



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:27 AM GMT

PDB ID : 2X4M  
Title : Yersinia Pestis Plasminogen Activator Pla  
Authors : Eren, E.; Murphy, M.; Goguen, J.; Van Den Berg, B.  
Deposited on : 2010-02-05  
Resolution : 2.55 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

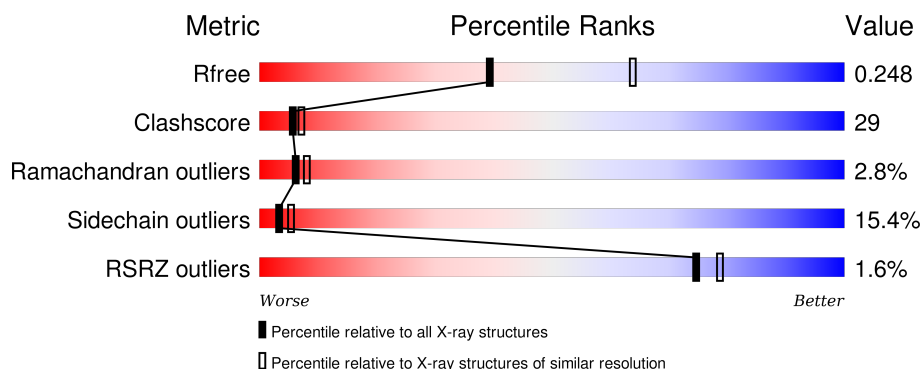
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.55 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	4549 (2.58-2.50)
Clashscore	102246	5292 (2.58-2.50)
Ramachandran outliers	100387	5194 (2.58-2.50)
Sidechain outliers	100360	5196 (2.58-2.50)
RSRZ outliers	91569	4561 (2.58-2.50)

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	298	 49% 41% 7% ..
1	B	298	 4% 52% 34% 9% .
1	C	298	 2% 50% 37% 11% .
1	D	298	 51% 38% 9% ..

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	B	1302	-	-	X	X
2	SO4	D	1295	-	-	-	X
3	C8E	A	1300	-	-	-	X
3	C8E	A	1301	-	-	-	X
3	C8E	A	1302	-	-	-	X
3	C8E	A	1304	-	-	-	X
3	C8E	B	1304	-	-	-	X
3	C8E	B	1306	-	-	-	X
3	C8E	C	1301	-	-	-	X
3	C8E	D	1303	-	-	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9482 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 COAGULASE/FIBRINOLYSIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	293	Total	C	N	O	S	0	0	0
			2305	1450	393	456	6			
1	B	286	Total	C	N	O	S	0	0	0
			2242	1409	384	443	6			
1	C	291	Total	C	N	O	S	0	0	0
			2262	1419	389	448	6			
1	D	293	Total	C	N	O	S	0	0	0
			2305	1450	393	456	6			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	86	ALA	ASP	ENGINEERED MUTATION	UNP P17811
B	86	ALA	ASP	ENGINEERED MUTATION	UNP P17811
C	86	ALA	ASP	ENGINEERED MUTATION	UNP P17811
D	86	ALA	ASP	ENGINEERED MUTATION	UNP P17811
A	293	GLY	-	EXPRESSION TAG	UNP P17811
A	294	GLY	-	EXPRESSION TAG	UNP P17811
A	295	GLY	-	EXPRESSION TAG	UNP P17811
A	296	GLY	-	EXPRESSION TAG	UNP P17811
A	297	GLY	-	EXPRESSION TAG	UNP P17811
A	298	GLY	-	EXPRESSION TAG	UNP P17811
B	293	GLY	-	EXPRESSION TAG	UNP P17811
B	294	GLY	-	EXPRESSION TAG	UNP P17811
B	295	GLY	-	EXPRESSION TAG	UNP P17811
B	296	GLY	-	EXPRESSION TAG	UNP P17811
B	297	GLY	-	EXPRESSION TAG	UNP P17811
B	298	GLY	-	EXPRESSION TAG	UNP P17811
C	293	GLY	-	EXPRESSION TAG	UNP P17811
C	294	GLY	-	EXPRESSION TAG	UNP P17811
C	295	GLY	-	EXPRESSION TAG	UNP P17811
C	296	GLY	-	EXPRESSION TAG	UNP P17811
C	297	GLY	-	EXPRESSION TAG	UNP P17811

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Chain	Residue	Modelled	Actual	Comment	Reference
C	298	GLY	-	EXPRESSION TAG	UNP P17811
D	293	GLY	-	EXPRESSION TAG	UNP P17811
D	294	GLY	-	EXPRESSION TAG	UNP P17811
D	295	GLY	-	EXPRESSION TAG	UNP P17811
D	296	GLY	-	EXPRESSION TAG	UNP P17811
D	297	GLY	-	EXPRESSION TAG	UNP P17811
D	298	GLY	-	EXPRESSION TAG	UNP P17811

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



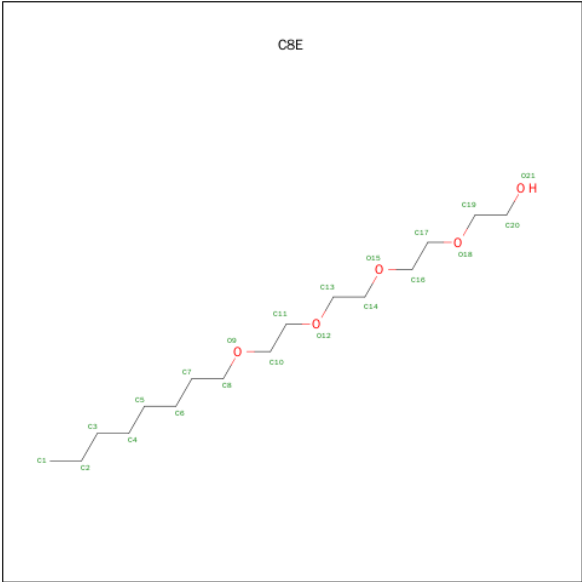
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	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	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
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 (HYDROXYETHYLOXY)TRI(ETHYLOXY)OCTANE (three-letter code: C8E) (formula: C<sub>16</sub>H<sub>34</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			11	10	1		
3	A	1	Total	C	O	0	0
			9	8	1		
3	A	1	Total	C	O	0	0
			9	8	1		
3	A	1	Total	C	O	0	0
			10	9	1		
3	A	1	Total	C		0	0
			8	8			
3	B	1	Total	C		0	0
			8	8			
3	B	1	Total	C	O	0	0
			8	7	1		
3	B	1	Total	C	O	0	0
			11	9	2		
3	C	1	Total	C	O	0	0
			11	10	1		
3	C	1	Total	C	O	0	0
			9	8	1		
3	C	1	Total	C	O	0	0
			9	8	1		
3	D	1	Total	C	O	0	0
			12	10	2		
3	D	1	Total	C	O	0	0
			9	8	1		
3	D	1	Total	C	O	0	0
			9	8	1		

- Molecule 4 is water.

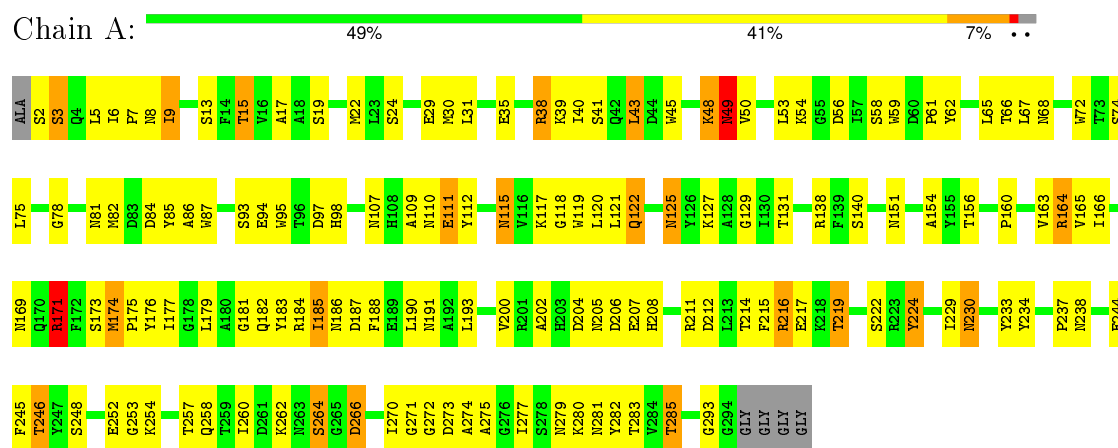
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	33	Total 33	O 33	0	0
4	B	30	Total 30	O 30	0	0
4	C	30	Total 30	O 30	0	0
4	D	27	Total 27	O 27	0	0

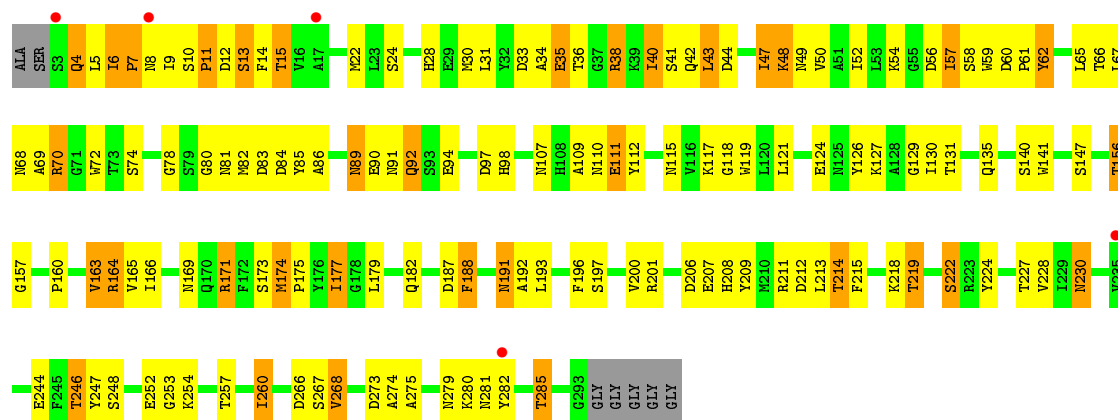


### 3 Residue-property plots

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.

