



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 26, 2026 – 01:08 PM EDT

PDB ID : 8EEE / pdb\_00008eee  
Title : Crystal structure of a NHP anti-ZIKV neutralizing antibody rhMZ104-d in complex with ZIKV E glycoprotein  
Authors : Sankhala, R.S.; Joyce, M.G.  
Deposited on : 2022-09-07  
Resolution : 2.82 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 2.0  
EDS : 3.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

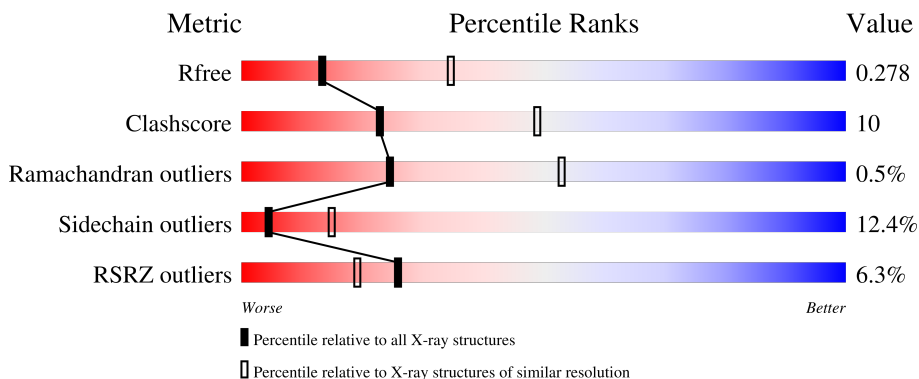
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.82 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	180053	4591 (2.84-2.80)
Clashscore	190562	5010 (2.84-2.80)
Ramachandran outliers	187476	4916 (2.84-2.80)
Sidechain outliers	187428	4918 (2.84-2.80)
RSRZ outliers	180081	4594 (2.84-2.80)

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

Mol	Chain	Length	Quality of chain
1	E	405	
1	Z	405	
2	B	220	
2	L	220	
3	A	228	

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Mol	Chain	Length	Quality of chain
3	H	228	 <p>A horizontal bar chart representing the quality of chain. The bar is divided into four segments: a small red segment (3%), a green segment (35%), a yellow segment (16%), and a grey segment (45%). A small black dot is located at the end of the yellow segment.</p>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11031 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 Envelope protein E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	Z	393	Total 2919	C 1826	N 499	O 569	S 25	0	0	0
1	E	392	Total 2929	C 1832	N 504	O 568	S 25	0	0	0

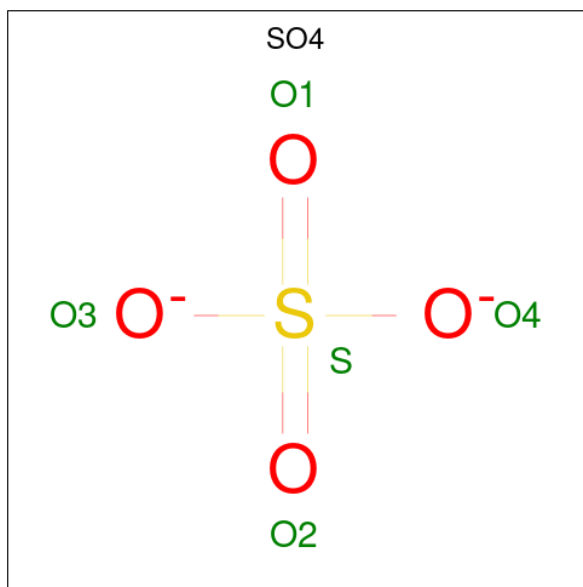
- Molecule 2 is a protein called rhMZ104-D antibody light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	L	115	Total 874	C 553	N 143	O 175	S 3	0	0	0
2	B	217	Total 1634	C 1029	N 269	O 331	S 5	0	0	0

- Molecule 3 is a protein called rhMZ104-D antibody heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	H	125	Total 963	C 608	N 166	O 183	S 6	0	0	0
3	A	226	Total 1702	C 1071	N 289	O 334	S 8	0	0	0

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O<sub>4</sub>S).

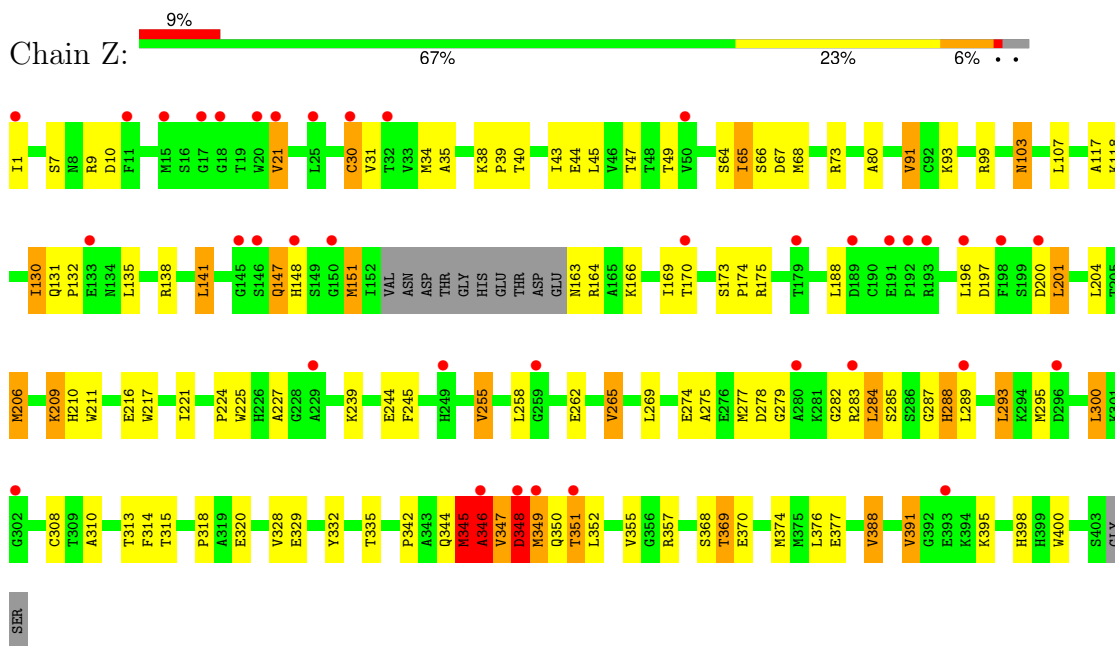


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	H	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		

