	0.49
1:A:597:GLU:O	1:A:598:ASN:HB2	2.13	0.49
1:D:490:THR:HG23	1:D:504:ILE:HD13	1.93	0.49
1:B:519:ALA:HA	1:B:614:LEU:HD22	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:333:ARG:NH1	1:A:333:ARG:CG	2.57	0.48
1:D:607:ASN:N	1:D:607:ASN:OD1	2.45	0.48
1:B:458:VAL:C	1:B:460:MET:H	2.21	0.48
1:A:554:SER:C	1:A:556:GLY:H	2.21	0.48
1:A:325:HIS:NE2	1:A:329:ILE:HD13	2.28	0.48
1:A:722:LEU:O	1:A:723:GLU:HG3	2.13	0.48
1:B:344:THR:O	1:B:346:LYS:HG2	2.13	0.48
1:C:584:HIS:ND1	1:C:586:LEU:HB2	2.28	0.48
1:D:353:LYS:CG	3:D:731:CL:CL	2.99	0.48
1:D:387:TRP:HB3	1:D:389:PHE:CE2	2.48	0.48
1:A:646:LYS:O	1:A:648:ASP:N	2.41	0.48
1:A:662:LEU:CD2	1:A:662:LEU:N	2.77	0.48
1:C:687:TYR:O	1:C:688:GLN:C	2.56	0.48
1:C:554:SER:C	1:C:556:GLY:N	2.72	0.48
1:A:540:VAL:HG22	1:A:578:VAL:HG12	1.95	0.48
1:D:637:GLN:O	1:D:664:GLY:HA3	2.14	0.47
1:B:663:PRO:HG3	1:B:694:PHE:CD2	2.49	0.47
1:C:485:PRO:HA	1:C:508:GLY:HA2	1.95	0.47
1:B:356:VAL:HG23	1:B:421:TRP:HA	1.96	0.47
1:D:325:HIS:NE2	1:D:329:ILE:HD11	2.28	0.47
1:D:347:GLU:O	1:D:436:ASN:ND2	2.47	0.47
1:B:651:LEU:O	1:B:651:LEU:HD23	2.15	0.47
1:C:316:VAL:HG23	1:D:331:LEU:HD22	1.96	0.47
1:D:378:LYS:HD3	1:D:379:TYR:CE2	2.49	0.47
1:A:453:ASN:HA	1:A:469:LYS:HD3	1.96	0.47
1:B:670:PRO:HD2	1:B:671:TYR:CD2	2.49	0.47
1:C:338:ARG:HD3	1:C:412:TYR:OH	2.13	0.47
1:C:420:HIS:CE1	1:C:718:ILE:HG22	2.49	0.47
1:D:375:TYR:C	1:D:375:TYR:CD2	2.93	0.47
1:A:515:LEU:HD12	1:A:632:ILE:HD12	1.96	0.47
1:C:695:TYR:C	1:C:695:TYR:CD2	2.92	0.47
1:D:365:TYR:CZ	1:D:370:LYS:HG3	2.50	0.47
1:D:663:PRO:HG3	1:D:694:PHE:CG	2.49	0.47
1:B:524:TYR:O	1:B:528:ILE:HG13	2.15	0.47
1:D:697:ARG:HD3	1:D:698:PHE:CE2	2.49	0.47
1:B:338:ARG:HD3	1:B:412:TYR:OH	2.14	0.47
1:B:669:GLU:HG2	1:B:671:TYR:H	1.79	0.47
1:D:465:THR:CG2	1:D:469:LYS:HE3	2.44	0.47
1:A:480:ASP:O	1:A:503:ARG:HG2	2.15	0.47
1:B:625:SER:HB3	2:B:730:SO4:O2	2.14	0.47
1:A:344:THR:O	1:A:346:LYS:HG3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:356:VAL:HG23	1:D:421:TRP:HA	1.97	0.47
1:A:406:ARG:O	1:A:407:ASN:HB2	2.14	0.46
1:A:484:SER:HA	1:A:485:PRO:HD3	1.73	0.46
1:C:450:ARG:HG3	1:C:653:GLY:O	2.15	0.46
1:D:651:LEU:HG	1:D:653:GLY:H	1.81	0.46
1:B:353:LYS:HA	1:B:718:ILE:HD12	1.98	0.46
1:B:639:PHE:N	1:B:639:PHE:CD2	2.83	0.46
1:D:340:LEU:O	1:D:344:THR:HG23	2.15	0.46