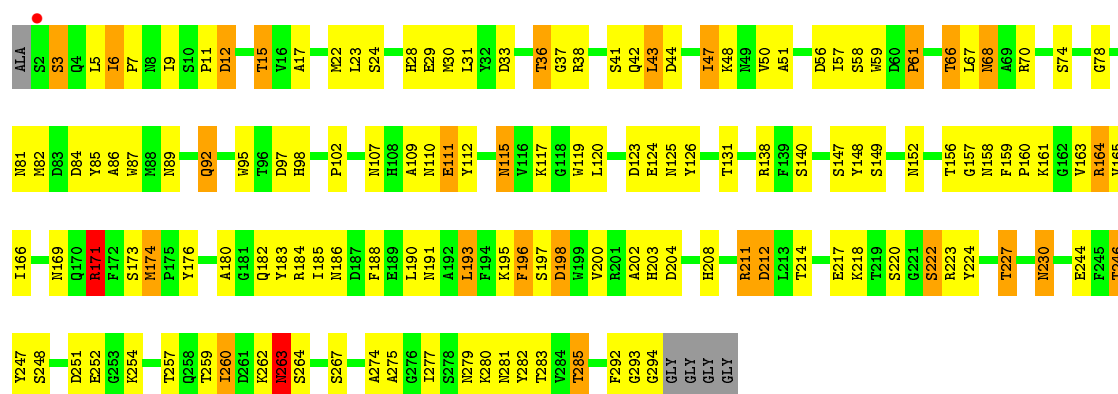
#### • Molecule 1: COAGULASE/FIBRINOLYSIN





• Molecule 1: COAGULASE/FIBRINOLYSIN

Chain D: 51% 38% 9% ..



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	69.91Å 127.82Å 107.17Å 90.00° 90.06° 90.00°	Depositor
Resolution (Å)	19.93 – 2.55 35.72 – 2.54	Depositor EDS
% Data completeness (in resolution range)	92.6 (19.93-2.55) 91.6 (35.72-2.54)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.64 (at 2.54Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, $R_{free}$	0.185 , 0.246 0.187 , 0.248	Depositor DCC
$R_{free}$ test set	1982 reflections (3.37%)	DCC
Wilson B-factor (Å <sup>2</sup> )	46.9	Xtriage
Anisotropy	0.510	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 36.2	EDS
Estimated twinning fraction	0.321 for H,-K,-L 0.288 for h,-k,-l	Xtriage
Reported twinning fraction	0.321 for H,-K,-L	Depositor
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.40$ , $\langle L^2 \rangle = 0.23$	Xtriage
Outliers	1 of 59361 reflections (0.002%)	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	9482	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.36% 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: C8E, 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	0.45	0/2366	0.65	2/3208 (0.1%)
1	B	0.45	0/2301	0.65	2/3116 (0.1%)
1	C	0.44	0/2321	0.80	3/3141 (0.1%)
1	D	0.46	0/2366	0.65	2/3208 (0.1%)
All	All	0.45	0/9354	0.69	9/12673 (0.1%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	171	ARG	NE-CZ-NH1	-18.99	110.81	120.30
1	C	171	ARG	NE-CZ-NH2	18.19	129.40	120.30
1	C	171	ARG	CD-NE-CZ	8.99	136.19	123.60
1	D	171	ARG	NE-CZ-NH2	-7.00	116.80	120.30
1	A	171	ARG	NE-CZ-NH2	-6.77	116.92	120.30
1	A	171	ARG	NE-CZ-NH1	6.26	123.43	120.30
1	D	171	ARG	NE-CZ-NH1	5.57	123.08	120.30
1	B	171	ARG	NE-CZ-NH1	5.28	122.94	120.30
1	B	171	ARG	NE-CZ-NH2	-5.13	117.73	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	2305	0	2141	129	1
1	B	2242	0	2077	131	2
1	C	2262	0	2070	135	2
1	D	2305	0	2141	139	1
2	A	25	0	0	2	0
2	B	25	0	0	2	0
2	C	30	0	0	3	0
2	D	35	0	0	2	0
3	A	47	0	85	7	0
3	B	27	0	43	3	0
3	C	29	0	53	0	0
3	D	30	0	55	0	0
4	A	33	0	0	4	0
4	B	30	0	0	5	0
4	C	30	0	0	2	0
4	D	27	0	0	2	0
All	All	9482	0	8665	526	3

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 29.

