



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 11:07 AM GMT

PDB ID : 3O4L  
Title : Genetic and structural basis for selection of a ubiquitous T cell receptor deployed in Epstein-Barr virus  
Authors : Miles, J.J.; Bulek, A.M.; Cole, D.K.; Gostick, E.; Schauenburg, J.A.; Dolton, G.; Venturi, V.; Davenport, M.P.; Tan, M.P.; Burrows, S.R.; Wooldridge, L.; Price, D.A.; Rizkallah, P.J.; Sewell, A.K.  
Deposited on : 2010-07-27  
Resolution : 2.54 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

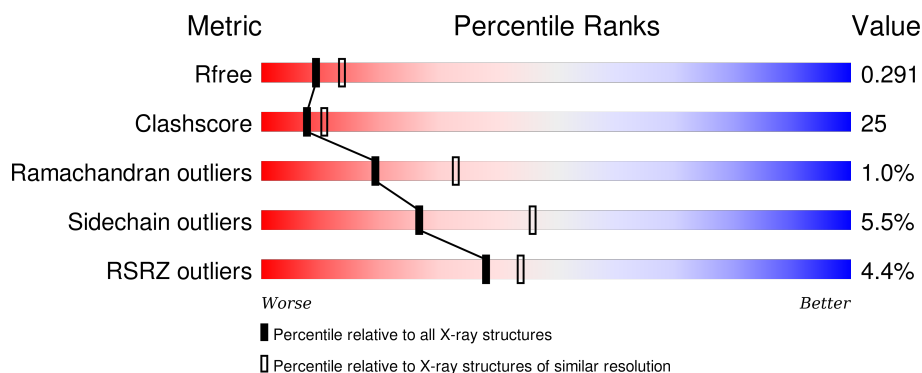
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.54 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	276	<div> <div>2%</div> <div>74%</div> <div>24%</div> <div>.</div> </div>
2	B	100	<div> <div>5%</div> <div>57%</div> <div>38%</div> <div>5%</div> </div>
3	C	9	<div> <div>67%</div> <div>33%</div> </div>
4	D	195	<div> <div>11%</div> <div>54%</div> <div>36%</div> <div>9%</div> <div>.</div> </div>
5	E	245	<div> <div>2%</div> <div>71%</div> <div>25%</div> <div>.</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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	GOL	A	279	-	-	-	X
6	GOL	D	202	-	-	X	X
6	GOL	D	6	-	-	X	-
6	GOL	E	1	-	-	-	X
6	GOL	E	247	-	-	-	X
6	GOL	E	250	-	-	X	X
7	SO4	E	252	-	-	-	X

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 7067 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 MHC class I antigen.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	276	Total	C	N	O	S	0	0	0
			2254	1408	410	427	9			

- Molecule 2 is a protein called Beta-2-microglobulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	100	Total	C	N	O	S	0	0	0
			834	530	140	159	5			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	MET	-	expression tag	UNP P61769
B	91	CYS	LYS	engineered	UNP P61769

- Molecule 3 is a protein called BSLF2/BMLF1 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	9	Total	C	N	O	S	0	0	0
			62	40	9	11	2			

- Molecule 4 is a protein called T-CELL RECEPTOR, ALPHA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	195	Total	C	N	O	S	0	0	0
			1538	960	254	314	10			

- Molecule 5 is a protein called T-CELL RECEPTOR, BETA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	245	Total	C	N	O	S	0	0	0
			1930	1215	331	375	9			

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			6	3	3		
6	A	1	Total	C	O	0	0
			6	3	3		
6	A	1	Total	C	O	0	0
			6	3	3		
6	B	1	Total	C	O	0	0
			6	3	3		
6	D	1	Total	C	O	0	0
			6	3	3		
6	D	1	Total	C	O	0	0
			6	3	3		
6	E	1	Total	C	O	0	0
			6	3	3		
6	E	1	Total	C	O	0	0
			6	3	3		
6	E	1	Total	C	O	0	0
			6	3	3		
6	E	1	Total	C	O	0	0
			6	3	3		

- Molecule 7 is SULFATE ION (three-letter code: SO4) (formula:  $O_4S$ ).



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

- Molecule 8 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: C<sub>6</sub>H<sub>13</sub>NO<sub>4</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

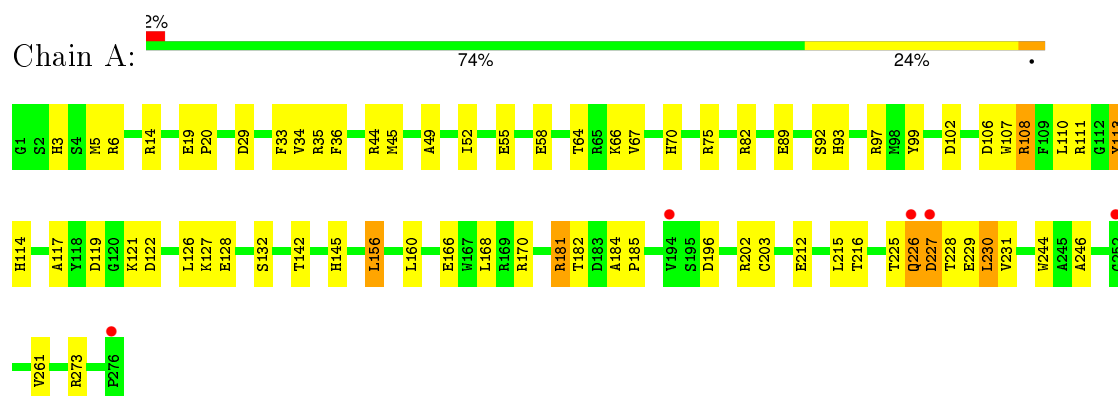
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	106	Total	O	0	0
			106	106		
9	B	48	Total	O	0	0
			48	48		
9	C	3	Total	O	0	0
			3	3		
9	D	76	Total	O	0	0
			76	76		
9	E	101	Total	O	0	2
			103	103		

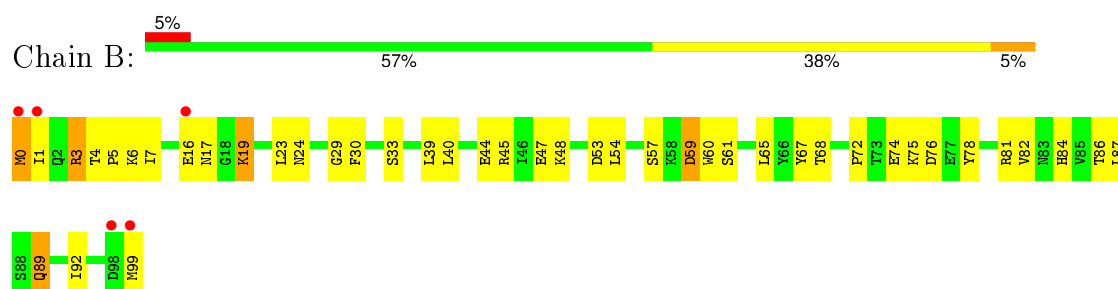
### 3 Residue-property plots

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.

