



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:12 AM GMT

PDB ID : 3L7I  
Title : Structure of the Wall Teichoic Acid Polymerase TagF  
Authors : Strynadka, N.C.J.; Lovering, A.L.  
Deposited on : 2009-12-28  
Resolution : 2.70 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

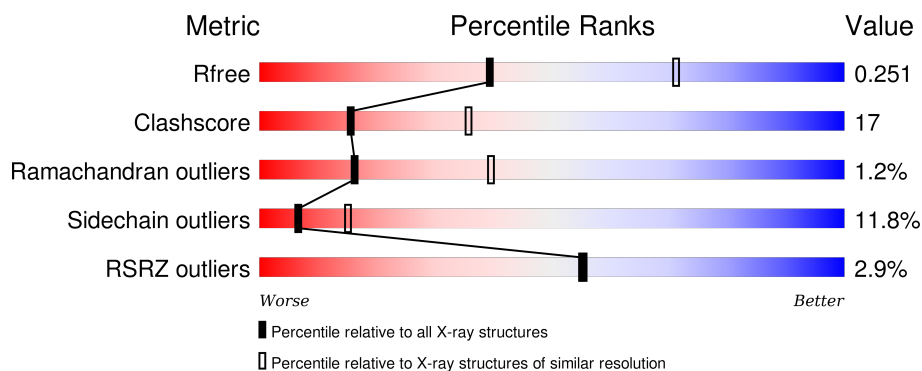
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)

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

Mol	Chain	Length	Quality of chain
1	A	729	 35% 18% • 44%
1	B	729	 2% 36% 17% • 44%
1	C	729	 2% 35% 17% • 44%
1	D	729	 35% 16% • 44%

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	CL	B	733	-	-	X	-
3	CL	B	737	-	-	X	-
3	CL	D	734	-	-	X	-
4	EDO	B	731	-	-	-	X
4	EDO	C	732	-	-	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 13962 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	411	Total	C	N	O	S	0	0	0
			3469	2229	579	650	11			
1	B	411	Total	C	N	O	S	0	0	0
			3469	2229	579	650	11			
1	C	411	Total	C	N	O	S	0	0	0
			3469	2229	579	650	11			
1	D	408	Total	C	N	O	S	0	0	0
			3451	2218	576	646	11			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
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	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	722	LEU	-	EXPRESSION TAG	UNP Q5HLM5
C	723	GLU	-	EXPRESSION TAG	UNP Q5HLM5
C	724	HIS	-	EXPRESSION TAG	UNP Q5HLM5
C	725	HIS	-	EXPRESSION TAG	UNP Q5HLM5
C	726	HIS	-	EXPRESSION TAG	UNP Q5HLM5

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Chain	Residue	Modelled	Actual	Comment	Reference
C	727	HIS	-	EXPRESSION TAG	UNP Q5HLM5
C	728	HIS	-	EXPRESSION TAG	UNP Q5HLM5
C	729	HIS	-	EXPRESSION TAG	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 (three-letter code: SO<sub>4</sub>) (formula: O<sub>4</sub>S).



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

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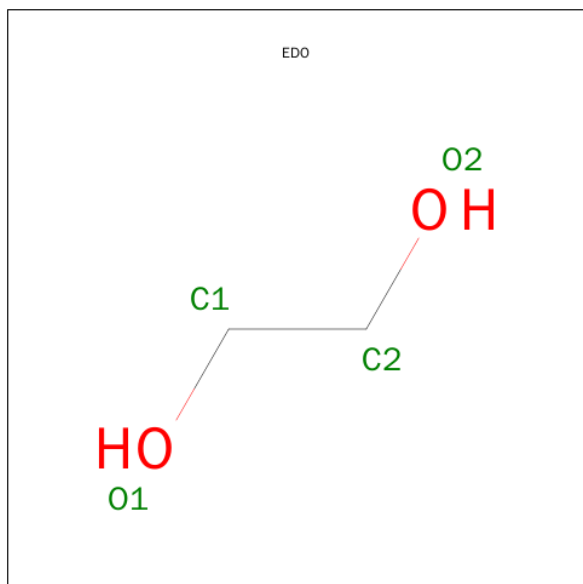
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	D	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	6	Total	Cl	0	0
			6	6		
3	A	12	Total	Cl	0	0
			12	12		
3	D	3	Total	Cl	0	0
			3	3		
3	C	5	Total	Cl	0	0
			5	5		

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



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

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

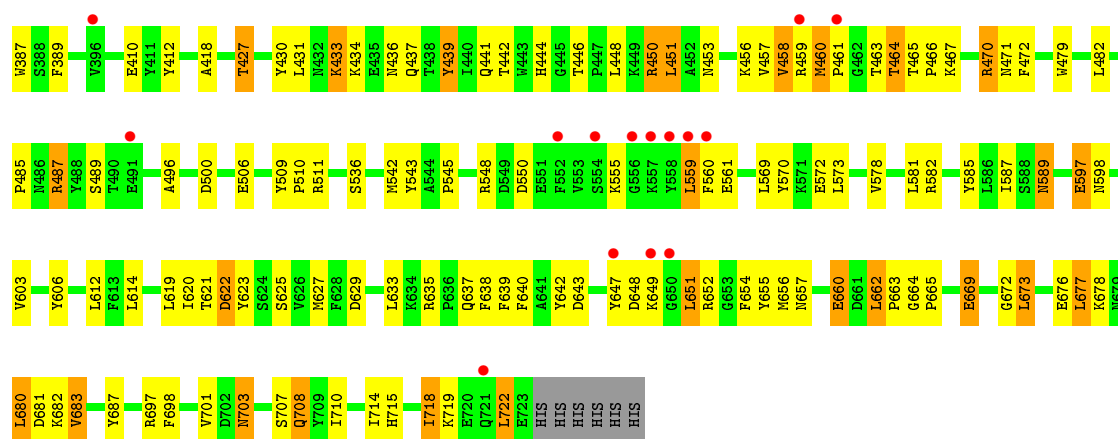
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	6	Total	O	0	0
			6	6		
5	B	4	Total	O	0	0
			4	4		
5	C	5	Total	O	0	0
			5	5		
5	D	3	Total	O	0	0
			3	3		

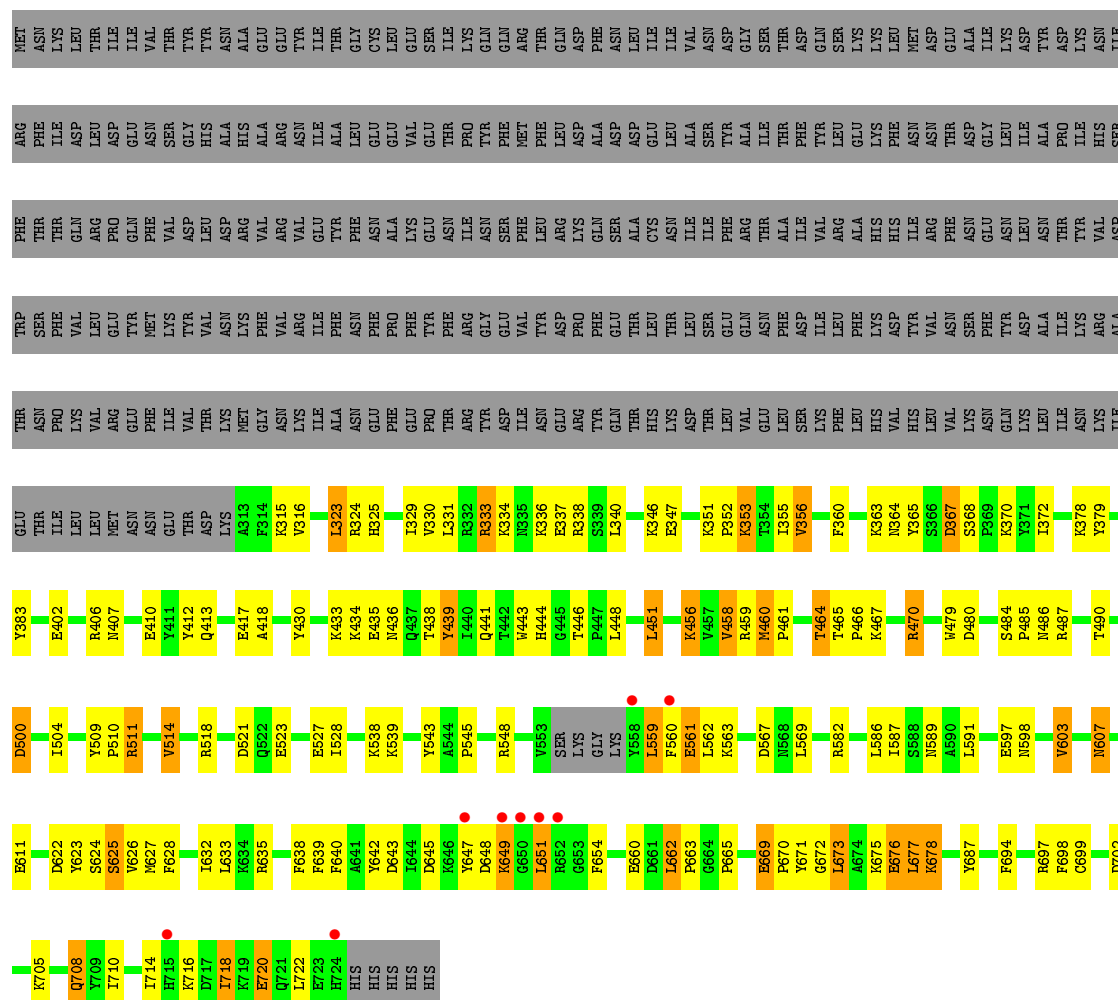
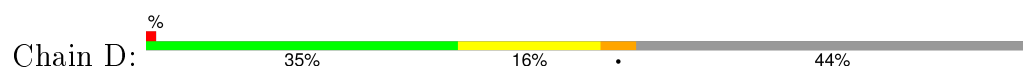