All (526) 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:C:38:ARG:HG3	1:C:38:ARG:HH11	1.01	1.17
1:C:13:SER:HB3	1:C:59:TRP:HZ3	1.08	1.09
1:A:164:ARG:HH11	1:A:164:ARG:HG2	1.11	1.08
1:C:13:SER:HB3	1:C:59:TRP:CZ3	1.93	1.03
1:D:117:LYS:HG3	1:D:131:THR:HG22	1.40	1.03
1:B:117:LYS:HG3	1:B:131:THR:HG22	1.41	1.02
1:B:234:TYR:HD2	4:B:2023:HOH:O	1.42	1.02
1:D:12:ASP:HB2	1:D:59:TRP:CZ3	1.95	1.01
1:A:117:LYS:HG3	1:A:131:THR:HG22	1.41	1.00
1:C:117:LYS:HG3	1:C:131:THR:HG22	1.45	0.98
1:B:164:ARG:HH11	1:B:164:ARG:HG3	1.27	0.98
1:D:12:ASP:HB2	1:D:59:TRP:HZ3	1.31	0.95
1:D:36:THR:HG22	1:D:38:ARG:H	1.32	0.94
1:C:57:ILE:HG22	1:C:69:ALA:HB3	1.50	0.93
1:A:13:SER:HA	1:A:293:GLY:HA2	1.51	0.92
1:C:248:SER:HB2	1:C:281:ASN:HB2	1.54	0.90
1:D:89:ASN:HB3	1:D:92:GLN:HB3	1.53	0.90
1:C:50:VAL:HG22	1:C:78:GLY:HA3	1.53	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:181:GLY:HA3	3:A:1302:C8E:H81	1.56	0.88
1:D:248:SER:HB2	1:D:281:ASN:HB2	1.56	0.87
1:C:267:SER:O	1:C:268:VAL:HG23	1.74	0.87
1:A:164:ARG:HG2	1:A:164:ARG:NH1	1.88	0.86
1:D:31:LEU:HB3	1:D:41:SER:HB3	1.58	0.86
1:B:248:SER:HB2	1:B:281:ASN:HB2	1.57	0.85
1:B:164:ARG:HH11	1:B:164:ARG:CG	1.89	0.85
1:C:38:ARG:HG3	1:C:38:ARG:NH1	1.81	0.85
1:B:24:SER:HB3	1:B:282:TYR:HD2	1.40	0.84
1:D:217:GLU:HB3	1:D:277:ILE:HD11	1.61	0.81
1:A:248:SER:HB2	1:A:281:ASN:HB2	1.62	0.81
1:D:263:ASN:C	1:D:263:ASN:HD22	1.84	0.80
1:B:24:SER:HB3	1:B:282:TYR:CD2	2.17	0.80
1:C:89:ASN:HD22	1:C:90:GLU:N	1.81	0.79
1:C:12:ASP:O	1:C:13:SER:HB2	1.81	0.78
1:C:147:SER:OG	1:D:6:ILE:HD11	1.83	0.78
1:B:59:TRP:HD1	1:B:67:LEU:HD12	1.49	0.78
1:A:204:ASP:OD1	1:A:217:GLU:HB2	1.83	0.78
1:A:164:ARG:HH11	1:A:164:ARG:CG	1.93	0.77
1:A:38:ARG:CZ	1:A:39:LYS:H	1.97	0.77
1:A:15:THR:HG22	1:A:58:SER:HB3	1.65	0.77
1:C:13:SER:CB	1:C:59:TRP:HZ3	1.95	0.76
1:B:56:ASP:OD2	1:B:57:ILE:N	2.19	0.76
1:B:234:TYR:CD2	4:B:2023:HOH:O	2.26	0.75
1:D:66:THR:HG23	1:D:119:TRP:HE1	1.51	0.74
1:A:200:VAL:HB	1:A:222:SER:OG	1.88	0.74
1:D:36:THR:HG22	1:D:38:ARG:N	2.03	0.73
1:A:54:LYS:CG	1:A:72:TRP:HB3	2.19	0.72
1:D:214:THR:HG23	1:D:260:ILE:HG23	1.71	0.72
1:B:54:LYS:HB3	1:B:54:LYS:NZ	2.02	0.72
1:D:185:ILE:O	1:D:185:ILE:HG23	1.90	0.71
1:C:38:ARG:CG	1:C:38:ARG:HH11	1.92	0.71
1:A:13:SER:HA	1:A:293:GLY:CA	2.20	0.70
1:D:92:GLN:HE22	1:D:152:ASN:HD21	1.39	0.70
1:C:227:THR:HG22	1:C:247:TYR:HB3	1.74	0.69
1:A:6:ILE:HD12	1:A:186:ASN:HA	1.74	0.69
1:B:194:PHE:CE2	1:B:196:PHE:CD1	2.80	0.69
1:B:190:LEU:HG	1:B:191:ASN:N	2.07	0.69
1:D:12:ASP:CB	1:D:59:TRP:CZ3	2.74	0.69
1:A:7:PRO:HG3	1:A:234:TYR:CD1	2.28	0.69
1:B:239:ALA:N	4:B:2023:HOH:O	2.26	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:54:LYS:HG3	1:A:72:TRP:HB3	1.75	0.68
1:D:148:TYR:CZ	1:D:157:GLY:HA3	2.28	0.68
1:C:12:ASP:O	1:C:13:SER:CB	2.42	0.68
1:C:57:ILE:CG2	1:C:69:ALA:HB3	2.23	0.67
1:C:9:ILE:H	1:C:14:PHE:HE1	1.43	0.67
1:D:117:LYS:HG3	1:D:131:THR:CG2	2.22	0.67
1:B:166:ILE:HD12	1:B:208:HIS:CE1	2.29	0.67
1:C:91:ASN:OD1	1:C:92:GLN:N	2.28	0.67
1:B:38:ARG:NH2	1:B:87:TRP:O	2.28	0.67
1:C:91:ASN:O	1:C:92:GLN:HB3	1.94	0.67
1:C:191:ASN:HD22	1:C:230:ASN:ND2	1.92	0.67
1:C:118:GLY:O	1:C:129:GLY:HA3	1.94	0.67
1:D:12:ASP:HB2	1:D:59:TRP:CH2	2.30	0.66
1:B:176:TYR:O	1:B:177:ILE:HD13	1.95	0.66
1:D:66:THR:CG2	1:D:119:TRP:HE1	2.09	0.66
1:C:191:ASN:HD22	1:C:230:ASN:HD21	1.43	0.66
1:C:38:ARG:HE	1:C:90:GLU:HG3	1.60	0.65
1:C:147:SER:HB2	1:C:157:GLY:O	1.96	0.65
1:D:59:TRP:O	1:D:61:PRO:HD3	1.96	0.65
1:D:92:GLN:HE22	1:D:152:ASN:ND2	1.94	0.65
1:A:160:PRO:HB2	1:A:163:VAL:HG21	1.79	0.65
1:B:212:ASP:C	1:B:262:LYS:HG2	2.17	0.65
1:B:59:TRP:CH2	1:B:296:GLY:O	2.50	0.65
1:B:40:ILE:O	1:B:86:ALA:HA	1.97	0.64
1:C:160:PRO:O	1:C:163:VAL:HG22	1.98	0.64
1:B:212:ASP:O	1:B:262:LYS:HG2	1.98	0.64
1:B:126:TYR:CZ	1:B:183:TYR:CE1	2.85	0.64
1:D:147:SER:HB3	1:D:158:ASN:HD22	1.63	0.63
1:B:61:PRO:HG2	1:B:65:LEU:HD23	1.80	0.63
1:C:219:THR:HG21	1:C:253:GLY:HA3	1.81	0.63
1:C:117:LYS:HG3	1:C:131:THR:CG2	2.26	0.62
1:D:160:PRO:HB2	1:D:163:VAL:HG21	1.81	0.62
1:A:175:PRO:HB2	3:A:1303:C8E:H61	1.82	0.62
1:C:191:ASN:ND2	1:C:230:ASN:HD21	1.98	0.62
1:A:6:ILE:CD1	1:A:186:ASN:HA	2.30	0.62
1:B:257:THR:HG22	1:B:275:ALA:HB2	1.82	0.62
1:D:36:THR:CG2	1:D:38:ARG:HB2	2.29	0.62
1:D:17:ALA:HB3	1:D:56:ASP:HB3	1.81	0.62
1:B:54:LYS:HD3	1:B:285:THR:HG21	1.82	0.62
1:B:182:GLN:HG2	1:B:183:TYR:N	2.15	0.62
1:A:15:THR:CG2	1:A:58:SER:HB3	2.29	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:15:THR:HG22	1:C:58:SER:HB2	1.83	0.61
1:A:9:ILE:HD12	1:A:184:ARG:NH1	2.16	0.61
1:B:200:VAL:HB	1:B:222:SER:OG	2.00	0.61
1:A:230:ASN:C	1:A:230:ASN:HD22	2.04	0.61
1:A:117:LYS:HG3	1:A:131:THR:CG2	2.24	0.61
1:A:205:ASN:HD21	1:A:216:ARG:NH2	1.98	0.61
1:B:117:LYS:HG3	1:B:131:THR:CG2	2.26	0.61
1:B:48:LYS:O	1:B:49:ASN:C	2.39	0.61
1:B:126:TYR:CZ	1:B:183:TYR:CD1	2.88	0.61
1:B:180:ALA:C	3:B:1306:C8E:H81	2.21	0.61
1:C:9:ILE:O	1:C:11:PRO:N	2.34	0.60
1:C:43:LEU:CD2	1:C:43:LEU:N	2.64	0.60
1:B:92:GLN:HG2	1:B:94:GLU:O	2.02	0.60
1:D:208:HIS:HB3	1:D:211:ARG:HG2	1.83	0.60
1:A:67:LEU:N	1:A:67:LEU:HD23	2.16	0.60
1:C:257:THR:HG22	1:C:275:ALA:HB2	1.82	0.60
1:A:214:THR:HB	1:A:260:ILE:HD13	1.84	0.60
1:A:29:GLU:HB3	1:A:43:LEU:HB2	1.84	0.60
1:D:164:ARG:HH11	1:D:164:ARG:CG	2.14	0.60
1:A:175:PRO:HD3	4:A:2016:HOH:O	2.03	0.59
1:D:200:VAL:HB	1:D:222:SER:HB2	1.84	0.59
1:D:257:THR:HG22	1:D:275:ALA:HB2	1.82	0.59
1:B:54:LYS:HG2	1:B:72:TRP:HB3	1.85	0.59
1:C:89:ASN:HD22	1:C:89:ASN:C	2.06	0.59
1:D:131:THR:CG2	1:D:180:ALA:HB2	2.33	0.59
1:B:188:PHE:CD2	1:B:189:GLU:N	2.71	0.59
1:C:268:VAL:O	1:C:268:VAL:HG12	2.01	0.59
1:A:188:PHE:CZ	1:A:190:LEU:HB2	2.37	0.59
1:A:257:THR:HG22	1:A:275:ALA:HB2	1.85	0.59
1:C:61:PRO:HB2	1:C:62:TYR:CD1	2.39	0.58
