



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 11:32 PM GMT

PDB ID : 1XP4  
Title : Crystal structure of a peptidoglycan synthesis regulatory factor (PBP3) from *Streptococcus pneumoniae*  
Authors : Morlot, C.; Pernot, L.; Le Gouellec, A.; Di Guilmi, A.M.; Vernet, T.; Dideberg, O.; Dessen, A.  
Deposited on : 2004-10-08  
Resolution : 2.80 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

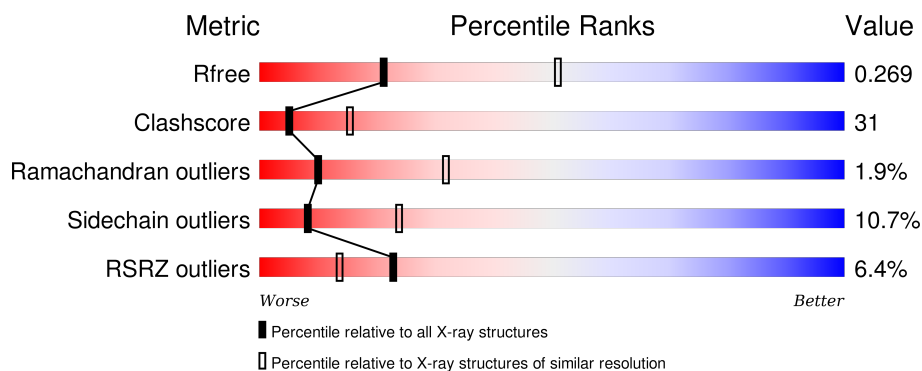
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	379	<div> <div>5%</div> <div>57% 32% 5% . .</div> </div>
1	B	379	<div> <div>7%</div> <div>48% 31% 7% . 11%</div> </div>
1	C	379	<div> <div>5%</div> <div>56% 32% 5% . 5%</div> </div>
1	D	379	<div> <div>5%</div> <div>45% 33% 5% . 15%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	A	464	-	-	-	X
3	IOD	A	468	-	-	X	-
3	IOD	B	472	-	-	X	-
3	IOD	C	476	-	-	X	-
3	IOD	D	481	-	-	X	-

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11150 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 D-alanyl-D-alanine carboxypeptidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	369	Total	C	N	O	Se	0	0	0
			2821	1775	457	580	9			
1	B	339	Total	C	N	O	Se	49	0	0
			2602	1642	420	531	9			
1	C	359	Total	C	N	O	Se	72	0	0
			2750	1731	445	565	9			
1	D	321	Total	C	N	O	Se	27	0	0
			2480	1571	398	502	9			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	101	MSE	MET	MODIFIED RESIDUE	UNP Q8DQ99
A	141	MSE	MET	MODIFIED RESIDUE	UNP Q8DQ99
A	142	MSE	MET	MODIFIED RESIDUE	UNP Q8DQ99
A	216	MSE	MET	MODIFIED RESIDUE	UNP Q8DQ99
A	224	MSE	MET	MODIFIED RESIDUE	UNP Q8DQ99
A	228	MSE	MET	MODIFIED RESIDUE	UNP Q8DQ99
A	259	MSE	MET	MODIFIED RESIDUE	UNP Q8DQ99
A	286	MSE	MET	MODIFIED RESIDUE	UNP Q8DQ99
A	386	MSE	MET	MODIFIED RESIDUE	UNP Q8DQ99
B	101	MSE	MET	MODIFIED RESIDUE	UNP Q8DQ99
B	141	MSE	MET	MODIFIED RESIDUE	UNP Q8DQ99
B	142	MSE	MET	MODIFIED RESIDUE	UNP Q8DQ99
B	216	MSE	MET	MODIFIED RESIDUE	UNP Q8DQ99
B	224	MSE	MET	MODIFIED RESIDUE	UNP Q8DQ99
B	228	MSE	MET	MODIFIED RESIDUE	UNP Q8DQ99
B	259	MSE	MET	MODIFIED RESIDUE	UNP Q8DQ99
B	286	MSE	MET	MODIFIED RESIDUE	UNP Q8DQ99
B	386	MSE	MET	MODIFIED RESIDUE	UNP Q8DQ99
C	101	MSE	MET	MODIFIED RESIDUE	UNP Q8DQ99
C	141	MSE	MET	MODIFIED RESIDUE	UNP Q8DQ99
C	142	MSE	MET	MODIFIED RESIDUE	UNP Q8DQ99

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Chain	Residue	Modelled	Actual	Comment	Reference
C	216	MSE	MET	MODIFIED RESIDUE	UNP Q8DQ99
C	224	MSE	MET	MODIFIED RESIDUE	UNP Q8DQ99
C	228	MSE	MET	MODIFIED RESIDUE	UNP Q8DQ99
C	259	MSE	MET	MODIFIED RESIDUE	UNP Q8DQ99
C	286	MSE	MET	MODIFIED RESIDUE	UNP Q8DQ99
C	386	MSE	MET	MODIFIED RESIDUE	UNP Q8DQ99
D	101	MSE	MET	MODIFIED RESIDUE	UNP Q8DQ99
D	141	MSE	MET	MODIFIED RESIDUE	UNP Q8DQ99
D	142	MSE	MET	MODIFIED RESIDUE	UNP Q8DQ99
D	216	MSE	MET	MODIFIED RESIDUE	UNP Q8DQ99
D	224	MSE	MET	MODIFIED RESIDUE	UNP Q8DQ99
D	228	MSE	MET	MODIFIED RESIDUE	UNP Q8DQ99
D	259	MSE	MET	MODIFIED RESIDUE	UNP Q8DQ99
D	286	MSE	MET	MODIFIED RESIDUE	UNP Q8DQ99
D	386	MSE	MET	MODIFIED RESIDUE	UNP Q8DQ99

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	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 IODIDE ION (three-letter code: IOD) (formula: I).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	4	Total I 4 4	0	0
3	A	4	Total I 4 4	0	0
3	D	4	Total I 4 4	0	0
3	C	4	Total I 4 4	0	0

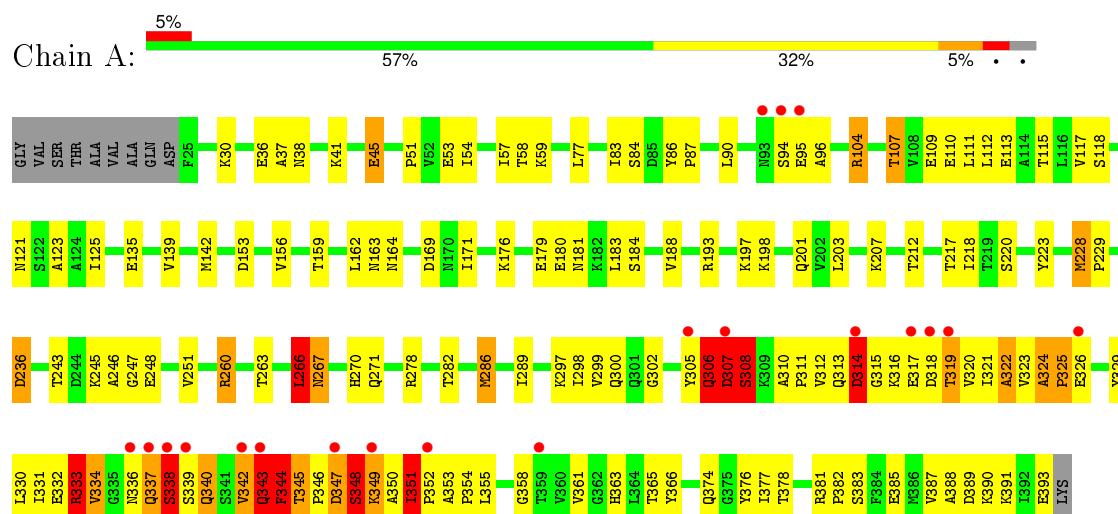
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	139	Total O 139 139	1	0
4	B	98	Total O 98 98	0	0
4	C	121	Total O 121 121	0	0
4	D	103	Total O 103 103	0	0