• Molecule 1: Teichoic acid biosynthesis protein F



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	223.74Å 223.74Å 100.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	74.84 – 2.70 74.84 – 2.70	Depositor EDS
% Data completeness (in resolution range)	98.0 (74.84-2.70) 98.0 (74.84-2.70)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.56 (at 2.69Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, $R_{free}$	0.210 , 0.260 0.196 , 0.251	Depositor DCC
$R_{free}$ test set	3483 reflections (5.05%)	DCC
Wilson B-factor (Å <sup>2</sup> )	67.5	Xtriage
Anisotropy	0.131	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 41.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 68992 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	13962	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.73% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CL, EDO, SO4

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	0.51	0/3559	0.65	0/4809
1	B	0.52	0/3559	0.66	2/4809 (0.0%)
1	C	0.48	0/3559	0.63	0/4809
1	D	0.48	0/3541	0.65	0/4786
All	All	0.50	0/14218	0.65	2/19213 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	662	LEU	CA-CB-CG	5.14	127.11	115.30
1	B	333	ARG	NE-CZ-NH1	5.12	122.86	120.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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	3469	0	3375	117	0
1	B	3469	0	3375	121	0
1	C	3469	0	3375	123	0
1	D	3451	0	3347	120	0
2	A	15	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	5	0	0	0	0
2	C	10	0	0	0	0
2	D	10	0	0	0	0
3	A	12	0	0	2	0
3	B	6	0	0	5	0
3	C	5	0	0	1	0
3	D	3	0	0	4	0
4	B	4	0	6	2	0
4	C	8	0	12	0	0
4	D	8	0	12	3	0
5	A	6	0	0	0	0
5	B	4	0	0	1	0
5	C	5	0	0	0	0
5	D	3	0	0	0	0
All	All	13962	0	13502	473	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 17.