1:C:65:LEU:HD12	1:C:117:LYS:O	2.03	0.58
1:B:31:LEU:HG	1:B:40:ILE:HD11	1.84	0.58
1:B:48:LYS:O	1:B:49:ASN:O	2.21	0.58
1:D:28:HIS:HD2	1:D:42:GLN:HE21	1.50	0.58
1:A:119:TRP:CE3	1:A:127:LYS:HG2	2.38	0.58
1:B:111:GLU:HG2	1:B:112:TYR:N	2.18	0.58
1:B:160:PRO:HB2	1:B:163:VAL:CG2	2.34	0.58
1:C:174:MET:CE	1:C:200:VAL:HG22	2.33	0.58
1:D:252:GLU:OE2	1:D:254:LYS:HE2	2.04	0.58
1:D:182:GLN:HG3	1:D:191:ASN:OD1	2.04	0.58
1:D:36:THR:HG21	1:D:38:ARG:NH1	2.19	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:192:ALA:HA	1:C:228:VAL:O	2.04	0.58
1:C:4:GLN:O	1:C:6:ILE:N	2.37	0.58
1:D:204:ASP:OD1	1:D:217:GLU:HB2	2.04	0.58
1:A:38:ARG:HA	1:A:38:ARG:NE	2.19	0.58
1:B:230:ASN:C	1:B:230:ASN:HD22	2.07	0.58
1:C:165:VAL:HG12	1:C:166:ILE:HG12	1.85	0.58
1:A:59:TRP:O	1:A:61:PRO:HD3	2.04	0.57
1:A:206:ASP:HB3	1:A:215:PHE:HB2	1.85	0.57
1:B:185:ILE:HG23	1:B:185:ILE:O	2.04	0.57
1:D:5:LEU:HD23	1:D:5:LEU:C	2.24	0.57
1:C:174:MET:HE3	1:C:200:VAL:HG22	1.84	0.57
1:C:84:ASP:O	1:C:98:HIS:HA	2.05	0.57
1:D:176:TYR:CE1	1:D:195:LYS:HG2	2.40	0.57
1:B:86:ALA:HB3	1:B:97:ASP:HB2	1.87	0.57
1:A:122:GLN:HG2	1:A:127:LYS:HG3	1.87	0.57
1:D:28:HIS:CD2	1:D:42:GLN:HE21	2.23	0.57
1:B:98:HIS:CE1	4:B:2005:HOH:O	2.57	0.57
1:D:164:ARG:HG2	1:D:164:ARG:HH11	1.70	0.57
1:B:97:ASP:OD2	2:B:1302:SO4:O2	2.23	0.57
1:D:263:ASN:ND2	1:D:263:ASN:C	2.56	0.56
1:C:22:MET:HE2	1:C:49:ASN:HA	1.87	0.56
1:A:84:ASP:O	1:A:98:HIS:HA	2.04	0.56
1:C:38:ARG:HH21	1:C:90:GLU:HG2	1.70	0.56
1:C:9:ILE:N	1:C:14:PHE:HE1	2.04	0.56
1:D:174:MET:CE	1:D:200:VAL:HG22	2.35	0.56
1:C:28:HIS:HD2	1:C:42:GLN:HE21	1.51	0.56
1:A:19:SER:O	1:A:53:LEU:HD12	2.06	0.56
1:D:131:THR:HG21	1:D:193:LEU:HD11	1.88	0.56
1:B:182:GLN:HG2	1:B:183:TYR:H	1.71	0.56
1:A:119:TRP:HB2	1:A:122:GLN:OE1	2.06	0.56
1:A:179:LEU:O	1:A:193:LEU:HD12	2.05	0.56
1:B:54:LYS:HB3	1:B:54:LYS:HZ2	1.71	0.55
1:C:212:ASP:O	1:C:213:LEU:HD23	2.06	0.55
1:B:56:ASP:O	1:B:57:ILE:HG13	2.06	0.55
1:D:230:ASN:C	1:D:230:ASN:HD22	2.09	0.55
1:C:50:VAL:CG2	1:C:78:GLY:HA3	2.33	0.55
1:D:6:ILE:HG22	1:D:7:PRO:HD2	1.86	0.55
1:D:174:MET:HE1	1:D:197:SER:HB3	1.88	0.55
1:D:161:LYS:HD3	2:D:1296:SO4:O1	2.07	0.55
1:B:188:PHE:CD2	1:B:188:PHE:C	2.78	0.55
1:B:165:VAL:HG12	1:B:166:ILE:HG12	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:68:ASN:HB2	1:D:115:ASN:OD1	2.06	0.55
1:B:160:PRO:HB2	1:B:163:VAL:HG21	1.89	0.55
1:C:59:TRP:NE1	1:C:61:PRO:HG3	2.21	0.55
1:A:257:THR:CG2	1:A:275:ALA:HB2	2.35	0.55
1:A:49:ASN:O	1:A:49:ASN:CG	2.44	0.55
1:B:30:MET:SD	1:B:42:GLN:HG3	2.47	0.55
1:C:187:ASP:O	1:C:188:PHE:CB	2.53	0.55
1:A:160:PRO:HB2	1:A:163:VAL:CG2	2.38	0.54
1:A:31:LEU:HB3	1:A:41:SER:HB3	1.88	0.54
1:B:214:THR:HG22	1:B:260:ILE:HG23	1.90	0.54
1:C:207:GLU:HG3	1:C:214:THR:HG23	1.90	0.54
1:A:279:ASN:CG	1:A:280:LYS:N	2.61	0.54
1:C:126:TYR:OH	2:C:1295:SO4:O1	2.18	0.54
1:B:61:PRO:O	1:B:297:GLY:HA3	2.07	0.54
1:A:177:ILE:HD11	3:A:1303:C8E:C5	2.36	0.54
1:D:160:PRO:HB2	1:D:163:VAL:CG2	2.38	0.54
1:D:257:THR:CG2	1:D:275:ALA:HB2	2.37	0.54
1:B:28:HIS:HD2	1:B:44:ASP:OD2	1.90	0.54
1:C:8:ASN:N	1:C:9:ILE:CA	2.70	0.54
1:B:125:ASN:O	1:B:126:TYR:CD1	2.60	0.54
1:C:257:THR:CG2	1:C:275:ALA:HB2	2.38	0.54
1:A:174:MET:CE	1:A:200:VAL:HG22	2.37	0.54
1:B:164:ARG:NH1	1:B:164:ARG:HG3	2.07	0.54
1:A:38:ARG:HA	1:A:38:ARG:HE	1.72	0.54
1:C:156:THR:CG2	1:D:9:ILE:HG12	2.37	0.54
1:A:54:LYS:HE2	1:A:244:GLU:OE2	2.07	0.54
1:A:6:ILE:HD13	1:A:6:ILE:N	2.22	0.54
1:C:48:LYS:HE3	1:C:80:GLY:O	2.08	0.53
1:C:7:PRO:CA	1:C:59:TRP:HH2	2.21	0.53
1:B:59:TRP:CD1	1:B:67:LEU:HD12	2.38	0.53
1:B:279:ASN:CG	1:B:280:LYS:N	2.61	0.53
1:D:279:ASN:CG	1:D:280:LYS:N	2.60	0.53
1:B:257:THR:CG2	1:B:275:ALA:HB2	2.37	0.53
1:D:56:ASP:O	1:D:57:ILE:HG13	2.09	0.53
1:A:94:GLU:H	1:A:94:GLU:CD	2.12	0.53
1:D:23:LEU:HG	1:D:47:ILE:HD11	1.90	0.53
1:C:127:LYS:HE3	1:C:182:GLN:HE21	1.73	0.53
1:C:38:ARG:NE	1:C:90:GLU:HG3	2.23	0.53
1:C:91:ASN:O	1:C:92:GLN:CB	2.57	0.53
1:B:212:ASP:HB3	1:B:262:LYS:HB2	1.90	0.53
1:D:84:ASP:O	1:D:98:HIS:HA	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:86:ALA:HB3	1:C:97:ASP:HB2	1.91	0.53
1:A:35:GLU:HG3	1:C:35:GLU:CG	2.38	0.53
1:D:292:PHE:O	1:D:294:GLY:N	2.40	0.53
1:D:102:PRO:HD2	4:D:2009:HOH:O	2.09	0.53
1:D:123:ASP:OD2	1:D:126:TYR:HB2	2.08	0.53
1:D:12:ASP:CB	1:D:59:TRP:HZ3	2.11	0.53
1:B:84:ASP:O	1:B:98:HIS:HA	2.09	0.52
1:D:198:ASP:OD1	1:D:223:ARG:NH2	2.41	0.52
1:C:111:GLU:HG2	1:C:112:TYR:N	2.25	0.52
1:D:246:THR:O	1:D:282:TYR:HA	2.10	0.52
1:C:70:ARG:NH2	2:C:1294:SO4:O4	2.42	0.52
1:A:35:GLU:HG3	1:C:35:GLU:HB3	1.92	0.52
1:C:279:ASN:CG	1:C:280:LYS:N	2.63	0.52
1:D:260:ILE:HG13	1:D:262:LYS:HG2	1.92	0.52
1:C:85:TYR:CE1	1:C:98:HIS:CD2	2.98	0.52
1:D:223:ARG:HG3	1:D:251:ASP:OD2	2.10	0.52
1:A:2:SER:O	1:A:3:SER:HB2	2.10	0.52
1:A:244:GLU:HB3	1:A:285:THR:HG22	1.92	0.52
2:B:1302:SO4:O3	2:B:1303:SO4:O3	2.27	0.52
1:A:118:GLY:O	1:A:129:GLY:HA3	2.10	0.52
1:B:54:LYS:HB3	1:B:54:LYS:HZ3	1.75	0.51
1:A:62:TYR:HD1	1:A:65:LEU:HD23	1.75	0.51
1:D:190:LEU:C	1:D:190:LEU:HD23	2.31	0.51
1:D:165:VAL:HG12	1:D:166:ILE:HG12	1.91	0.51
1:C:59:TRP:CZ2	1:C:61:PRO:HA	2.46	0.51
1:A:191:ASN:O	1:A:229:ILE:HA	2.10	0.51
1:D:164:ARG:HG2	1:D:164:ARG:NH1	2.25	0.51
1:C:22:MET:HG2	1:C:49:ASN:HA	1.92	0.51
1:C:230:ASN:HD22	1:C:230:ASN:C	2.14	0.51
1:A:216:ARG:HB2	1:A:258:GLN:HB3	1.93	0.51
1:B:164:ARG:HG2	1:B:209:TYR:CD1	2.46	0.51
1:B:31:LEU:HD12	1:B:274:ALA:O	2.11	0.51
1:D:111:GLU:HG2	1:D:112:TYR:N	2.26	0.51
1:A:216:ARG:NH2	2:A:1296:SO4:O2	2.43	0.51
1:C:43:LEU:N	1:C:43:LEU:HD23	2.26	0.51
1:D:230:ASN:ND2	4:D:2020:HOH:O	2.44	0.51
1:D:279:ASN:CG	1:D:280:LYS:H	2.14	0.51
1:C:244:GLU:HB3	1:C:285:THR:HG22	1.91	0.51
1:C:6:ILE:O	1:C:61:PRO:O	2.28	0.51
1:D:148:TYR:OH	1:D:157:GLY:HA3	2.10	0.51