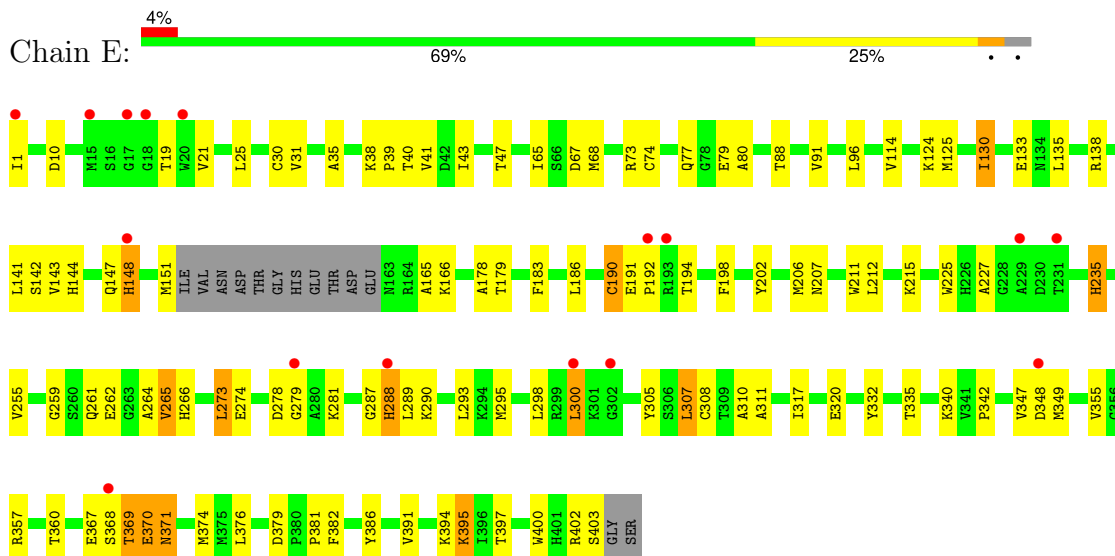
### 3 Residue-property plots i

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

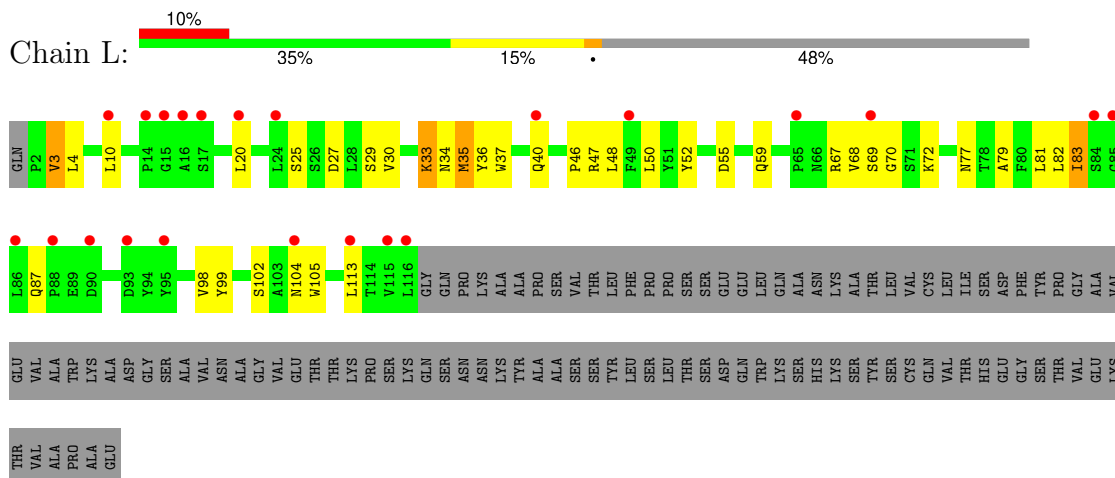
- Molecule 1: Envelope protein E



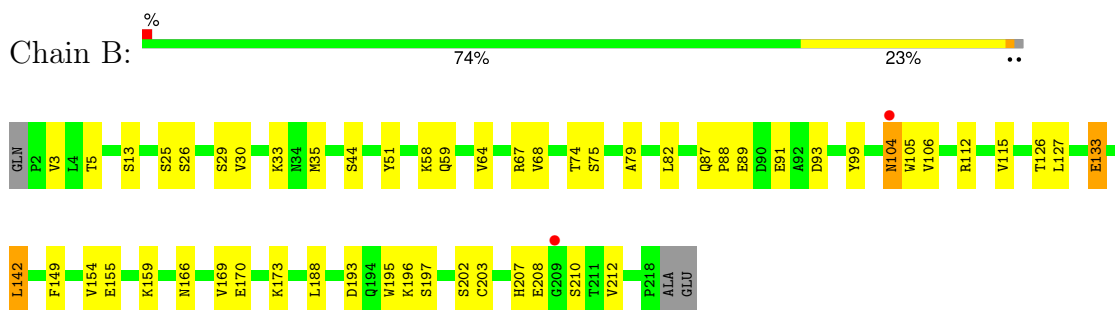
- Molecule 1: Envelope protein E



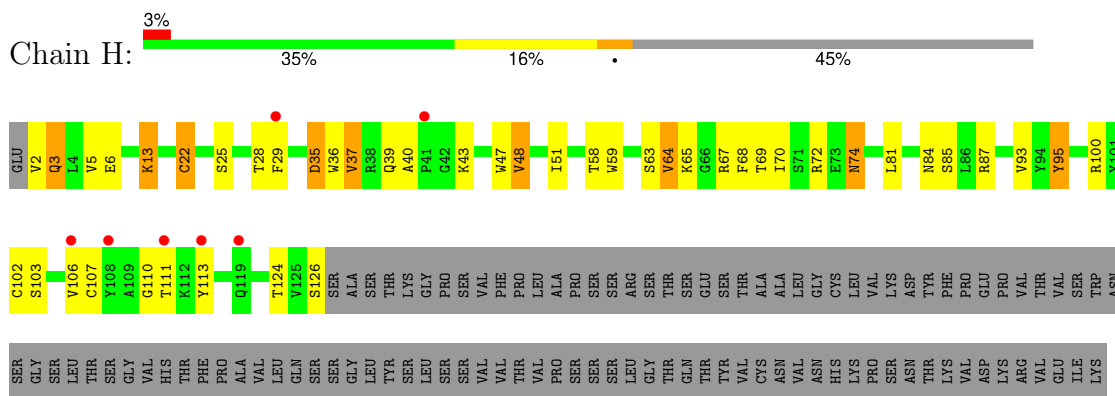
- Molecule 2: rhMZ104-D antibody light chain



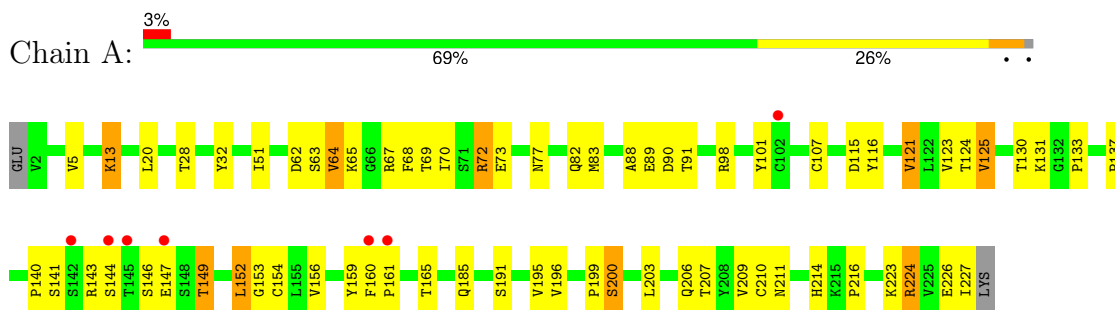
- Molecule 2: rhMZ104-D antibody light chain



- Molecule 3: rhMZ104-D antibody heavy chain



- Molecule 3: rhMZ104-D antibody heavy chain



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	85.32Å 130.42Å 109.71Å 90.00° 104.17° 90.00°	Depositor
Resolution (Å)	14.99 – 2.82 14.99 – 2.82	Depositor EDS
% Data completeness (in resolution range)	73.1 (14.99-2.82) 72.6 (14.99-2.82)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.76 (at 2.81Å)	Xtrriage
Refinement program	PHENIX 1.11.1_2575	Depositor
R, $R_{free}$	0.217 , 0.275 0.221 , 0.278	Depositor DCC
$R_{free}$ test set	2000 reflections (3.56%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	44.4	Xtrriage