All (473) 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:B:563:LYS:HD2	1:B:563:LYS:H	1.07	1.19
1:C:542:MET:HE1	1:C:612:LEU:HB3	1.29	1.14
1:D:383:TYR:CE2	1:D:718:ILE:HD11	1.92	1.04
1:B:470:ARG:HG2	1:B:470:ARG:HH11	1.20	1.02
1:D:333:ARG:HH11	1:D:333:ARG:HG2	1.25	0.97
1:A:648:ASP:HB2	1:A:651:LEU:HB2	1.42	0.97
1:B:382:ASN:N	1:B:382:ASN:HD22	1.62	0.92
1:B:346:LYS:HG3	1:B:349:ASN:ND2	1.85	0.91
1:A:333:ARG:HG2	1:A:333:ARG:HH11	1.32	0.90
1:C:648:ASP:HB2	1:C:651:LEU:HB3	1.54	0.89
1:D:353:LYS:HG3	3:D:734:CL:CL	2.09	0.89
1:B:563:LYS:HD2	1:B:563:LYS:N	1.88	0.88
1:C:383:TYR:CZ	1:C:718:ILE:HD11	2.09	0.88
1:C:383:TYR:CE2	1:C:718:ILE:HD11	2.10	0.86
1:B:346:LYS:HG3	1:B:349:ASN:HD21	1.41	0.81
1:B:470:ARG:NH1	1:B:470:ARG:HG2	1.96	0.80
1:A:353:LYS:HG2	3:A:733:CL:CL	2.19	0.79
1:B:382:ASN:HD22	1:B:382:ASN:H	1.26	0.79
1:B:548:ARG:HD3	1:B:643:ASP:OD2	1.82	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:722:LEU:O	1:B:723:GLU:HG3	1.83	0.79
1:C:470:ARG:HG2	1:C:470:ARG:HH11	1.48	0.79
1:D:665:PRO:HG3	1:D:687:TYR:CZ	2.18	0.78
1:A:722:LEU:O	1:A:723:GLU:HG3	1.84	0.77
1:B:333:ARG:HG2	1:B:333:ARG:HH11	1.50	0.77
1:A:338:ARG:HD2	1:A:430:TYR:CD1	2.19	0.77
1:B:467:LYS:HE3	1:B:470:ARG:NH2	1.99	0.77
1:C:367:ASP:HB2	1:C:511:ARG:HD3	1.66	0.75
1:D:333:ARG:CG	1:D:333:ARG:HH11	1.98	0.75
1:B:648:ASP:HB2	1:B:651:LEU:HB3	1.68	0.75
1:A:648:ASP:CB	1:A:651:LEU:HB2	2.16	0.74
1:C:427:THR:HG23	1:C:439:TYR:OH	1.88	0.74
1:A:467:LYS:HE3	1:A:470:ARG:HH22	1.53	0.73
1:C:543:TYR:CZ	1:C:545:PRO:HG3	2.23	0.73
1:B:382:ASN:ND2	1:B:382:ASN:N	2.36	0.73
1:B:470:ARG:CG	1:B:470:ARG:HH11	2.00	0.72
1:D:714:ILE:O	1:D:718:ILE:HG23	1.88	0.72
1:D:383:TYR:CZ	1:D:718:ILE:HD11	2.24	0.72
1:B:561:GLU:HB2	3:B:735:CL:CL	2.27	0.71
1:D:651:LEU:HD21	1:D:654:PHE:CD2	2.25	0.71
1:B:382:ASN:ND2	1:B:382:ASN:H	1.89	0.71
1:D:662:LEU:H	1:D:662:LEU:HD23	1.55	0.71
1:C:620:ILE:HD13	1:C:673:LEU:HD11	1.73	0.71
1:D:464:THR:OG1	1:D:466:PRO:HD2	1.91	0.70
1:A:542:MET:HE1	1:A:613:PHE:CD1	2.26	0.70
1:A:662:LEU:HD23	1:A:662:LEU:H	1.56	0.70
1:A:485:PRO:HG3	1:A:509:TYR:CE2	2.27	0.70
1:D:324:ARG:HH11	4:D:732:EDO:H12	1.56	0.69
1:C:648:ASP:HB2	1:C:651:LEU:CB	2.21	0.69
1:C:450:ARG:HA	1:C:655:TYR:CE2	2.27	0.69
1:A:333:ARG:CG	1:A:333:ARG:HH11	2.06	0.69
1:B:663:PRO:HG3	1:B:694:PHE:CD2	2.28	0.68
1:C:367:ASP:CG	1:C:368:SER:H	1.96	0.68
1:B:346:LYS:NZ	1:C:332:ARG:HH12	1.91	0.68
1:C:347:GLU:HG3	1:C:436:ASN:HB2	1.74	0.68
1:A:338:ARG:HD3	1:A:412:TYR:OH	1.93	0.68
1:D:624:SER:OG	1:D:626:VAL:HG22	1.93	0.68
1:D:333:ARG:HG2	1:D:333:ARG:NH1	2.03	0.68
1:D:338:ARG:HD2	1:D:430:TYR:CD1	2.29	0.68
1:A:703:ASN:HB3	1:A:705:LYS:HB2	1.75	0.68
1:D:548:ARG:NH2	1:D:622:ASP:OD1	2.20	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:451:LEU:HD12	1:D:451:LEU:N	2.09	0.68
1:A:662:LEU:HB2	1:A:663:PRO:CD	2.24	0.67
1:B:443:TRP:HB3	5:B:741:HOH:O	1.94	0.67
1:C:714:ILE:O	1:C:718:ILE:HG23	1.94	0.67
1:B:543:TYR:CZ	1:B:545:PRO:HG3	2.29	0.67
1:C:451:LEU:H	1:C:451:LEU:HD12	1.59	0.67
1:B:624:SER:OG	1:B:626:VAL:HG22	1.93	0.67
1:D:543:TYR:CZ	1:D:545:PRO:HG3	2.30	0.67
1:C:665:PRO:HG3	1:C:687:TYR:CZ	2.30	0.67
1:C:446:THR:O	1:C:625:SER:HB2	1.95	0.67
1:C:372:ILE:HD13	1:C:710:ILE:HG21	1.76	0.66
1:B:480:ASP:O	1:B:503:ARG:HG2	1.95	0.66
1:A:451:LEU:HD12	1:A:451:LEU:H	1.61	0.66
1:B:563:LYS:CD	1:B:563:LYS:H	1.93	0.66
1:A:662:LEU:HB2	1:A:663:PRO:HD3	1.76	0.66
1:B:383:TYR:CE2	1:B:718:ILE:HD11	2.31	0.66
1:B:338:ARG:HD2	1:B:430:TYR:CD1	2.31	0.66
1:B:648:ASP:HB2	1:B:651:LEU:CB	2.25	0.65
1:A:542:MET:HE1	1:A:613:PHE:CE1	2.32	0.65
1:C:665:PRO:HG3	1:C:687:TYR:CE1	2.32	0.65
1:C:464:THR:OG1	1:C:466:PRO:HD2	1.96	0.65
1:C:703:ASN:ND2	1:C:703:ASN:H	1.94	0.65
1:D:365:TYR:CZ	1:D:370:LYS:HG3	2.32	0.65
1:C:375:TYR:CE1	1:C:708:GLN:HB2	2.31	0.65
1:C:458:VAL:HG13	1:C:460:MET:HE2	1.80	0.64
1:B:513:ASP:HA	1:B:704:GLY:HA2	1.78	0.64
1:D:325:HIS:CE1	1:D:329:ILE:HD11	2.32	0.64
1:B:663:PRO:HG3	1:B:694:PHE:CG	2.32	0.64
1:B:333:ARG:HH11	1:B:333:ARG:CG	2.11	0.64
1:B:353:LYS:HG3	3:B:733:CL:CL	2.35	0.63
1:A:467:LYS:HE3	1:A:470:ARG:NH2	2.12	0.63
1:C:382:ASN:H	1:C:382:ASN:ND2	1.95	0.63
1:A:548:ARG:HD3	1:A:643:ASP:OD2	1.98	0.63
1:D:638:PHE:HE1	1:D:676:GLU:HG2	1.63	0.63
1:B:451:LEU:H	1:B:451:LEU:HD12	1.64	0.62
1:A:648:ASP:OD2	1:A:651:LEU:HD12	1.98	0.62
1:D:352:PRO:HD2	3:D:734:CL:CL	2.36	0.62
1:B:383:TYR:CE2	1:B:718:ILE:CD1	2.83	0.62
1:B:482:LEU:HD23	1:B:499:MET:HG3	1.81	0.62
1:A:641:ALA:HB1	1:A:644:ILE:HB	1.81	0.61
1:D:446:THR:O	1:D:625:SER:HB2	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:638:PHE:HE1	1:B:676:GLU:HG2	1.64	0.61
1:B:679:ASN:HD22	1:B:682:LYS:HE3	1.65	0.61
1:B:665:PRO:HG3	1:B:687:TYR:CZ	2.35	0.61
1:D:451:LEU:HD12	1:D:451:LEU:H	1.65	0.61
1:D:514:VAL:HG12	1:D:518:ARG:HG3	1.81	0.61
1:C:639:PHE:CE2	1:C:663:PRO:HD2	2.35	0.61
1:D:597:GLU:O	1:D:598:ASN:HB2	2.01	0.61
1:A:372:ILE:HD13	1:A:710:ILE:HG21	1.80	0.61
1:C:338:ARG:HD2	1:C:430:TYR:CD1	2.36	0.61
1:B:426:ARG:HD3	4:B:731:EDO:H22	1.81	0.60
1:C:444:HIS:C	1:C:511:ARG:HH11	2.05	0.60
1:D:607:ASN:H	1:D:607:ASN:ND2	1.99	0.60
1:D:372:ILE:HD13	1:D:710:ILE:HG21	1.83	0.60
1:D:338:ARG:HD3	1:D:412:TYR:OH	2.02	0.60
1:C:662:LEU:H	1:C:662:LEU:HD23	1.67	0.60
1:D:633:LEU:HB3	1:D:635:ARG:HD3	1.84	0.59
1:C:511:ARG:HH22	1:C:629:ASP:CG	2.06	0.59