1:B:445:GLY:HA2	1:B:509:TYR:CE2	2.50	0.46
1:C:470:ARG:NH1	1:C:471:ASN:OD1	2.48	0.46
1:D:494:ARG:HA	1:D:499:MET:HB2	1.96	0.46
1:C:353:LYS:HA	1:C:718:ILE:HD12	1.97	0.46
1:D:345:ASP:OD2	1:D:434:LYS:HE3	2.15	0.46
1:A:490:THR:HG23	1:A:504:ILE:HD13	1.98	0.46
1:B:532:LEU:HD21	1:B:606:TYR:CE2	2.50	0.46
1:D:639:PHE:HZ	1:D:663:PRO:HD2	1.73	0.46
1:B:662:LEU:HB2	1:B:663:PRO:CD	2.46	0.46
1:B:673:LEU:HD22	1:B:677:LEU:HD22	1.97	0.46
1:B:714:ILE:O	1:B:718:ILE:HG23	2.15	0.46
1:A:352:PRO:HA	1:A:419:SER:HB3	1.97	0.45
1:B:317:ASN:O	1:B:321:LYS:HG3	2.17	0.45
1:A:450:ARG:HA	1:A:655:TYR:CE2	2.52	0.45
1:A:509:TYR:HB3	1:A:511:ARG:HG2	1.96	0.45
1:C:652:ARG:C	1:C:654:PHE:N	2.73	0.45
1:D:458:VAL:C	1:D:460:MET:HE2	2.41	0.45
1:B:451:LEU:HD12	1:B:451:LEU:N	2.32	0.45
1:B:652:ARG:C	1:B:654:PHE:N	2.71	0.45
1:C:323:LEU:HD12	1:C:323:LEU:HA	1.75	0.45
1:B:638:PHE:CZ	1:B:683:VAL:HG11	2.52	0.45
1:D:325:HIS:CE1	1:D:329:ILE:CD1	2.98	0.45
1:D:652:ARG:C	1:D:654:PHE:N	2.72	0.45
1:D:675:LYS:O	1:D:678:LYS:HB2	2.17	0.45
1:A:458:VAL:C	1:A:460:MET:HE2	2.42	0.45
1:C:470:ARG:NH1	1:C:470:ARG:CG	2.75	0.45
1:B:380:TYR:N	1:B:381:PRO:HD3	2.31	0.45
1:B:531:HIS:CD2	1:B:531:HIS:O	2.70	0.45
1:C:663:PRO:HG3	1:C:694:PHE:CD2	2.52	0.45
1:A:519:ALA:HA	1:A:614:LEU:HD22	1.98	0.45
1:B:418:ALA:O	1:B:437:GLN:HG2	2.17	0.45
1:B:488:TYR:OH	1:B:655:TYR:HB2	2.16	0.45
1:A:385:TYR:O	1:A:401:ALA:HA	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:329:ILE:HD12	1:B:336:LYS:HB2	1.98	0.44
1:B:347:GLU:HG3	1:B:436:ASN:HB2	1.98	0.44
1:C:316:VAL:HG23	1:D:331:LEU:CD2	2.47	0.44
1:D:325:HIS:HE1	1:D:340:LEU:HB2	1.81	0.44
1:C:680:LEU:HD23	1:C:680:LEU:HA	1.80	0.44
1:D:548:ARG:NH1	1:D:643:ASP:OD1	2.50	0.44
1:B:560:PHE:O	1:B:561:GLU:C	2.60	0.44
1:A:345:ASP:OD1	1:A:434:LYS:CE	2.66	0.44
1:B:607:ASN:OD1	1:B:607:ASN:N	2.50	0.44
1:D:450:ARG:HA	1:D:655:TYR:CE2	2.52	0.44
1:A:607:ASN:OD1	1:A:607:ASN:N	2.48	0.44
1:B:405:LYS:O	1:B:411:TYR:HB2	2.18	0.44
1:B:403:LYS:CE	3:B:736:CL:CL	3.01	0.44
1:D:525:LEU:O	1:D:529:ARG:HG3	2.18	0.44
1:A:472:PHE:O	1:A:476:THR:HG23	2.18	0.44
1:C:353:LYS:HG2	3:C:733:CL:CL	2.54	0.44
1:C:470:ARG:HD2	1:C:474:ARG:HH21	1.83	0.44
1:B:340:LEU:O	1:B:344:THR:HG23	2.18	0.43
1:B:554:SER:C	1:B:556:GLY:N	2.75	0.43
1:C:560:PHE:O	1:C:561:GLU:C	2.61	0.43
1:C:585:TYR:O	1:C:589:ASN:OD1	2.36	0.43