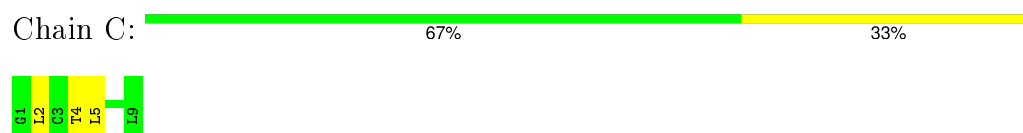
- Molecule 1: MHC class I antigen



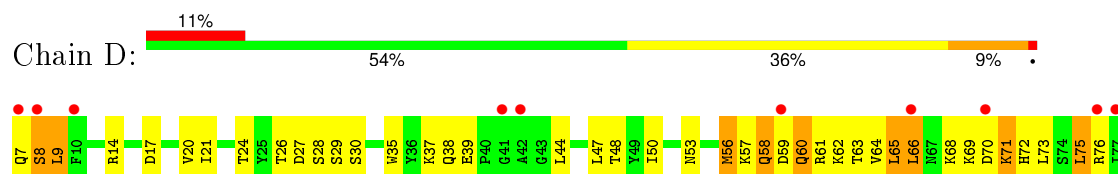
- Molecule 2: Beta-2-microglobulin



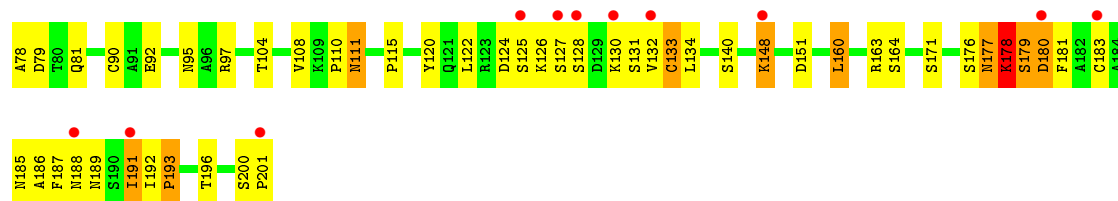
- Molecule 3: BSLF2/BMLF1 protein



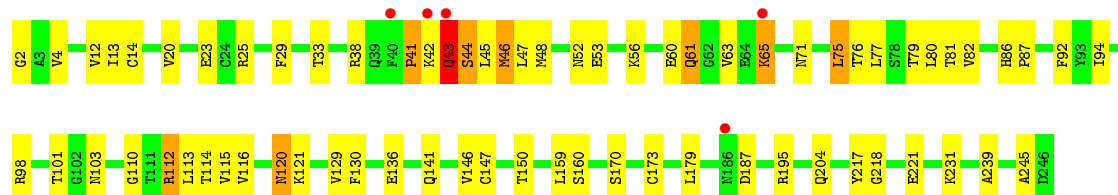
- Molecule 4: T-CELL RECEPTOR, ALPHA CHAIN







• Molecule 5: T-CELL RECEPTOR, BETA CHAIN



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	94.08 Å 122.50 Å 82.37 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	61.25 – 2.54 61.25 – 2.54	Depositor EDS
% Data completeness (in resolution range)	100.0 (61.25-2.54) 99.0 (61.25-2.54)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.16	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.64 (at 2.55 Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.221 , 0.296 0.218 , 0.291	Depositor DCC
$R_{free}$ test set	1603 reflections (5.31%)	DCC
Wilson B-factor (Å <sup>2</sup> )	30.3	Xtriage
Anisotropy	0.476	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 36.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 31773 reflections	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	7067	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.13% 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: GOL, SO4, MES

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	0.79	4/2320 (0.2%)	0.54	0/3149
2	B	0.74	0/857	0.60	1/1159 (0.1%)
3	C	0.73	0/61	0.63	0/80
4	D	0.94	4/1568 (0.3%)	0.68	3/2123 (0.1%)
5	E	0.80	2/1981 (0.1%)	0.63	2/2695 (0.1%)
All	All	0.82	10/6787 (0.1%)	0.61	6/9206 (0.1%)

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	133	CYS	CB-SG	-14.49	1.57	1.82
4	D	183	CYS	CB-SG	-9.50	1.66	1.82
1	A	166	GLU	CG-CD	6.07	1.61	1.51
1	A	203	CYS	CB-SG	-5.67	1.72	1.81
4	D	133	CYS	CA-CB	-5.39	1.42	1.53
5	E	147	CYS	CB-SG	-5.33	1.73	1.81
1	A	58	GLU	CG-CD	5.21	1.59	1.51
4	D	183	CYS	CA-CB	-5.16	1.42	1.53
1	A	113	TYR	CB-CG	-5.08	1.44	1.51
5	E	14	CYS	CB-SG	-5.08	1.73	1.81

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	183	CYS	CA-CB-SG	-7.03	101.35	114.00
5	E	43	GLN	N-CA-C	6.18	127.68	111.00
5	E	44	SER	N-CA-C	5.54	125.95	111.00
4	D	178	LYS	N-CA-C	-5.52	96.09	111.00
4	D	179	SER	N-CA-C	5.34	125.42	111.00
2	B	59	ASP	N-CA-C	-5.10	97.24	111.00

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2254	0	2103	73	0
2	B	834	0	795	50	1
3	C	62	0	73	2	0
4	D	1538	0	1466	135	0
5	E	1930	0	1837	100	1
6	A	18	0	24	5	0
6	B	6	0	8	1	0
6	D	12	0	16	8	0
6	E	30	0	40	9	0
7	A	10	0	0	0	0
7	B	10	0	0	1	0
7	E	15	0	0	0	0
8	B	12	0	12	0	0
9	A	106	0	0	5	0
9	B	48	0	0	2	0
9	C	3	0	0	0	0
9	D	76	0	0	2	0
9	E	103	0	0	2	0
All	All	7067	0	6374	330	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 25.