Anisotropy	0.044	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.25 , 25.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	11031	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	55.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.56% 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, 0.333 respectively for untwinned datasets, and 0.375, 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: 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	E	0.18	0/2992	0.51	0/4065
1	Z	0.21	0/2981	0.57	7/4053 (0.2%)
2	B	0.15	0/1677	0.39	0/2289
2	L	0.14	0/898	0.40	0/1225
3	A	0.15	0/1743	0.40	0/2371
3	H	0.13	0/986	0.41	0/1333
All	All	0.17	0/11277	0.48	7/15336 (0.0%)

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	E	0	2
1	Z	0	5
All	All	0	7

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Z	346	ALA	CA-C-N	6.10	132.95	121.97
1	Z	346	ALA	C-N-CA	6.10	132.95	121.97
1	Z	345	MET	CA-C-N	5.60	132.23	121.54
1	Z	345	MET	C-N-CA	5.60	132.23	121.54
1	Z	347	VAL	N-CA-C	5.38	120.53	109.34
1	Z	196	LEU	CA-C-N	5.30	131.66	121.54
1	Z	196	LEU	C-N-CA	5.30	131.66	121.54

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	190	CYS	Peptide
1	E	349	MET	Peptide
1	Z	197	ASP	Peptide
1	Z	345	MET	Peptide
1	Z	346	ALA	Peptide
1	Z	348	ASP	Peptide
1	Z	351	THR	Peptide