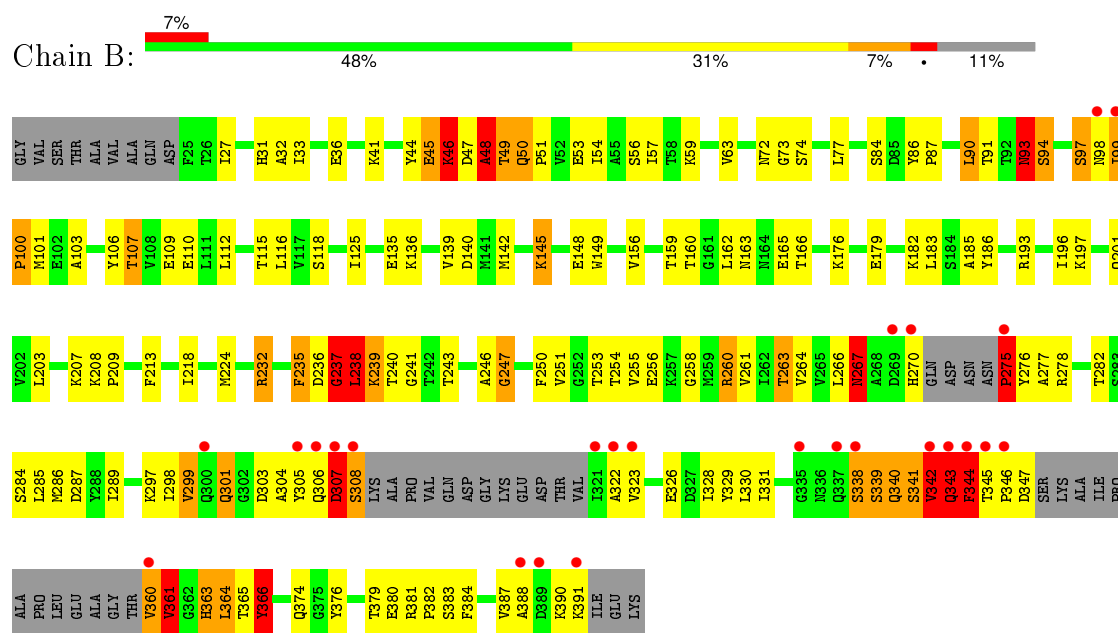
### 3 Residue-property plots

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

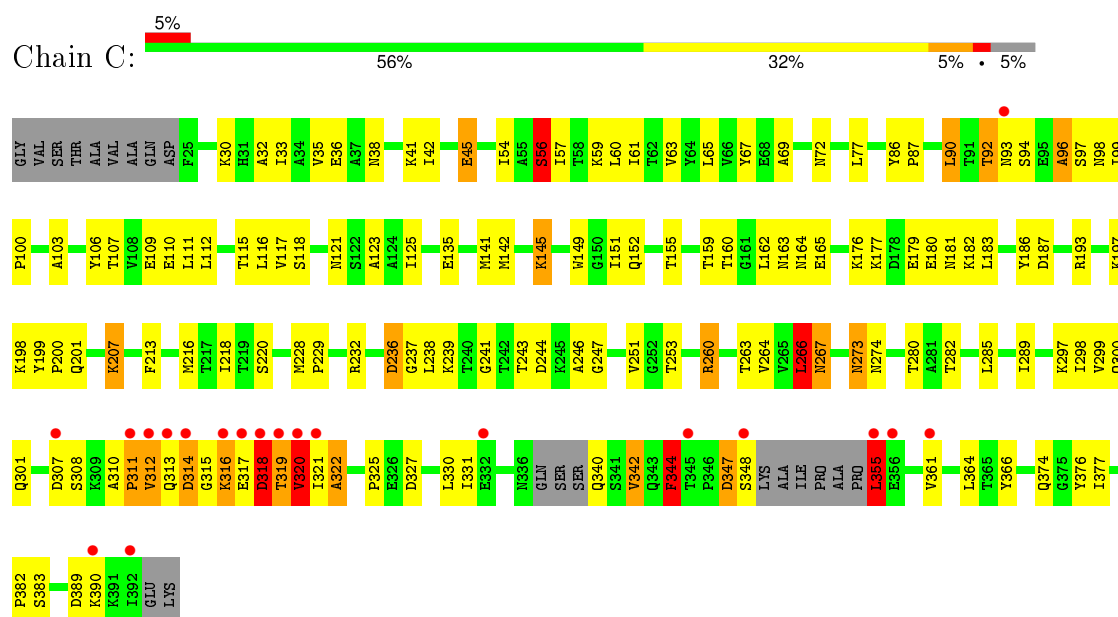
#### • Molecule 1: D-alanyl-D-alanine carboxypeptidase



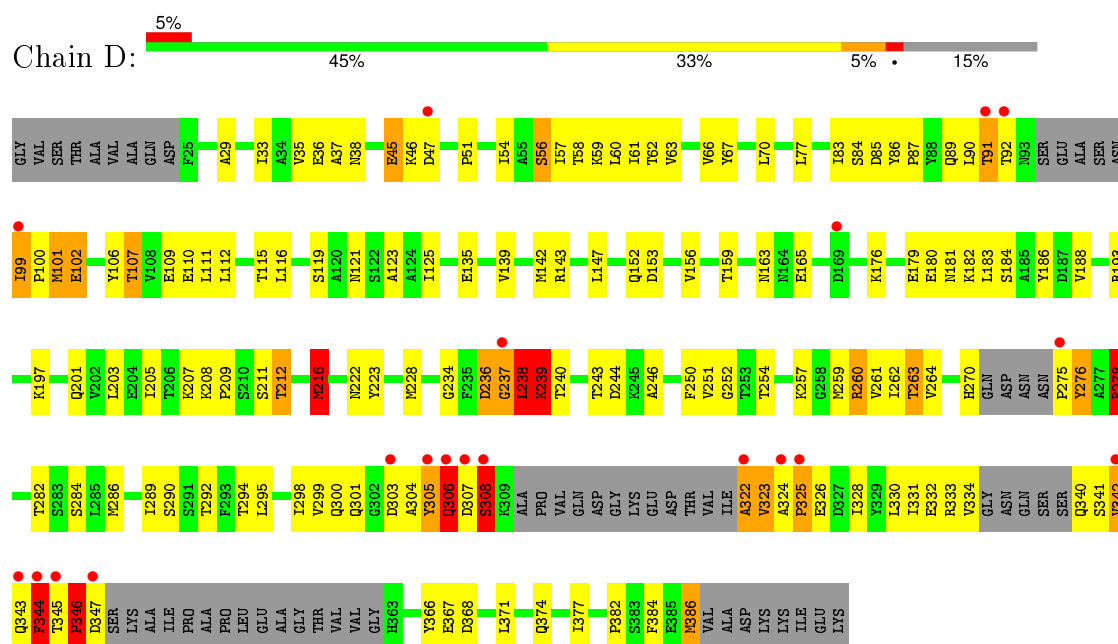
#### • Molecule 1: D-alanyl-D-alanine carboxypeptidase



#### • Molecule 1: D-alanyl-D-alanine carboxypeptidase



- Molecule 1: D-alanyl-D-alanine carboxypeptidase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	87.61Å 120.84Å 177.08Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	65.84 – 2.80 65.84 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.8 (65.84-2.80) 99.9 (65.84-2.80)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.69 (at 2.81Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.237 , 0.278 0.232 , 0.269	Depositor DCC
$R_{free}$ test set	3309 reflections (7.57%)	DCC
Wilson B-factor (Å <sup>2</sup> )	25.8	Xtriage
Anisotropy	0.904	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 47.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.52$ , $\langle L^2 \rangle = 0.36$	Xtriage
Outliers	1 of 47009 reflections (0.002%)	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	11150	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 43.43 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 1.7648e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: IOD, 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	0.62	1/2857 (0.0%)	1.02	16/3868 (0.4%)
1	B	0.50	0/2632	0.96	12/3555 (0.3%)
1	C	0.55	1/2782 (0.0%)	0.91	11/3762 (0.3%)
1	D	0.48	0/2508	0.91	11/3384 (0.3%)
All	All	0.54	2/10779 (0.0%)	0.95	50/14569 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	14
1	B	0	15
1	C	2	8
1	D	0	6
All	All	2	43

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	344	PHE	C-N	18.73	1.77	1.34
1	C	266	LEU	C-O	16.93	1.55	1.23

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	338	SER	O-C-N	-17.82	94.19	122.70
1	C	266	LEU	O-C-N	-17.40	94.86	122.70
1	B	275	PRO	CA-N-CD	-16.95	87.76	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	275	PRO	CA-N-CD	-16.85	87.91	111.50
1	C	311	PRO	CA-N-CD	-14.77	90.82	111.50
1	A	351	ILE	O-C-N	-12.77	96.83	121.10
1	A	338	SER	CA-C-N	-12.20	90.37	117.20
1	C	266	LEU	C-N-CA	-10.84	94.61	121.70
1	C	340	GLN	C-N-CA	-10.15	96.31	121.70
1	C	320	VAL	O-C-N	-10.04	106.64	122.70
1	A	322	ALA	O-C-N	9.57	138.01	122.70
1	A	308	SER	O-C-N	-9.29	107.84	122.70
1	A	344	PHE	C-N-CA	-8.79	99.71	121.70
1	A	322	ALA	CA-C-N	-8.57	98.35	117.20
1	B	94	SER	O-C-N	-8.56	109.01	122.70
1	C	266	LEU	CA-C-O	-8.42	102.41	120.10
1	A	306	GLN	CA-CB-CG	-7.53	96.84	113.40
1	B	366	TYR	O-C-N	-7.35	110.94	122.70
1	D	305	TYR	CA-C-N	-7.20	101.35	117.20
1	D	92	THR	N-CA-C	-7.15	91.69	111.00
1	B	338	SER	N-CA-C	7.10	130.16	111.00
1	D	344	PHE	CB-CG-CD1	-6.99	115.91	120.80
1	B	308	SER	CB-CA-C	6.92	123.26	110.10
1	B	48	ALA	CA-C-N	-6.84	102.15	117.20
1	B	237	GLY	C-N-CA	6.83	138.78	121.70
1	B	361	VAL	C-N-CA	-6.76	108.11	122.30
1	A	318	ASP	C-N-CA	6.65	138.33	121.70
1	A	324	ALA	C-N-CD	6.62	142.30	128.40
1	A	343	GLN	C-N-CA	-6.47	105.53	121.70
1	D	346	PRO	O-C-N	-6.31	112.60	122.70
1	D	278	ARG	CD-NE-CZ	-6.25	114.84	123.60
1	A	344	PHE	CA-C-N	-6.15	103.67	117.20
1	D	308	SER	CA-C-N	-6.13	103.71	117.20
1	C	355	LEU	O-C-N	-5.99	113.11	122.70
1	A	344	PHE	O-C-N	5.98	132.27	122.70
1	B	366	TYR	CA-C-N	-5.91	104.19	117.20
1	A	306	GLN	CB-CA-C	5.69	121.78	110.40
1	D	344	PHE	CB-CG-CD2	-5.57	116.90	120.80
1	D	216	MSE	O-C-N	-5.57	113.79	122.70
1	D	278	ARG	O-C-N	5.54	131.57	122.70
1	C	318	ASP	N-CA-C	5.51	125.88	111.00
1	B	366	TYR	CB-CG-CD2	-5.45	117.73	121.00
1	B	342	VAL	CA-C-N	-5.41	105.29	117.20
1	A	333	ARG	CD-NE-CZ	-5.38	116.06	123.60
1	B	94	SER	CA-C-N	5.29	128.83	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	305	TYR	O-C-N	5.28	131.15	122.70
1	C	322	ALA	O-C-N	5.27	131.13	122.70
1	A	344	PHE	CB-CG-CD2	-5.12	117.21	120.80
1	C	313	GLN	C-N-CA	5.00	134.21	121.70
1	C	96	ALA	N-CA-C	-5.00	97.50	111.00

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	C	318	ASP	CA
1	C	343	GLN	CA

All (43) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	266	LEU	Peptide
1	A	308	SER	Mainchain
1	A	314	ASP	Sidechain
1	A	315	GLY	Peptide
1	A	317	GLU	Mainchain
1	A	319	THR	Peptide
1	A	338	SER	Mainchain,Peptide
1	A	339	SER	Peptide
1	A	343	GLN	Peptide
1	A	344	PHE	Sidechain
1	A	348	SER	Peptide
1	A	350	ALA	Peptide
1	A	351	ILE	Mainchain
1	B	100	PRO	Mainchain
1	B	213	PHE	Sidechain
1	B	237	GLY	Peptide
1	B	258	GLY	Mainchain
1	B	342	VAL	Mainchain
1	B	343	GLN	Peptide
1	B	344	PHE	Sidechain
1	B	366	TYR	Sidechain,Mainchain
1	B	46	LYS	Peptide
1	B	48	ALA	Mainchain
1	B	49	THR	Mainchain
1	B	93	ASN	Peptide
1	B	94	SER	Peptide
1	B	97	SER	Peptide

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Mol	Chain	Res	Type	Group
1	C	266	LEU	Mainchain,Peptide
1	C	316	LYS	Peptide
1	C	318	ASP	Peptide
1	C	320	VAL	Mainchain
1	C	342	VAL	Peptide
1	C	344	PHE	Sidechain
1	C	355	LEU	Mainchain
1	D	216	MSE	Mainchain
1	D	239	LYS	Mainchain
1	D	322	ALA	Peptide
1	D	325	PRO	Mainchain
1	D	344	PHE	Sidechain
1	D	346	PRO	Mainchain

## 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	2821	0	2801	178	0
1	B	2602	0	2586	168	1
1	C	2750	0	2728	139	1
1	D	2480	0	2467	173	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
2	D	5	0	0	0	0
3	A	4	0	0	2	0
3	B	4	0	0	2	0
3	C	4	0	0	2	0
3	D	4	0	0	3	0
4	A	139	0	0	6	0
4	B	98	0	0	2	0
4	C	121	0	0	8	0
4	D	103	0	0	5	0
All	All	11150	0	10582	646	1

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 31.