1:D:325:HIS:O	1:D:329:ILE:HD13	2.17	0.43
1:C:356:VAL:HG22	1:C:418:ALA:CB	2.48	0.43
1:A:450:ARG:HD2	1:A:653:GLY:HA2	2.01	0.43
1:B:352:PRO:HA	1:B:419:SER:HB3	2.00	0.43
1:C:325:HIS:CE1	1:C:340:LEU:HB2	2.53	0.43
1:C:347:GLU:CG	1:C:436:ASN:HB2	2.49	0.43
1:C:431:LEU:HD23	1:C:431:LEU:HA	1.60	0.43
1:C:443:TRP:CD1	1:C:444:ASN:H	2.36	0.43
1:C:718:ILE:O	1:C:722:LEU:HD22	2.19	0.43
1:B:376:MET:HE2	1:B:376:MET:HB3	1.84	0.43
1:A:443:TRP:CG	1:A:444:ASN:N	2.86	0.43
1:C:441:GLN:HG2	1:C:479:TRP:CE2	2.53	0.43
1:D:542:MET:HE1	1:D:612:LEU:HB3	2.01	0.43
1:B:663:PRO:HG3	1:B:694:PHE:CD1	2.53	0.43
1:C:341:TYR:CD1	1:C:412:TYR:HB3	2.53	0.43
1:C:722:LEU:O	1:C:723:GLU:HG3	2.19	0.43
1:C:316:VAL:CG1	1:C:317:ASN:N	2.81	0.43
1:C:511:ARG:NH2	1:C:629:ASP:CG	2.76	0.43
1:B:626:VAL:C	1:B:628:PHE:N	2.75	0.43
1:D:446:THR:HB	1:D:628:PHE:CD2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:638:PHE:N	1:D:638:PHE:CD2	2.87	0.43
1:A:356:VAL:HG23	1:A:421:TRP:HA	2.01	0.43
1:B:345:ASP:OD2	1:B:434:LYS:HE3	2.19	0.43
1:D:515:LEU:HD12	1:D:632:ILE:HD12	2.01	0.43
1:D:624:SER:OG	1:D:626:VAL:HG22	2.19	0.43
1:C:378:LYS:HD3	1:C:379:TYR:CE2	2.53	0.42
1:D:458:VAL:C	1:D:460:MET:H	2.26	0.42
1:A:627:MET:HE3	1:A:628:PHE:CZ	2.54	0.42
1:B:484:SER:HA	1:B:485:PRO:HD3	1.78	0.42
1:C:444:ASN:C	1:C:511:ARG:HH11	2.27	0.42
1:C:458:VAL:HG13	1:C:460:MET:HE3	2.01	0.42
1:D:458:VAL:HG12	1:D:460:MET:HB2	2.00	0.42
1:A:380:TYR:N	1:A:381:PRO:HD3	2.34	0.42
1:B:618:CYS:HB2	1:B:636:PRO:O	2.18	0.42
1:C:458:VAL:HG13	1:C:460:MET:CE	2.48	0.42
1:C:586:LEU:HD23	1:C:586:LEU:HA	1.88	0.42
1:C:671:TYR:O	1:C:675:LYS:HG2	2.20	0.42
1:C:722:LEU:HD12	1:C:722:LEU:HA	1.70	0.42
1:D:633:LEU:HB3	1:D:635:ARG:HD3	2.01	0.42
1:B:662:LEU:H	1:B:662:LEU:CD2	2.32	0.42
1:A:591:LEU:HD23	1:A:591:LEU:HA	1.91	0.42
1:A:651:LEU:HG	1:A:653:GLY:H	1.84	0.42
1:D:562:LEU:H	1:D:562:LEU:HG	1.67	0.42
1:A:459:ARG:O	1:A:459:ARG:HG3	2.19	0.42
1:B:460:MET:HA	1:B:461:PRO:HD2	1.77	0.42
1:B:542:MET:HE1	1:B:612:LEU:CB	2.50	0.42
1:C:448:LEU:HD13	1:C:627:MET:HE1	2.01	0.42
1:D:480:ASP:O	1:D:503:ARG:HG2	2.20	0.42
1:B:648:ASP:O	1:B:649:LYS:HB2	2.20	0.42
1:C:569:LEU:HD23	1:C:569:LEU:HA	1.83	0.42
1:A:450:ARG:HG3	1:A:653:GLY:O	2.20	0.42
1:A:639:PHE:CZ	1:A:663:PRO:HD2	2.55	0.42
1:A:669:GLU:HA	1:A:670:PRO:HD3	1.89	0.42