## 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	E	2929	0	2795	64	0
1	Z	2919	0	2777	71	0
2	B	1634	0	1576	20	0
2	L	874	0	838	21	0
3	A	1702	0	1647	32	0
3	H	963	0	916	30	0
4	A	5	0	0	0	0
4	H	5	0	0	0	0
All	All	11031	0	10549	225	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (225) 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:E:88:THR:HG23	3:H:106:VAL:HG12	1.39	1.04
1:Z:30:CYS:SG	1:Z:31:VAL:N	2.53	0.80
1:Z:262:GLU:HG2	1:E:259:GLY:HA3	1.65	0.78
1:Z:206:MET:HE1	1:Z:262:GLU:HG3	1.68	0.76
3:H:106:VAL:HG12	3:H:106:VAL:O	1.85	0.75
3:H:3:GLN:HE21	3:H:25:SER:HB2	1.53	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:225:TRP:HZ3	1:E:227:ALA:HB2	1.55	0.70
1:E:30:CYS:SG	1:E:31:VAL:N	2.65	0.69
1:Z:93:LYS:HD3	1:Z:245:PHE:HB2	1.76	0.68
2:L:40:GLN:HB2	2:L:46:PRO:HB3	1.76	0.68
1:E:320:GLU:HB2	1:E:400:TRP:HZ2	1.60	0.67
1:E:41:VAL:HG22	1:E:143:VAL:HG12	1.77	0.66
1:Z:318:PRO:HB3	1:Z:328:VAL:HG22	1.76	0.66
1:Z:35:ALA:HB3	1:Z:38:LYS:HB2	1.77	0.65
3:A:185:GLN:HG2	2:B:170:GLU:HG3	1.76	0.65
1:E:47:THR:HB	1:E:138:ARG:HB3	1.78	0.65
1:E:10:ASP:HB2	1:E:31:VAL:HG12	1.77	0.65
1:E:88:THR:HG23	3:H:106:VAL:CG1	2.22	0.65
1:E:347:VAL:HB	1:E:355:VAL:HG21	1.79	0.64
1:Z:244:GLU:HG3	1:Z:258:LEU:HD11	1.79	0.64
1:E:35:ALA:HB3	1:E:38:LYS:HB2	1.80	0.64
2:L:25:SER:O	2:L:77:ASN:ND2	2.30	0.64
1:Z:200:ASP:OD1	1:Z:201:LEU:N	2.27	0.63
3:H:74:ASN:N	3:H:74:ASN:OD1	2.29	0.63
2:L:30:VAL:HG22	2:L:72:LYS:HD2	1.78	0.63
1:Z:10:ASP:HB2	1:Z:31:VAL:HG12	1.80	0.63
1:E:39:PRO:HD3	1:E:300:LEU:HA	1.81	0.62
3:A:149:THR:HG22	3:A:199:PRO:HA	1.81	0.62
1:E:43:ILE:HG12	1:E:141:LEU:HD23	1.81	0.62
1:Z:47:THR:HB	1:Z:138:ARG:HB3	1.81	0.61
1:Z:225:TRP:HZ3	1:Z:227:ALA:HB2	1.65	0.61
2:L:36:TYR:OH	3:H:111:THR:O	2.18	0.61
1:Z:43:ILE:HG12	1:Z:141:LEU:HD12	1.83	0.61
1:Z:351:THR:HG23	1:Z:352:LEU:HB2	1.82	0.61
1:E:307:LEU:HD13	1:E:342:PRO:HG3	1.83	0.60
2:L:3:VAL:O	2:L:25:SER:OG	2.14	0.60
3:A:153:GLY:HA3	3:A:195:VAL:HG12	1.82	0.60
2:L:69:SER:HB3	2:L:82:LEU:HD13	1.83	0.60
1:E:273:LEU:HD23	1:E:273:LEU:H	1.66	0.59
1:Z:335:THR:HG23	1:Z:369:THR:HB	1.84	0.59
2:B:87:GLN:HG2	2:B:88:PRO:HD2	1.85	0.58
1:E:73:ARG:HD2	1:E:80:ALA:HA	1.85	0.58
2:L:33:LYS:NZ	2:L:99:TYR:O	2.37	0.57
3:A:115:ASP:HB3	3:A:116:TYR:HD2	1.69	0.57
1:E:311:ALA:HB2	1:E:394:LYS:HB3	1.86	0.57
2:B:3:VAL:H	2:B:25:SER:HB3	1.69	0.57
1:Z:348:ASP:OD1	1:Z:349:MET:N	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:21:VAL:HG13	1:Z:293:LEU:HB2	1.86	0.56
1:Z:39:PRO:HD3	1:Z:300:LEU:HA	1.87	0.56
1:E:73:ARG:NH1	1:E:79:GLU:O	2.35	0.56
1:E:355:VAL:HG12	1:E:381:PRO:HG3	1.86	0.56
3:A:63:SER:O	3:A:67:ARG:NH2	2.38	0.56
1:Z:148:HIS:ND1	1:Z:329:GLU:OE1	2.39	0.56
2:B:207:HIS:CD2	2:B:208:GLU:HG2	2.41	0.56
3:H:6:GLU:HG2	3:H:22:CYS:HB2	1.88	0.56
1:Z:258:LEU:O	1:E:266:HIS:ND1	2.34	0.55
1:Z:275:ALA:HB1	1:Z:283:ARG:O	2.06	0.55
1:E:144:HIS:HB3	1:E:360:THR:HG23	1.89	0.55
1:E:206:MET:HE1	1:E:262:GLU:HG3	1.89	0.55
1:Z:320:GLU:HB2	1:Z:400:TRP:CZ2	2.42	0.54
3:A:140:PRO:HD3	3:A:152:LEU:HB3	1.89	0.54
1:Z:66:SER:HB3	1:Z:118:LYS:HB3	1.88	0.54
1:Z:320:GLU:HB2	1:Z:400:TRP:HZ2	1.73	0.54
3:H:64:VAL:HG13	3:H:68:PHE:HB2	1.89	0.54
1:E:212:LEU:HB2	1:E:273:LEU:HG	1.89	0.54
3:H:39:GLN:OE1	3:H:95:TYR:OH	2.26	0.54
2:B:195:TRP:CD1	2:B:196:LYS:HG3	2.43	0.54
1:Z:130:ILE:HD13	1:Z:130:ILE:H	1.72	0.53
1:Z:209:LYS:HZ2	1:Z:209:LYS:HB2	1.73	0.53
1:E:147:GLN:HG2	1:E:148:HIS:H	1.74	0.53
1:E:206:MET:HB2	1:E:211:TRP:HZ3	1.72	0.53
3:A:83:MET:HE1	3:A:123:VAL:HG11	1.89	0.53