All (646) 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:344:PHE:C	1:A:345:THR:N	1.77	1.38
1:C:243:THR:HG22	1:C:246:ALA:CB	1.63	1.27
1:B:305:TYR:OH	1:B:343:GLN:HB3	1.28	1.25
1:B:237:GLY:HA3	1:B:253:THR:CG2	1.67	1.24
1:B:342:VAL:CG2	1:B:342:VAL:O	1.81	1.24
1:A:305:TYR:OH	1:A:343:GLN:HG3	1.39	1.23
1:B:307:ASP:O	1:B:307:ASP:OD1	1.57	1.23
1:B:237:GLY:CA	1:B:253:THR:HG22	1.71	1.20
1:A:333:ARG:CB	1:A:336:ASN:HD21	1.54	1.20
1:D:243:THR:HG22	1:D:246:ALA:CB	1.73	1.17
1:D:222:ASN:ND2	1:D:237:GLY:HA3	1.58	1.15
1:A:243:THR:HG22	1:A:246:ALA:CB	1.74	1.15
1:A:333:ARG:HB3	1:A:336:ASN:HD21	1.12	1.13
1:D:243:THR:CG2	1:D:246:ALA:H	1.61	1.13
1:B:342:VAL:O	1:B:342:VAL:HG23	1.37	1.12
1:B:304:ALA:HB2	1:B:323:VAL:HG12	1.12	1.11
1:C:243:THR:CG2	1:C:246:ALA:HB3	1.80	1.09
1:D:243:THR:HG23	1:D:246:ALA:H	0.96	1.08
1:C:243:THR:CG2	1:C:246:ALA:CB	2.32	1.08
1:A:243:THR:CG2	1:A:246:ALA:HB3	1.85	1.07
1:B:243:THR:HG23	1:B:246:ALA:H	1.08	1.07
1:A:347:ASP:N	1:A:347:ASP:OD1	1.86	1.06
1:D:139:VAL:HA	1:D:142:MSE:HE3	1.38	1.04
1:C:243:THR:HG23	1:C:246:ALA:H	0.94	1.04
1:D:304:ALA:CB	1:D:322:ALA:HB1	1.88	1.04
1:A:336:ASN:O	1:A:337:GLN:O	1.77	1.03
1:B:330:LEU:HD13	1:B:342:VAL:HG11	1.43	1.01
1:D:243:THR:HG22	1:D:246:ALA:HB3	1.03	1.01
1:A:243:THR:HG23	1:A:246:ALA:H	1.19	1.01
1:A:243:THR:CG2	1:A:246:ALA:CB	2.38	1.00
1:B:243:THR:HG22	1:B:246:ALA:HB3	1.43	1.00
1:D:222:ASN:HD21	1:D:237:GLY:HA3	1.26	0.99
1:C:243:THR:CG2	1:C:246:ALA:H	1.74	0.99
1:B:330:LEU:CD1	1:B:342:VAL:HG11	1.94	0.98
1:A:333:ARG:HB3	1:A:336:ASN:ND2	1.79	0.98
1:B:305:TYR:CZ	1:B:343:GLN:HB3	1.98	0.98
1:D:243:THR:CG2	1:D:246:ALA:CB	2.42	0.97
1:B:63:VAL:HG21	1:B:116:LEU:HD21	1.42	0.97
1:C:243:THR:HG23	1:C:246:ALA:N	1.78	0.97
1:A:243:THR:HG22	1:A:246:ALA:HB3	0.98	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:304:ALA:HB1	1:D:322:ALA:CB	1.93	0.97
1:C:63:VAL:HG21	1:C:116:LEU:HD21	1.48	0.95
1:D:243:THR:CG2	1:D:246:ALA:HB3	1.95	0.95
1:C:317:GLU:O	1:C:318:ASP:CB	2.15	0.95
1:D:341:SER:C	1:D:343:GLN:H	1.69	0.94
1:D:243:THR:HG23	1:D:246:ALA:N	1.81	0.94
1:B:48:ALA:HB1	1:B:185:ALA:HB3	1.50	0.92
1:D:237:GLY:O	1:D:238:LEU:HB2	1.66	0.92
1:B:298:ILE:HD12	1:B:299:VAL:HG22	1.52	0.91
1:B:243:THR:CG2	1:B:246:ALA:H	1.82	0.91
1:B:107:THR:HG22	1:B:110:GLU:HG3	1.50	0.90
1:D:304:ALA:CB	1:D:322:ALA:CB	2.48	0.90
1:D:222:ASN:HD21	1:D:237:GLY:CA	1.82	0.90
1:A:330:LEU:CD1	1:A:342:VAL:HG11	2.01	0.90
1:C:60:LEU:HD21	1:C:238:LEU:CD1	2.02	0.89
1:D:330:LEU:HD11	1:D:342:VAL:HB	1.55	0.89
1:B:342:VAL:O	1:B:342:VAL:HG22	1.70	0.88
1:B:345:THR:HA	1:B:363:HIS:O	1.75	0.87
1:B:247:GLY:HA3	1:B:267:ASN:HB2	1.56	0.87
1:A:346:PRO:HD2	1:A:363:HIS:O	1.75	0.87
1:B:176:LYS:HB2	1:B:179:GLU:HG3	1.55	0.86
1:B:304:ALA:CB	1:B:323:VAL:HG12	2.01	0.86
1:A:305:TYR:OH	1:A:343:GLN:CG	2.23	0.86
1:C:243:THR:HG22	1:C:246:ALA:HB3	0.88	0.86
1:C:60:LEU:CD2	1:C:238:LEU:CD1	2.53	0.86
1:B:196:ILE:HD11	1:B:238:LEU:HD21	1.55	0.86
1:D:107:THR:HG22	1:D:110:GLU:H	1.41	0.86
1:A:333:ARG:CB	1:A:336:ASN:ND2	2.38	0.86
1:D:107:THR:HG22	1:D:110:GLU:HG3	1.58	0.85
1:A:306:GLN:O	1:A:308:SER:HB3	1.75	0.85
1:B:346:PRO:HD2	1:B:363:HIS:O	1.77	0.85
1:D:239:LYS:NZ	1:D:240:THR:O	2.10	0.85
1:B:304:ALA:HB2	1:B:323:VAL:CG1	2.03	0.84
1:C:317:GLU:O	1:C:318:ASP:CG	2.15	0.84
1:A:349:LYS:O	1:A:351:ILE:HG22	1.78	0.84
1:B:305:TYR:OH	1:B:343:GLN:CB	2.21	0.84
1:A:344:PHE:C	1:A:345:THR:CA	2.44	0.84
1:A:330:LEU:HD11	1:A:342:VAL:HG11	1.59	0.84
1:A:107:THR:HG22	1:A:110:GLU:H	1.43	0.83
1:C:263:THR:HG21	1:C:282:THR:HG23	1.60	0.83
1:D:243:THR:CG2	1:D:246:ALA:N	2.40	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:298:ILE:CD1	1:D:342:VAL:HG21	2.08	0.83
1:A:343:GLN:O	1:A:344:PHE:HB2	1.78	0.82
1:D:176:LYS:HB2	1:D:179:GLU:HG3	1.61	0.82
1:A:305:TYR:HD1	1:A:305:TYR:O	1.61	0.82
1:D:99:ILE:O	1:D:99:ILE:HG12	1.78	0.82
1:D:142:MSE:CE	1:D:159:THR:HG22	2.10	0.82
1:D:263:THR:HG21	1:D:282:THR:HG23	1.62	0.82
1:A:271:GLN:OE1	1:B:73:GLY:HA3	1.80	0.81
1:D:90:LEU:O	1:D:90:LEU:HG	1.80	0.81
1:C:176:LYS:HB2	1:C:179:GLU:HG3	1.62	0.81
1:B:261:VAL:HG11	1:B:286:MSE:HE1	1.63	0.81
1:B:107:THR:HG22	1:B:110:GLU:H	1.45	0.81
1:A:243:THR:HG23	1:A:246:ALA:N	1.97	0.80
1:A:313:GLN:HG3	1:A:313:GLN:O	1.80	0.80
1:B:243:THR:CG2	1:B:246:ALA:HB3	2.10	0.80
1:B:53:GLU:HB2	1:B:246:ALA:HB2	1.63	0.80
1:D:63:VAL:HG21	1:D:116:LEU:HD21	1.63	0.80
1:A:107:THR:HB	1:A:110:GLU:HG3	1.62	0.80
1:D:182:LYS:O	1:D:183:LEU:HD12	1.80	0.80
1:D:298:ILE:HD12	1:D:342:VAL:HG21	1.62	0.79
1:A:361:VAL:HG21	1:A:388:ALA:HB2	1.64	0.79
1:B:48:ALA:CB	1:B:185:ALA:HB3	2.11	0.79
1:C:317:GLU:O	1:C:318:ASP:HB3	1.82	0.79
1:B:298:ILE:HG12	1:B:330:LEU:CD1	2.12	0.79
1:B:263:THR:HG21	1:B:282:THR:HG23	1.63	0.78
1:A:286:MSE:HE3	1:A:286:MSE:HA	1.65	0.78
1:B:247:GLY:CA	1:B:267:ASN:HB2	2.14	0.78
1:B:243:THR:HG23	1:B:246:ALA:N	1.94	0.78
1:A:374:GLN:HG3	3:A:468:IOD:I	2.55	0.77
1:C:145:LYS:HE3	4:C:569:HOH:O	1.83	0.77
1:D:301:GLN:HG3	1:D:325:PRO:O	1.83	0.77
1:D:305:TYR:OH	1:D:343:GLN:HG2	1.84	0.77
1:A:390:LYS:HE3	1:C:325:PRO:O	1.83	0.77
1:D:341:SER:C	1:D:343:GLN:N	2.37	0.76
1:D:305:TYR:CE2	1:D:343:GLN:HA	2.20	0.76
1:B:53:GLU:CB	1:B:246:ALA:HB2	2.16	0.75
1:A:349:LYS:HG2	1:D:147:LEU:HD11	1.68	0.75
1:C:374:GLN:HG3	3:C:476:IOD:I	2.57	0.74
1:B:286:MSE:HE2	1:B:289:ILE:HD12	1.69	0.74
1:A:305:TYR:O	1:A:305:TYR:CD1	2.40	0.74
1:B:308:SER:CB	1:B:322:ALA:O	2.35	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:139:VAL:HA	1:D:142:MSE:CE	2.16	0.74
1:A:333:ARG:HB2	1:A:336:ASN:HD21	1.51	0.73
1:D:222:ASN:HD22	1:D:237:GLY:HA3	1.51	0.73
1:C:297:LYS:HE3	1:C:300:GLN:HB3	1.69	0.73
1:A:336:ASN:C	1:A:337:GLN:O	2.27	0.72
1:B:86:TYR:HB3	1:B:87:PRO:HD3	1.70	0.72
1:D:38:ASN:HA	1:D:197:LYS:HE3	1.71	0.72
1:C:243:THR:CG2	1:C:246:ALA:N	2.45	0.72
1:D:142:MSE:HE2	1:D:159:THR:HG22	1.72	0.72
1:C:312:VAL:HG21	1:C:320:VAL:HG22	1.70	0.72
1:A:263:THR:HG21	1:A:282:THR:HG23	1.72	0.71
1:B:107:THR:CG2	1:B:110:GLU:HG3	2.20	0.71
1:B:342:VAL:HA	1:B:366:TYR:HA	1.72	0.71
1:C:59:LYS:O	1:C:63:VAL:HG23	1.89	0.71
1:C:107:THR:HB	1:C:110:GLU:HG3	1.71	0.71
1:D:323:VAL:C	1:D:386:MSE:CE	2.59	0.71
1:D:342:VAL:O	1:D:342:VAL:HG22	1.89	0.71
1:A:77:LEU:O	1:A:107:THR:HG23	1.91	0.71
1:C:312:VAL:CG2	1:C:320:VAL:HG22	2.21	0.70
1:C:60:LEU:HD21	1:C:238:LEU:HD13	1.74	0.70
1:C:107:THR:HG21	4:C:599:HOH:O	1.91	0.70
1:D:86:TYR:HB3	1:D:87:PRO:HD3	1.72	0.70
1:C:298:ILE:HD13	1:C:330:LEU:HD11	1.73	0.70
1:D:304:ALA:HB1	1:D:322:ALA:HB1	1.55	0.70
1:A:316:LYS:HE3	1:C:301:GLN:CG	2.21	0.70
1:A:243:THR:CG2	1:A:246:ALA:HB2	2.22	0.70
1:A:90:LEU:O	1:A:94:SER:HB2	1.91	0.70
1:B:298:ILE:HD12	1:B:299:VAL:CG2	2.21	0.70
1:D:286:MSE:HE2	1:D:289:ILE:HD12	1.74	0.69
1:A:343:GLN:O	1:A:344:PHE:CB	2.40	0.69
1:A:358:GLY:HA2	1:A:387:VAL:CG1	2.23	0.69
1:A:325:PRO:O	1:A:326:GLU:HG3	1.93	0.68
1:A:344:PHE:CA	1:A:345:THR:N	2.57	0.68
1:D:374:GLN:HG3	3:D:481:IOD:I	2.64	0.68
1:C:273:ASN:HB2	4:C:488:HOH:O	1.94	0.67
1:A:41:LYS:HD3	1:A:331:ILE:HD12	1.76	0.67
1:C:243:THR:CG2	1:C:246:ALA:HB2	2.24	0.67
1:B:307:ASP:O	1:B:307:ASP:CG	2.32	0.67
1:A:363:HIS:NE2	1:A:385:GLU:HG2	2.09	0.67