1:A:669:GLU:HG2	1:A:671:TYR:H	1.67	0.59
1:C:633:LEU:HB3	1:C:635:ARG:HD3	1.84	0.59
1:C:458:VAL:HG13	1:C:460:MET:SD	2.43	0.59
1:D:347:GLU:HG3	1:D:436:ASN:HB2	1.85	0.59
1:D:458:VAL:HG12	1:D:460:MET:HB2	1.84	0.58
1:A:480:ASP:O	1:A:503:ARG:HG2	2.03	0.58
1:D:413:GLN:O	1:D:417:GLU:HG3	2.03	0.58
1:B:475:GLU:OE1	1:B:478:ARG:NH1	2.36	0.58
1:A:325:HIS:CE1	1:A:329:ILE:CD1	2.86	0.58
1:A:651:LEU:HD21	1:A:654:PHE:CD1	2.39	0.58
1:D:582:ARG:HD3	3:D:736:CL:CL	2.40	0.58
1:B:315:LYS:HB2	1:D:315:LYS:HD3	1.86	0.58
1:C:458:VAL:HG13	1:C:460:MET:CE	2.33	0.58
1:A:665:PRO:HG3	1:A:687:TYR:CZ	2.39	0.58
1:B:675:LYS:O	1:B:678:LYS:HB2	2.04	0.58
1:D:662:LEU:H	1:D:662:LEU:CD2	2.16	0.58
1:D:438:THR:HA	1:D:480:ASP:OD2	2.04	0.57
1:D:670:PRO:HD2	1:D:671:TYR:CD2	2.40	0.57
1:B:346:LYS:HZ1	1:C:332:ARG:HH12	1.52	0.57
1:C:410:GLU:H	1:C:410:GLU:CD	2.08	0.57
1:C:459:ARG:O	1:C:459:ARG:HG3	2.04	0.57
1:D:465:THR:HB	1:D:466:PRO:HD3	1.87	0.56
1:D:325:HIS:CE1	1:D:329:ILE:CD1	2.88	0.56
1:A:451:LEU:HD12	1:A:451:LEU:N	2.19	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:607:ASN:N	1:B:607:ASN:OD1	2.34	0.56
1:B:662:LEU:H	1:B:662:LEU:HD23	1.71	0.56
1:B:620:ILE:HD11	1:B:677:LEU:HD21	1.87	0.56
1:C:347:GLU:CG	1:C:436:ASN:HB2	2.35	0.56
1:D:355:ILE:HD13	1:D:714:ILE:HG21	1.87	0.56
1:C:458:VAL:O	1:C:458:VAL:HG12	2.05	0.56
1:B:347:GLU:O	1:B:436:ASN:ND2	2.39	0.56
1:D:434:LYS:C	1:D:436:ASN:H	2.09	0.56
1:A:420:HIS:CD2	1:A:438:THR:HB	2.40	0.56
1:A:624:SER:O	1:A:627:MET:HG2	2.05	0.56
1:C:338:ARG:HD3	1:C:412:TYR:OH	2.07	0.55
1:B:583:MET:HE2	1:B:587:ILE:HG21	1.88	0.55
1:A:569:LEU:HD22	1:A:573:LEU:HD12	1.89	0.55
1:D:640:PHE:CE2	1:D:642:TYR:HB3	2.41	0.55
1:A:323:LEU:HD23	1:B:327:LYS:HB2	1.87	0.55
1:C:585:TYR:O	1:C:589:ASN:OD1	2.25	0.55
1:A:352:PRO:O	1:A:718:ILE:HG21	2.06	0.55
1:A:485:PRO:HG3	1:A:509:TYR:CZ	2.41	0.55
1:B:559:LEU:HD13	1:B:559:LEU:O	2.06	0.55
1:D:324:ARG:NH1	4:D:732:EDO:H12	2.21	0.54
1:C:347:GLU:O	1:C:436:ASN:ND2	2.41	0.54
1:B:349:ASN:N	1:B:349:ASN:HD22	2.04	0.54
1:C:353:LYS:HG3	3:C:734:CL:CL	2.45	0.54
1:B:679:ASN:ND2	1:B:682:LYS:HB2	2.22	0.54
1:B:434:LYS:C	1:B:436:ASN:H	2.10	0.54
1:B:442:THR:HA	1:B:483:ILE:HG13	1.90	0.54
1:C:652:ARG:C	1:C:654:PHE:H	2.09	0.54
1:C:485:PRO:HD2	1:C:489:SER:HB2	1.88	0.54
1:D:485:PRO:HG3	1:D:509:TYR:CE2	2.43	0.54
1:C:470:ARG:HG2	1:C:470:ARG:NH1	2.15	0.54
1:A:313:ALA:HB2	3:A:743:CL:CL	2.45	0.54
1:B:338:ARG:HD3	1:B:412:TYR:OH	2.08	0.53
1:D:324:ARG:HD3	4:D:732:EDO:O1	2.09	0.53
1:A:569:LEU:CD2	1:A:573:LEU:HD12	2.38	0.53
1:D:490:THR:HG23	1:D:504:ILE:HD13	1.90	0.53
1:D:563:LYS:HD2	1:D:563:LYS:N	2.22	0.53
1:C:465:THR:HB	1:C:466:PRO:HD3	1.90	0.53
1:A:427:THR:HG23	1:A:439:TYR:OH	2.08	0.53
1:A:405:LYS:O	1:A:411:TYR:HB2	2.08	0.53
1:B:595:GLY:N	1:B:597:GLU:OE2	2.38	0.53
1:D:446:THR:HB	1:D:628:PHE:CD2	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:485:PRO:HG3	1:C:509:TYR:CE2	2.44	0.53
1:A:585:TYR:O	1:A:589:ASN:OD1	2.27	0.53
1:D:662:LEU:CD2	1:D:662:LEU:N	2.71	0.52
1:D:663:PRO:HG3	1:D:694:PHE:CG	2.44	0.52
1:A:458:VAL:HA	1:A:460:MET:HE2	1.90	0.52
1:B:652:ARG:C	1:B:654:PHE:H	2.11	0.52
1:C:572:GLU:O	1:C:678:LYS:HE3	2.10	0.52
1:B:673:LEU:HD22	1:B:677:LEU:HD22	1.91	0.52
1:B:347:GLU:HG3	1:B:436:ASN:HB2	1.91	0.52
1:A:350:VAL:CG2	1:A:436:ASN:HD22	2.23	0.52
1:D:378:LYS:HD3	1:D:379:TYR:CE2	2.45	0.52
1:A:597:GLU:O	1:A:598:ASN:HB2	2.09	0.52
1:C:548:ARG:HD3	1:C:643:ASP:OD2	2.09	0.52
1:C:467:LYS:CE	1:C:470:ARG:HH22	2.23	0.52
1:D:697:ARG:HD3	1:D:698:PHE:CE2	2.45	0.52
1:A:662:LEU:HD23	1:A:662:LEU:N	2.22	0.52
1:C:662:LEU:H	1:C:662:LEU:CD2	2.23	0.52
1:B:325:HIS:CE1	1:B:329:ILE:HD13	2.44	0.52
1:D:651:LEU:HD21	1:D:654:PHE:CE2	2.45	0.52
1:D:356:VAL:HG22	1:D:418:ALA:CB	2.40	0.52
1:A:351:LYS:HD2	1:A:417:GLU:OE1	2.10	0.52
1:C:597:GLU:O	1:C:598:ASN:HB2	2.10	0.52
1:C:322:THR:O	1:C:326:VAL:HG23	2.11	0.51
1:C:673:LEU:HD22	1:C:677:LEU:HD22	1.91	0.51
1:B:662:LEU:H	1:B:662:LEU:CD2	2.23	0.51
1:D:470:ARG:HG2	1:D:470:ARG:HH11	1.74	0.51
1:A:514:VAL:HG12	1:A:518:ARG:HG3	1.92	0.51
1:D:669:GLU:OE2	1:D:672:GLY:N	2.43	0.51
1:D:439:TYR:N	1:D:480:ASP:OD2	2.33	0.51
1:A:481:TYR:CE2	1:A:713:LEU:HD21	2.45	0.51
1:B:380:TYR:HA	1:B:382:ASN:HD21	1.76	0.51
1:B:378:LYS:HB3	1:B:379:TYR:CD2	2.46	0.51
1:D:603:VAL:HG13	1:D:603:VAL:O	2.09	0.51
1:D:639:PHE:CZ	1:D:663:PRO:HD2	2.46	0.51
1:B:572:GLU:OE1	1:B:678:LYS:HE3	2.11	0.51
1:C:559:LEU:HD23	1:C:587:ILE:HG23	1.92	0.51
1:C:444:HIS:O	1:C:511:ARG:NH1	2.43	0.51
1:D:697:ARG:HD3	1:D:698:PHE:CZ	2.46	0.51
1:A:451:LEU:HA	1:A:455:MET:HE3	1.93	0.51
1:D:325:HIS:CE1	1:D:340:LEU:HB2	2.46	0.51
1:D:648:ASP:O	1:D:649:LYS:HB2	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:637:GLN:O	1:C:664:GLY:HA3	2.10	0.51
1:B:380:TYR:N	1:B:381:PRO:HD3	2.26	0.50
1:D:662:LEU:HB2	1:D:663:PRO:CD	2.41	0.50
1:D:368:SER:O	1:D:372:ILE:HG13	2.11	0.50
1:C:451:LEU:HD12	1:C:451:LEU:N	2.26	0.50
1:B:450:ARG:HA	1:B:655:TYR:CE2	2.47	0.50
1:A:470:ARG:HH11	1:A:470:ARG:HG2	1.77	0.50
1:C:662:LEU:HB2	1:C:663:PRO:HD3	1.94	0.50
1:C:657:ASN:ND2	1:C:660:GLU:OE1	2.44	0.50
1:A:652:ARG:C	1:A:654:PHE:H	2.14	0.50
1:B:646:LYS:O	1:B:648:ASP:N	2.41	0.50
1:A:458:VAL:HG13	1:A:460:MET:CE	2.42	0.50
1:A:662:LEU:N	1:A:662:LEU:CD2	2.75	0.50
1:B:345:ASP:OD1	1:B:434:LYS:HE2	2.12	0.50
1:B:456:LYS:HA	1:B:456:LYS:HE2	1.93	0.50