1:C:467:LYS:HE3	1:C:470:ARG:NH2	2.33	0.42
1:D:356:VAL:HG22	1:D:418:ALA:CB	2.50	0.42
1:D:443:TRP:CG	1:D:444:ASN:H	2.38	0.42
1:A:353:LYS:HB2	1:A:383:TYR:CD2	2.55	0.41
1:A:375:TYR:CD2	1:A:375:TYR:C	2.98	0.41
1:B:325:HIS:CE1	1:B:340:LEU:HB2	2.55	0.41
1:B:458:VAL:C	1:B:460:MET:HE2	2.45	0.41
1:B:540:VAL:HG22	1:B:578:VAL:HG12	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:597:GLU:O	1:B:598:ASN:HB2	2.19	0.41
1:B:665:PRO:HB2	1:B:667:TYR:CE2	2.55	0.41
1:D:682:LYS:HE3	1:D:682:LYS:HB2	1.93	0.41
1:A:582:ARG:NH2	1:A:606:TYR:O	2.53	0.41
1:A:660:GLU:HB3	1:A:661:ASP:H	1.53	0.41
1:C:329:ILE:HG22	1:C:330:VAL:N	2.32	0.41
1:C:451:LEU:H	1:C:451:LEU:HD12	1.85	0.41
1:C:597:GLU:O	1:C:598:ASN:HB2	2.21	0.41
1:D:431:LEU:HD23	1:D:431:LEU:HA	1.88	0.41
1:D:501:GLU:HA	1:D:504:ILE:HD12	2.03	0.41
1:A:722:LEU:C	1:A:723:GLU:HG3	2.45	0.41
1:B:431:LEU:HD23	1:B:431:LEU:HA	1.68	0.41
1:C:353:LYS:CG	3:C:733:CL:CL	3.06	0.41
1:C:720:GLU:C	1:C:722:LEU:N	2.77	0.41
1:D:586:LEU:HA	1:D:586:LEU:HD23	1.65	0.41
1:A:352:PRO:HB2	1:A:722:LEU:HD11	2.02	0.41
1:A:353:LYS:HA	1:A:718:ILE:HD12	2.02	0.41
1:D:554:SER:C	1:D:556:GLY:H	2.28	0.41
1:A:325:HIS:HB2	1:A:339:SER:HB2	2.02	0.41
1:A:470:ARG:NH1	1:A:470:ARG:CG	2.79	0.41
1:B:410:GLU:OE1	1:B:410:GLU:N	2.47	0.41
1:C:427:THR:HA	1:C:428:PRO:HD3	1.91	0.41
1:D:677:LEU:HD12	1:D:677:LEU:HA	1.87	0.41
1:A:438:THR:HA	1:A:480:ASP:OD2	2.21	0.41
1:D:351:LYS:HA	1:D:352:PRO:HD3	1.87	0.41
1:B:338:ARG:HD2	1:B:430:TYR:CG	2.56	0.41
1:B:350:VAL:HA	1:B:417:GLU:O	2.20	0.41
1:B:351:LYS:HB3	3:B:732:CL:CL	2.57	0.41
1:C:554:SER:O	1:C:555:LYS:HB2	2.20	0.41
1:C:559:LEU:CD1	1:C:559:LEU:C	2.94	0.41
1:C:566:LEU:HD23	1:C:566:LEU:HA	1.86	0.41
1:D:434:LYS:C	1:D:436:ASN:N	2.78	0.41
1:D:444:ASN:C	1:D:511:ARG:HH12	2.29	0.41
1:A:434:LYS:C	1:A:436:ASN:H	2.29	0.41
1:A:543:TYR:CE2	1:A:545:PRO:HG3	2.55	0.41
1:C:484:SER:HA	1:C:485:PRO:HD3	1.86	0.41
1:D:458:VAL:HG12	1:D:458:VAL:O	2.21	0.41
1:A:669:GLU:HG2	1:A:671:TYR:H	1.86	0.40
1:B:446:THR:HA	1:B:447:PRO:HD3	1.90	0.40
1:A:452:ALA:CB	1:A:496:ALA:O	2.70	0.40
1:C:448:LEU:HD13	1:C:627:MET:CE	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:373:TYR:OH	1:D:398:PRO:O	2.37	0.40
1:D:453:ASN:HA	1:D:469:LYS:HD3	2.02	0.40
1:B:396:VAL:HA	3:B:736:CL:CL	2.59	0.40
1:B:443:TRP:CG	1:B:444:ASN:N	2.89	0.40