1:A:22:MET:SD	1:A:49:ASN:ND2	2.84	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:36:THR:CG2	1:C:38:ARG:HB2	2.41	0.50
1:B:188:PHE:HD1	1:B:233:TYR:CZ	2.29	0.50
1:B:38:ARG:NH1	1:B:40:ILE:HG22	2.26	0.50
1:A:279:ASN:CG	1:A:280:LYS:H	2.15	0.50
1:D:198:ASP:OD1	1:D:223:ARG:NE	2.42	0.50
1:B:65:LEU:HD12	1:B:117:LYS:O	2.11	0.50
1:B:54:LYS:HE3	1:B:244:GLU:OE2	2.11	0.50
1:A:230:ASN:C	1:A:230:ASN:ND2	2.63	0.50
1:B:279:ASN:CG	1:B:280:LYS:H	2.15	0.50
1:C:31:LEU:HB3	1:C:41:SER:HB2	1.94	0.50
1:A:219:THR:HG21	1:A:253:GLY:HA3	1.94	0.50
1:A:87:TRP:CE2	1:A:95:TRP:HB3	2.46	0.50
1:D:203:HIS:HA	1:D:217:GLU:O	2.12	0.50
1:B:244:GLU:HB3	1:B:285:THR:HG22	1.92	0.50
1:B:194:PHE:CE2	1:B:196:PHE:HD1	2.27	0.50
1:B:185:ILE:HG22	1:B:188:PHE:HB3	1.92	0.50
1:D:15:THR:HG22	1:D:58:SER:H	1.76	0.50
1:A:22:MET:HG3	1:A:49:ASN:HD22	1.76	0.50
1:A:224:TYR:C	1:A:224:TYR:CD2	2.86	0.49
1:C:174:MET:HE1	1:C:224:TYR:HB3	1.93	0.49
1:D:125:ASN:O	1:D:183:TYR:HA	2.12	0.49
1:D:36:THR:HG21	1:D:38:ARG:HH11	1.76	0.49
1:D:9:ILE:CD1	1:D:184:ARG:HH12	2.25	0.49
1:A:50:VAL:HG22	1:A:78:GLY:HA3	1.94	0.49
1:B:230:ASN:C	1:B:230:ASN:ND2	2.66	0.49
1:C:89:ASN:C	1:C:89:ASN:ND2	2.66	0.49
1:A:230:ASN:ND2	4:A:2023:HOH:O	2.44	0.49
1:D:185:ILE:O	1:D:185:ILE:CG2	2.60	0.49
1:C:28:HIS:CD2	1:C:42:GLN:HE21	2.29	0.49
1:C:279:ASN:CG	1:C:280:LYS:H	2.15	0.49
1:D:86:ALA:HB3	1:D:97:ASP:HB2	1.95	0.49
1:D:31:LEU:HD12	1:D:274:ALA:O	2.13	0.48
1:A:87:TRP:CD1	1:A:93:SER:O	2.66	0.48
1:A:111:GLU:HG2	1:A:112:TYR:N	2.27	0.48
1:B:180:ALA:CA	3:B:1306:C8E:H81	2.43	0.48
1:B:203:HIS:NE2	1:B:218:LYS:HE3	2.29	0.48
1:D:230:ASN:C	1:D:230:ASN:ND2	2.66	0.48
1:A:85:TYR:CE1	1:A:98:HIS:CD2	3.02	0.48
1:B:203:HIS:CD2	1:B:218:LYS:HG3	2.48	0.48
1:A:187:ASP:O	1:A:233:TYR:HA	2.14	0.48
1:C:9:ILE:N	1:C:14:PHE:CE1	2.72	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:182:GLN:HG2	1:A:183:TYR:N	2.28	0.48
1:C:252:GLU:OE2	1:C:254:LYS:HE2	2.13	0.48
1:A:81:ASN:OD1	1:A:82:MET:N	2.47	0.48
1:C:56:ASP:OD2	1:C:57:ILE:N	2.47	0.48
1:A:17:ALA:HB3	1:A:56:ASP:HB3	1.94	0.48
1:B:214:THR:CG2	1:B:260:ILE:HG23	2.44	0.48
1:B:28:HIS:CD2	1:B:44:ASP:OD2	2.66	0.48
1:A:151:ASN:HB3	1:A:154:ALA:HB3	1.95	0.48
1:D:147:SER:HB3	1:D:158:ASN:ND2	2.29	0.47
1:A:165:VAL:HG12	1:A:166:ILE:HG12	1.95	0.47
1:B:65:LEU:HG	1:B:66:THR:N	2.28	0.47
1:C:166:ILE:HD12	1:C:208:HIS:CE1	2.49	0.47
1:C:222:SER:HB2	4:C:2026:HOH:O	2.14	0.47
1:A:31:LEU:HD12	1:A:274:ALA:O	2.14	0.47
1:B:246:THR:HB	1:B:283:THR:OG1	2.14	0.47
1:B:122:GLN:HG3	1:B:127:LYS:HE2	1.96	0.47
1:D:244:GLU:HB3	1:D:285:THR:HG22	1.97	0.47
1:D:33:ASP:O	1:D:37:GLY:N	2.40	0.47
1:D:263:ASN:HD22	1:D:264:SER:N	2.12	0.47
1:C:164:ARG:HH11	1:C:164:ARG:CG	2.28	0.47
1:D:12:ASP:CB	1:D:59:TRP:CH2	2.96	0.47
1:D:174:MET:HE3	1:D:200:VAL:HG22	1.97	0.47
1:D:43:LEU:N	1:D:43:LEU:CD2	2.77	0.47
1:A:7:PRO:HG3	1:A:234:TYR:CE1	2.49	0.47
1:C:9:ILE:CA	1:C:14:PHE:HE1	2.28	0.47
1:A:179:LEU:N	1:A:179:LEU:HD22	2.30	0.47
1:A:246:THR:O	1:A:282:TYR:HA	2.15	0.47
1:A:117:LYS:HE3	1:A:117:LYS:HB2	1.65	0.47
1:B:40:ILE:HG12	1:B:41:SER:N	2.29	0.47
1:C:174:MET:HE1	1:C:197:SER:HB3	1.97	0.47
1:C:107:ASN:HB2	1:C:140:SER:HB3	1.95	0.47
1:B:54:LYS:HA	1:B:72:TRP:HB3	1.96	0.47
1:A:54:LYS:HG2	1:A:72:TRP:HB3	1.95	0.46
1:A:112:TYR:HB2	3:A:1300:C8E:H62	1.98	0.46
1:B:15:THR:O	1:B:57:ILE:HA	2.16	0.46
1:A:45:TRP:CZ3	1:A:82:MET:HG3	2.50	0.46
1:B:252:GLU:OE2	1:B:254:LYS:HE2	2.14	0.46
1:A:202:ALA:HB3	1:A:219:THR:HB	1.97	0.46
1:C:246:THR:O	1:C:282:TYR:HA	2.15	0.46
1:B:138:ARG:HG2	1:B:171:ARG:HG3	1.96	0.46
1:D:68:ASN:OD1	1:D:70:ARG:HD2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:181:GLY:CA	3:A:1302:C8E:H81	2.38	0.46
1:C:156:THR:HG22	1:D:9:ILE:H	1.81	0.46
1:D:260:ILE:O	1:D:260:ILE:HG13	2.14	0.46
1:B:295:GLY:O	1:B:296:GLY:C	2.54	0.46
1:A:48:LYS:O	1:A:49:ASN:C	2.54	0.46
1:D:44:ASP:O	1:D:82:MET:HA	2.16	0.46
1:D:196:PHE:HA	1:D:224:TYR:O	2.15	0.46
1:B:259:THR:O	1:B:267:SER:HA	2.16	0.46
1:B:117:LYS:HB2	1:B:117:LYS:HE3	1.61	0.46
1:B:188:PHE:CZ	1:B:231:ALA:HB1	2.50	0.46
1:B:174:MET:CE	1:B:200:VAL:HG22	2.46	0.46
1:B:44:ASP:O	1:B:82:MET:HA	2.16	0.46
1:B:263:ASN:HD22	1:B:263:ASN:H	1.63	0.46
1:A:54:LYS:CE	1:A:244:GLU:OE2	2.64	0.46
1:D:115:ASN:HB2	1:D:176:TYR:OH	2.16	0.46
1:B:217:GLU:HG2	1:B:275:ALA:HB1	1.98	0.45
1:D:15:THR:O	1:D:57:ILE:HA	2.16	0.45
1:B:174:MET:HE1	1:B:197:SER:HB3	1.97	0.45
1:C:31:LEU:HD12	1:C:274:ALA:O	2.16	0.45
1:D:50:VAL:HG12	1:D:51:ALA:O	2.16	0.45
1:D:246:THR:HB	1:D:283:THR:OG1	2.16	0.45
1:C:47:ILE:HG22	1:C:141:TRP:HZ2	1.82	0.45
1:A:49:ASN:ND2	1:A:49:ASN:C	2.70	0.45
1:A:175:PRO:CB	3:A:1303:C8E:H61	2.47	0.45
1:D:214:THR:CG2	1:D:262:LYS:HD3	2.47	0.45
1:C:230:ASN:C	1:C:230:ASN:ND2	2.69	0.45
1:C:164:ARG:HB3	1:C:209:TYR:CD1	2.51	0.45
1:D:81:ASN:OD1	1:D:82:MET:N	2.50	0.45
1:A:206:ASP:OD1	1:A:208:HIS:ND1	2.44	0.45
1:B:47:ILE:HD11	1:B:141:TRP:CZ2	2.52	0.45
1:D:56:ASP:C	1:D:57:ILE:HG13	2.37	0.45
1:C:94:GLU:OE1	1:D:123:ASP:HB2	2.16	0.45
1:D:223:ARG:CG	1:D:251:ASP:OD2	2.64	0.45
1:A:87:TRP:CD1	1:A:95:TRP:HA	2.51	0.45
1:A:264:SER:OG	1:A:266:ASP:HB2	2.17	0.45
1:D:6:ILE:CG2	1:D:7:PRO:HD2	2.46	0.45
1:C:157:GLY:HA2	1:D:7:PRO:O	2.17	0.45
1:D:185:ILE:O	1:D:186:ASN:HB2	2.16	0.45
1:D:138:ARG:HG2	1:D:171:ARG:HG3	1.99	0.45
1:B:31:LEU:HB3	1:B:41:SER:HB3	1.99	0.45
1:D:85:TYR:CE1	1:D:98:HIS:CD2	3.04	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:107:ASN:HB2	1:A:140:SER:HB3	1.99	0.45
1:C:156:THR:HG23	1:C:157:GLY:N	2.32	0.45
1:D:87:TRP:CD1	1:D:95:TRP:HA	2.52	0.45
1:C:33:ASP:HB3	1:C:36:THR:HB	1.99	0.44
1:B:24:SER:HA	1:B:47:ILE:O	2.18	0.44
1:A:121:LEU:C	1:A:122:GLN:HG3	2.37	0.44
1:A:86:ALA:HB3	1:A:97:ASP:HB2	1.98	0.44