All (330) 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)
4:D:7:GLN:O	5:E:43:GLN:HG2	1.31	1.29
4:D:26:THR:HG22	4:D:92:GLU:OE2	1.36	1.24
4:D:192:ILE:CD1	4:D:196:THR:HG21	1.68	1.22
4:D:61:ARG:HG3	4:D:62:LYS:HG3	1.32	1.12
4:D:61:ARG:HG3	4:D:62:LYS:H	1.12	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:61:ARG:CG	4:D:62:LYS:H	1.60	1.09
4:D:192:ILE:HD13	4:D:196:THR:HG21	1.20	1.07
5:E:112:ARG:HG2	5:E:112:ARG:HH21	1.15	1.06
4:D:7:GLN:HG2	4:D:8:SER:H	1.22	1.02
5:E:43:GLN:O	5:E:44:SER:HB2	1.60	0.99
4:D:58:GLN:O	4:D:58:GLN:HG2	1.60	0.98
4:D:7:GLN:O	5:E:43:GLN:CG	2.11	0.97
4:D:177:ASN:O	4:D:178:LYS:HB3	1.64	0.94
4:D:178:LYS:O	4:D:178:LYS:HG2	1.68	0.91
1:A:108:ARG:HH11	1:A:108:ARG:HG2	1.36	0.90
4:D:60:GLN:HG3	4:D:61:ARG:N	1.83	0.89
1:A:226:GLN:O	1:A:227:ASP:HB2	1.73	0.88
5:E:101:THR:HG22	9:E:343:HOH:O	1.72	0.87
4:D:192:ILE:CD1	4:D:196:THR:CG2	2.52	0.87
4:D:76:ARG:NH2	4:D:78:ALA:HB2	1.90	0.87
4:D:61:ARG:CG	4:D:62:LYS:N	2.36	0.86
2:B:29:GLY:HA2	2:B:61:SER:OG	1.75	0.86
4:D:60:GLN:CG	4:D:61:ARG:N	2.39	0.86
5:E:43:GLN:HE21	5:E:43:GLN:N	1.74	0.85
4:D:66:LEU:HD12	4:D:66:LEU:O	1.74	0.85
1:A:114:HIS:CD2	1:A:156:LEU:HD11	2.11	0.85
4:D:177:ASN:H	4:D:177:ASN:HD22	1.25	0.85
1:A:49:ALA:O	1:A:52:ILE:HG22	1.77	0.84
5:E:112:ARG:CG	5:E:112:ARG:HH21	1.89	0.84
4:D:57:LYS:O	4:D:65:LEU:HD13	1.78	0.84
2:B:4:THR:OG1	2:B:86:THR:HG21	1.78	0.84
5:E:112:ARG:HG2	5:E:112:ARG:NH2	1.91	0.84
4:D:132:VAL:HG21	5:E:146:VAL:HG21	1.59	0.84
1:A:226:GLN:HG2	1:A:226:GLN:O	1.75	0.84
4:D:61:ARG:HG3	4:D:62:LYS:CG	2.09	0.83
4:D:61:ARG:HG3	4:D:62:LYS:N	1.91	0.82
4:D:61:ARG:CG	4:D:62:LYS:HG3	2.08	0.82
5:E:71:ASN:OD1	5:E:79:THR:HB	1.79	0.82
4:D:131:SER:HG	6:D:6:GOL:HO2	1.17	0.82
1:A:108:ARG:HH11	1:A:108:ARG:CG	1.94	0.81
1:A:230:LEU:HD21	9:A:296:HOH:O	1.80	0.80
5:E:159:LEU:HD23	5:E:160:SER:N	1.96	0.80
1:A:97:ARG:HE	1:A:114:HIS:HE1	1.30	0.79
1:A:230:LEU:C	1:A:230:LEU:CD2	2.51	0.78
4:D:37:LYS:NZ	4:D:39:GLU:OE2	2.16	0.78
4:D:68:LYS:O	4:D:70:ASP:N	2.17	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:230:LEU:O	1:A:230:LEU:HD22	1.85	0.77
5:E:56:LYS:H	5:E:56:LYS:HD2	1.49	0.77
5:E:129:VAL:HG23	5:E:239:ALA:HB3	1.67	0.77
4:D:7:GLN:HG2	4:D:8:SER:N	1.99	0.77
4:D:124:ASP:CG	4:D:126:LYS:O	2.24	0.76
4:D:26:THR:CG2	4:D:92:GLU:OE2	2.28	0.76
4:D:160:LEU:O	4:D:160:LEU:HD12	1.87	0.75
1:A:6:ARG:NH2	1:A:102:ASP:OD1	2.20	0.75
4:D:65:LEU:HD13	4:D:65:LEU:N	2.01	0.75
4:D:148:LYS:HB2	4:D:148:LYS:NZ	2.01	0.75
4:D:7:GLN:HA	5:E:43:GLN:HB2	1.68	0.75
5:E:130:PHE:HB2	5:E:146:VAL:HG22	1.71	0.73
5:E:45:LEU:HD21	5:E:94:ILE:HD12	1.71	0.72
5:E:38:ARG:HG3	5:E:48:MET:SD	2.29	0.72
4:D:95:ASN:N	6:D:202:GOL:O2	2.17	0.72
4:D:65:LEU:N	4:D:65:LEU:CD1	2.53	0.72
5:E:25:ARG:HG3	5:E:76:THR:HG22	1.71	0.71
5:E:221:GLU:HA	5:E:231:LYS:HZ3	1.55	0.71
4:D:177:ASN:ND2	4:D:177:ASN:O	2.22	0.71
4:D:97:ARG:HD2	5:E:47:LEU:CD2	2.21	0.70
5:E:43:GLN:NE2	5:E:43:GLN:N	2.40	0.69
4:D:7:GLN:CA	5:E:43:GLN:HB2	2.23	0.69
5:E:42:LYS:HB3	5:E:43:GLN:NE2	2.08	0.68
5:E:43:GLN:O	5:E:44:SER:CB	2.33	0.68
1:A:215:LEU:O	1:A:216:THR:HG23	1.94	0.68
4:D:192:ILE:HD11	4:D:196:THR:HG21	1.74	0.67
4:D:191:ILE:HD13	4:D:191:ILE:C	2.15	0.67
2:B:0:MET:CE	2:B:0:MET:N	2.58	0.67
4:D:65:LEU:HD13	4:D:65:LEU:H	1.61	0.66
1:A:230:LEU:C	1:A:230:LEU:HD22	2.15	0.66
5:E:12:VAL:HG13	5:E:113:LEU:CD1	2.25	0.66
4:D:7:GLN:CG	4:D:8:SER:H	1.94	0.66
4:D:160:LEU:HD12	4:D:160:LEU:C	2.16	0.66
1:A:229:GLU:O	1:A:229:GLU:HG3	1.96	0.66
4:D:66:LEU:HD12	4:D:66:LEU:C	2.16	0.65
5:E:221:GLU:HA	5:E:231:LYS:NZ	2.11	0.65