1:D:107:THR:CG2	1:D:110:GLU:HG3	2.25	0.67
1:B:36:GLU:HG3	1:B:331:ILE:HD11	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:222:ASN:ND2	1:D:237:GLY:CA	2.42	0.67
1:C:312:VAL:CG2	1:C:320:VAL:CG2	2.72	0.67
1:C:347:ASP:OD1	1:C:347:ASP:N	2.26	0.67
1:B:246:ALA:O	1:B:247:GLY:O	2.12	0.67
1:B:344:PHE:O	1:B:346:PRO:HD3	1.94	0.66
1:A:358:GLY:HA2	1:A:387:VAL:HG11	1.76	0.66
1:B:303:ASP:O	1:B:323:VAL:HB	1.96	0.66
1:C:60:LEU:HD22	1:C:238:LEU:CD1	2.25	0.66
1:A:349:LYS:HG2	1:D:147:LEU:CD1	2.26	0.66
1:D:305:TYR:HE2	1:D:343:GLN:HA	1.58	0.66
1:B:297:LYS:HA	1:B:329:TYR:HA	1.78	0.66
1:C:298:ILE:HG21	1:C:330:LEU:CD1	2.26	0.65
1:D:298:ILE:HD13	1:D:330:LEU:HG	1.78	0.65
1:A:314:ASP:HB2	1:A:353:ALA:HB3	1.78	0.65
1:B:308:SER:HB3	1:B:322:ALA:O	1.96	0.65
1:A:333:ARG:NH2	4:A:600:HOH:O	2.29	0.65
1:D:83:ILE:HD11	1:D:106:TYR:HD1	1.59	0.65
1:A:306:GLN:O	1:A:308:SER:CB	2.44	0.65
1:C:247:GLY:HA3	1:C:267:ASN:ND2	2.12	0.65
1:D:323:VAL:C	1:D:386:MSE:HE3	2.17	0.65
1:B:238:LEU:HD12	1:B:251:VAL:HG11	1.79	0.65
1:C:86:TYR:HB3	1:C:87:PRO:HD3	1.79	0.64
1:A:314:ASP:O	1:A:393:GLU:HB2	1.98	0.64
1:D:304:ALA:CA	1:D:322:ALA:HB1	2.28	0.64
1:B:330:LEU:HD11	1:B:342:VAL:HG11	1.76	0.64
1:A:316:LYS:HE3	1:C:301:GLN:HG2	1.79	0.64
1:B:237:GLY:HA3	1:B:253:THR:HG22	0.79	0.63
1:A:353:ALA:HB1	1:A:354:PRO:HA	1.80	0.63
1:B:341:SER:HA	1:B:343:GLN:NE2	2.14	0.63
1:C:60:LEU:HD22	1:C:238:LEU:HD11	1.80	0.63
1:D:99:ILE:O	1:D:99:ILE:CG1	2.47	0.62
1:A:286:MSE:CE	1:A:286:MSE:HA	2.28	0.62
1:B:308:SER:HB2	1:B:322:ALA:O	1.98	0.62
1:B:224:MSE:HE2	1:B:232:ARG:HB2	1.80	0.62
1:D:257:LYS:HE2	1:D:290:SER:O	2.00	0.62
1:B:298:ILE:HG12	1:B:330:LEU:HD11	1.81	0.62
1:C:60:LEU:CD2	1:C:238:LEU:HD12	2.28	0.62
1:C:77:LEU:O	1:C:107:THR:HG23	1.99	0.61
1:D:263:THR:HG21	1:D:282:THR:CG2	2.30	0.61
1:D:111:LEU:HD22	1:D:123:ALA:HA	1.83	0.61
1:A:286:MSE:HE3	1:A:289:ILE:HB	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:342:VAL:HG22	1:A:342:VAL:O	2.00	0.60
1:C:160:THR:CG2	1:C:162:LEU:HG	2.31	0.60
1:C:60:LEU:HD21	1:C:238:LEU:HD12	1.80	0.60
1:C:298:ILE:HG21	1:C:330:LEU:HD11	1.83	0.60
1:A:203:LEU:O	1:A:207:LYS:HB2	2.01	0.60
1:C:63:VAL:HG13	1:C:112:LEU:HD11	1.83	0.60
1:D:261:VAL:HG11	1:D:286:MSE:HE1	1.82	0.60
1:A:83:ILE:O	1:A:104:ARG:NH1	2.34	0.60
1:B:203:LEU:O	1:B:207:LYS:HB2	2.01	0.60
1:B:31:His:HB2	1:B:266:LEU:HB2	1.82	0.60
1:D:323:VAL:H	1:D:386:MSE:HE2	1.67	0.60
1:C:107:THR:HG22	1:C:109:GLU:N	2.15	0.60
1:C:237:GLY:HA3	1:C:253:THR:HG22	1.84	0.60
1:B:139:VAL:HA	1:B:142:MSE:HG2	1.83	0.60
1:B:346:PRO:CD	1:B:363:HIS:O	2.48	0.60
1:A:176:LYS:HB2	1:A:179:GLU:HG3	1.84	0.60
1:A:142:MSE:HE2	1:A:156:VAL:HG11	1.83	0.60
1:D:135:GLU:HG3	1:D:159:THR:HG23	1.82	0.60
1:D:142:MSE:HE1	1:D:159:THR:HG22	1.83	0.60
1:D:243:THR:CG2	1:D:246:ALA:HB2	2.31	0.59
1:B:275:PRO:HB2	1:B:276:TYR:CD2	2.36	0.59
1:D:163:ASN:OD1	1:D:165:GLU:HG3	2.02	0.59
1:C:160:THR:HG21	1:C:162:LEU:HG	1.83	0.59
1:B:330:LEU:HD11	1:B:342:VAL:HG21	1.85	0.59
1:B:243:THR:CG2	1:B:246:ALA:N	2.59	0.59
1:B:196:ILE:HD11	1:B:238:LEU:CD2	2.31	0.59
1:C:65:LEU:HD13	1:C:141:MSE:HE2	1.84	0.59
1:D:135:GLU:O	1:D:139:VAL:HG23	2.02	0.59
1:B:298:ILE:HG12	1:B:330:LEU:HD12	1.85	0.58
1:D:57:ILE:HD13	1:D:251:VAL:HG23	1.84	0.58
1:D:36:GLU:HG3	1:D:331:ILE:HD11	1.85	0.58
1:A:90:LEU:HD12	1:A:94:SER:OG	2.03	0.58
1:A:342:VAL:CG2	1:A:342:VAL:O	2.51	0.58
1:D:163:ASN:HD22	1:D:180:GLU:HG3	1.67	0.58
1:A:38:ASN:HA	1:A:197:LYS:HE2	1.85	0.58
1:B:341:SER:C	1:B:343:GLN:H	2.06	0.58
1:D:308:SER:HB2	1:D:322:ALA:HB2	1.85	0.58
1:B:305:TYR:CZ	1:B:343:GLN:CB	2.83	0.58
1:A:316:LYS:HE3	1:C:301:GLN:HG3	1.86	0.58
1:C:60:LEU:CD1	1:C:238:LEU:HD12	2.34	0.58
1:C:60:LEU:HD11	1:C:238:LEU:HD12	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:86:TYR:O	1:B:90:LEU:HB2	2.03	0.57
1:A:266:LEU:O	1:A:267:ASN:HB2	2.02	0.57
1:A:87:PRO:HG3	1:A:125:ILE:HG21	1.86	0.57
1:D:163:ASN:ND2	1:D:180:GLU:HG3	2.20	0.57
1:C:198:LYS:HB2	4:C:590:HOH:O	2.03	0.57
1:C:56:SER:HB2	1:C:241:GLY:HA2	1.87	0.57
1:D:276:TYR:N	1:D:276:TYR:CD1	2.72	0.57
1:A:267:ASN:HD22	1:A:267:ASN:C	2.06	0.57
1:A:86:TYR:HB3	1:A:87:PRO:HD3	1.87	0.57
1:D:91:THR:OG1	1:D:91:THR:O	2.16	0.57
1:A:310:ALA:HB3	1:A:361:VAL:CG1	2.35	0.57
1:C:152:GLN:HA	4:C:546:HOH:O	2.05	0.57
1:A:153:ASP:HB3	1:D:344:PHE:CE1	2.40	0.56
1:D:33:ILE:HG22	1:D:264:VAL:HB	1.87	0.56
1:B:263:THR:HG21	1:B:282:THR:CG2	2.35	0.56
1:A:310:ALA:HB3	1:A:361:VAL:HG12	1.87	0.56
1:A:322:ALA:HA	1:A:387:VAL:O	2.06	0.56
1:D:193:ARG:O	1:D:197:LYS:HB2	2.06	0.56
1:B:374:GLN:HG3	3:B:472:IOD:I	2.75	0.56
1:D:77:LEU:HB3	1:D:109:GLU:HB2	1.86	0.56
1:D:304:ALA:HB2	1:D:322:ALA:CB	2.33	0.56
1:A:59:LYS:HD3	1:A:115:THR:HG23	1.87	0.56
1:B:243:THR:CG2	1:B:246:ALA:CB	2.81	0.56
1:D:330:LEU:HD11	1:D:342:VAL:CB	2.34	0.56
1:B:363:HIS:HD2	1:B:383:SER:HB2	1.70	0.56
1:B:59:LYS:HD3	1:B:115:THR:HG23	1.88	0.56
1:B:45:GLU:HG3	4:B:492:HOH:O	2.07	0.55
1:D:35:VAL:HG12	1:D:262:ILE:HB	1.88	0.55
1:C:266:LEU:O	1:C:267:ASN:HB2	2.07	0.55
1:A:193:ARG:HH21	1:A:197:LYS:HE3	1.70	0.55
1:B:263:THR:OG1	1:B:286:MSE:HE3	2.06	0.55
1:A:361:VAL:CG2	1:A:388:ALA:HB2	2.36	0.55
1:B:297:LYS:HB3	1:B:329:TYR:CD2	2.41	0.55
1:C:244:ASP:HB2	4:C:591:HOH:O	2.06	0.55
1:C:247:GLY:HA3	1:C:267:ASN:HD21	1.71	0.55
1:D:107:THR:CG2	1:D:110:GLU:H	2.18	0.55
1:A:107:THR:HB	1:A:110:GLU:CG	2.36	0.55
1:A:193:ARG:NH2	1:A:197:LYS:HE3	2.22	0.55
1:C:207:LYS:HB3	1:C:236:ASP:HB2	1.88	0.55
1:A:198:LYS:HB2	4:A:478:HOH:O	2.06	0.54
1:C:155:THR:O	1:C:181:ASN:HA	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:135:GLU:HG3	1:C:159:THR:HG23	1.89	0.54
1:D:115:THR:O	1:D:119:SER:HA	2.07	0.54
1:A:365:THR:HG22	1:A:383:SER:HB2	1.88	0.54
1:B:390:LYS:HG2	1:B:391:LYS:N	2.23	0.54
1:A:306:GLN:O	1:A:308:SER:CA	2.55	0.54
1:A:348:SER:O	1:A:349:LYS:O	2.26	0.54
1:D:139:VAL:CA	1:D:142:MSE:HE3	2.27	0.54
1:A:307:ASP:N	1:A:307:ASP:OD1	2.39	0.54
1:A:358:GLY:C	1:A:387:VAL:HG13	2.28	0.54
1:A:243:THR:CG2	1:A:246:ALA:H	2.06	0.54
1:B:135:GLU:HG3	1:B:159:THR:HG23	1.90	0.54
1:A:305:TYR:HH	1:A:343:GLN:HG3	1.65	0.54
1:D:238:LEU:HD23	1:D:251:VAL:HG12	1.90	0.54
1:A:330:LEU:HD11	1:A:342:VAL:HG21	1.89	0.54
1:A:365:THR:HG22	1:A:383:SER:CB	2.37	0.54
1:C:228:MSE:HB3	1:C:229:PRO:HD2	1.89	0.54
1:A:305:TYR:C	1:A:305:TYR:CD1	2.82	0.53
1:A:336:ASN:O	1:A:337:GLN:C	2.38	0.53
1:D:276:TYR:HB3	3:D:482:IOD:I	2.77	0.53
1:B:250:PHE:HB2	1:B:278:ARG:CD	2.38	0.53
1:B:160:THR:OG1	1:B:162:LEU:HD12	2.07	0.53
1:C:243:THR:HG21	1:C:246:ALA:HB2	1.90	0.53
1:C:285:LEU:O	1:C:289:ILE:HG12	2.08	0.53
1:C:251:VAL:HA	1:C:263:THR:O	2.08	0.53
1:B:163:ASN:OD1	1:B:165:GLU:HG3	2.08	0.53
1:A:248:GLU:HG2	1:A:278:ARG:HH21	1.72	0.53
1:D:236:ASP:OD1	1:D:260:ARG:NH2	2.41	0.53
1:B:193:ARG:O	1:B:197:LYS:HG3	2.07	0.53
1:C:274:ASN:ND2	1:C:280:THR:OG1	2.38	0.53
1:D:303:ASP:O	1:D:323:VAL:HA	2.09	0.53
1:D:257:LYS:CE	1:D:290:SER:O	2.57	0.53
1:C:111:LEU:HD22	1:C:123:ALA:HA	1.90	0.53
1:A:332:GLU:HG2	1:A:333:ARG:O	2.08	0.53
1:B:267:ASN:O	1:B:267:ASN:ND2	2.41	0.53
1:C:107:THR:HG22	1:C:109:GLU:H	1.73	0.53
1:B:342:VAL:HB	1:B:366:TYR:HB2	1.90	0.52