1:Z:170:THR:HB	1:Z:173:SER:HB3	1.91	0.53
2:L:20:LEU:HB2	2:L:83:ILE:HD11	1.89	0.53
1:E:357:ARG:HG2	1:E:379:ASP:HB3	1.91	0.53
3:H:29:PHE:O	3:H:72:ARG:NH1	2.41	0.53
1:Z:9:ARG:NH2	1:Z:377:GLU:OE2	2.39	0.53
1:E:279:GLY:C	1:E:281:LYS:H	2.17	0.53
3:A:32:TYR:CE1	3:A:101:TYR:HB2	2.44	0.53
1:E:320:GLU:HB2	1:E:400:TRP:CZ2	2.42	0.52
3:A:51:ILE:HD13	3:A:72:ARG:HB3	1.91	0.52
1:Z:342:PRO:HG2	1:Z:391:VAL:HG13	1.92	0.52
1:E:194:THR:HA	1:E:288:HIS:O	2.10	0.52
1:E:261:GLN:HG3	1:E:264:ALA:HB3	1.92	0.52
1:Z:132:PRO:HA	1:Z:135:LEU:HD13	1.93	0.51
1:Z:344:GLN:HG3	1:Z:388:VAL:HG13	1.91	0.51
3:A:67:ARG:NH1	3:A:90:ASP:OD2	2.44	0.51
1:Z:348:ASP:CG	1:Z:349:MET:N	2.69	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:142:LEU:HB2	2:B:188:LEU:HB3	1.92	0.51
1:E:88:THR:HG23	3:H:106:VAL:O	2.11	0.51
3:H:67:ARG:HB3	3:H:84:ASN:O	2.11	0.51
3:A:130:THR:HG23	3:A:161:PRO:HG3	1.93	0.50
3:H:37:VAL:HA	3:H:48:VAL:HG23	1.93	0.50
1:Z:99:ARG:NE	1:Z:103:ASN:OD1	2.29	0.50
3:A:69:THR:HB	3:A:82:GLN:HB3	1.94	0.50
2:B:35:MET:HE3	2:B:79:ALA:HB2	1.94	0.50
2:B:195:TRP:HD1	2:B:196:LYS:HG3	1.76	0.50
1:Z:30:CYS:HB2	1:Z:44:GLU:HB2	1.94	0.50
1:E:348:ASP:HB3	1:E:386:TYR:CD1	2.47	0.50
3:A:64:VAL:HG13	3:A:68:PHE:HB2	1.92	0.50
1:Z:91:VAL:HG22	1:Z:239:LYS:HD2	1.93	0.49
1:Z:335:THR:HA	1:Z:368:SER:O	2.12	0.49
3:A:144:SER:O	3:A:200:SER:OG	2.24	0.49
1:Z:225:TRP:CZ3	1:Z:227:ALA:HB2	2.47	0.49
1:E:88:THR:CG2	3:H:106:VAL:HG12	2.26	0.49
1:Z:34:MET:HE1	1:Z:357:ARG:HH21	1.78	0.49
2:L:99:TYR:HB2	2:L:105:TRP:CZ3	2.48	0.48
1:Z:204:LEU:HD22	1:Z:211:TRP:HE3	1.78	0.48
3:H:51:ILE:HG13	3:H:58:THR:HG22	1.96	0.48
1:E:1:ILE:N	1:E:142:SER:OG	2.45	0.48
3:H:40:ALA:HB3	3:H:43:LYS:HB3	1.95	0.48
2:B:29:SER:O	2:B:33:LYS:HG2	2.14	0.48
2:B:91:GLU:HG2	2:B:115:VAL:HG23	1.96	0.47
1:E:125:MET:HE1	1:E:265:VAL:HG11	1.96	0.47
1:E:202:TYR:CE2	1:E:215:LYS:HG2	2.49	0.47
3:A:32:TYR:O	3:A:72:ARG:NH2	2.47	0.47
1:Z:369:THR:HA	1:Z:370:GLU:HA	1.70	0.47
1:Z:206:MET:HG3	1:Z:211:TRP:HZ3	1.79	0.47
2:L:27:ASP:OD1	2:L:27:ASP:N	2.42	0.47
3:A:88:ALA:HA	3:A:125:VAL:HG22	1.96	0.47
3:A:209:VAL:HA	3:A:224:ARG:HA	1.97	0.47
2:B:64:VAL:HG12	2:B:68:VAL:HG11	1.96	0.47
3:A:62:ASP:HA	3:A:65:LYS:HD2	1.97	0.46
1:Z:210:HIS:NE2	1:Z:277:MET:HB3	2.31	0.46
1:E:395:LYS:H	1:E:395:LYS:HD3	1.80	0.46
1:Z:369:THR:OG1	1:Z:370:GLU:HB3	2.15	0.46
1:E:135:LEU:HD11	1:E:198:PHE:HE1	1.79	0.46
2:B:193:ASP:O	2:B:197:SER:OG	2.33	0.46
1:Z:350:GLN:HA	1:Z:351:THR:HA	1.69	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:214:HIS:NE2	3:A:216:PRO:HG2	2.31	0.46
1:E:374:MET:HE1	1:E:376:LEU:HB3	1.97	0.46
3:A:144:SER:HB2	3:A:203:LEU:HD12	1.97	0.46
1:Z:175:ARG:HA	1:Z:188:LEU:O	2.16	0.46
1:E:308:CYS:HB3	1:E:332:TYR:CE2	2.51	0.45
2:L:34:ASN:ND2	3:H:110:GLY:O	2.50	0.45
2:L:67:ARG:NH1	2:L:87:GLN:OE1	2.49	0.45
1:Z:209:LYS:HB2	1:Z:209:LYS:NZ	2.31	0.45
3:A:207:THR:HB	3:A:224:ARG:NH1	2.31	0.45
3:H:63:SER:O	3:H:67:ARG:NH2	2.48	0.45
3:A:98:ARG:NH2	3:A:115:ASP:OD2	2.50	0.45
1:Z:169:ILE:HG23	1:Z:174:PRO:HA	1.98	0.45
1:Z:374:MET:HE1	1:Z:376:LEU:HD23	1.99	0.45
1:E:370:GLU:OE2	1:E:371:ASN:HB2	2.16	0.45
3:A:147:GLU:H	3:A:147:GLU:CD	2.25	0.45
1:E:25:LEU:HB2	1:E:289:LEU:HD23	1.99	0.44
3:H:111:THR:HB	3:H:113:TYR:CD1	2.52	0.44
3:A:143:ARG:HG3	3:A:146:SER:OG	2.17	0.44
2:L:104:ASN:HD21	3:H:59:TRP:CD1	2.36	0.44
1:E:165:ALA:HB1	1:E:178:ALA:HB1	2.00	0.44
1:E:235:HIS:ND1	1:E:235:HIS:C	2.74	0.44
3:H:102:CYS:HA	3:H:107:CYS:HB3	2.00	0.44
1:E:192:PRO:HD2	1:E:290:LYS:CB	2.48	0.44
3:H:106:VAL:O	3:H:106:VAL:CG1	2.57	0.44