1:A:344:THR:O	1:A:346:LYS:HG3	2.12	0.49
1:B:542:MET:HE1	1:B:613:PHE:HD1	1.77	0.49
1:D:470:ARG:HG2	1:D:470:ARG:NH1	2.27	0.49
1:D:548:ARG:HD3	1:D:643:ASP:OD2	2.13	0.49
1:A:670:PRO:HG2	1:A:671:TYR:CE2	2.48	0.49
1:C:356:VAL:HG23	1:C:418:ALA:HB2	1.93	0.49
1:B:669:GLU:OE2	1:B:672:GLY:N	2.36	0.49
1:D:329:ILE:HD12	1:D:336:LYS:HB2	1.95	0.49
1:C:639:PHE:CZ	1:C:663:PRO:HD2	2.47	0.49
1:B:434:LYS:C	1:B:436:ASN:N	2.65	0.49
1:B:378:LYS:HD3	1:B:379:TYR:CE2	2.47	0.49
1:B:350:VAL:HB	1:B:436:ASN:ND2	2.28	0.49
1:B:333:ARG:NH1	1:B:333:ARG:HG2	2.22	0.48
1:C:543:TYR:CE2	1:C:545:PRO:HG3	2.48	0.48
1:A:509:TYR:HB3	1:A:511:ARG:HG3	1.95	0.48
1:B:457:VAL:HG11	1:B:459:ARG:NH2	2.28	0.48
1:C:662:LEU:CD2	1:C:662:LEU:N	2.76	0.48
1:B:542:MET:HE1	1:B:613:PHE:CD1	2.49	0.48
1:A:510:PRO:HA	1:A:706:ALA:HB3	1.94	0.48
1:C:487:ARG:HA	1:C:506:GLU:OE2	2.13	0.48
1:C:464:THR:HG23	1:C:467:LYS:CB	2.43	0.48
1:D:675:LYS:O	1:D:678:LYS:HB2	2.14	0.48
1:C:703:ASN:HD22	1:C:703:ASN:H	1.60	0.48
1:D:444:HIS:C	1:D:511:ARG:NH1	2.67	0.48
1:A:554:SER:O	1:A:555:LYS:HB2	2.13	0.48
1:A:572:GLU:O	1:A:678:LYS:HE3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:456:LYS:HE2	1:D:456:LYS:HA	1.95	0.48
1:C:510:PRO:HB3	1:C:707:SER:OG	2.14	0.48
1:D:441:GLN:HG2	1:D:479:TRP:CE2	2.49	0.48
1:A:697:ARG:HD3	1:A:698:PHE:CZ	2.49	0.48
1:B:511:ARG:HH22	1:B:629:ASP:CG	2.17	0.48
1:C:697:ARG:HD3	1:C:698:PHE:CE2	2.49	0.48
1:A:456:LYS:HA	1:A:456:LYS:HE2	1.95	0.48
1:B:540:VAL:HG22	1:B:578:VAL:HG12	1.96	0.47
1:A:679:ASN:ND2	1:A:682:LYS:HE3	2.29	0.47
1:C:621:THR:HG23	1:C:622:ASP:N	2.29	0.47
1:D:485:PRO:HG3	1:D:509:TYR:CZ	2.49	0.47
1:A:352:PRO:HA	1:A:419:SER:HB3	1.96	0.47
1:D:559:LEU:HD13	1:D:560:PHE:O	2.15	0.47
1:A:543:TYR:CZ	1:A:545:PRO:HG3	2.49	0.47
1:C:367:ASP:CG	1:C:368:SER:N	2.61	0.47
1:B:383:TYR:CE2	1:B:718:ILE:HD13	2.50	0.47
1:B:347:GLU:CG	1:B:436:ASN:HB2	2.44	0.47
1:B:716:LYS:O	1:B:720:GLU:HG2	2.15	0.47
1:D:459:ARG:HG3	1:D:459:ARG:O	2.15	0.47
1:A:638:PHE:HE1	1:A:676:GLU:HG2	1.78	0.47
1:C:347:GLU:HA	1:C:434:LYS:HD3	1.95	0.47
1:D:451:LEU:CD1	1:D:451:LEU:N	2.76	0.47
1:A:333:ARG:NH1	1:A:333:ARG:HG2	2.12	0.47
1:B:427:THR:HG1	1:B:439:TYR:HH	1.63	0.47
1:A:387:TRP:HB3	1:A:389:PHE:CE2	2.50	0.47
1:C:441:GLN:O	1:C:482:LEU:HA	2.15	0.47
1:C:470:ARG:NH1	1:C:471:ASN:OD1	2.49	0.46
1:C:442:THR:O	1:C:509:TYR:HE1	1.98	0.46
1:B:446:THR:O	1:B:625:SER:HB2	2.14	0.46
1:A:490:THR:HG23	1:A:504:ILE:HD13	1.97	0.46
1:D:353:LYS:CG	3:D:734:CL:CL	2.91	0.46
1:A:662:LEU:H	1:A:662:LEU:CD2	2.27	0.46
1:C:662:LEU:HB2	1:C:663:PRO:CD	2.45	0.46
1:C:680:LEU:HD23	1:C:680:LEU:HA	1.69	0.46
1:B:351:LYS:HB3	3:B:733:CL:CL	2.52	0.46
1:C:382:ASN:N	1:C:382:ASN:ND2	2.62	0.46
1:B:403:LYS:HE3	3:B:737:CL:CL	2.52	0.46
1:C:597:GLU:H	1:C:597:GLU:HG2	1.15	0.46
1:D:559:LEU:O	1:D:559:LEU:HD12	2.15	0.46
1:D:560:PHE:O	1:D:561:GLU:C	2.54	0.46
1:B:384:ARG:NH2	1:B:417:GLU:OE1	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:485:PRO:HB2	1:D:486:ASN:ND2	2.31	0.46
1:C:582:ARG:NH2	1:C:606:TYR:O	2.48	0.46
1:C:433:LYS:HD2	1:C:439:TYR:HB2	1.98	0.46
1:A:561:GLU:H	1:A:561:GLU:HG2	1.55	0.46
1:B:387:TRP:HB3	1:B:389:PHE:CE2	2.50	0.46
1:A:470:ARG:HD2	1:A:474:ARG:HH21	1.81	0.45
1:D:591:LEU:HA	1:D:591:LEU:HD23	1.77	0.45
1:B:458:VAL:HG12	1:B:460:MET:HB2	1.97	0.45
1:C:638:PHE:HE1	1:C:676:GLU:HG2	1.81	0.45
1:D:673:LEU:HD22	1:D:677:LEU:HD22	1.98	0.45
1:D:360:PHE:HB2	1:D:363:LYS:HG2	1.97	0.45
1:A:345:ASP:OD2	1:A:434:LYS:HE3	2.16	0.45
1:C:316:VAL:HG13	1:C:317:ASN:N	2.30	0.45
1:D:458:VAL:O	1:D:458:VAL:HG12	2.16	0.45
1:D:490:THR:HG23	1:D:504:ILE:HG21	1.99	0.45
1:A:651:LEU:HD23	1:A:651:LEU:O	2.16	0.45
1:D:367:ASP:HB2	1:D:511:ARG:CB	2.46	0.45
1:A:458:VAL:CA	1:A:460:MET:HE2	2.47	0.45
1:C:378:LYS:HB3	1:C:379:TYR:CD2	2.52	0.45
1:C:434:LYS:C	1:C:436:ASN:H	2.18	0.45
1:A:350:VAL:CG2	1:A:436:ASN:ND2	2.80	0.45
1:C:350:VAL:HG21	1:C:436:ASN:ND2	2.31	0.45
1:D:632:ILE:HG12	1:D:699:CYS:HB3	1.98	0.45
1:C:581:LEU:O	1:C:603:VAL:HG12	2.17	0.45
1:D:368:SER:OG	1:D:510:PRO:HD2	2.16	0.45
1:A:350:VAL:HG21	1:A:436:ASN:HD22	1.82	0.45
1:C:418:ALA:O	1:C:437:GLN:HG2	2.17	0.45
1:A:633:LEU:HB3	1:A:635:ARG:HD3	1.98	0.45
1:D:718:ILE:HG13	1:D:718:ILE:O	2.15	0.45
1:C:648:ASP:O	1:C:649:LYS:HB2	2.17	0.45
1:C:652:ARG:C	1:C:654:PHE:N	2.70	0.45
1:D:648:ASP:HB2	1:D:651:LEU:HB2	1.98	0.45
1:B:543:TYR:CE2	1:B:545:PRO:HG3	2.52	0.45
1:A:714:ILE:O	1:A:718:ILE:HG12	2.16	0.44
1:C:559:LEU:HD12	1:C:559:LEU:O	2.17	0.44
1:B:680:LEU:HD23	1:B:680:LEU:HA	1.78	0.44
1:C:441:GLN:HG2	1:C:479:TRP:CE2	2.52	0.44
1:B:458:VAL:C	1:B:460:MET:H	2.20	0.44
1:B:456:LYS:HA	1:B:456:LYS:CE	2.48	0.44
1:B:559:LEU:C	1:B:559:LEU:HD13	2.37	0.44
1:C:638:PHE:CZ	1:C:683:VAL:HG11	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:665:PRO:HG3	1:D:687:TYR:OH	2.17	0.44
1:B:403:LYS:CE	3:B:737:CL:CL	3.03	0.44
1:A:406:ARG:O	1:A:407:ASN:HB2	2.16	0.44
1:A:341:TYR:CD1	1:A:412:TYR:HB3	2.52	0.44
1:B:443:TRP:HH2	4:B:731:EDO:H11	1.82	0.44
1:C:316:VAL:HG23	1:D:331:LEU:HD22	2.00	0.44
1:D:500:ASP:OD1	1:D:500:ASP:N	2.50	0.44
1:C:353:LYS:HB3	1:C:383:TYR:CD2	2.53	0.44
1:D:367:ASP:HB2	1:D:511:ARG:HD3	1.99	0.44
1:B:648:ASP:O	1:B:649:LYS:HB2	2.16	0.43
1:A:470:ARG:NH1	1:A:470:ARG:HG2	2.33	0.43
1:B:353:LYS:HA	1:B:718:ILE:HD12	2.00	0.43
1:D:347:GLU:O	1:D:436:ASN:ND2	2.51	0.43