1:C:48:LYS:CE	1:C:81:ASN:HB2	2.46	0.44
1:C:119:TRP:CE3	1:C:127:LYS:HG3	2.52	0.44
1:B:261:ASP:HB3	1:B:264:SER:HB2	1.99	0.44
1:D:9:ILE:HG13	1:D:184:ARG:HH12	1.81	0.44
1:D:107:ASN:HB2	1:D:140:SER:HB3	1.99	0.44
1:A:212:ASP:O	1:A:262:LYS:HB2	2.17	0.44
1:C:68:ASN:N	1:C:68:ASN:ND2	2.65	0.44
1:D:259:THR:O	1:D:267:SER:HA	2.17	0.44
1:D:184:ARG:HA	1:D:188:PHE:O	2.17	0.44
1:C:163:VAL:O	1:C:165:VAL:HG23	2.17	0.44
1:A:185:ILE:O	1:A:185:ILE:HG23	2.17	0.44
1:D:211:ARG:O	1:D:212:ASP:C	2.54	0.44
1:A:208:HIS:HB3	1:A:211:ARG:HG2	1.99	0.44
1:A:8:ASN:HB2	1:A:237:PRO:HB3	1.99	0.44
1:C:267:SER:O	1:C:268:VAL:CG2	2.58	0.44
1:B:59:TRP:HH2	1:B:296:GLY:O	2.00	0.44
1:B:125:ASN:C	1:B:126:TYR:CD1	2.91	0.44
1:B:174:MET:HB2	1:B:174:MET:HE2	1.73	0.44
1:C:174:MET:HB2	1:C:174:MET:HE2	1.70	0.44
1:C:201:ARG:NH2	4:C:2020:HOH:O	2.50	0.44
1:A:138:ARG:HG2	1:A:171:ARG:HG3	1.98	0.44
1:A:5:LEU:O	1:A:187:ASP:HB3	2.17	0.44
1:B:190:LEU:HD12	1:B:230:ASN:O	2.18	0.44
1:C:219:THR:CG2	1:C:253:GLY:HA3	2.47	0.44
1:C:43:LEU:HA	1:C:83:ASP:O	2.18	0.44
1:C:33:ASP:OD1	1:C:33:ASP:C	2.56	0.44
1:B:126:TYR:CE2	1:B:183:TYR:CD1	3.06	0.44
1:C:28:HIS:HD2	1:C:44:ASP:OD2	2.01	0.44
1:D:203:HIS:CE1	2:D:1297:SO4:O4	2.71	0.43
1:C:187:ASP:O	1:C:188:PHE:HB2	2.16	0.43
1:A:8:ASN:ND2	4:A:2001:HOH:O	2.28	0.43
1:A:184:ARG:O	1:A:185:ILE:HB	2.18	0.43
1:C:74:SER:HB2	1:C:109:ALA:H	1.83	0.43
1:A:122:GLN:HB2	1:A:122:GLN:HE21	1.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:190:LEU:HD23	1:D:191:ASN:N	2.34	0.43
1:C:117:LYS:HE3	1:C:117:LYS:HB2	1.63	0.43
1:B:194:PHE:HE2	1:B:196:PHE:CD1	2.32	0.43
1:C:121:LEU:O	1:C:127:LYS:HB2	2.18	0.43
1:A:125:ASN:O	1:A:183:TYR:HA	2.18	0.43
1:C:135:GLN:HB3	1:C:135:GLN:HE21	1.65	0.43
1:A:127:LYS:HB2	1:A:127:LYS:HE3	1.87	0.43
1:A:252:GLU:OE2	1:A:254:LYS:HE2	2.19	0.43
1:A:54:LYS:HG3	1:A:72:TRP:CB	2.47	0.43
1:B:191:ASN:ND2	1:B:191:ASN:N	2.66	0.43
1:A:245:PHE:CE1	1:A:282:TYR:HB2	2.54	0.43
1:B:263:ASN:N	1:B:263:ASN:HD22	2.17	0.43
1:C:156:THR:HG21	1:D:9:ILE:HG12	2.00	0.43
1:D:204:ASP:OD1	1:D:204:ASP:C	2.58	0.43
1:D:148:TYR:CZ	1:D:157:GLY:CA	3.00	0.43
1:A:246:THR:HB	1:A:283:THR:OG1	2.19	0.43
1:A:115:ASN:HB2	1:A:176:TYR:OH	2.19	0.43
1:B:14:PHE:CD2	1:B:59:TRP:CE3	3.07	0.42
1:D:174:MET:HE2	1:D:200:VAL:HG22	2.02	0.42
1:A:87:TRP:HD1	1:A:93:SER:O	2.02	0.42
1:A:273:ASP:N	1:A:273:ASP:OD2	2.51	0.42
1:C:54:LYS:HG3	1:C:72:TRP:HB3	2.01	0.42
1:B:185:ILE:HD13	1:B:186:ASN:OD1	2.20	0.42
1:B:188:PHE:HD2	1:B:188:PHE:C	2.22	0.42
1:C:206:ASP:HB3	1:C:215:PHE:HB2	1.99	0.42
1:A:222:SER:HB2	4:A:2027:HOH:O	2.18	0.42
1:C:166:ILE:HD12	1:C:208:HIS:CD2	2.54	0.42
1:B:160:PRO:HB2	1:B:163:VAL:HG23	2.02	0.42
1:B:203:HIS:CE1	4:B:2016:HOH:O	2.72	0.42
1:C:13:SER:CB	1:C:59:TRP:CZ3	2.82	0.42
1:C:156:THR:CG2	1:D:7:PRO:O	2.67	0.42
1:B:14:PHE:CE2	1:B:59:TRP:CE3	3.07	0.42
1:A:217:GLU:HB3	1:A:277:ILE:HD11	2.00	0.42
1:D:15:THR:HG22	1:D:58:SER:N	2.35	0.42
1:A:166:ILE:HD12	1:A:208:HIS:NE2	2.34	0.42
1:B:107:ASN:HB2	1:B:140:SER:HB3	2.01	0.42
1:C:61:PRO:HB2	1:C:62:TYR:CE1	2.54	0.42
1:D:89:ASN:CB	1:D:92:GLN:HB3	2.37	0.42
1:A:166:ILE:HD12	1:A:208:HIS:CD2	2.55	0.42
1:A:112:TYR:CB	3:A:1300:C8E:H62	2.50	0.42
1:A:174:MET:HE3	1:A:200:VAL:HG22	1.99	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:177:ILE:HD11	1:C:196:PHE:HD1	1.84	0.42
1:D:33:ASP:HB3	1:D:36:THR:HB	2.02	0.42
1:D:202:ALA:O	1:D:218:LYS:HA	2.20	0.42
1:B:125:ASN:OD1	1:B:184:ARG:O	2.38	0.42
1:B:81:ASN:OD1	1:B:82:MET:N	2.51	0.42
1:D:74:SER:HB2	1:D:109:ALA:H	1.85	0.42
1:C:38:ARG:HE	1:C:90:GLU:CG	2.30	0.42
1:C:57:ILE:HD13	1:C:58:SER:N	2.35	0.42
1:D:59:TRP:CD1	1:D:67:LEU:HD12	2.55	0.41
1:B:275:ALA:HB1	3:B:1304:C8E:H11	2.02	0.41
1:A:74:SER:HB2	1:A:109:ALA:H	1.85	0.41
1:A:174:MET:HA	1:A:175:PRO:HD3	1.95	0.41
1:D:147:SER:O	1:D:159:PHE:HE1	2.04	0.41
1:B:174:MET:HA	1:B:175:PRO:HD3	1.94	0.41
1:B:34:ALA:HB1	1:B:272:GLY:O	2.20	0.41
1:B:164:ARG:NH1	1:B:164:ARG:CG	2.59	0.41
1:C:40:ILE:O	1:C:86:ALA:HA	2.20	0.41
1:A:270:ILE:CG2	1:A:271:GLY:N	2.83	0.41
1:B:29:GLU:HB3	1:B:43:LEU:HB2	2.01	0.41
1:B:43:LEU:N	1:B:43:LEU:CD2	2.83	0.41
1:A:238:ASN:ND2	2:A:1295:SO4:O4	2.54	0.41
1:D:203:HIS:CD2	1:D:218:LYS:HG2	2.55	0.41
1:C:34:ALA:HB2	1:C:274:ALA:HB2	2.02	0.41
1:B:122:GLN:HG3	1:B:127:LYS:HB3	2.02	0.41
1:D:29:GLU:HB3	1:D:43:LEU:HB2	2.01	0.41
1:D:50:VAL:HG22	1:D:78:GLY:HA3	2.01	0.41
1:D:281:ASN:HD22	1:D:281:ASN:HA	1.65	0.41
1:B:187:ASP:O	1:B:233:TYR:HA	2.20	0.41
1:D:214:THR:CG2	1:D:260:ILE:HG23	2.47	0.41
1:B:188:PHE:HE2	1:B:190:LEU:HB2	1.86	0.41
1:D:15:THR:CG2	1:D:58:SER:HB3	2.50	0.41
1:D:74:SER:CB	1:D:109:ALA:H	2.34	0.41
1:D:227:THR:HG23	1:D:247:TYR:HB3	2.03	0.41
1:A:204:ASP:OD1	1:A:217:GLU:OE1	2.38	0.41
1:A:43:LEU:CD2	1:A:43:LEU:N	2.84	0.41
1:C:164:ARG:HD3	2:C:1298:SO4:O2	2.20	0.41
1:B:17:ALA:O	1:B:56:ASP:N	2.49	0.41
1:B:185:ILE:CG2	1:B:188:PHE:HB3	2.51	0.41
1:B:214:THR:HG22	1:B:260:ILE:CG2	2.49	0.41
1:A:125:ASN:OD1	1:A:125:ASN:N	2.53	0.41
1:B:74:SER:HB2	1:B:109:ALA:H	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:117:LYS:HB2	1:D:117:LYS:HE3	1.72	0.41
1:B:115:ASN:HB2	1:B:176:TYR:OH	2.21	0.41
1:C:214:THR:HB	1:C:260:ILE:HG23	2.02	0.41
1:B:56:ASP:OD2	1:B:68:ASN:ND2	2.54	0.41
1:C:130:ILE:HG22	1:C:179:LEU:HD13	2.02	0.41
1:D:262:LYS:HE2	1:D:262:LYS:HB3	1.86	0.40
1:C:130:ILE:HG22	1:C:179:LEU:CD1	2.51	0.40
1:B:61:PRO:O	1:B:297:GLY:CA	2.69	0.40
1:C:200:VAL:HG23	1:C:222:SER:O	2.21	0.40
1:C:174:MET:CE	1:C:224:TYR:HB3	2.52	0.40
1:D:23:LEU:HG	1:D:47:ILE:CD1	2.52	0.40
1:C:54:LYS:NZ	1:C:70:ARG:HH12	2.20	0.40
1:D:87:TRP:CE2	1:D:95:TRP:HB3	2.56	0.40
1:D:204:ASP:OD1	1:D:217:GLU:OE1	2.40	0.40
1:C:81:ASN:OD1	1:C:82:MET:N	2.54	0.40
1:A:75:LEU:HD23	1:A:75:LEU:HA	1.90	0.40