2:B:99:TYR:HB2	2:B:105:TRP:CZ3	2.53	0.44
1:Z:346:ALA:HB3	1:Z:355:VAL:HG21	1.99	0.44
3:A:141:SER:O	3:A:141:SER:OG	2.33	0.44
1:Z:49:THR:HA	1:Z:282:GLY:O	2.17	0.44
1:E:369:THR:HA	1:E:370:GLU:HA	1.66	0.44
1:Z:314:PHE:CE2	1:Z:398:HIS:HB2	2.53	0.44
3:H:13:LYS:HG2	3:H:126:SER:C	2.43	0.44
2:B:104:ASN:O	2:B:105:TRP:CG	2.71	0.44
1:Z:308:CYS:HB3	1:Z:332:TYR:CE1	2.52	0.43
1:E:190:CYS:O	1:E:191:GLU:HG3	2.18	0.43
1:Z:310:ALA:HB3	1:Z:332:TYR:CZ	2.53	0.43
1:E:206:MET:O	1:E:207:ASN:C	2.62	0.43
2:L:48:LEU:HG	3:H:113:TYR:CE2	2.53	0.43
3:H:87:ARG:HA	3:H:87:ARG:HD2	1.84	0.43
1:Z:65:ILE:HD12	1:Z:65:ILE:HA	1.76	0.43
1:E:305:TYR:HB2	1:E:340:LYS:HG3	2.00	0.43
2:B:51:TYR:HB3	2:B:59:GLN:HB3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:217:TRP:CH2	1:Z:221:ILE:HD11	2.54	0.43
1:E:382:PHE:HA	1:E:402:ARG:HB3	2.00	0.43
2:L:50:LEU:HD23	2:L:81:LEU:HD12	2.00	0.43
1:Z:348:ASP:CG	1:Z:349:MET:H	2.21	0.43
1:Z:151:MET:HE2	1:Z:151:MET:HB2	1.78	0.43
1:E:403:SER:O	1:E:403:SER:OG	2.26	0.42
2:B:127:LEU:HD13	2:B:203:CYS:HB2	2.00	0.42
1:Z:45:LEU:HD22	1:Z:289:LEU:HD22	2.01	0.42
1:E:310:ALA:HB3	1:E:332:TYR:CZ	2.54	0.42
1:E:317:ILE:HD12	1:E:317:ILE:H	1.84	0.42
3:H:64:VAL:HA	3:H:67:ARG:NH2	2.34	0.42
1:Z:204:LEU:HD22	1:Z:211:TRP:CE3	2.54	0.42
3:A:98:ARG:O	3:A:115:ASP:N	2.51	0.42
1:Z:163:ASN:HB3	1:Z:164:ARG:H	1.41	0.42
1:E:74:CYS:HB2	1:E:77:GLN:HG3	2.02	0.42
1:E:278:ASP:HA	1:E:279:GLY:HA2	1.78	0.42
1:Z:274:GLU:HG2	1:Z:275:ALA:H	1.84	0.42
1:Z:103:ASN:ND2	1:Z:103:ASN:H	2.16	0.42
1:Z:265:VAL:O	1:Z:269:LEU:HD23	2.19	0.42
1:E:19:THR:CB	1:E:295:MET:H	2.32	0.42
1:E:225:TRP:CZ3	1:E:227:ALA:HB2	2.43	0.42
3:H:35:ASP:OD1	3:H:47:TRP:NE1	2.45	0.42
3:H:51:ILE:HD12	3:H:70:ILE:HG23	2.02	0.42
3:A:91:THR:HG23	3:A:124:THR:HA	2.01	0.42
3:A:137:PRO:HG3	3:A:223:LYS:HG2	2.02	0.42
1:Z:278:ASP:HA	1:Z:279:GLY:HA2	1.67	0.42
1:Z:287:GLY:C	1:Z:288:HIS:CG	2.98	0.42
1:Z:284:LEU:HD23	1:Z:285:SER:H	1.85	0.42
3:A:133:PRO:HB3	3:A:159:TYR:HB3	2.02	0.41
1:E:335:THR:HA	1:E:368:SER:O	2.21	0.41
2:L:37:TRP:CG	2:L:81:LEU:HD13	2.55	0.41
2:B:159:LYS:HB2	2:B:202:SER:OG	2.20	0.41
2:B:93:ASP:OD1	2:B:112:ARG:HD3	2.21	0.41
2:B:149:PHE:CE2	2:B:154:VAL:HG13	2.56	0.41
1:Z:147:GLN:HG2	1:Z:148:HIS:H	1.84	0.41
3:A:13:LYS:HB2	3:A:13:LYS:HE2	1.85	0.41
1:Z:65:ILE:HG13	1:Z:117:ALA:HB1	2.03	0.41
2:L:33:LYS:HA	2:L:33:LYS:HD2	1.78	0.41
2:B:133:GLU:CD	2:B:133:GLU:H	2.28	0.41
1:Z:147:GLN:HG2	1:Z:148:HIS:N	2.36	0.41
1:E:183:PHE:O	1:E:298:LEU:HD23	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:20:LEU:HD22	3:A:121:VAL:HG21	2.03	0.41
1:Z:73:ARG:HG3	1:Z:80:ALA:HA	2.03	0.40
1:E:348:ASP:HB3	1:E:386:TYR:CE1	2.55	0.40
3:A:160:PHE:HB3	3:A:161:PRO:HD3	2.02	0.40
1:Z:65:ILE:HG12	1:Z:255:VAL:HG11	2.02	0.40
3:H:36:TRP:NE1	3:H:81:LEU:HB2	2.36	0.40
1:Z:224:PRO:HG3	1:Z:239:LYS:HA	2.03	0.40
1:E:88:THR:CG2	3:H:106:VAL:CG1	2.93	0.40
1:E:287:GLY:C	1:E:288:HIS:CG	2.99	0.40
2:L:52:TYR:CD1	2:L:70:GLY:HA3	2.56	0.40
1:E:73:ARG:NH2	2:L:102:SER:HB2	2.36	0.40
1:E:130:ILE:H	1:E:130:ILE:HG12	1.77	0.40
2:L:35:MET:HE2	2:L:79:ALA:HB2	2.04	0.40
2:L:104:ASN:O	2:L:105:TRP:CG	2.75	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	388/405 (96%)	344 (89%)	43 (11%)	1 (0%)	36	64
1	Z	389/405 (96%)	344 (88%)	39 (10%)	6 (2%)	8	26
2	B	215/220 (98%)	205 (95%)	10 (5%)	0	100	100
2	L	113/220 (51%)	103 (91%)	10 (9%)	0	100	100
3	A	224/228 (98%)	206 (92%)	18 (8%)	0	100	100
3	H	123/228 (54%)	112 (91%)	11 (9%)	0	100	100
All	All	1452/1706 (85%)	1314 (90%)	131 (9%)	7 (0%)	24	53