1:D:523:GLU:O	1:D:527:GLU:HG3	2.18	0.43
1:D:410:GLU:N	1:D:410:GLU:OE1	2.42	0.43
1:A:457:VAL:HG22	1:A:458:VAL:N	2.33	0.43
1:A:350:VAL:HG21	1:A:436:ASN:ND2	2.33	0.43
1:A:350:VAL:HB	1:A:436:ASN:ND2	2.33	0.43
1:B:446:THR:HA	1:B:447:PRO:HD3	1.87	0.43
1:A:484:SER:HA	1:A:485:PRO:HD3	1.71	0.43
1:A:680:LEU:HD23	1:A:680:LEU:HA	1.80	0.43
1:C:387:TRP:HB3	1:C:389:PHE:CE2	2.53	0.43
1:B:418:ALA:O	1:B:437:GLN:HG2	2.18	0.43
2:A:731:SO4:O1	1:B:320:ARG:NH1	2.44	0.43
1:C:550:ASP:C	1:C:550:ASP:OD1	2.56	0.43
1:A:333:ARG:NH1	1:A:333:ARG:CG	2.75	0.43
1:B:338:ARG:HD2	1:B:430:TYR:CG	2.54	0.43
1:B:372:ILE:HD13	1:B:710:ILE:HG21	2.00	0.43
1:C:718:ILE:O	1:C:722:LEU:HD22	2.17	0.43
1:B:380:TYR:C	1:B:382:ASN:ND2	2.72	0.43
1:A:448:LEU:HD13	1:A:627:MET:HE1	2.00	0.43
1:A:624:SER:OG	1:A:626:VAL:HG22	2.18	0.43
1:B:559:LEU:CD1	1:B:559:LEU:O	2.66	0.43
1:D:562:LEU:HD11	1:D:591:LEU:HD11	1.99	0.43
1:A:619:LEU:HB2	1:A:630:TYR:CD2	2.53	0.43
1:C:448:LEU:HD13	1:C:627:MET:CE	2.48	0.43
1:D:434:LYS:C	1:D:436:ASN:N	2.70	0.43
1:D:363:LYS:HE2	1:D:364:ASN:OD1	2.19	0.43
1:B:484:SER:HA	1:B:485:PRO:HD3	1.68	0.43
1:C:715:HIS:NE2	1:C:719:LYS:HE3	2.34	0.43
1:D:539:LYS:HB2	1:D:539:LYS:HE3	1.85	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:327:LYS:O	1:C:331:LEU:HB2	2.19	0.43
1:D:528:ILE:HD13	1:D:611:GLU:HB3	1.99	0.43
1:C:569:LEU:HD22	1:C:573:LEU:HD12	1.99	0.43
1:D:383:TYR:CZ	1:D:718:ILE:CD1	2.99	0.42
1:D:662:LEU:HB2	1:D:663:PRO:HD3	2.01	0.42
1:C:323:LEU:HD12	1:C:323:LEU:HA	1.68	0.42
1:A:458:VAL:HG13	1:A:460:MET:HE2	2.00	0.42
1:C:460:MET:HA	1:C:461:PRO:HD2	1.79	0.42
1:D:464:THR:HG23	1:D:467:LYS:HB3	2.01	0.42
1:A:329:ILE:HG22	1:A:330:VAL:N	2.34	0.42
1:D:560:PHE:O	1:D:561:GLU:O	2.38	0.42
1:C:453:ASN:HB3	1:C:496:ALA:HA	2.01	0.42
1:A:670:PRO:HG2	1:A:671:TYR:CD2	2.54	0.42
1:A:352:PRO:O	1:A:718:ILE:CG2	2.67	0.42
1:A:347:GLU:HG3	1:A:436:ASN:HB2	2.01	0.42
1:A:682:LYS:HB2	1:A:682:LYS:HE3	1.74	0.42
1:C:344:THR:O	1:C:346:LYS:HG3	2.19	0.42
1:A:314:PHE:HB2	1:C:314:PHE:CZ	2.55	0.42
1:C:364:ASN:HD22	1:C:366:SER:HB3	1.85	0.42
1:A:331:LEU:O	1:A:332:ARG:HB2	2.19	0.42
1:B:651:LEU:O	1:B:651:LEU:HG	2.20	0.42
1:C:614:LEU:HA	1:C:614:LEU:HD23	1.88	0.42
1:C:431:LEU:HA	1:C:431:LEU:HD23	1.65	0.42
1:A:460:MET:HA	1:A:461:PRO:HD2	1.80	0.42
1:A:619:LEU:HB2	1:A:630:TYR:CE2	2.54	0.42
1:B:367:ASP:O	1:B:370:LYS:HB3	2.20	0.42
1:B:531:HIS:CD2	1:B:531:HIS:O	2.73	0.42
1:D:355:ILE:CD1	1:D:714:ILE:HG21	2.50	0.41
1:A:703:ASN:HB3	1:A:705:LYS:H	1.85	0.41
1:C:640:PHE:CE2	1:C:642:TYR:HB3	2.55	0.41
1:B:662:LEU:N	1:B:662:LEU:CD2	2.84	0.41
1:D:367:ASP:O	1:D:370:LYS:HB3	2.21	0.41
1:C:697:ARG:HD3	1:C:698:PHE:CZ	2.54	0.41
1:C:380:TYR:CE1	1:C:715:HIS:CE1	3.09	0.41
1:C:701:VAL:O	1:C:701:VAL:HG12	2.20	0.41
1:B:697:ARG:HD3	1:B:698:PHE:CE2	2.55	0.41
1:B:532:LEU:HD21	1:B:606:TYR:CE2	2.56	0.41
1:A:446:THR:HB	1:A:628:PHE:CD2	2.55	0.41
1:C:367:ASP:O	1:C:370:LYS:HB3	2.20	0.41
1:C:350:VAL:CG2	1:C:436:ASN:ND2	2.84	0.41
1:A:434:LYS:HG3	1:A:437:GLN:OE1	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:515:LEU:HA	1:B:614:LEU:HD21	2.02	0.41
1:A:708:GLN:HE21	1:A:708:GLN:HB2	1.61	0.41
1:D:586:LEU:HA	1:D:586:LEU:HD23	1.45	0.41
1:B:346:LYS:HZ3	1:C:332:ARG:HH12	1.67	0.41
1:A:509:TYR:HB3	1:A:511:ARG:CG	2.51	0.41
1:A:378:LYS:HD3	1:A:379:TYR:CE2	2.55	0.41
1:D:705:LYS:O	1:D:708:GLN:HG2	2.21	0.41
1:A:578:VAL:HG22	1:A:599:PHE:O	2.20	0.41
1:A:470:ARG:NH1	1:A:474:ARG:NH2	2.69	0.41
1:D:716:LYS:O	1:D:720:GLU:HG2	2.20	0.41
1:B:579:ILE:O	1:B:579:ILE:HG23	2.21	0.41
1:A:651:LEU:HG	1:A:653:GLY:H	1.86	0.41
1:A:485:PRO:HB2	1:A:486:ASN:ND2	2.35	0.41
1:A:458:VAL:HG12	1:A:458:VAL:O	2.21	0.41
1:B:697:ARG:HD3	1:B:698:PHE:CZ	2.55	0.41
1:C:485:PRO:HG3	1:C:509:TYR:CZ	2.55	0.41
1:B:406:ARG:O	1:B:407:ASN:HB2	2.21	0.41
1:A:534:LEU:HA	1:A:535:PRO:HD2	1.97	0.41
1:C:464:THR:HG23	1:C:467:LYS:HB3	2.03	0.40
1:D:467:LYS:CE	1:D:470:ARG:HH22	2.34	0.40
1:D:484:SER:HA	1:D:485:PRO:HD3	1.77	0.40
1:C:364:ASN:HD22	1:C:366:SER:CB	2.35	0.40
1:C:560:PHE:O	1:C:561:GLU:C	2.59	0.40
1:D:347:GLU:CG	1:D:436:ASN:HB2	2.50	0.40
1:A:501:GLU:HA	1:A:504:ILE:HD12	2.02	0.40
1:C:316:VAL:CG1	1:C:317:ASN:N	2.83	0.40
1:A:314:PHE:CE2	1:D:330:VAL:O	2.74	0.40
1:D:406:ARG:O	1:D:407:ASN:HB2	2.21	0.40
1:B:465:THR:N	1:B:466:PRO:CD	2.84	0.40
1:C:669:GLU:OE2	1:C:672:GLY:N	2.54	0.40
1:A:722:LEU:HA	1:A:722:LEU:HD12	1.76	0.40
1:D:444:HIS:O	1:D:511:ARG:NH1	2.55	0.40
1:A:634:LYS:HE2	1:A:695:TYR:CE1	2.56	0.40
1:B:358:GLU:O	1:B:423:SER:HB2	2.20	0.40
1:D:351:LYS:HE3	1:D:417:GLU:OE1	2.21	0.40
1:A:660:GLU:HB3	1:A:661:ASP:H	1.74	0.40
1:D:448:LEU:HD13	1:D:627:MET:HE1	2.02	0.40
1:A:508:GLY:HA3	1:A:702:ASP:OD1	2.22	0.40
1:B:662:LEU:HB2	1:B:663:PRO:CD	2.51	0.40
1:A:347:GLU:O	1:A:436:ASN:ND2	2.55	0.40
1:B:720:GLU:HG2	1:B:720:GLU:H	1.62	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:355:ILE:HG22	1:B:357:PHE:CE2	2.56	0.40
1:D:569:LEU:HA	1:D:569:LEU:HD23	1.85	0.40
1:D:323:LEU:HA	1:D:323:LEU:HD12	1.74	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	409/729 (56%)	381 (93%)	23 (6%)	5 (1%)	16	39
1	B	409/729 (56%)	376 (92%)	29 (7%)	4 (1%)	19	45
1	C	409/729 (56%)	367 (90%)	39 (10%)	3 (1%)	26	55
1	D	404/729 (55%)	370 (92%)	26 (6%)	8 (2%)	9	24
All	All	1631/2916 (56%)	1494 (92%)	117 (7%)	20 (1%)	16	39