4:D:30:SER:HA	6:D:202:GOL:H2	1.79	0.65
2:B:0:MET:HE3	2:B:0:MET:N	2.12	0.64
4:D:68:LYS:C	4:D:70:ASP:H	2.00	0.64
5:E:60:GLU:O	5:E:63:VAL:HG22	1.98	0.64
5:E:56:LYS:N	5:E:56:LYS:HD2	2.12	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:82:ARG:HD2	1:A:89:GLU:HA	1.80	0.64
2:B:84:HIS:HB3	2:B:87:LEU:HD23	1.80	0.63
2:B:47:GLU:O	2:B:48:LYS:HG3	1.98	0.63
5:E:179:LEU:HD12	5:E:179:LEU:C	2.18	0.62
5:E:20:VAL:CG1	5:E:82:VAL:HB	2.29	0.62
4:D:60:GLN:HG3	4:D:61:ARG:H	1.62	0.62
2:B:24:ASN:HD22	2:B:67:TYR:HB3	1.65	0.62
4:D:177:ASN:N	4:D:177:ASN:HD22	1.96	0.62
4:D:21:ILE:HD12	4:D:21:ILE:N	2.15	0.62
4:D:192:ILE:HD13	4:D:196:THR:CG2	2.13	0.62
5:E:33:THR:OG1	5:E:52:ASN:ND2	2.33	0.61
4:D:97:ARG:HD2	5:E:47:LEU:HD23	1.82	0.61
1:A:35:ARG:HG2	1:A:36:PHE:N	2.13	0.61
5:E:204:GLN:O	5:E:245:ALA:HB2	2.01	0.60
4:D:124:ASP:OD2	4:D:128:SER:HB2	2.01	0.60
4:D:148:LYS:HZ2	4:D:148:LYS:HB2	1.63	0.60
4:D:122:LEU:CD2	5:E:146:VAL:HG13	2.31	0.60
4:D:200:SER:HB2	4:D:201:PRO:HD2	1.82	0.60
5:E:179:LEU:O	5:E:179:LEU:HD12	2.02	0.60
4:D:47:LEU:O	4:D:48:THR:HG23	2.02	0.60
5:E:218:GLY:O	6:E:250:GOL:H2	2.02	0.60
5:E:116:VAL:HB	5:E:121:LYS:HD3	1.83	0.59
5:E:46:MET:HE2	5:E:46:MET:HA	1.83	0.59
4:D:64:VAL:HB	4:D:76:ARG:HB3	1.84	0.59
4:D:47:LEU:H	4:D:47:LEU:HD23	1.68	0.59
5:E:12:VAL:HG13	5:E:113:LEU:HD13	1.84	0.59
1:A:226:GLN:HG3	1:A:227:ASP:OD2	2.03	0.59
4:D:61:ARG:HG2	4:D:62:LYS:H	1.60	0.59
1:A:3:HIS:ND1	1:A:29:ASP:OD2	2.28	0.58
5:E:29:PHE:HA	6:E:249:GOL:H2	1.85	0.58
1:A:117:ALA:HB2	2:B:60:TRP:CE2	2.39	0.58
1:A:19:GLU:HG3	1:A:20:PRO:HD2	1.86	0.58
5:E:75:LEU:N	5:E:75:LEU:HD12	2.19	0.57
5:E:43:GLN:NE2	5:E:43:GLN:CA	2.66	0.57
1:A:114:HIS:HD2	1:A:156:LEU:HD11	1.69	0.57
4:D:179:SER:C	4:D:181:PHE:H	2.07	0.56
5:E:103:ASN:HA	6:E:247:GOL:O2	2.06	0.56
4:D:58:GLN:O	4:D:58:GLN:CG	2.33	0.56
4:D:79:ASP:OD1	4:D:79:ASP:O	2.23	0.56
1:A:35:ARG:HG3	2:B:53:ASP:OD2	2.06	0.56
4:D:7:GLN:CG	4:D:8:SER:N	2.61	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:66:LEU:C	4:D:66:LEU:CD1	2.75	0.56
1:A:66:LYS:O	1:A:70:HIS:HD2	1.89	0.55
1:A:75:ARG:NH2	5:E:53:GLU:O	2.39	0.55
2:B:0:MET:HA	2:B:0:MET:HE2	1.89	0.55
4:D:180:ASP:C	4:D:180:ASP:OD2	2.43	0.55
5:E:25:ARG:HG3	5:E:76:THR:CG2	2.37	0.55
5:E:159:LEU:C	5:E:159:LEU:HD23	2.27	0.55
5:E:221:GLU:HG2	5:E:231:LYS:HZ3	1.72	0.55
5:E:20:VAL:HG12	5:E:82:VAL:HB	1.89	0.55
5:E:23:GLU:HB3	5:E:77:LEU:HD11	1.89	0.55
5:E:80:LEU:HD23	5:E:81:THR:N	2.22	0.55
4:D:47:LEU:O	4:D:48:THR:CG2	2.55	0.55
2:B:6:LYS:NZ	2:B:6:LYS:HB2	2.22	0.54
1:A:215:LEU:O	1:A:216:THR:CG2	2.55	0.54
5:E:44:SER:OG	5:E:45:LEU:N	2.41	0.54
5:E:12:VAL:CG1	5:E:113:LEU:HD13	2.37	0.54
4:D:111:ASN:N	4:D:111:ASN:HD22	2.05	0.54
5:E:2:GLY:O	5:E:4:VAL:HG23	2.06	0.54
2:B:57:SER:O	2:B:59:ASP:O	2.26	0.54
1:A:156:LEU:HD22	1:A:160:LEU:HG	1.87	0.54
5:E:45:LEU:CD2	5:E:94:ILE:HD12	2.36	0.54
5:E:12:VAL:HG13	5:E:113:LEU:HD12	1.89	0.54
4:D:111:ASN:HD22	4:D:111:ASN:H	1.56	0.54
1:A:230:LEU:HD23	1:A:230:LEU:C	2.26	0.53
2:B:24:ASN:HB3	2:B:65:LEU:HD11	1.88	0.53
1:A:127:LYS:HD3	1:A:132:SER:HB3	1.90	0.53
5:E:12:VAL:HA	6:E:250:GOL:H11	1.90	0.53
1:A:114:HIS:CD2	1:A:156:LEU:CD1	2.88	0.53
1:A:6:ARG:NH2	1:A:113:TYR:CE1	2.76	0.53
2:B:89:GLN:NE2	9:B:122:HOH:O	2.40	0.53
2:B:0:MET:H2	2:B:0:MET:HE3	1.73	0.53
5:E:112:ARG:CG	5:E:112:ARG:NH2	2.58	0.53
4:D:7:GLN:O	5:E:43:GLN:CB	2.56	0.53
4:D:59:ASP:O	4:D:59:ASP:OD2	2.27	0.53
4:D:192:ILE:HD12	4:D:193:PRO:O	2.09	0.53
4:D:47:LEU:N	4:D:47:LEU:HD23	2.24	0.53
4:D:130:LYS:HZ2	5:E:150:THR:HG21	1.75	0.52