All (3) 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:266:ASP:OD2	1:C:97:ASP:OD2[2_544]	2.10	0.10
1:B:97:ASP:OD2	1:C:266:ASP:OD2[2_544]	2.14	0.06
1:A:266:ASP:OD2	1:D:97:ASP:OD2[2_554]	2.18	0.02

## 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	291/298 (98%)	267 (92%)	18 (6%)	6 (2%)	9	13
1	B	284/298 (95%)	261 (92%)	16 (6%)	7 (2%)	7	10

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	289/298 (97%)	263 (91%)	14 (5%)	12 (4%)	3	3
1	D	291/298 (98%)	269 (92%)	15 (5%)	7 (2%)	7	11
All	All	1155/1192 (97%)	1060 (92%)	63 (6%)	32 (3%)	6	8

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3	SER
1	A	185	ILE
1	A	264	SER
1	B	49	ASN
1	C	5	LEU
1	C	7	PRO
1	C	10	SER
1	C	188	PHE
1	C	268	VAL
1	D	12	ASP
1	A	49	ASN
1	A	272	GLY
1	C	11	PRO
1	C	13	SER
1	C	92	GLN
1	D	293	GLY
1	A	266	ASP
1	B	123	ASP
1	B	125	ASN
1	C	124	GLU
1	C	273	ASP
1	D	11	PRO
1	D	263	ASN
1	B	186	ASN
1	B	296	GLY
1	D	3	SER
1	C	4	GLN
1	D	61	PRO
1	D	212	ASP
1	B	272	GLY
1	C	6	ILE
1	B	295	GLY

### 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	239/240 (100%)	209 (87%)	30 (13%)	5	9
1	B	229/240 (95%)	192 (84%)	37 (16%)	3	5
1	C	229/240 (95%)	189 (82%)	40 (18%)	2	4
1	D	239/240 (100%)	202 (84%)	37 (16%)	3	5
All	All	936/960 (98%)	792 (85%)	144 (15%)	3	5

All (144) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	ILE
1	A	15	THR
1	A	24	SER
1	A	30	MET
1	A	38	ARG
1	A	40	ILE
1	A	43	LEU
1	A	48	LYS
1	A	49	ASN
1	A	66	THR
1	A	68	ASN
1	A	110	ASN
1	A	111	GLU
1	A	115	ASN
1	A	120	LEU
1	A	122	GLN
1	A	125	ASN
1	A	156	THR
1	A	164	ARG
1	A	169	ASN
1	A	171	ARG
1	A	173	SER
1	A	174	MET
1	A	207	GLU

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Mol	Chain	Res	Type
1	A	216	ARG
1	A	219	THR
1	A	224	TYR
1	A	230	ASN
1	A	246	THR
1	A	285	THR
1	B	15	THR
1	B	24	SER
1	B	30	MET
1	B	40	ILE
1	B	43	LEU
1	B	58	SER
1	B	66	THR
1	B	70	ARG
1	B	110	ASN
1	B	111	GLU
1	B	115	ASN
1	B	120	LEU
1	B	123	ASP
1	B	124	GLU
1	B	156	THR
1	B	164	ARG
1	B	169	ASN
1	B	171	ARG
1	B	173	SER
1	B	174	MET
1	B	182	GLN
1	B	185	ILE
1	B	190	LEU
1	B	191	ASN
1	B	193	LEU
1	B	196	PHE
1	B	214	THR
1	B	219	THR
1	B	224	TYR
1	B	227	THR
1	B	230	ASN
1	B	246	THR
1	B	260	ILE
1	B	282	TYR
1	B	285	THR
1	B	291	ARG

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Mol	Chain	Res	Type
1	B	292	PHE
1	C	15	THR
1	C	24	SER
1	C	30	MET
1	C	35	GLU
1	C	38	ARG
1	C	40	ILE
1	C	43	LEU
1	C	47	ILE
1	C	48	LYS
1	C	52	ILE
1	C	57	ILE
1	C	60	ASP
1	C	62	TYR
1	C	66	THR
1	C	67	LEU
1	C	70	ARG
1	C	89	ASN
1	C	110	ASN
1	C	111	GLU
1	C	115	ASN
1	C	156	THR
1	C	163	VAL
1	C	164	ARG
1	C	169	ASN
1	C	171	ARG
1	C	173	SER
1	C	174	MET
1	C	175	PRO
1	C	177	ILE
1	C	191	ASN
1	C	193	LEU
1	C	211	ARG
1	C	214	THR
1	C	218	LYS
1	C	219	THR
1	C	222	SER
1	C	230	ASN
1	C	246	THR
1	C	260	ILE
1	C	285	THR
1	D	3	SER

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Mol	Chain	Res	Type
1	D	6	ILE
1	D	15	THR
1	D	22	MET
1	D	24	SER
1	D	30	MET
1	D	36	THR
1	D	43	LEU
1	D	47	ILE
1	D	48	LYS
1	D	66	THR
1	D	68	ASN
1	D	92	GLN
1	D	110	ASN
1	D	111	GLU
1	D	115	ASN
1	D	120	LEU
1	D	124	GLU
1	D	149	SER
1	D	156	THR
1	D	164	ARG
1	D	169	ASN
1	D	171	ARG
1	D	173	SER
1	D	174	MET
1	D	193	LEU
1	D	196	PHE
1	D	198	ASP
1	D	211	ARG
1	D	220	SER
1	D	222	SER
1	D	227	THR
1	D	230	ASN
1	D	246	THR
1	D	260	ILE
1	D	263	ASN
1	D	285	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	49	ASN
1	A	98	HIS

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Mol	Chain	Res	Type
1	A	107	ASN
1	A	108	HIS
1	A	110	ASN
1	A	158	ASN
1	A	186	ASN
1	A	205	ASN
1	A	230	ASN
1	A	281	ASN
1	B	28	HIS
1	B	98	HIS
1	B	107	ASN
1	B	110	ASN
1	B	122	GLN
1	B	182	GLN
1	B	191	ASN
1	B	230	ASN
1	B	263	ASN
1	B	281	ASN
1	C	28	HIS
1	C	49	ASN
1	C	89	ASN
1	C	107	ASN
1	C	110	ASN
1	C	125	ASN
1	C	182	GLN
1	C	230	ASN
1	C	263	ASN
1	C	281	ASN
1	D	28	HIS
1	D	98	HIS
1	D	107	ASN
1	D	110	ASN
1	D	152	ASN
1	D	158	ASN
1	D	203	HIS
1	D	230	ASN
1	D	263	ASN
1	D	281	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.



## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

37 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	SO4	A	1295	-	4,4,4	0.17	0	6,6,6	0.21	0
2	SO4	A	1296	-	4,4,4	0.21	0	6,6,6	0.22	0
2	SO4	A	1297	-	4,4,4	0.21	0	6,6,6	0.16	0
2	SO4	A	1298	-	4,4,4	0.10	0	6,6,6	0.21	0
2	SO4	A	1299	-	4,4,4	0.09	0	6,6,6	0.31	0
3	C8E	A	1300	-	10,10,20	0.37	0	9,9,19	0.46	0
3	C8E	A	1301	-	8,8,20	0.32	0	7,7,19	0.53	0
3	C8E	A	1302	-	8,8,20	0.34	0	7,7,19	0.36	0
3	C8E	A	1303	-	9,9,20	0.36	0	8,8,19	0.37	0
3	C8E	A	1304	-	7,7,20	0.39	0	6,6,19	0.18	0
2	SO4	B	1299	-	4,4,4	0.21	0	6,6,6	0.38	0
2	SO4	B	1300	-	4,4,4	0.22	0	6,6,6	0.25	0
2	SO4	B	1301	-	4,4,4	0.12	0	6,6,6	0.17	0
2	SO4	B	1302	-	4,4,4	0.25	0	6,6,6	0.39	0
2	SO4	B	1303	-	4,4,4	0.25	0	6,6,6	0.25	0
3	C8E	B	1304	-	7,7,20	0.30	0	6,6,19	0.44	0
3	C8E	B	1305	-	7,7,20	0.32	0	6,6,19	0.43	0
3	C8E	B	1306	-	10,10,20	0.34	0	9,9,19	0.42	0
2	SO4	C	1294	-	4,4,4	0.17	0	6,6,6	0.21	0
2	SO4	C	1295	-	4,4,4	0.26	0	6,6,6	0.46	0
2	SO4	C	1296	-	4,4,4	0.27	0	6,6,6	0.24	0
2	SO4	C	1297	-	4,4,4	0.19	0	6,6,6	0.14	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	SO4	C	1298	-	4,4,4	0.24	0	6,6,6	0.27	0
2	SO4	C	1299	-	4,4,4	0.12	0	6,6,6	0.23	0
3	C8E	C	1300	-	10,10,20	0.39	0	9,9,19	0.38	0
3	C8E	C	1301	-	8,8,20	0.36	0	7,7,19	0.39	0
3	C8E	C	1302	-	8,8,20	0.35	0	7,7,19	0.46	0
2	SO4	D	1295	-	4,4,4	0.07	0	6,6,6	0.10	0
2	SO4	D	1296	-	4,4,4	0.18	0	6,6,6	0.11	0
2	SO4	D	1297	-	4,4,4	0.12	0	6,6,6	0.14	0
2	SO4	D	1298	-	4,4,4	0.19	0	6,6,6	0.19	0
2	SO4	D	1299	-	4,4,4	0.16	0	6,6,6	0.28	0
2	SO4	D	1300	-	4,4,4	0.17	0	6,6,6	0.29	0
2	SO4	D	1301	-	4,4,4	0.16	0	6,6,6	0.28	0
3	C8E	D	1302	-	11,11,20	0.34	0	10,10,19	0.49	0
3	C8E	D	1303	-	8,8,20	0.30	0	7,7,19	0.46	0
3	C8E	D	1304	-	8,8,20	0.34	0	7,7,19	0.37	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	1295	-	-	0/0/0/0	0/0/0/0
2	SO4	A	1296	-	-	0/0/0/0	0/0/0/0
2	SO4	A	1297	-	-	0/0/0/0	0/0/0/0
2	SO4	A	1298	-	-	0/0/0/0	0/0/0/0
2	SO4	A	1299	-	-	0/0/0/0	0/0/0/0
3	C8E	A	1300	-	-	0/8/8/18	0/0/0/0
3	C8E	A	1301	-	-	0/6/6/18	0/0/0/0
3	C8E	A	1302	-	-	0/6/6/18	0/0/0/0
3	C8E	A	1303	-	-	0/7/7/18	0/0/0/0
3	C8E	A	1304	-	-	0/5/5/18	0/0/0/0
2	SO4	B	1299	-	-	0/0/0/0	0/0/0/0
2	SO4	B	1300	-	-	0/0/0/0	0/0/0/0
2	SO4	B	1301	-	-	0/0/0/0	0/0/0/0
2	SO4	B	1302	-	-	0/0/0/0	0/0/0/0
2	SO4	B	1303	-	-	0/0/0/0	0/0/0/0
3	C8E	B	1304	-	-	0/5/5/18	0/0/0/0
3	C8E	B	1305	-	-	0/5/5/18	0/0/0/0
3	C8E	B	1306	-	-	0/8/8/18	0/0/0/0
2	SO4	C	1294	-	-	0/0/0/0	0/0/0/0
2	SO4	C	1295	-	-	0/0/0/0	0/0/0/0
2	SO4	C	1296	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SO4	C	1297	-	-	0/0/0/0	0/0/0/0
2	SO4	C	1298	-	-	0/0/0/0	0/0/0/0
2	SO4	C	1299	-	-	0/0/0/0	0/0/0/0
3	C8E	C	1300	-	-	0/8/8/18	0/0/0/0
3	C8E	C	1301	-	-	0/6/6/18	0/0/0/0
3	C8E	C	1302	-	-	0/6/6/18	0/0/0/0
2	SO4	D	1295	-	-	0/0/0/0	0/0/0/0
2	SO4	D	1296	-	-	0/0/0/0	0/0/0/0
2	SO4	D	1297	-	-	0/0/0/0	0/0/0/0
2	SO4	D	1298	-	-	0/0/0/0	0/0/0/0
2	SO4	D	1299	-	-	0/0/0/0	0/0/0/0
2	SO4	D	1300	-	-	0/0/0/0	0/0/0/0
2	SO4	D	1301	-	-	0/0/0/0	0/0/0/0
3	C8E	D	1302	-	-	0/9/9/18	0/0/0/0
3	C8E	D	1303	-	-	0/6/6/18	0/0/0/0
3	C8E	D	1304	-	-	0/6/6/18	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.

14 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1295	SO4	1	0
2	A	1296	SO4	1	0
3	A	1300	C8E	2	0
3	A	1302	C8E	2	0
3	A	1303	C8E	3	0
2	B	1302	SO4	2	0
2	B	1303	SO4	1	0
3	B	1304	C8E	1	0
3	B	1306	C8E	2	0
2	C	1294	SO4	1	0
2	C	1295	SO4	1	0
2	C	1298	SO4	1	0
2	D	1296	SO4	1	0
2	D	1297	SO4	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	293/298 (98%)	0.18	0 100 100	36, 48, 63, 76	0
1	B	286/298 (95%)	0.29	13 (4%) 37 43	34, 50, 77, 97	0
1	C	291/298 (97%)	0.24	5 (1%) 73 77	35, 49, 74, 91	0
1	D	293/298 (98%)	0.14	1 (0%) 94 95	31, 49, 66, 92	0
All	All	1163/1192 (97%)	0.21	19 (1%) 74 79	31, 49, 71, 97	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	3	SER	4.5
1	C	235	VAL	4.0
1	B	291	ARG	3.8
1	B	63	SER	3.7
1	B	235	VAL	3.7
1	B	282	TYR	3.7
1	B	14	PHE	3.1
1	B	246	THR	3.1
1	B	292	PHE	3.0
1	C	282	TYR	2.4
1	B	247	TYR	2.4
1	C	8	ASN	2.4
1	B	194	PHE	2.3
1	B	227	THR	2.3
1	B	62	TYR	2.2
1	B	155	TYR	2.2
1	C	17	ALA	2.1
1	D	2	SER	2.1
1	B	185	ILE	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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(Å <sup>2</sup> )	Q<0.9
3	C8E	B	1306	11/21	0.83	0.51	5.60	47,54,62,63	0
3	C8E	A	1304	8/21	0.82	0.27	4.32	36,43,46,48	0
3	C8E	D	1303	9/21	0.90	0.23	3.67	40,46,63,67	0
3	C8E	A	1300	11/21	0.87	0.28	2.84	39,49,68,68	0
3	C8E	A	1301	9/21	0.92	0.25	2.79	39,45,49,58	0
3	C8E	A	1302	9/21	0.93	0.23	2.50	40,44,53,62	0
3	C8E	C	1301	9/21	0.93	0.21	2.42	39,46,56,63	0
2	SO4	B	1302	5/5	0.93	0.19	2.25	43,61,70,70	0
2	SO4	D	1295	5/5	0.97	0.28	2.12	61,74,82,90	0
3	C8E	B	1304	8/21	0.91	0.20	2.08	36,40,46,46	0
2	SO4	B	1301	5/5	0.82	0.23	1.92	79,80,99,110	0
3	C8E	D	1304	9/21	0.89	0.20	1.41	34,49,52,56	0
3	C8E	C	1300	11/21	0.88	0.19	1.30	41,43,49,51	0
3	C8E	D	1302	12/21	0.88	0.22	1.05	39,50,68,71	0
2	SO4	C	1294	5/5	0.91	0.17	0.85	69,70,84,84	0
2	SO4	D	1297	5/5	0.88	0.19	0.21	74,76,85,100	0
2	SO4	B	1299	5/5	0.95	0.17	0.05	43,69,78,78	0
2	SO4	A	1297	5/5	0.98	0.18	-0.01	57,70,77,84	0
2	SO4	B	1303	5/5	0.91	0.14	-0.05	55,57,65,72	0
2	SO4	D	1300	5/5	0.94	0.18	-0.18	56,62,83,84	0
3	C8E	B	1305	8/21	0.90	0.15	-0.19	32,40,45,47	0
3	C8E	C	1302	9/21	0.90	0.15	-0.29	37,41,48,57	0
2	SO4	C	1295	5/5	0.98	0.13	-0.52	41,51,51,52	0
2	SO4	D	1296	5/5	0.94	0.14	-0.69	62,67,72,79	0
2	SO4	D	1301	5/5	0.96	0.13	-0.75	46,66,79,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	SO4	C	1299	5/5	0.96	0.14	-0.75	49,63,72,75	0
2	SO4	A	1298	5/5	0.97	0.14	-0.82	56,62,77,82	0
3	C8E	A	1303	10/21	0.90	0.14	-0.88	37,42,46,58	0
2	SO4	C	1296	5/5	0.97	0.14	-0.92	38,56,70,72	0
2	SO4	A	1299	5/5	0.88	0.12	-1.51	49,64,85,96	0
2	SO4	C	1298	5/5	0.95	0.28	-	45,49,64,65	0
2	SO4	A	1296	5/5	0.95	0.17	-	64,66,83,91	0
2	SO4	C	1297	5/5	0.94	0.12	-	65,67,79,86	0
2	SO4	D	1299	5/5	0.88	0.16	-	72,91,94,101	0
2	SO4	A	1295	5/5	0.92	0.17	-	61,74,93,105	0
2	SO4	B	1300	5/5	0.93	0.14	-	58,73,75,79	0
2	SO4	D	1298	5/5	0.96	0.12	-	69,75,83,87	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.