1:B:297:LYS:HB3	1:B:329:TYR:CE2	2.44	0.52
1:D:107:THR:HG22	1:D:110:GLU:N	2.19	0.52
1:A:217:THR:HG23	4:A:510:HOH:O	2.08	0.52
1:B:145:LYS:HD2	1:B:149:TRP:CE2	2.44	0.52
1:A:299:VAL:CG2	1:A:305:TYR:HB2	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:341:SER:O	1:D:367:GLU:HG3	2.09	0.52
1:B:243:THR:HG22	1:B:246:ALA:CB	2.26	0.52
1:D:323:VAL:O	1:D:386:MSE:HE3	2.09	0.52
1:D:107:THR:HG23	1:D:109:GLU:N	2.25	0.52
1:D:107:THR:HG23	1:D:109:GLU:H	1.74	0.52
1:D:45:GLU:HG3	3:D:481:IOD:I	2.79	0.52
1:B:341:SER:C	1:B:343:GLN:HG2	2.30	0.52
1:C:312:VAL:HG22	1:C:320:VAL:CG2	2.40	0.52
1:A:286:MSE:CE	1:A:289:ILE:HB	2.39	0.52
1:B:36:GLU:CG	1:B:331:ILE:HD11	2.39	0.52
1:A:180:GLU:OE2	1:A:245:LYS:HD2	2.10	0.52
1:D:184:SER:O	1:D:188:VAL:HG23	2.09	0.52
1:C:315:GLY:N	1:C:318:ASP:OD2	2.41	0.52
1:D:63:VAL:HG21	1:D:116:LEU:CD2	2.36	0.52
1:A:163:ASN:HD22	1:A:180:GLU:HG3	1.74	0.52
1:C:165:GLU:HG3	1:C:177:LYS:O	2.10	0.52
1:D:323:VAL:N	1:D:386:MSE:HE2	2.24	0.52
1:D:83:ILE:CD1	1:D:106:TYR:HD1	2.22	0.52
1:D:56:SER:HB2	4:D:585:HOH:O	2.09	0.52
1:D:67:TYR:HA	1:D:70:LEU:HD12	1.92	0.52
1:A:310:ALA:CB	1:A:361:VAL:HG12	2.39	0.51
1:A:247:GLY:HA3	1:A:267:ASN:ND2	2.25	0.51
1:D:51:PRO:HG3	1:D:153:ASP:OD2	2.11	0.51
1:B:90:LEU:HD22	1:B:91:THR:N	2.24	0.51
1:C:41:LYS:HB2	1:C:376:TYR:CE2	2.46	0.51
1:D:100:PRO:O	1:D:102:GLU:N	2.43	0.51
1:D:203:LEU:O	1:D:207:LYS:HB2	2.11	0.51
1:A:333:ARG:HB3	1:A:336:ASN:CG	2.31	0.51
1:B:247:GLY:N	1:B:267:ASN:HB2	2.26	0.51
1:D:308:SER:CB	1:D:322:ALA:HB2	2.40	0.51
1:D:366:TYR:CE2	1:D:368:ASP:HB2	2.46	0.51
1:D:294:THR:HG22	1:D:295:LEU:N	2.26	0.51
1:A:297:LYS:HB2	1:A:329:TYR:CE2	2.46	0.51
1:D:304:ALA:CB	1:D:322:ALA:HB3	2.40	0.51
1:D:263:THR:OG1	1:D:286:MSE:HE3	2.10	0.51
1:D:101:MSE:HB2	1:D:106:TYR:CE1	2.45	0.51
1:C:243:THR:CG2	1:C:246:ALA:CA	2.88	0.51
1:B:162:LEU:HD22	1:B:166:THR:HG21	1.93	0.51
1:A:58:THR:HG21	1:A:181:ASN:ND2	2.26	0.51
1:A:334:VAL:O	1:A:334:VAL:CG2	2.59	0.51
1:C:121:ASN:O	1:C:125:ILE:HG13	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:45:GLU:HG3	3:B:472:IOD:I	2.82	0.50
1:B:63:VAL:HG21	1:B:116:LEU:CD2	2.30	0.50
1:A:84:SER:O	1:A:87:PRO:HD2	2.12	0.50
1:C:163:ASN:HD22	1:C:180:GLU:HG3	1.76	0.50
1:C:121:ASN:ND2	1:C:162:LEU:HD21	2.27	0.50
1:C:63:VAL:HG21	1:C:116:LEU:CD2	2.30	0.50
1:B:47:ASP:O	1:B:47:ASP:OD1	2.29	0.50
1:A:346:PRO:HB3	1:D:152:GLN:HB3	1.94	0.50
1:A:95:GLU:HA	1:A:95:GLU:OE1	2.11	0.50
1:A:299:VAL:HG22	1:A:305:TYR:HB2	1.94	0.50
1:B:299:VAL:CG2	1:B:328:ILE:HB	2.41	0.50
1:B:107:THR:HG23	1:B:109:GLU:N	2.27	0.50
1:C:298:ILE:HG21	1:C:330:LEU:HD12	1.92	0.50
1:A:286:MSE:HE3	1:A:289:ILE:HD12	1.93	0.50
1:A:139:VAL:HA	1:A:142:MSE:CG	2.41	0.50
1:B:27:ILE:HG22	1:B:46:LYS:HD2	1.94	0.50
1:A:355:LEU:O	1:A:391:LYS:HA	2.11	0.50
1:A:306:GLN:O	1:A:308:SER:N	2.45	0.49
1:B:87:PRO:HG3	1:B:125:ILE:CG2	2.43	0.49
1:C:121:ASN:OD1	1:C:160:THR:HG23	2.10	0.49
1:D:223:TYR:CD1	1:D:228:MSE:HE3	2.47	0.49
1:B:360:VAL:O	1:B:360:VAL:HG22	2.12	0.49
1:C:117:VAL:O	1:C:220:SER:HA	2.12	0.49
1:B:238:LEU:HD12	1:B:251:VAL:CG1	2.43	0.49
1:B:33:ILE:HG22	1:B:264:VAL:HB	1.94	0.49
1:B:261:VAL:CG1	1:B:286:MSE:HE1	2.40	0.49
1:B:27:ILE:HD12	1:B:285:LEU:HD22	1.93	0.49
1:B:107:THR:CG2	1:B:110:GLU:H	2.22	0.49
1:D:182:LYS:C	1:D:183:LEU:HD12	2.32	0.49
1:D:83:ILE:HD13	1:D:101:MSE:SE	2.62	0.49
1:B:142:MSE:HE2	1:B:156:VAL:HG11	1.94	0.49
1:A:87:PRO:HG3	1:A:125:ILE:CG2	2.42	0.49
1:B:238:LEU:O	1:B:239:LYS:HB3	2.12	0.49
1:D:323:VAL:N	1:D:386:MSE:CE	2.76	0.49
1:D:324:ALA:HA	1:D:386:MSE:HE3	1.93	0.49
1:C:86:TYR:CB	1:C:87:PRO:HD3	2.43	0.49
1:A:153:ASP:HB3	1:D:344:PHE:CZ	2.47	0.49
1:A:358:GLY:CA	1:A:387:VAL:HG13	2.43	0.49
1:C:236:ASP:OD1	1:C:260:ARG:NH2	2.45	0.49
1:A:270:HIS:O	1:B:74:SER:HA	2.13	0.49
1:B:56:SER:O	1:B:239:LYS:HD3	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:121:ASN:OD1	1:C:160:THR:CG2	2.60	0.49
1:D:243:THR:HG21	1:D:246:ALA:HB2	1.95	0.49
1:A:176:LYS:H	1:A:179:GLU:HG3	1.78	0.49
1:D:304:ALA:HB2	1:D:322:ALA:HB1	1.86	0.48
1:C:54:ILE:HD13	1:C:183:LEU:HB2	1.95	0.48
1:D:54:ILE:HD13	1:D:183:LEU:HD22	1.95	0.48
1:C:182:LYS:O	1:C:183:LEU:HD12	2.13	0.48
1:C:151:ILE:HG23	1:C:187:ASP:OD1	2.13	0.48
1:C:32:ALA:HA	1:C:264:VAL:O	2.14	0.48
1:D:259:MSE:HE3	1:D:261:VAL:HG22	1.96	0.48
1:B:86:TYR:CZ	1:B:125:ILE:HD13	2.49	0.48
1:D:59:LYS:HD3	1:D:115:THR:HG23	1.95	0.48
1:B:182:LYS:O	1:B:183:LEU:HD12	2.14	0.48
1:A:366:TYR:HB3	1:A:382:PRO:HG2	1.94	0.48
1:A:135:GLU:HG3	1:A:159:THR:HG23	1.95	0.48
1:B:303:ASP:C	1:B:323:VAL:HB	2.34	0.48
1:D:299:VAL:HG12	1:D:324:ALA:HB2	1.95	0.48
1:C:312:VAL:O	1:C:318:ASP:HB2	2.13	0.48
1:A:306:GLN:O	1:A:307:ASP:C	2.51	0.48
1:D:324:ALA:HB1	1:D:328:ILE:HD12	1.95	0.48
1:C:65:LEU:HD21	1:C:145:LYS:HG3	1.95	0.48
1:A:94:SER:O	1:A:96:ALA:N	2.42	0.48
1:A:36:GLU:HG3	1:A:331:ILE:HD11	1.96	0.48
1:A:142:MSE:HE2	1:A:156:VAL:CG1	2.43	0.48
1:A:358:GLY:CA	1:A:387:VAL:CG1	2.92	0.48
1:C:145:LYS:HD2	1:C:149:TRP:CE2	2.48	0.48
1:C:298:ILE:CG2	1:C:330:LEU:HD12	2.43	0.48
1:D:243:THR:CG2	1:D:246:ALA:CA	2.92	0.47
1:C:182:LYS:C	1:C:183:LEU:HD12	2.35	0.47
1:A:107:THR:HG22	1:A:110:GLU:N	2.21	0.47
1:A:45:GLU:CG	4:A:480:HOH:O	2.62	0.47
1:A:117:VAL:O	1:A:220:SER:HA	2.14	0.47
1:C:198:LYS:C	1:C:200:PRO:HD3	2.34	0.47
1:D:332:GLU:HB2	1:D:340:GLN:NE2	2.28	0.47
1:A:45:GLU:HG2	4:A:480:HOH:O	2.14	0.47
1:B:384:PHE:CD1	1:B:384:PHE:N	2.83	0.47
1:C:90:LEU:HD23	1:C:90:LEU:HA	1.76	0.47
1:B:77:LEU:HB3	1:B:109:GLU:HB2	1.96	0.47
1:C:267:ASN:ND2	4:C:575:HOH:O	2.47	0.47
1:C:297:LYS:HD2	1:C:327:ASP:OD2	2.14	0.47
1:D:342:VAL:HA	1:D:366:TYR:HA	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:360:VAL:O	1:B:360:VAL:CG2	2.63	0.47
1:B:107:THR:HG22	1:B:110:GLU:N	2.21	0.47
1:B:238:LEU:O	1:B:239:LYS:CB	2.60	0.47
1:A:107:THR:HG22	1:A:109:GLU:N	2.30	0.47
1:D:234:GLY:O	1:D:254:THR:HA	2.15	0.47
1:D:84:SER:O	1:D:87:PRO:HD2	2.15	0.47
1:C:30:LYS:HB2	1:C:267:ASN:HB3	1.97	0.47
1:D:62:THR:O	1:D:66:VAL:HG23	2.15	0.47
1:C:237:GLY:CA	1:C:253:THR:HG22	2.44	0.47
1:A:223:TYR:CD1	1:A:228:MSE:HE2	2.50	0.47
1:C:59:LYS:HD3	1:C:115:THR:HG23	1.97	0.46
1:B:107:THR:HG23	1:B:109:GLU:H	1.80	0.46
1:D:139:VAL:HG22	1:D:142:MSE:CE	2.44	0.46
1:C:86:TYR:CZ	1:C:125:ILE:HD13	2.51	0.46
1:A:297:LYS:HD3	1:A:329:TYR:CZ	2.50	0.46
1:C:87:PRO:HG3	1:C:125:ILE:CG2	2.46	0.46
1:D:37:ALA:HB3	1:D:260:ARG:HG2	1.97	0.46
1:B:27:ILE:CG2	1:B:46:LYS:HD2	2.45	0.46
1:C:193:ARG:NH2	1:C:197:LYS:HE3	2.30	0.46
1:A:163:ASN:HD22	1:A:180:GLU:CG	2.29	0.46
1:B:299:VAL:HG23	1:B:328:ILE:HB	1.97	0.46
1:D:85:ASP:O	1:D:89:GLN:HG3	2.16	0.46
1:A:111:LEU:HD22	1:A:123:ALA:HA	1.97	0.46
1:D:58:THR:HG21	1:D:181:ASN:ND2	2.30	0.46
1:C:57:ILE:HD13	1:C:251:VAL:HG23	1.96	0.46
1:A:313:GLN:O	1:A:314:ASP:CG	2.54	0.46
1:B:232:ARG:NH1	1:B:256:GLU:OE2	2.48	0.46
1:A:30:LYS:HB2	1:A:267:ASN:HB3	1.97	0.46
1:D:384:PHE:CD1	1:D:384:PHE:N	2.83	0.46
1:C:310:ALA:O	1:C:320:VAL:HG23	2.16	0.46
1:D:259:MSE:SE	1:D:295:LEU:HD11	2.66	0.46
1:B:84:SER:O	1:B:87:PRO:HD2	2.16	0.46
1:A:361:VAL:HG12	1:A:361:VAL:O	2.16	0.46
1:A:325:PRO:O	1:A:326:GLU:CG	2.63	0.46
1:D:36:GLU:CG	1:D:331:ILE:HD11	2.45	0.46