5:E:217:TYR:HB3	6:E:250:GOL:H31	1.90	0.52
1:A:106:ASP:O	1:A:107:TRP:HB2	2.09	0.52
4:D:68:LYS:HB3	4:D:72:HIS:HB3	1.91	0.52
4:D:179:SER:C	4:D:181:PHE:N	2.62	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:61:GLN:C	5:E:61:GLN:NE2	2.63	0.52
4:D:134:LEU:HD11	4:D:171:SER:HB2	1.92	0.52
2:B:1:ILE:N	2:B:1:ILE:HD12	2.24	0.52
1:A:119:ASP:O	2:B:1:ILE:HD13	2.09	0.52
1:A:14:ARG:NH1	9:A:357:HOH:O	2.38	0.52
4:D:120:TYR:CE1	5:E:136:GLU:HA	2.46	0.51
4:D:7:GLN:C	5:E:43:GLN:HB2	2.30	0.51
1:A:114:HIS:HD2	1:A:156:LEU:CD1	2.23	0.51
4:D:131:SER:OG	6:D:6:GOL:O2	2.01	0.51
4:D:35:TRP:O	4:D:47:LEU:HD23	2.10	0.51
4:D:73:LEU:HD23	4:D:90:CYS:HB2	1.92	0.51
4:D:63:THR:HG23	4:D:75:LEU:HD21	1.91	0.51
2:B:16:GLU:HB3	2:B:19:LYS:HG2	1.92	0.51
4:D:127:SER:HG	6:D:6:GOL:HO1	1.50	0.51
4:D:9:LEU:HD12	4:D:104:THR:HG23	1.93	0.51
2:B:29:GLY:HA2	2:B:61:SER:HG	1.75	0.50
1:A:97:ARG:HE	1:A:114:HIS:CE1	2.18	0.50
4:D:124:ASP:C	4:D:126:LYS:H	2.14	0.50
1:A:181:ARG:HG2	1:A:182:THR:N	2.25	0.50
4:D:122:LEU:HD12	4:D:122:LEU:N	2.27	0.50
2:B:29:GLY:CA	2:B:61:SER:OG	2.55	0.50
5:E:56:LYS:CD	5:E:56:LYS:H	2.21	0.50
2:B:24:ASN:ND2	2:B:67:TYR:HB3	2.26	0.50
4:D:177:ASN:O	4:D:178:LYS:CB	2.43	0.50
1:A:228:THR:HA	1:A:246:ALA:O	2.11	0.50
5:E:43:GLN:HE21	5:E:43:GLN:CA	2.25	0.49
1:A:225:THR:OG1	1:A:226:GLN:N	2.43	0.49
2:B:4:THR:HG22	2:B:5:PRO:HD2	1.93	0.49
2:B:24:ASN:HD22	2:B:67:TYR:CB	2.25	0.49
1:A:244:TRP:NE1	2:B:99:MET:HG3	2.28	0.49
4:D:130:LYS:NZ	5:E:150:THR:HG21	2.28	0.49
4:D:95:ASN:H	6:D:202:GOL:HO2	1.51	0.49
1:A:202:ARG:HD3	1:A:244:TRP:CE3	2.47	0.49
4:D:111:ASN:H	4:D:111:ASN:ND2	2.10	0.49
1:A:111:ARG:NH1	1:A:128:GLU:HG3	2.28	0.49
2:B:4:THR:CG2	2:B:5:PRO:HD2	2.43	0.49
1:A:226:GLN:O	1:A:227:ASP:CB	2.48	0.48
2:B:39:LEU:CD1	2:B:68:THR:HG22	2.44	0.48
4:D:68:LYS:C	4:D:70:ASP:N	2.65	0.48
5:E:65:LYS:HD3	5:E:65:LYS:O	2.12	0.48
2:B:76:ASP:HB3	2:B:78:TYR:CE2	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:97:ARG:NE	1:A:114:HIS:HE1	2.06	0.48
5:E:42:LYS:HB3	5:E:43:GLN:HE21	1.79	0.48
4:D:151:ASP:OD1	4:D:151:ASP:N	2.46	0.48
1:A:145:HIS:HB2	6:A:279:GOL:H32	1.96	0.48
4:D:124:ASP:O	4:D:126:LYS:N	2.47	0.48
1:A:230:LEU:CD2	9:A:296:HOH:O	2.51	0.47
1:A:145:HIS:CB	6:A:279:GOL:H32	2.44	0.47
2:B:40:LEU:HA	2:B:44:GLU:O	2.14	0.47
1:A:108:ARG:NH1	1:A:108:ARG:CG	2.63	0.47
2:B:87:LEU:HD22	2:B:87:LEU:N	2.29	0.47
1:A:231:VAL:HG13	1:A:244:TRP:CZ2	2.49	0.47
2:B:33:SER:HB2	2:B:54:LEU:HD21	1.96	0.47
4:D:124:ASP:C	4:D:126:LYS:N	2.67	0.47
5:E:45:LEU:O	5:E:46:MET:HE3	2.14	0.47
1:A:126:LEU:HD22	1:A:156:LEU:HD13	1.98	0.46
1:A:127:LYS:HE3	6:A:278:GOL:H11	1.97	0.46
4:D:44:LEU:HD11	5:E:45:LEU:HD11	1.97	0.46
4:D:38:GLN:HB2	4:D:44:LEU:HD23	1.97	0.46
1:A:142:THR:HG23	6:A:279:GOL:H12	1.97	0.46
4:D:97:ARG:CD	5:E:47:LEU:CD2	2.94	0.46
1:A:55:GLU:OE2	1:A:170:ARG:NH1	2.47	0.46
5:E:86:HIS:HB3	5:E:87:PRO:CD	2.46	0.46
2:B:5:PRO:HB3	2:B:30:PHE:HB3	1.97	0.46
4:D:160:LEU:CD1	4:D:160:LEU:C	2.83	0.46
1:A:75:ARG:NH1	5:E:53:GLU:OE1	2.49	0.46
4:D:122:LEU:HD22	5:E:146:VAL:HG13	1.97	0.46
1:A:231:VAL:CG1	1:A:244:TRP:CZ2	2.99	0.46
2:B:0:MET:HE2	2:B:0:MET:CA	2.45	0.46
1:A:5:MET:HB2	1:A:168:LEU:HD13	1.97	0.46
1:A:117:ALA:HB2	2:B:60:TRP:CD2	2.51	0.45
4:D:185:ASN:O	4:D:188:ASN:HB3	2.16	0.45
4:D:185:ASN:OD1	4:D:186:ALA:N	2.50	0.45
1:A:111:ARG:HH12	1:A:128:GLU:CG	2.28	0.45
4:D:24:THR:HA	4:D:71:LYS:O	2.16	0.45
2:B:0:MET:H1	2:B:0:MET:CE	2.28	0.45
4:D:56:MET:HA	4:D:65:LEU:O	2.17	0.45
4:D:37:LYS:HB2	4:D:47:LEU:HD22	1.99	0.45
4:D:163:ARG:HG2	5:E:170:SER:OG	2.16	0.45
1:A:127:LYS:HB3	6:A:278:GOL:C1	2.47	0.45