1:D:323:LEU:HA	1:D:323:LEU:HD12	1.75	0.40
1:C:317:ASN:O	1:C:321:LYS:HG3	2.21	0.40
1:D:484:SER:HA	1:D:485:PRO:HD3	1.84	0.40
1:D:541:ILE:HG12	1:D:618:CYS:SG	2.61	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	408/729 (56%)	384 (94%)	21 (5%)	3 (1%)	18	45
1	B	410/729 (56%)	378 (92%)	30 (7%)	2 (0%)	24	53
1	C	409/729 (56%)	370 (90%)	36 (9%)	3 (1%)	18	45
1	D	409/729 (56%)	376 (92%)	26 (6%)	7 (2%)	7	23
All	All	1636/2916 (56%)	1508 (92%)	113 (7%)	15 (1%)	14	38

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	647	TYR
1	D	561	GLU
1	A	535	PRO
1	B	345	ASP
1	B	649	LYS
1	D	649	LYS
1	C	521	ASP

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Mol	Chain	Res	Type
1	C	649	LYS
1	D	521	ASP
1	D	562	LEU
1	D	565	ASP
1	A	649	LYS
1	C	443	TRP
1	D	458	VAL
1	D	603	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	379/675 (56%)	342 (90%)	37 (10%)	7	24
1	B	380/675 (56%)	331 (87%)	49 (13%)	4	14
1	C	379/675 (56%)	338 (89%)	41 (11%)	6	20
1	D	380/675 (56%)	343 (90%)	37 (10%)	8	24
All	All	1518/2700 (56%)	1354 (89%)	164 (11%)	6	20

All (164) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	316	VAL
1	A	322	THR
1	A	323	LEU
1	A	329	ILE
1	A	333	ARG
1	A	356	VAL
1	A	402	GLU
1	A	403	LYS
1	A	433	LYS
1	A	448	LEU
1	A	451	LEU
1	A	456	LYS
1	A	460	MET

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Mol	Chain	Res	Type
1	A	487	ARG
1	A	488	TYR
1	A	511	ARG
1	A	514	VAL
1	A	555	LYS
1	A	559	LEU
1	A	578	VAL
1	A	589	ASN
1	A	594	SER
1	A	597	GLU
1	A	607	ASN
1	A	619	LEU
1	A	635	ARG
1	A	645	ASP
1	A	651	LEU
1	A	656	MET
1	A	659	MET
1	A	660	GLU
1	A	662	LEU
1	A	669	GLU
1	A	673	LEU
1	A	677	LEU
1	A	678	LYS
1	A	718	ILE
1	B	315	LYS
1	B	316	VAL
1	B	323	LEU
1	B	329	ILE
1	B	333	ARG
1	B	343	LEU
1	B	346	LYS
1	B	356	VAL
1	B	368	SER
1	B	402	GLU
1	B	403	LYS
1	B	407	ASN
1	B	423	SER
1	B	433	LYS
1	B	449	LYS
1	B	451	LEU
1	B	456	LYS
1	B	460	MET

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Mol	Chain	Res	Type
1	B	465	THR
1	B	470	ARG
1	B	487	ARG
1	B	491	GLU
1	B	514	VAL
1	B	548	ARG
1	B	555	LYS
1	B	559	LEU
1	B	579	ILE
1	B	594	SER
1	B	597	GLU
1	B	607	ASN
1	B	619	LEU
1	B	622	ASP
1	B	625	SER
1	B	635	ARG
1	B	651	LEU
1	B	656	MET
1	B	661	ASP
1	B	662	LEU
1	B	668	THR
1	B	669	GLU
1	B	673	LEU
1	B	677	LEU
1	B	680	LEU
1	B	699	CYS
1	B	702	ASP
1	B	718	ILE
1	B	720	GLU