1:B:87:PRO:HG3	1:B:125:ILE:HG21	1.98	0.46
1:A:45:GLU:HG3	3:A:468:IOD:I	2.86	0.45
1:C:77:LEU:O	1:C:107:THR:CG2	2.64	0.45
4:A:604:HOH:O	1:D:45:GLU:HG2	2.16	0.45
1:A:247:GLY:HA3	1:A:267:ASN:HD21	1.81	0.45
1:D:278:ARG:HH11	1:D:278:ARG:HD3	1.56	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:143:ARG:HG2	1:D:156:VAL:CG1	2.46	0.45
1:D:257:LYS:HE3	4:D:487:HOH:O	2.15	0.45
1:D:292:THR:O	1:D:334:VAL:HG23	2.16	0.45
1:C:110:GLU:HB3	1:C:213:PHE:CE1	2.51	0.45
1:B:260:ARG:HD2	4:B:570:HOH:O	2.17	0.45
1:C:145:LYS:HD2	1:C:149:TRP:CZ2	2.51	0.45
1:B:142:MSE:HE2	1:B:156:VAL:CG1	2.46	0.45
1:B:56:SER:HB2	1:B:241:GLY:HA2	1.98	0.45
1:C:298:ILE:HG13	1:C:299:VAL:N	2.30	0.45
1:B:118:SER:OG	1:B:218:ILE:HB	2.16	0.45
1:D:305:TYR:O	1:D:306:GLN:O	2.34	0.45
1:B:182:LYS:C	1:B:183:LEU:HD12	2.37	0.45
1:A:378:THR:O	1:A:381:ARG:NH1	2.50	0.45
1:B:86:TYR:CB	1:B:87:PRO:HD3	2.41	0.45
1:A:228:MSE:HE2	1:A:229:PRO:HD2	1.98	0.45
1:D:116:LEU:HD12	1:D:205:ILE:HG21	1.99	0.45
1:A:298:ILE:HD13	1:A:330:LEU:HD11	1.98	0.45
1:A:223:TYR:HD1	1:A:228:MSE:HE2	1.82	0.45
1:D:119:SER:HB3	1:D:239:LYS:CE	2.48	0.44
1:C:107:THR:HB	1:C:110:GLU:CG	2.43	0.44
1:A:193:ARG:HD2	1:A:377:ILE:HD11	1.98	0.44
1:C:364:LEU:O	1:C:383:SER:HA	2.18	0.44
1:A:96:ALA:HB1	1:A:121:ASN:HD22	1.82	0.44
1:C:321:ILE:O	1:C:389:ASP:HB2	2.17	0.44
1:C:263:THR:HG21	1:C:282:THR:CG2	2.38	0.44
1:B:360:VAL:HA	1:B:387:VAL:HA	2.00	0.44
1:A:302:GLY:C	1:A:323:VAL:HG13	2.38	0.44
1:A:139:VAL:HA	1:A:142:MSE:HG2	2.00	0.44
1:C:193:ARG:HD3	4:C:491:HOH:O	2.18	0.44
1:B:361:VAL:HG21	1:B:388:ALA:HB2	1.99	0.44
1:A:343:GLN:O	1:A:344:PHE:CD2	2.70	0.44
1:B:390:LYS:HG2	1:B:391:LYS:H	1.81	0.44
1:B:32:ALA:HA	1:B:264:VAL:O	2.16	0.44
1:A:57:ILE:HD13	1:A:251:VAL:HG23	2.00	0.44
1:B:54:ILE:HB	1:B:57:ILE:HB	2.00	0.44
1:B:365:THR:HA	1:B:382:PRO:O	2.17	0.44
1:B:107:THR:CG2	1:B:109:GLU:HB3	2.47	0.44
1:A:271:GLN:HA	1:B:73:GLY:O	2.18	0.44
1:C:87:PRO:HG3	1:C:125:ILE:HG21	2.00	0.44
1:D:156:VAL:HA	1:D:181:ASN:OD1	2.18	0.44
1:A:312:VAL:HG22	1:A:351:ILE:HD13	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:121:ASN:ND2	1:A:162:LEU:HD21	2.32	0.44
1:D:304:ALA:HA	1:D:322:ALA:HB1	2.00	0.44
1:A:236:ASP:N	1:A:236:ASP:OD1	2.51	0.44
1:D:333:ARG:NH2	4:D:547:HOH:O	2.41	0.43
1:C:61:ILE:HD11	1:C:183:LEU:HD21	2.00	0.43
1:C:92:THR:OG1	1:C:93:ASN:N	2.50	0.43
1:D:324:ALA:HB1	1:D:326:GLU:O	2.17	0.43
1:D:61:ILE:HD11	1:D:183:LEU:HD21	2.00	0.43
1:A:387:VAL:CG1	1:A:388:ALA:N	2.80	0.43
1:B:341:SER:CA	1:B:343:GLN:HG2	2.48	0.43
1:A:163:ASN:ND2	1:A:180:GLU:HG3	2.33	0.43
1:A:53:GLU:HG2	1:A:245:LYS:HB2	1.99	0.43
1:A:95:GLU:OE1	1:A:95:GLU:CA	2.67	0.43
1:B:72:ASN:C	1:B:72:ASN:OD1	2.57	0.43
1:D:371:LEU:HA	4:D:514:HOH:O	2.18	0.43
1:A:351:ILE:O	1:A:352:PRO:C	2.57	0.43
1:A:393:GLU:HG2	1:A:393:GLU:O	2.18	0.43
1:B:301:GLN:HG3	1:B:326:GLU:HA	1.99	0.43
1:C:69:ALA:HA	1:C:72:ASN:HD22	1.84	0.43
1:D:60:LEU:HD21	1:D:239:LYS:HB2	2.00	0.43
1:B:239:LYS:HG3	1:B:240:THR:O	2.19	0.43
1:B:364:LEU:O	1:B:384:PHE:HD1	2.01	0.43
1:D:250:PHE:HB2	1:D:278:ARG:CD	2.48	0.43
1:B:53:GLU:HB3	1:B:246:ALA:HB2	2.00	0.43
1:C:314:ASP:OD1	1:C:314:ASP:O	2.37	0.43
1:B:237:GLY:CA	1:B:253:THR:CG2	2.54	0.42
1:C:45:GLU:HG3	3:C:476:IOD:I	2.89	0.42
1:B:41:LYS:HB2	1:B:376:TYR:CE2	2.53	0.42
1:A:344:PHE:C	1:A:345:THR:HA	2.32	0.42
1:B:253:THR:HG23	1:B:253:THR:O	2.18	0.42
1:D:238:LEU:HB3	1:D:239:LYS:H	1.65	0.42
1:D:237:GLY:O	1:D:252:GLY:HA2	2.18	0.42
1:A:243:THR:HG21	1:A:246:ALA:HB2	2.00	0.42
1:B:145:LYS:HD3	1:B:148:GLU:OE1	2.20	0.42
1:B:236:ASP:OD1	1:B:260:ARG:NH2	2.52	0.42
1:C:67:TYR:HB3	1:C:199:TYR:CD1	2.54	0.42
1:C:316:LYS:O	1:C:317:GLU:HG3	2.19	0.42
1:C:176:LYS:CB	1:C:179:GLU:HG3	2.40	0.42
1:A:51:PRO:HG3	1:A:153:ASP:OD2	2.20	0.42
1:C:364:LEU:HA	1:C:364:LEU:HD23	1.91	0.42
1:B:136:LYS:NZ	1:B:140:ASP:OD2	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:100:PRO:HD2	1:C:216:MSE:SE	2.69	0.42
1:D:366:TYR:HB3	1:D:382:PRO:HB2	2.00	0.42
1:A:107:THR:CB	1:A:110:GLU:HG3	2.40	0.42
1:C:163:ASN:HA	1:C:180:GLU:HG2	2.01	0.42
1:A:118:SER:OG	1:A:218:ILE:HB	2.19	0.42
1:B:232:ARG:HB3	1:B:235:PHE:HD2	1.85	0.42
1:C:33:ILE:HG22	1:C:264:VAL:HB	2.02	0.42
1:D:286:MSE:CE	1:D:289:ILE:HD12	2.46	0.42
1:B:380:GLU:O	1:B:381:ARG:HD2	2.19	0.42
1:D:211:SER:OG	1:D:212:THR:N	2.50	0.42
1:B:340:GLN:HB2	1:B:342:VAL:HG12	2.01	0.42
1:D:386:MSE:HB3	1:D:386:MSE:HE2	1.77	0.42
1:B:48:ALA:O	1:B:186:TYR:HB2	2.20	0.42
1:C:142:MSE:SE	1:C:159:THR:HG22	2.70	0.42
1:A:323:VAL:CG1	1:A:324:ALA:N	2.83	0.42
1:C:36:GLU:HG3	1:C:331:ILE:HD11	2.02	0.42
1:A:86:TYR:CZ	1:A:125:ILE:HD13	2.55	0.41
1:C:298:ILE:CG2	1:C:330:LEU:CD1	2.97	0.41
1:B:33:ILE:HA	1:B:44:TYR:O	2.20	0.41
1:B:254:THR:OG1	1:B:255:VAL:N	2.53	0.41
1:C:35:VAL:HG12	1:C:42:ILE:HA	2.02	0.41
1:B:50:GLN:HA	1:B:51:PRO:HD3	1.84	0.41
1:B:99:ILE:HA	1:B:100:PRO:HD3	1.82	0.41
1:B:86:TYR:CE2	1:B:125:ILE:HD13	2.55	0.41
1:D:292:THR:C	1:D:334:VAL:HG23	2.41	0.41
1:C:103:ALA:HB3	1:C:106:TYR:CZ	2.54	0.41
1:D:341:SER:O	1:D:343:GLN:N	2.49	0.41
1:C:38:ASN:HA	1:C:197:LYS:HE2	2.02	0.41
1:A:344:PHE:HA	1:A:345:THR:N	2.33	0.41
1:B:286:MSE:CE	1:B:289:ILE:HD12	2.43	0.41
1:C:96:ALA:HB1	1:C:121:ASN:HD22	1.85	0.41
1:D:37:ALA:CB	1:D:260:ARG:HG2	2.50	0.41
1:B:308:SER:HB3	1:B:322:ALA:HB3	2.02	0.41
1:C:273:ASN:HD22	1:C:273:ASN:HA	1.60	0.41
1:A:164:ASN:HB3	1:A:171:ILE:HG21	2.02	0.41
1:A:37:ALA:CB	1:A:260:ARG:HG2	2.50	0.41
1:D:322:ALA:O	1:D:323:VAL:HB	2.21	0.41
1:D:342:VAL:CG2	1:D:342:VAL:O	2.62	0.41
1:A:86:TYR:CB	1:A:87:PRO:HD3	2.50	0.41
1:B:59:LYS:HD3	1:B:115:THR:CG2	2.50	0.41
1:A:54:ILE:HD13	1:A:183:LEU:HB2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:298:ILE:HD13	1:D:330:LEU:CG	2.48	0.41
1:A:41:LYS:HB2	1:A:376:TYR:CE2	2.56	0.41
1:B:232:ARG:NH2	1:B:287:ASP:OD1	2.54	0.41
1:D:102:GLU:H	1:D:102:GLU:HG2	1.49	0.41
1:A:321:ILE:HG22	1:A:323:VAL:HG23	2.03	0.41
1:A:54:ILE:CD1	1:A:183:LEU:HD13	2.51	0.41
1:B:208:LYS:HA	1:B:209:PRO:HD3	1.76	0.41
1:D:47:ASP:HA	4:D:506:HOH:O	2.20	0.41
1:C:308:SER:HB2	1:C:322:ALA:O	2.20	0.41
1:A:184:SER:O	1:A:188:VAL:HG23	2.20	0.41
1:C:186:TYR:CE1	1:C:377:ILE:HG22	2.56	0.41
1:A:313:GLN:CG	1:A:313:GLN:O	2.52	0.41
1:D:83:ILE:HD11	1:D:106:TYR:CD1	2.47	0.41
1:D:208:LYS:HA	1:D:209:PRO:HD3	1.91	0.41
1:D:121:ASN:O	1:D:125:ILE:HG13	2.21	0.41
1:B:139:VAL:HA	1:B:142:MSE:CG	2.51	0.40
1:C:310:ALA:CB	1:C:361:VAL:CG2	2.99	0.40
1:D:86:TYR:CB	1:D:87:PRO:HD3	2.47	0.40
1:D:83:ILE:CD1	1:D:106:TYR:CD1	3.03	0.40
1:C:366:TYR:HB3	1:C:382:PRO:HB2	2.02	0.40
1:D:186:TYR:CE1	1:D:377:ILE:HG22	2.57	0.40
1:C:164:ASN:HD22	1:C:179:GLU:HB2	1.85	0.40
1:B:145:LYS:HD3	1:B:145:LYS:HA	1.83	0.40
1:D:29:ALA:O	1:D:46:LYS:HE2	2.21	0.40
1:C:118:SER:OG	1:C:218:ILE:HB	2.22	0.40
1:D:139:VAL:HG13	1:D:156:VAL:HG22	2.02	0.40
1:D:304:ALA:HB2	1:D:322:ALA:HB3	2.02	0.40
1:A:363:HIS:CD2	1:A:385:GLU:HG2	2.56	0.40
1:B:57:ILE:HG12	1:B:251:VAL:HG23	2.04	0.40
1:A:334:VAL:HG23	1:A:334:VAL:O	2.21	0.40
1:A:340:GLN:HG3	1:A:340:GLN:H	1.65	0.40
1:B:103:ALA:HB3	1:B:106:TYR:CZ	2.56	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:51:PRO:CD	1:C:344:PHE:CZ[3_545]	1.79	0.41