5:E:86:HIS:HB3	5:E:87:PRO:HD2	1.98	0.45
1:A:33:PHE:CD2	1:A:34:VAL:HG13	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:176:SER:OG	4:D:178:LYS:HD3	2.17	0.44
4:D:132:VAL:C	4:D:133:CYS:SG	2.95	0.44
5:E:25:ARG:HA	5:E:76:THR:O	2.17	0.44
4:D:110:PRO:O	4:D:140:SER:OG	2.33	0.44
4:D:185:ASN:OD1	4:D:185:ASN:C	2.55	0.44
2:B:4:THR:CB	2:B:86:THR:HG21	2.48	0.44
1:A:93:HIS:HD2	1:A:119:ASP:OD1	2.01	0.44
2:B:23:LEU:O	2:B:67:TYR:HA	2.18	0.44
4:D:20:VAL:C	4:D:21:ILE:HD12	2.38	0.44
4:D:14:ARG:HB2	4:D:17:ASP:OD1	2.18	0.44
1:A:82:ARG:NH1	9:A:300:HOH:O	2.50	0.43
5:E:92:PHE:CZ	5:E:110:GLY:HA3	2.53	0.43
2:B:5:PRO:HD2	2:B:87:LEU:HD21	2.00	0.43
1:A:122:ASP:OD1	2:B:60:TRP:NE1	2.43	0.43
4:D:97:ARG:HD2	5:E:47:LEU:HD21	1.98	0.43
5:E:120:ASN:HD22	5:E:121:LYS:N	2.16	0.43
2:B:39:LEU:HD12	2:B:68:THR:HG22	2.00	0.43
4:D:50:ILE:HD12	4:D:65:LEU:HD22	2.00	0.43
4:D:148:LYS:HZ3	4:D:148:LYS:HB2	1.82	0.43
4:D:97:ARG:CD	5:E:47:LEU:HD21	2.49	0.43
5:E:120:ASN:HD22	5:E:120:ASN:C	2.21	0.43
5:E:221:GLU:HB3	9:E:259:HOH:O	2.18	0.43
5:E:221:GLU:CA	5:E:231:LYS:HZ3	2.27	0.43
4:D:47:LEU:C	4:D:48:THR:HG23	2.39	0.43
4:D:191:ILE:CD1	4:D:191:ILE:C	2.85	0.43
2:B:81:ARG:HG3	2:B:92:ILE:CD1	2.49	0.43
2:B:17:ASN:HA	2:B:72:PRO:O	2.17	0.43
2:B:84:HIS:CD2	2:B:86:THR:H	2.36	0.43
4:D:127:SER:OG	6:D:6:GOL:O1	2.21	0.43
5:E:75:LEU:H	5:E:75:LEU:HD12	1.83	0.43
4:D:9:LEU:HA	4:D:9:LEU:HD22	1.69	0.43
5:E:121:LYS:NZ	5:E:187:ASP:OD1	2.45	0.42
2:B:40:LEU:CD1	2:B:40:LEU:N	2.82	0.42
4:D:111:ASN:O	4:D:111:ASN:ND2	2.52	0.42
4:D:71:LYS:HD3	4:D:71:LYS:N	2.34	0.42
5:E:75:LEU:N	5:E:75:LEU:CD1	2.82	0.42
1:A:45:MET:HE1	3:C:2:LEU:HD11	2.02	0.42
5:E:13:ILE:H	6:E:250:GOL:H11	1.83	0.42
4:D:187:PHE:C	4:D:189:ASN:H	2.21	0.42
7:B:102:SO4:O1	9:B:169:HOH:O	2.21	0.42
5:E:179:LEU:CD1	5:E:179:LEU:C	2.86	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:196:ASP:O	1:A:196:ASP:OD1	2.38	0.42
4:D:81:GLN:O	4:D:108:VAL:HG21	2.20	0.42
1:A:212:GLU:OE2	1:A:212:GLU:HA	2.20	0.42
4:D:60:GLN:HG2	4:D:61:ARG:CB	2.50	0.42
5:E:141:GLN:HA	5:E:141:GLN:NE2	2.34	0.42
5:E:98:ARG:NH2	6:E:247:GOL:O1	2.53	0.42
5:E:114:THR:HG23	6:E:1:GOL:O2	2.20	0.42
4:D:196:THR:HG23	9:D:235:HOH:O	2.20	0.41
4:D:160:LEU:HB3	5:E:173:CYS:HB2	2.01	0.41
2:B:74:GLU:C	2:B:74:GLU:OE1	2.59	0.41
1:A:6:ARG:HH22	1:A:113:TYR:HE1	1.64	0.41
4:D:29:SER:HB3	6:D:202:GOL:H12	2.03	0.41
2:B:7:ILE:HD13	2:B:82:VAL:HG21	2.03	0.41
2:B:57:SER:C	2:B:59:ASP:O	2.59	0.41
2:B:59:ASP:OD1	2:B:61:SER:HB3	2.20	0.41
1:A:99:TYR:HB3	1:A:114:HIS:ND1	2.36	0.41
1:A:215:LEU:CD2	1:A:261:VAL:HG22	2.51	0.41
1:A:92:SER:N	9:A:284:HOH:O	2.53	0.41
4:D:124:ASP:CB	4:D:126:LYS:O	2.69	0.41
5:E:221:GLU:CG	5:E:231:LYS:HZ3	2.33	0.41
2:B:0:MET:CA	2:B:0:MET:CE	2.98	0.41
5:E:20:VAL:HG13	5:E:82:VAL:HB	2.02	0.41
5:E:87:PRO:HA	5:E:115:VAL:HB	2.01	0.41
4:D:27:ASP:OD2	4:D:28:SER:N	2.54	0.41
4:D:62:LYS:HB3	4:D:78:ALA:HB3	2.03	0.41
4:D:97:ARG:HG3	5:E:47:LEU:HD21	2.03	0.41
4:D:111:ASN:N	4:D:111:ASN:ND2	2.68	0.41
1:A:184:ALA:HA	1:A:185:PRO:HD3	1.91	0.41
2:B:3:ARG:HB3	6:B:101:GOL:H31	2.03	0.41
1:A:108:ARG:NH1	1:A:108:ARG:HG2	2.16	0.40
2:B:24:ASN:ND2	2:B:67:TYR:CB	2.85	0.40
1:A:64:THR:O	1:A:67:VAL:HG12	2.20	0.40
4:D:7:GLN:O	5:E:43:GLN:HB2	2.20	0.40
1:A:215:LEU:C	1:A:216:THR:HG23	2.42	0.40
3:C:4:THR:O	6:E:247:GOL:H11	2.21	0.40
4:D:164:SER:HB3	9:D:207:HOH:O	2.21	0.40
5:E:63:VAL:O	5:E:63:VAL:HG23	2.21	0.40
5:E:75:LEU:H	5:E:75:LEU:CD1	2.34	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)
2:B:45:ARG:NH2	5:E:221:GLU:OE2[2_565]	1.88	0.32