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	Z	347	VAL
1	Z	348	ASP
1	Z	300	LEU
1	Z	346	ALA
1	Z	349	MET
1	E	300	LEU
1	Z	131	GLN

### 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	E	312/338 (92%)	281 (90%)	31 (10%)	7 23
1	Z	310/338 (92%)	275 (89%)	35 (11%)	5 18
2	B	183/185 (99%)	161 (88%)	22 (12%)	5 16
2	L	98/185 (53%)	85 (87%)	13 (13%)	4 13
3	A	188/190 (99%)	161 (86%)	27 (14%)	3 10
3	H	98/190 (52%)	79 (81%)	19 (19%)	1 4
All	All	1189/1426 (83%)	1042 (88%)	147 (12%)	4 15

All (147) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	Z	1	ILE
1	Z	7	SER
1	Z	21	VAL
1	Z	30	CYS
1	Z	40	THR
1	Z	64	SER
1	Z	65	ILE
1	Z	67	ASP
1	Z	68	MET
1	Z	91	VAL
1	Z	103	ASN
1	Z	107	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	Z	130	ILE
1	Z	141	LEU
1	Z	147	GLN
1	Z	151	MET
1	Z	166	LYS
1	Z	201	LEU
1	Z	206	MET
1	Z	209	LYS
1	Z	216	GLU
1	Z	255	VAL
1	Z	265	VAL
1	Z	284	LEU
1	Z	288	HIS
1	Z	293	LEU
1	Z	295	MET
1	Z	313	THR
1	Z	315	THR
1	Z	345	MET
1	Z	348	ASP
1	Z	369	THR
1	Z	388	VAL
1	Z	391	VAL
1	Z	395	LYS
1	E	21	VAL
1	E	40	THR
1	E	65	ILE
1	E	67	ASP
1	E	68	MET
1	E	91	VAL
1	E	96	LEU
1	E	114	VAL
1	E	124	LYS
1	E	130	ILE
1	E	133	GLU
1	E	148	HIS
1	E	151	MET
1	E	166	LYS
1	E	179	THR
1	E	186	LEU
1	E	235	HIS
1	E	255	VAL
1	E	265	VAL

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	E	273	LEU
1	E	274	GLU
1	E	288	HIS
1	E	293	LEU
1	E	307	LEU
1	E	367	GLU
1	E	369	THR
1	E	370	GLU
1	E	371	ASN
1	E	391	VAL
1	E	395	LYS
1	E	397	THR
2	L	3	VAL
2	L	4	LEU
2	L	10	LEU
2	L	29	SER
2	L	33	LYS
2	L	35	MET
2	L	47	ARG
2	L	55	ASP
2	L	59	GLN
2	L	68	VAL
2	L	83	ILE
2	L	98	VAL
2	L	113	LEU
3	H	2	VAL
3	H	3	GLN
3	H	5	VAL
3	H	13	LYS
3	H	22	CYS
3	H	28	THR
3	H	35	ASP
3	H	37	VAL
3	H	48	VAL
3	H	64	VAL
3	H	65	LYS
3	H	69	THR
3	H	74	ASN
3	H	85	SER
3	H	93	VAL
3	H	95	TYR
3	H	100	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
3	H	103	SER
3	H	124	THR
3	A	5	VAL
3	A	13	LYS
3	A	28	THR
3	A	64	VAL
3	A	70	ILE
3	A	72	ARG
3	A	73	GLU
3	A	77	ASN
3	A	89	GLU
3	A	107	CYS
3	A	121	VAL
3	A	125	VAL
3	A	131	LYS
3	A	149	THR
3	A	152	LEU
3	A	154	CYS
3	A	156	VAL
3	A	165	THR
3	A	191	SER
3	A	196	VAL
3	A	200	SER
3	A	206	GLN
3	A	210	CYS
3	A	211	ASN
3	A	224	ARG
3	A	226	GLU
3	A	227	ILE
2	B	5	THR
2	B	13	SER
2	B	26	SER
2	B	30	VAL
2	B	44	SER
2	B	58	LYS
2	B	67	ARG
2	B	74	THR
2	B	75	SER
2	B	82	LEU
2	B	89	GLU
2	B	104	ASN
2	B	106	VAL