1	B	721	GLN
1	B	722	LEU
1	C	315	LYS
1	C	322	THR
1	C	323	LEU
1	C	329	ILE
1	C	333	ARG
1	C	338	ARG
1	C	339	SER
1	C	356	VAL
1	C	403	LYS
1	C	433	LYS
1	C	451	LEU

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Mol	Chain	Res	Type
1	C	456	LYS
1	C	460	MET
1	C	463	THR
1	C	470	ARG
1	C	487	ARG
1	C	491	GLU
1	C	511	ARG
1	C	518	ARG
1	C	536	SER
1	C	559	LEU
1	C	562	LEU
1	C	567	ASP
1	C	589	ASN
1	C	597	GLU
1	C	619	LEU
1	C	635	ARG
1	C	651	LEU
1	C	656	MET
1	C	660	GLU
1	C	662	LEU
1	C	669	GLU
1	C	673	LEU
1	C	677	LEU
1	C	680	LEU
1	C	683	VAL
1	C	702	ASP
1	C	714	ILE
1	C	718	ILE
1	C	720	GLU
1	C	722	LEU
1	D	316	VAL
1	D	323	LEU
1	D	333	ARG
1	D	346	LYS
1	D	356	VAL
1	D	403	LYS
1	D	413	GLN
1	D	433	LYS
1	D	451	LEU
1	D	456	LYS
1	D	460	MET
1	D	470	ARG

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Mol	Chain	Res	Type
1	D	487	ARG
1	D	491	GLU
1	D	511	ARG
1	D	514	VAL
1	D	518	ARG
1	D	548	ARG
1	D	559	LEU
1	D	594	SER
1	D	597	GLU
1	D	607	ASN
1	D	619	LEU
1	D	622	ASP
1	D	635	ARG
1	D	645	ASP
1	D	651	LEU
1	D	656	MET
1	D	660	GLU
1	D	662	LEU
1	D	669	GLU
1	D	673	LEU
1	D	677	LEU
1	D	678	LYS
1	D	702	ASP
1	D	718	ILE
1	D	722	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	349	ASN
1	A	391	ASN
1	A	420	HIS
1	A	679	ASN
1	A	708	GLN
1	B	349	ASN
1	B	436	ASN
1	B	531	HIS
1	B	568	ASN
1	B	686	GLN
1	C	318	GLN
1	C	349	ASN
1	C	436	ASN

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Mol	Chain	Res	Type
1	C	531	HIS
1	C	684	GLN
1	C	688	GLN
1	D	349	ASN
1	D	413	GLN
1	D	531	HIS
1	D	686	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 40 ligands modelled in this entry, 32 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	C	730	-	4,4,4	0.24	0	6,6,6	0.24	0
2	SO4	C	731	-	4,4,4	0.22	0	6,6,6	0.13	0
2	SO4	C	732	-	4,4,4	0.23	0	6,6,6	0.13	0
2	SO4	D	730	-	4,4,4	0.24	0	6,6,6	0.09	0
2	SO4	B	730	-	4,4,4	0.20	0	6,6,6	0.15	0
2	SO4	A	731	-	4,4,4	0.20	0	6,6,6	0.33	0
2	SO4	A	730	-	4,4,4	0.27	0	6,6,6	0.20	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	SO4	A	732	-	4,4,4	0.26	0	6,6,6	0.05	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	730	SO4	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [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%)	-0.49	1 (0%) 91 89	50, 73, 143, 221	0
1	B	412/729 (56%)	-0.48	3 (0%) 84 78	51, 72, 158, 239	0