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	274/276 (99%)	264 (96%)	9 (3%)	1 (0%)	39	60
2	B	98/100 (98%)	91 (93%)	7 (7%)	0	100	100
3	C	7/9 (78%)	7 (100%)	0	0	100	100
4	D	193/195 (99%)	170 (88%)	17 (9%)	6 (3%)	5	6
5	E	243/245 (99%)	228 (94%)	14 (6%)	1 (0%)	39	60
All	All	815/825 (99%)	760 (93%)	47 (6%)	8 (1%)	19	33

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	60	GLN
4	D	69	LYS
4	D	178	LYS
1	A	227	ASP
4	D	193	PRO
4	D	8	SER
4	D	125	SER
5	E	41	PRO

### 5.3.2 Protein sidechains [i](#)

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	232/232 (100%)	223 (96%)	9 (4%)	39	64
2	B	95/95 (100%)	90 (95%)	5 (5%)	28	48
3	C	7/7 (100%)	6 (86%)	1 (14%)	4	7
4	D	178/178 (100%)	162 (91%)	16 (9%)	12	21
5	E	213/213 (100%)	204 (96%)	9 (4%)	36	60
All	All	725/725 (100%)	685 (94%)	40 (6%)	27	46

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	ARG
1	A	108	ARG
1	A	110	LEU
1	A	121	LYS
1	A	156	LEU
1	A	181	ARG
1	A	226	GLN
1	A	230	LEU
1	A	273	ARG
2	B	0	MET
2	B	3	ARG
2	B	19	LYS
2	B	75	LYS
2	B	89	GLN
3	C	5	LEU
4	D	9	LEU
4	D	53	ASN
4	D	56	MET
4	D	58	GLN
4	D	65	LEU
4	D	66	LEU
4	D	71	LYS
4	D	75	LEU
4	D	111	ASN
4	D	115	PRO
4	D	148	LYS
4	D	160	LEU
4	D	177	ASN
4	D	178	LYS

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Mol	Chain	Res	Type
4	D	180	ASP
4	D	191	ILE
5	E	41	PRO
5	E	43	GLN
5	E	46	MET
5	E	61	GLN
5	E	65	LYS
5	E	75	LEU
5	E	112	ARG
5	E	120	ASN
5	E	195	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	70	HIS
1	A	93	HIS
1	A	114	HIS
1	A	115	GLN
1	A	174	ASN
1	A	224	GLN
1	A	242	GLN
1	A	253	GLN
1	A	262	GLN
2	B	24	ASN
2	B	51	HIS
2	B	84	HIS
4	D	22	ASN
4	D	38	GLN
4	D	53	ASN
4	D	111	ASN
4	D	143	ASN
4	D	146	GLN
4	D	177	ASN
5	E	39	GLN
5	E	43	GLN
5	E	52	ASN
5	E	61	GLN
5	E	86	HIS
5	E	120	ASN
5	E	141	GLN
5	E	215	GLN

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Mol	Chain	Res	Type
5	E	222	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 ⓘ