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Mol	Chain	Res	Type
2	B	126	THR
2	B	133	GLU
2	B	142	LEU
2	B	155	GLU
2	B	166	ASN
2	B	169	VAL
2	B	173	LYS
2	B	210	SER
2	B	212	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	Z	237	ASN
1	Z	253	GLN
1	Z	331	GLN
1	E	401	HIS
2	L	6	GLN
3	H	3	GLN
3	H	77	ASN
3	A	82	GLN
3	A	84	ASN
2	B	104	ASN
2	B	204	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

2 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	$\# Z  > 2$
4	SO4	H	301	-	4,4,4	0.23	0	6,6,6	0.08	0
4	SO4	A	301	-	4,4,4	0.24	0	6,6,6	0.07	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	E	392/405 (96%)	0.17	16 (4%) 41 32	15, 41, 84, 116	0
1	Z	393/405 (97%)	0.57	38 (9%) 13 9	15, 62, 102, 128	0
2	B	217/220 (98%)	-0.27	2 (0%) 81 74	12, 36, 68, 98	0
2	L	115/220 (52%)	1.14	22 (19%) 3 2	44, 98, 179, 199	0
3	A	226/228 (99%)	-0.07	7 (3%) 51 41	13, 39, 93, 127	0
3	H	125/228 (54%)	0.70	7 (5%) 30 23	51, 79, 93, 113	0
All	All	1468/1706 (86%)	0.29	92 (6%) 26 19	12, 49, 105, 199	0

All (92) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	192	PRO	8.9
2	L	116	LEU	6.8
1	Z	15	MET	5.7
2	L	65	PRO	5.5
3	A	145	THR	5.3
1	E	18	GLY	5.2
2	L	86	LEU	4.9
1	E	193	ARG	4.7
3	H	106	VAL	4.6
1	Z	150	GLY	4.4
1	Z	229	ALA	4.3
2	L	15	GLY	4.3
1	Z	170	THR	4.3
1	Z	146	SER	4.1
2	L	90	ASP	4.0
1	Z	30	CYS	4.0
1	Z	346	ALA	3.9
1	Z	259	GLY	3.9
1	Z	198	PHE	3.7

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	Z	196	LEU	3.6
2	L	95	TYR	3.6
2	L	10	LEU	3.4
2	L	17	SER	3.3
1	Z	18	GLY	3.3
1	E	15	MET	3.3
1	E	229	ALA	3.3
1	E	348	ASP	3.2
1	E	288	HIS	3.2
1	E	20	TRP	3.2
1	Z	32	THR	3.2
3	A	144	SER	3.2
1	E	231	THR	3.1
1	Z	20	TRP	3.1
1	Z	348	ASP	3.0
2	L	93	ASP	2.9
1	E	17	GLY	2.9
1	Z	302	GLY	2.8
1	Z	145	GLY	2.8
1	Z	21	VAL	2.7
1	Z	17	GLY	2.7
1	E	300	LEU	2.7
2	L	115	VAL	2.7
3	H	113	TYR	2.7
1	Z	11	PHE	2.6
1	Z	296	ASP	2.6
3	A	160	PHE	2.6
1	E	1	ILE	2.6
2	L	16	ALA	2.6
2	L	104	ASN	2.6
3	A	102	CYS	2.5
1	Z	193	ARG	2.5
2	L	84	SER	2.5
3	A	147	GLU	2.5
2	L	88	PRO	2.5
2	L	85	GLY	2.5
1	Z	283	ARG	2.5
3	A	161	PRO	2.4
2	L	49	PHE	2.4
1	Z	393	GLU	2.4
1	Z	200	ASP	2.4
3	H	29	PHE	2.4

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Mol	Chain	Res	Type	RSRZ
2	L	20	LEU	2.4
3	H	108	TYR	2.4
1	Z	25	LEU	2.3
1	Z	179	THR	2.3
1	Z	50	VAL	2.3
1	Z	189	ASP	2.3
1	Z	1	ILE	2.3
1	E	148	HIS	2.2
3	H	111	THR	2.2
1	Z	133	GLU	2.2
3	H	119	GLN	2.2
1	Z	148	HIS	2.2
3	H	41	PRO	2.2
1	E	302	GLY	2.2
2	L	24	LEU	2.2
2	B	104	ASN	2.1
2	L	14	PRO	2.1
1	Z	351	THR	2.1
1	Z	192	PRO	2.1
1	E	279	GLY	2.1
1	Z	289	LEU	2.1
1	Z	280	ALA	2.1
1	Z	191	GLU	2.1
2	L	113	LEU	2.1
2	B	209	GLY	2.1
2	L	69	SER	2.1
3	A	142	SER	2.1
2	L	40	GLN	2.1
1	Z	249	HIS	2.1
1	Z	349	MET	2.1
1	E	368	SER	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.4 Ligands [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. 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	B-factors(Å <sup>2</sup> )	Q<0.9
4	SO4	H	301	5/5	0.84	0.10	90,91,93,94	0
4	SO4	A	301	5/5	0.89	0.10	68,68,72,73	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.