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	647	TYR
1	C	367	ASP
1	C	647	TYR
1	D	367	ASP
1	D	561	GLU
1	A	443	TRP
1	B	443	TRP
1	A	647	TYR
1	A	649	LYS
1	B	649	LYS
1	B	722	LEU
1	D	521	ASP

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Mol	Chain	Res	Type
1	D	649	LYS
1	D	458	VAL
1	C	458	VAL
1	D	443	TRP
1	D	647	TYR
1	A	535	PRO
1	D	461	PRO
1	A	461	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%)	335 (88%)	44 (12%)	7	16
1	B	379/675 (56%)	333 (88%)	46 (12%)	6	14
1	C	379/675 (56%)	334 (88%)	45 (12%)	6	15
1	D	377/675 (56%)	333 (88%)	44 (12%)	7	15
All	All	1514/2700 (56%)	1335 (88%)	179 (12%)	6	15

All (179) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	316	VAL
1	A	323	LEU
1	A	329	ILE
1	A	333	ARG
1	A	356	VAL
1	A	367	ASP
1	A	388	SER
1	A	402	GLU
1	A	413	GLN
1	A	433	LYS
1	A	439	TYR
1	A	451	LEU
1	A	456	LYS

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Mol	Chain	Res	Type
1	A	460	MET
1	A	472	PHE
1	A	486	ASN
1	A	487	ARG
1	A	502	GLU
1	A	511	ARG
1	A	514	VAL
1	A	538	LYS
1	A	542	MET
1	A	549	ASP
1	A	553	VAL
1	A	555	LYS
1	A	559	LEU
1	A	578	VAL
1	A	587	ILE
1	A	594	SER
1	A	597	GLU
1	A	610	SER
1	A	619	LEU
1	A	622	ASP
1	A	645	ASP
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	676	GLU
1	A	677	LEU
1	A	718	ILE
1	A	722	LEU
1	B	316	VAL
1	B	323	LEU
1	B	329	ILE
1	B	332	ARG
1	B	333	ARG
1	B	343	LEU
1	B	349	ASN
1	B	353	LYS
1	B	356	VAL
1	B	363	LYS
1	B	367	ASP

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Mol	Chain	Res	Type
1	B	382	ASN
1	B	423	SER
1	B	433	LYS
1	B	439	TYR
1	B	450	ARG
1	B	451	LEU
1	B	456	LYS
1	B	460	MET
1	B	470	ARG
1	B	491	GLU
1	B	511	ARG
1	B	514	VAL
1	B	549	ASP
1	B	555	LYS
1	B	559	LEU
1	B	563	LYS
1	B	578	VAL
1	B	594	SER
1	B	607	ASN
1	B	619	LEU
1	B	622	ASP
1	B	623	TYR
1	B	645	ASP
1	B	651	LEU
1	B	656	MET
1	B	661	ASP
1	B	662	LEU
1	B	669	GLU
1	B	673	LEU
1	B	676	GLU
1	B	677	LEU
1	B	702	ASP
1	B	703	ASN
1	B	718	ILE
1	B	722	LEU
1	C	315	LYS
1	C	332	ARG
1	C	348	ASP
1	C	353	LYS
1	C	367	ASP
1	C	382	ASN
1	C	427	THR

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Mol	Chain	Res	Type
1	C	433	LYS
1	C	439	TYR
1	C	450	ARG
1	C	451	LEU
1	C	456	LYS
1	C	457	VAL
1	C	460	MET
1	C	463	THR
1	C	464	THR
1	C	470	ARG
1	C	472	PHE
1	C	487	ARG
1	C	500	ASP
1	C	536	SER
1	C	555	LYS
1	C	559	LEU
1	C	570	TYR
1	C	578	VAL
1	C	589	ASN
1	C	597	GLU
1	C	619	LEU
1	C	622	ASP
1	C	623	TYR
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	681	ASP
1	C	682	LYS
1	C	683	VAL
1	C	703	ASN
1	C	708	GLN
1	C	718	ILE
1	C	722	LEU
1	D	316	VAL
1	D	323	LEU
1	D	333	ARG
1	D	334	LYS

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Mol	Chain	Res	Type
1	D	337	GLU
1	D	346	LYS
1	D	353	LYS
1	D	356	VAL
1	D	402	GLU
1	D	433	LYS
1	D	435	GLU
1	D	439	TYR
1	D	451	LEU
1	D	456	LYS
1	D	460	MET
1	D	464	THR
1	D	470	ARG
1	D	487	ARG
1	D	500	ASP
1	D	511	ARG
1	D	514	VAL
1	D	538	LYS
1	D	559	LEU
1	D	567	ASP
1	D	587	ILE
1	D	589	ASN
1	D	603	VAL
1	D	607	ASN
1	D	623	TYR
1	D	625	SER
1	D	645	ASP
1	D	651	LEU
1	D	660	GLU
1	D	662	LEU
1	D	669	GLU
1	D	673	LEU
1	D	676	GLU
1	D	677	LEU
1	D	678	LYS
1	D	702	ASP
1	D	708	GLN
1	D	718	ILE
1	D	720	GLU
1	D	722	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	349	ASN
1	A	436	ASN
1	A	531	HIS
1	A	708	GLN
1	B	349	ASN
1	B	382	ASN
1	B	436	ASN
1	B	531	HIS
1	B	568	ASN
1	B	679	ASN
1	B	686	GLN
1	C	349	ASN
1	C	364	ASN
1	C	382	ASN
1	C	395	ASN
1	C	436	ASN
1	C	686	GLN
1	C	703	ASN
1	D	349	ASN
1	D	413	GLN
1	D	436	ASN
1	D	531	HIS
1	D	607	ASN
1	D	703	ASN
1	D	708	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