19 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	$\# Z  > 2$
6	GOL	A	277	-	5,5,5	0.55	0	5,5,5	0.11	0
6	GOL	A	278	-	5,5,5	0.48	0	5,5,5	0.26	0
6	GOL	A	279	-	5,5,5	0.42	0	5,5,5	0.18	0
7	SO4	A	280	-	4,4,4	0.15	0	6,6,6	0.15	0
7	SO4	A	281	-	4,4,4	0.19	0	6,6,6	0.14	0
8	MES	B	100	-	11,12,12	0.79	0	14,16,16	2.54	7 (50%)
6	GOL	B	101	-	5,5,5	0.40	0	5,5,5	0.19	0
7	SO4	B	102	-	4,4,4	0.16	0	6,6,6	0.12	0
7	SO4	B	103	-	4,4,4	0.13	0	6,6,6	0.07	0
6	GOL	D	202	-	5,5,5	0.59	0	5,5,5	0.19	0
6	GOL	D	6	-	5,5,5	0.54	0	5,5,5	0.23	0
6	GOL	E	1	-	5,5,5	0.41	0	5,5,5	0.21	0
6	GOL	E	247	-	5,5,5	0.70	0	5,5,5	0.26	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	GOL	E	248	-	5,5,5	0.42	0	5,5,5	0.26	0
6	GOL	E	249	-	5,5,5	0.60	0	5,5,5	0.22	0
6	GOL	E	250	-	5,5,5	0.36	0	5,5,5	0.31	0
7	SO4	E	251	-	4,4,4	0.15	0	6,6,6	0.05	0
7	SO4	E	252	-	4,4,4	0.14	0	6,6,6	0.07	0
7	SO4	E	253	-	4,4,4	0.14	0	6,6,6	0.12	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
6	GOL	A	277	-	-	0/4/4/4	0/0/0/0
6	GOL	A	278	-	-	0/4/4/4	0/0/0/0
6	GOL	A	279	-	-	0/4/4/4	0/0/0/0
7	SO4	A	280	-	-	0/0/0/0	0/0/0/0
7	SO4	A	281	-	-	0/0/0/0	0/0/0/0
8	MES	B	100	-	-	0/6/14/14	0/1/1/1
6	GOL	B	101	-	-	0/4/4/4	0/0/0/0
7	SO4	B	102	-	-	0/0/0/0	0/0/0/0
7	SO4	B	103	-	-	0/0/0/0	0/0/0/0
6	GOL	D	202	-	-	0/4/4/4	0/0/0/0
6	GOL	D	6	-	-	0/4/4/4	0/0/0/0
6	GOL	E	1	-	-	0/4/4/4	0/0/0/0
6	GOL	E	247	-	-	0/4/4/4	0/0/0/0
6	GOL	E	248	-	-	0/4/4/4	0/0/0/0
6	GOL	E	249	-	-	0/4/4/4	0/0/0/0
6	GOL	E	250	-	-	0/4/4/4	0/0/0/0
7	SO4	E	251	-	-	0/0/0/0	0/0/0/0
7	SO4	E	252	-	-	0/0/0/0	0/0/0/0
7	SO4	E	253	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	100	MES	C6-C5-N4	-2.87	105.77	110.12
8	B	100	MES	C2-C3-N4	-2.65	106.11	110.12
8	B	100	MES	O2S-S-C8	2.47	109.01	106.91
8	B	100	MES	C7-N4-C3	3.43	120.07	111.27
8	B	100	MES	C7-N4-C5	3.68	120.70	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	100	MES	O1S-S-C8	3.95	110.27	106.91
8	B	100	MES	C5-N4-C3	4.76	119.22	108.90

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

10 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	278	GOL	2	0
6	A	279	GOL	3	0
6	B	101	GOL	1	0
7	B	102	SO4	1	0
6	D	202	GOL	4	0
6	D	6	GOL	4	0
6	E	1	GOL	1	0
6	E	247	GOL	3	0
6	E	249	GOL	1	0
6	E	250	GOL	4	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	276/276 (100%)	-0.02	5 (1%) 71 76	6, 20, 60, 77	0
2	B	100/100 (100%)	0.30	5 (5%) 32 38	11, 30, 58, 63	0
3	C	9/9 (100%)	-0.39	0 100 100	7, 11, 19, 21	0
4	D	195/195 (100%)	0.61	21 (10%) 8 8	10, 32, 66, 76	0
5	E	245/245 (100%)	0.02	5 (2%) 68 73	7, 18, 43, 60	0
All	All	825/825 (100%)	0.18	36 (4%) 38 44	6, 24, 59, 77	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	8	SER	6.4
4	D	59	ASP	5.5
4	D	7	GLN	5.4
4	D	188	ASN	4.1
2	B	99	MET	3.8
4	D	66	LEU	3.6
4	D	191	ILE	3.4
5	E	43	GLN	3.2
1	A	252	GLY	3.1
4	D	128	SER	3.0
1	A	276	PRO	2.9
1	A	194	VAL	2.8
4	D	41	GLY	2.8
4	D	148	LYS	2.8
4	D	201	PRO	2.7
4	D	42	ALA	2.7
4	D	127	SER	2.7
2	B	0	MET	2.6
4	D	76	ARG	2.5
4	D	125	SER	2.5

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Mol	Chain	Res	Type	RSRZ
2	B	1	ILE	2.5
4	D	70	ASP	2.4
5	E	40	PHE	2.4
4	D	180	ASP	2.4
5	E	42	LYS	2.4
2	B	16	GLU	2.4
2	B	98	ASP	2.3
4	D	130	LYS	2.3
4	D	77	ILE	2.3
5	E	186	ASN	2.2
5	E	65	LYS	2.2
1	A	227	ASP	2.1
4	D	183	CYS	2.1
4	D	10	PHE	2.1
1	A	226	GLN	2.1
4	D	132	VAL	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no 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(Å <sup>2</sup> )	Q<0.9
6	GOL	A	279	6/6	0.78	0.29	9.84	48,52,52,52	0
6	GOL	E	250	6/6	0.82	0.37	9.20	41,44,45,46	0
6	GOL	D	202	6/6	0.89	0.40	9.18	46,50,52,54	0
6	GOL	E	247	6/6	0.83	0.27	7.12	22,29,31,34	0
6	GOL	E	1	6/6	0.77	0.24	4.98	52,55,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
7	SO4	E	252	5/5	0.77	0.38	2.26	77,79,79,80	0
7	SO4	E	253	5/5	0.87	0.21	1.56	64,65,66,67	0
6	GOL	A	277	6/6	0.85	0.23	0.44	36,37,39,41	0
7	SO4	A	280	5/5	0.90	0.16	-1.40	47,48,52,52	0
6	GOL	E	248	6/6	0.88	0.20	-	56,58,58,58	0
7	SO4	A	281	5/5	0.84	0.27	-	66,67,67,68	0
6	GOL	B	101	6/6	0.72	0.23	-	63,63,63,63	0
6	GOL	D	6	6/6	0.21	0.37	-	57,58,58,59	0
7	SO4	B	103	5/5	0.43	0.63	-	99,99,100,100	0
7	SO4	B	102	5/5	0.86	0.23	-	70,71,72,72	0
8	MES	B	100	12/12	0.29	0.43	-	97,98,100,100	0
6	GOL	A	278	6/6	0.72	0.28	-	37,39,41,43	0
6	GOL	E	249	6/6	0.67	0.49	-	45,50,51,51	0
7	SO4	E	251	5/5	0.93	0.19	-	55,55,56,56	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.