1	C	411/729 (56%)	-0.45	2 (0%) 87 82	56, 79, 158, 237	0
1	D	411/729 (56%)	-0.42	4 (0%) 79 72	57, 78, 159, 221	0
All	All	1644/2916 (56%)	-0.46	10 (0%) 85 80	50, 76, 154, 239	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	560	PHE	4.5
1	D	560	PHE	4.1
1	A	560	PHE	3.5
1	C	560	PHE	3.3
1	D	651	LEU	3.1
1	B	537	ASP	2.6
1	D	556	GLY	2.5
1	D	555	LYS	2.4
1	B	559	LEU	2.4
1	C	458	VAL	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 ⓘ

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	730	5/5	0.61	0.11	174,174,176,176	0
2	SO4	C	732	5/5	0.64	0.12	177,177,178,178	0
2	SO4	A	732	5/5	0.70	0.17	155,155,156,157	0
2	SO4	D	730	5/5	0.71	0.13	188,188,189,190	0
3	CL	D	735	1/1	0.80	0.10	103,103,103,103	0
3	CL	B	734	1/1	0.83	0.10	104,104,104,104	0
3	CL	B	733	1/1	0.85	0.09	111,111,111,111	0
3	CL	B	732	1/1	0.86	0.12	99,99,99,99	0
3	CL	A	733	1/1	0.87	0.17	97,97,97,97	0
3	CL	A	734	1/1	0.87	0.09	108,108,108,108	0
3	CL	D	736	1/1	0.87	0.08	93,93,93,93	0
2	SO4	C	731	5/5	0.88	0.07	118,119,121,121	0
3	CL	B	736	1/1	0.90	0.08	103,103,103,103	0
3	CL	C	733	1/1	0.90	0.06	105,105,105,105	0
3	CL	C	736	1/1	0.90	0.10	92,92,92,92	0
3	CL	C	738	1/1	0.90	0.16	87,87,87,87	0
3	CL	A	741	1/1	0.90	0.07	91,91,91,91	0
2	SO4	C	730	5/5	0.90	0.09	113,114,115,116	0
3	CL	D	731	1/1	0.91	0.08	90,90,90,90	0
3	CL	D	732	1/1	0.91	0.08	86,86,86,86	0
3	CL	C	737	1/1	0.92	0.06	92,92,92,92	0
3	CL	D	733	1/1	0.92	0.07	96,96,96,96	0
3	CL	D	734	1/1	0.92	0.09	93,93,93,93	0
3	CL	A	740	1/1	0.92	0.08	95,95,95,95	0
2	SO4	A	731	5/5	0.92	0.09	87,87,88,91	0
2	SO4	A	730	5/5	0.93	0.07	99,100,102,103	0
3	CL	A	737	1/1	0.93	0.11	93,93,93,93	0
3	CL	A	743	1/1	0.93	0.08	99,99,99,99	0
3	CL	C	739	1/1	0.93	0.09	99,99,99,99	0
3	CL	A	738	1/1	0.93	0.06	98,98,98,98	0
3	CL	B	735	1/1	0.94	0.09	103,103,103,103	0
3	CL	C	735	1/1	0.94	0.06	81,81,81,81	0
3	CL	A	735	1/1	0.94	0.15	98,98,98,98	0
3	CL	B	738	1/1	0.94	0.06	97,97,97,97	0
3	CL	A	742	1/1	0.95	0.07	95,95,95,95	0
3	CL	A	736	1/1	0.95	0.12	82,82,82,82	0
3	CL	C	734	1/1	0.96	0.04	93,93,93,93	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	CL	B	737	1/1	0.96	0.10	86,86,86,86	0
3	CL	A	739	1/1	0.98	0.10	68,68,68,68	0
3	CL	B	731	1/1	0.99	0.13	50,50,50,50	0

6.5 Other polymers [i](#)

There are no such residues in this entry.