Of 39 ligands modelled in this entry, 26 are monoatomic - leaving 13 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	A	730	-	4,4,4	0.18	0	6,6,6	0.15	0
2	SO4	A	731	-	4,4,4	0.20	0	6,6,6	0.30	0
2	SO4	A	732	-	4,4,4	0.13	0	6,6,6	0.07	0
2	SO4	B	730	-	4,4,4	0.14	0	6,6,6	0.32	0
4	EDO	B	731	-	3,3,3	0.80	0	2,2,2	0.18	0
2	SO4	C	730	-	4,4,4	0.17	0	6,6,6	0.15	0
2	SO4	C	731	-	4,4,4	0.15	0	6,6,6	0.24	0
4	EDO	C	732	-	3,3,3	0.68	0	2,2,2	0.24	0
4	EDO	C	733	-	3,3,3	0.57	0	2,2,2	0.33	0
2	SO4	D	730	-	4,4,4	0.16	0	6,6,6	0.19	0
2	SO4	D	731	-	4,4,4	0.14	0	6,6,6	0.23	0
4	EDO	D	732	-	3,3,3	0.43	0	2,2,2	0.54	0
4	EDO	D	733	-	3,3,3	0.71	0	2,2,2	0.28	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
2	SO4	A	730	-	-	0/0/0/0	0/0/0/0
2	SO4	A	731	-	-	0/0/0/0	0/0/0/0
2	SO4	A	732	-	-	0/0/0/0	0/0/0/0
2	SO4	B	730	-	-	0/0/0/0	0/0/0/0
4	EDO	B	731	-	-	0/1/1/1	0/0/0/0
2	SO4	C	730	-	-	0/0/0/0	0/0/0/0
2	SO4	C	731	-	-	0/0/0/0	0/0/0/0
4	EDO	C	732	-	-	0/1/1/1	0/0/0/0
4	EDO	C	733	-	-	0/1/1/1	0/0/0/0
2	SO4	D	730	-	-	0/0/0/0	0/0/0/0
2	SO4	D	731	-	-	0/0/0/0	0/0/0/0
4	EDO	D	732	-	-	0/1/1/1	0/0/0/0
4	EDO	D	733	-	-	0/1/1/1	0/0/0/0

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.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	731	SO4	1	0
4	B	731	EDO	2	0
4	D	732	EDO	3	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	411/729 (56%)	0.25	9 (2%) 65 66	52, 67, 111, 170	0
1	B	411/729 (56%)	0.32	14 (3%) 49 49	55, 68, 125, 182	0
1	C	411/729 (56%)	0.27	15 (3%) 46 46	51, 73, 133, 181	0
1	D	408/729 (55%)	0.28	9 (2%) 65 66	55, 71, 129, 196	0
All	All	1641/2916 (56%)	0.28	47 (2%) 55 55	51, 70, 127, 196	0

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	558	TYR	8.6
1	C	558	TYR	7.8
1	D	558	TYR	7.5
1	D	560	PHE	6.3
1	D	649	LYS	4.7
1	B	652	ARG	4.6
1	C	557	LYS	4.5
1	B	560	PHE	4.2
1	B	557	LYS	4.2
1	A	558	TYR	4.1
1	C	649	LYS	4.1
1	D	651	LEU	4.0
1	A	557	LYS	4.0
1	D	652	ARG	3.8
1	A	458	VAL	3.6
1	B	552	PHE	3.4
1	D	647	TYR	3.3
1	B	649	LYS	3.3
1	C	721	GLN	3.2
1	C	650	GLY	3.2
1	B	459	ARG	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	715	HIS	3.1
1	B	537	ASP	3.0
1	C	554	SER	3.0
1	D	724	HIS	2.9
1	C	556	GLY	2.9
1	C	560	PHE	2.8
1	B	561	GLU	2.8
1	A	717	ASP	2.5
1	A	560	PHE	2.5
1	D	715	HIS	2.5
1	C	552	PHE	2.5
1	B	647	TYR	2.5
1	B	559	LEU	2.3
1	C	647	TYR	2.3
1	C	559	LEU	2.2
1	C	459	ARG	2.2
1	A	459	ARG	2.2
1	A	647	TYR	2.1
1	B	648	ASP	2.1
1	D	650	GLY	2.1
1	C	396	VAL	2.1
1	B	555	LYS	2.1
1	C	491	GLU	2.0
1	A	313	ALA	2.0
1	C	461	PRO	2.0
1	A	652	ARG	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors

of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	EDO	B	731	4/4	0.84	0.30	6.06	53,53,53,53	0
4	EDO	C	732	4/4	0.82	0.24	3.93	58,58,58,58	0
2	SO4	C	731	5/5	0.90	0.19	0.27	116,116,116,116	0
2	SO4	D	730	5/5	0.97	0.19	-0.19	87,87,87,87	0
2	SO4	A	732	5/5	0.97	0.16	-0.39	92,92,92,92	0
2	SO4	D	731	5/5	0.90	0.16	-0.71	113,113,113,113	0
3	CL	A	739	1/1	0.98	0.14	-1.00	61,61,61,61	0
3	CL	A	743	1/1	0.95	0.12	-1.34	74,74,74,74	0
3	CL	A	736	1/1	0.85	0.14	-1.69	78,78,78,78	0
2	SO4	B	730	5/5	0.94	0.12	-1.95	100,100,100,100	0
2	SO4	A	730	5/5	0.97	0.15	-3.38	76,76,76,76	0
3	CL	B	732	1/1	0.99	0.13	-6.15	39,39,39,39	0
3	CL	B	734	1/1	0.95	0.07	-	83,83,83,83	0
3	CL	C	736	1/1	0.97	0.14	-	64,64,64,64	0
3	CL	D	734	1/1	0.95	0.08	-	71,71,71,71	0
3	CL	C	737	1/1	0.85	0.15	-	80,80,80,80	0
3	CL	A	742	1/1	0.94	0.20	-	85,85,85,85	0
2	SO4	A	731	5/5	0.97	0.14	-	78,78,78,78	0
3	CL	A	734	1/1	0.77	0.14	-	84,84,84,84	0
3	CL	D	736	1/1	0.94	0.07	-	80,80,80,80	0
3	CL	B	733	1/1	0.86	0.24	-	82,82,82,82	0
4	EDO	D	732	4/4	0.95	0.23	-	76,76,76,76	0
4	EDO	C	733	4/4	0.87	0.22	-	77,77,77,77	0
3	CL	B	736	1/1	0.89	0.11	-	81,81,81,81	0
3	CL	D	735	1/1	0.97	0.06	-	73,73,73,73	0
2	SO4	C	730	5/5	0.99	0.13	-	95,95,95,95	0
3	CL	A	744	1/1	0.70	0.19	-	88,88,88,88	0
4	EDO	D	733	4/4	0.85	0.33	-	52,52,52,52	0
3	CL	A	733	1/1	0.89	0.26	-	75,75,75,75	0
3	CL	B	735	1/1	0.66	0.15	-	92,92,92,92	0
3	CL	A	737	1/1	0.90	0.19	-	79,79,79,79	0
3	CL	B	737	1/1	0.92	0.28	-	90,90,90,90	0
3	CL	A	740	1/1	0.95	0.17	-	73,73,73,73	0
3	CL	A	741	1/1	0.91	0.07	-	73,73,73,73	0
3	CL	C	735	1/1	0.95	0.10	-	78,78,78,78	0
3	CL	A	735	1/1	0.97	0.37	-	69,69,69,69	0
3	CL	C	738	1/1	0.89	0.12	-	79,79,79,79	0
3	CL	A	738	1/1	0.96	0.09	-	72,72,72,72	0
3	CL	C	734	1/1	0.95	0.17	-	78,78,78,78	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.