## 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	367/379 (97%)	329 (90%)	31 (8%)	7 (2%)	10	32
1	B	331/379 (87%)	290 (88%)	33 (10%)	8 (2%)	7	25
1	C	353/379 (93%)	320 (91%)	29 (8%)	4 (1%)	17	50
1	D	309/379 (82%)	280 (91%)	22 (7%)	7 (2%)	8	26
All	All	1360/1516 (90%)	1219 (90%)	115 (8%)	26 (2%)	10	32

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	307	ASP
1	A	337	GLN
1	B	93	ASN
1	B	247	GLY
1	B	306	GLN
1	B	307	ASP
1	C	314	ASP
1	C	319	THR
1	D	101	MSE
1	D	238	LEU
1	D	306	GLN
1	A	314	ASP
1	A	325	PRO
1	B	238	LEU
1	B	267	ASN
1	D	237	GLY
1	A	236	ASP
1	A	343	GLN
1	D	307	ASP
1	A	306	GLN
1	B	277	ALA
1	B	339	SER

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Mol	Chain	Res	Type
1	C	56	SER
1	C	236	ASP
1	D	342	VAL
1	D	346	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	310/308 (101%)	279 (90%)	31 (10%)	9	27
1	B	286/308 (93%)	247 (86%)	39 (14%)	5	14
1	C	302/308 (98%)	275 (91%)	27 (9%)	12	34
1	D	272/308 (88%)	244 (90%)	28 (10%)	9	26
All	All	1170/1232 (95%)	1045 (89%)	125 (11%)	8	24

All (125) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	GLU
1	A	104	ARG
1	A	107	THR
1	A	112	LEU
1	A	113	GLU
1	A	169	ASP
1	A	201	GLN
1	A	212	THR
1	A	228	MSE
1	A	260	ARG
1	A	266	LEU
1	A	267	ASN
1	A	286	MSE
1	A	300	GLN
1	A	307	ASP
1	A	311	PRO
1	A	319	THR

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Mol	Chain	Res	Type
1	A	320	VAL
1	A	333	ARG
1	A	334	VAL
1	A	338	SER
1	A	340	GLN
1	A	342	VAL
1	A	343	GLN
1	A	344	PHE
1	A	345	THR
1	A	347	ASP
1	A	348	SER
1	A	349	LYS
1	A	351	ILE
1	A	389	ASP
1	B	45	GLU
1	B	46	LYS
1	B	49	THR
1	B	50	GLN
1	B	90	LEU
1	B	93	ASN
1	B	97	SER
1	B	98	ASN
1	B	99	ILE
1	B	101	MSE
1	B	107	THR
1	B	112	LEU
1	B	145	LYS
1	B	201	GLN
1	B	232	ARG
1	B	235	PHE
1	B	238	LEU
1	B	239	LYS
1	B	260	ARG
1	B	263	THR
1	B	267	ASN
1	B	270	HIS
1	B	275	PRO
1	B	284	SER
1	B	299	VAL
1	B	301	GLN
1	B	307	ASP
1	B	338	SER

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Mol	Chain	Res	Type
1	B	339	SER
1	B	340	GLN
1	B	341	SER
1	B	343	GLN
1	B	344	PHE
1	B	347	ASP
1	B	360	VAL
1	B	361	VAL
1	B	363	HIS
1	B	364	LEU
1	B	379	THR
1	C	45	GLU
1	C	56	SER
1	C	90	LEU
1	C	92	THR
1	C	94	SER
1	C	97	SER
1	C	98	ASN
1	C	99	ILE
1	C	145	LYS
1	C	201	GLN
1	C	207	LYS
1	C	232	ARG
1	C	239	LYS
1	C	260	ARG
1	C	267	ASN
1	C	273	ASN
1	C	307	ASP
1	C	311	PRO
1	C	312	VAL
1	C	319	THR
1	C	320	VAL
1	C	342	VAL
1	C	344	PHE
1	C	347	ASP
1	C	348	SER
1	C	355	LEU
1	C	390	LYS
1	D	45	GLU
1	D	56	SER
1	D	91	THR
1	D	99	ILE

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Mol	Chain	Res	Type
1	D	102	GLU
1	D	107	THR
1	D	112	LEU
1	D	201	GLN
1	D	212	THR
1	D	216	MSE
1	D	236	ASP
1	D	238	LEU
1	D	239	LYS
1	D	244	ASP
1	D	260	ARG
1	D	263	THR
1	D	270	HIS
1	D	276	TYR
1	D	278	ARG
1	D	284	SER
1	D	300	GLN
1	D	306	GLN
1	D	308	SER
1	D	323	VAL
1	D	344	PHE
1	D	345	THR
1	D	347	ASP
1	D	386	MSE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	50	GLN
1	A	152	GLN
1	A	267	ASN
1	A	313	GLN
1	A	336	ASN
1	A	337	GLN
1	A	343	GLN
1	B	170	ASN
1	B	340	GLN
1	B	343	GLN
1	B	363	HIS
1	C	72	ASN
1	C	267	ASN
1	C	273	ASN

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Mol	Chain	Res	Type
1	C	274	ASN
1	D	50	GLN
1	D	300	GLN
1	D	306	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 20 ligands modelled in this entry, 16 are monoatomic - leaving 4 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	464	-	4,4,4	0.25	0	6,6,6	0.15	0
2	SO4	B	465	-	4,4,4	0.22	0	6,6,6	0.17	0
2	SO4	C	466	-	4,4,4	0.24	0	6,6,6	0.13	0
2	SO4	D	467	-	4,4,4	0.21	0	6,6,6	0.08	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	464	-	-	0/0/0/0	0/0/0/0
2	SO4	B	465	-	-	0/0/0/0	0/0/0/0
2	SO4	C	466	-	-	0/0/0/0	0/0/0/0
2	SO4	D	467	-	-	0/0/0/0	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.

No monomer is involved in short contacts.

## 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	360/379 (94%)	0.11	20 (5%) 28 18	7, 20, 65, 82	0
1	B	323/379 (85%)	0.25	25 (7%) 16 8	9, 22, 72, 85	0
1	C	341/379 (89%)	0.18	20 (5%) 26 16	9, 23, 67, 88	0
1	D	309/379 (81%)	0.07	20 (6%) 22 13	7, 20, 61, 88	0
All	All	1333/1516 (87%)	0.15	85 (6%) 23 14	7, 22, 68, 88	0

All (85) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	337	GLN	8.3
1	A	318	ASP	7.8
1	C	316	LYS	6.7
1	C	318	ASP	6.1
1	A	338	SER	6.0
1	B	307	ASP	6.0
1	C	317	GLU	5.9
1	A	342	VAL	5.3
1	A	337	GLN	5.0
1	B	308	SER	4.9
1	D	91	THR	4.8
1	B	275	PRO	4.7
1	A	336	ASN	4.6
1	A	314	ASP	4.6
1	C	312	VAL	4.6
1	A	319	THR	4.5
1	B	322	ALA	4.4
1	A	343	GLN	4.4
1	D	342	VAL	4.4
1	B	269	ASP	4.3
1	C	361	VAL	4.2

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Mol	Chain	Res	Type	RSRZ
1	D	347	ASP	4.2
1	C	93	ASN	4.1
1	A	349	LYS	4.1
1	B	321	ILE	4.0
1	D	345	THR	3.9
1	B	342	VAL	3.9
1	B	270	HIS	3.8
1	B	306	GLN	3.8
1	D	322	ALA	3.8
1	C	319	THR	3.8
1	C	355	LEU	3.8
1	A	339	SER	3.7
1	B	344	PHE	3.6
1	C	356	GLU	3.5
1	D	307	ASP	3.5
1	D	344	PHE	3.5
1	C	313	GLN	3.5
1	C	311	PRO	3.4
1	B	323	VAL	3.3
1	A	359	THR	3.3
1	D	306	GLN	3.2
1	A	317	GLU	3.2
1	B	98	ASN	3.2
1	B	343	GLN	3.1
1	D	343	GLN	3.0
1	D	92	THR	3.0
1	B	388	ALA	3.0
1	B	389	ASP	2.9
1	B	391	LYS	2.9
1	D	237	GLY	2.9
1	B	305	TYR	2.8
1	A	307	ASP	2.7
1	D	99	ILE	2.7
1	A	305	TYR	2.6
1	D	303	ASP	2.6
1	B	345	THR	2.5
1	C	320	VAL	2.5
1	D	308	SER	2.5
1	A	347	ASP	2.5
1	A	93	ASN	2.4
1	C	321	ILE	2.4
1	D	169	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	324	ALA	2.4
1	B	300	GLN	2.3
1	B	335	GLY	2.3
1	A	326	GLU	2.3
1	B	346	PRO	2.3
1	C	392	ILE	2.2
1	D	47	ASP	2.2
1	C	345	THR	2.2
1	B	338	SER	2.1
1	C	348	SER	2.1
1	A	95	GLU	2.1
1	A	352	PRO	2.1
1	D	275	PRO	2.1
1	D	325	PRO	2.1
1	C	390	LYS	2.1
1	C	314	ASP	2.1
1	B	99	ILE	2.1
1	D	305	TYR	2.1
1	B	360	VAL	2.1
1	C	307	ASP	2.0
1	A	94	SER	2.0
1	C	332	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 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
2	SO4	A	464	5/5	0.95	0.20	2.54	48,52,54,54	0
2	SO4	D	467	5/5	0.96	0.19	1.21	38,39,41,41	0
2	SO4	C	466	5/5	0.94	0.20	0.81	60,61,63,63	0
2	SO4	B	465	5/5	0.92	0.18	-0.01	48,49,51,52	0
3	IOD	B	474	1/1	0.97	0.24	-0.32	9,9,9,9	1
3	IOD	A	468	1/1	1.00	0.15	-1.26	19,19,19,19	0
3	IOD	D	482	1/1	0.95	0.09	-2.13	56,56,56,56	1
3	IOD	C	476	1/1	1.00	0.12	-2.70	22,22,22,22	0
3	IOD	D	481	1/1	1.00	0.13	-2.96	17,17,17,17	0
3	IOD	B	472	1/1	1.00	0.12	-3.21	19,19,19,19	0
3	IOD	D	483	1/1	0.97	0.15	-	44,44,44,44	1
3	IOD	B	475	1/1	0.94	0.11	-	56,56,56,56	1
3	IOD	A	470	1/1	0.92	0.11	-	66,66,66,66	1
3	IOD	C	477	1/1	0.99	0.10	-	38,38,38,38	0
3	IOD	C	479	1/1	0.94	0.12	-	44,44,44,44	1
3	IOD	C	478	1/1	0.85	0.13	-	76,76,76,76	1
3	IOD	A	471	1/1	0.98	0.14	-	38,38,38,38	1
3	IOD	B	473	1/1	0.99	0.08	-	43,43,43,43	0
3	IOD	D	480	1/1	0.99	0.11	-	43,43,43,43	0
3	IOD	A	469	1/1	0.99	0.12	-	39,39,39,39	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.