



# Full wwPDB X-ray Structure Validation Report ⓘ

Jul 11, 2017 – 11:23 AM EDT

PDB ID : 3CFK  
Title : Crystal structure of catalytic elimination antibody 34E4, triclinic crystal form  
Authors : Debler, E.W.; Wilson, I.A.  
Deposited on : unknown  
Resolution : 2.60 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.

---

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

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20029824  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : rb-20029824

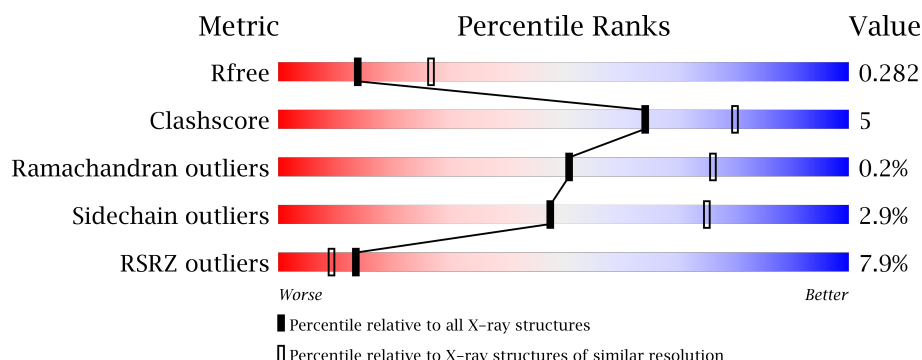
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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))
$R_{free}$	100719	2542 (2.60-2.60)
Clashscore	112137	2895 (2.60-2.60)
Ramachandran outliers	110173	2848 (2.60-2.60)
Sidechain outliers	110143	2848 (2.60-2.60)
RSRZ outliers	101464	2550 (2.60-2.60)

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	216	
1	C	216	
1	E	216	
1	G	216	
1	J	216	

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
1	L	216	
1	M	216	
1	O	216	
2	B	227	
2	D	227	
2	F	227	
2	H	227	
2	I	227	
2	K	227	
2	N	227	
2	P	227	

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
3	CD	K	304	-	-	X	-
3	CD	L	319	-	-	-	X
5	B3P	O	502	-	-	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 27118 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 CATALYTIC ANTIBODY FAB 34E4 LIGHT CHAIN, Uncharacterized protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	215	Total	C	N	O	S	0	0	0
			1628	1016	277	331	4			
1	A	215	Total	C	N	O	S	0	0	0
			1628	1016	277	331	4			
1	C	215	Total	C	N	O	S	0	0	0
			1628	1016	277	331	4			
1	E	215	Total	C	N	O	S	0	0	0
			1628	1016	277	331	4			
1	G	215	Total	C	N	O	S	0	0	0
			1628	1016	277	331	4			
1	J	215	Total	C	N	O	S	0	0	0
			1628	1016	277	331	4			
1	M	215	Total	C	N	O	S	0	0	0
			1628	1016	277	331	4			
1	O	215	Total	C	N	O	S	0	0	0
			1628	1016	277	331	4			

- Molecule 2 is a protein called CATALYTIC ANTIBODY FAB 34E4 HEAVY CHAIN, Uncharacterized protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	224	Total	C	N	O	S	0	0	0
			1718	1093	288	331	6			
2	B	224	Total	C	N	O	S	0	0	0
			1718	1093	288	331	6			
2	D	224	Total	C	N	O	S	0	0	0
			1718	1093	288	331	6			
2	F	224	Total	C	N	O	S	0	0	0
			1718	1093	288	331	6			
2	I	224	Total	C	N	O	S	0	0	0
			1718	1093	288	331	6			

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	K	224	Total	C	N	O	S	0	0	0
			1718	1093	288	331	6			
2	N	224	Total	C	N	O	S	0	0	0
			1718	1093	288	331	6			
2	P	224	Total	C	N	O	S	0	0	0
			1718	1093	288	331	6			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	108	SER	THR	engineered mutation	UNP A8K008
B	108	SER	THR	engineered mutation	UNP A8K008
D	108	SER	THR	engineered mutation	UNP A8K008
F	108	SER	THR	engineered mutation	UNP A8K008
I	108	SER	THR	engineered mutation	UNP A8K008
K	108	SER	THR	engineered mutation	UNP A8K008
N	108	SER	THR	engineered mutation	UNP A8K008
P	108	SER	THR	engineered mutation	UNP A8K008

- Molecule 3 is CADMIUM ION (three-letter code: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	G	4	Total	Cd	0	0
			4	4		
3	J	3	Total	Cd	0	0
			3	3		
3	D	2	Total	Cd	0	0
			2	2		
3	K	1	Total	Cd	0	0
			1	1		
3	E	2	Total	Cd	0	0
			2	2		
3	B	1	Total	Cd	0	0
			1	1		
3	C	3	Total	Cd	0	0
			3	3		
3	A	2	Total	Cd	0	0
			2	2		
3	O	1	Total	Cd	0	0
			1	1		
3	L	3	Total	Cd	0	0
			3	3		

*Continued on next page...*

Continued from previous page...

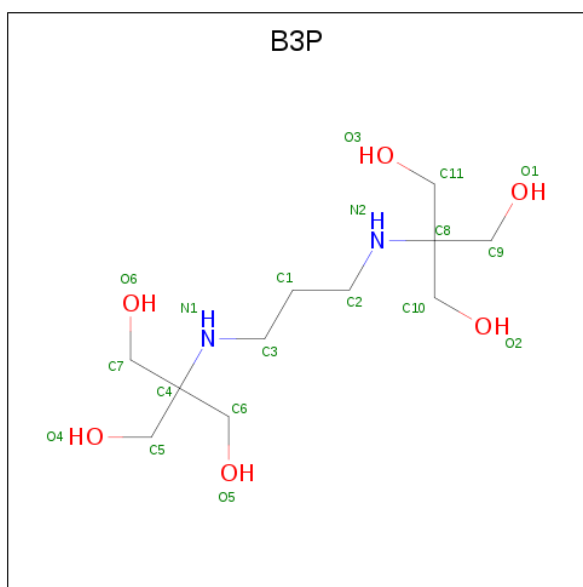
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	M	1	Total	Cd	0	0
			1	1		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



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

- Molecule 5 is 2-[3-(2-HYDROXY-1,1-DIHYDROXYMETHYL-ETHYLAMINO)-PROPYL AMINO]-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: B3P) (formula:  $C_{11}H_{26}N_2O_6$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	M	1	Total	C	N	O	0	0
			19	11	2	6		
5	O	1	Total	C	N	O	0	0
			19	11	2	6		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	L	26	Total	O	0	0
			26	26		
6	H	13	Total	O	0	0
			13	13		
6	A	16	Total	O	0	0
			16	16		
6	B	14	Total	O	0	0
			14	14		
6	C	35	Total	O	0	0
			35	35		
6	D	16	Total	O	0	0
			16	16		
6	E	13	Total	O	0	0
			13	13		
6	F	10	Total	O	0	0
			10	10		
6	G	27	Total	O	0	0
			27	27		
6	I	15	Total	O	0	0
			15	15		

*Continued on next page...*

*Continued from previous page...*

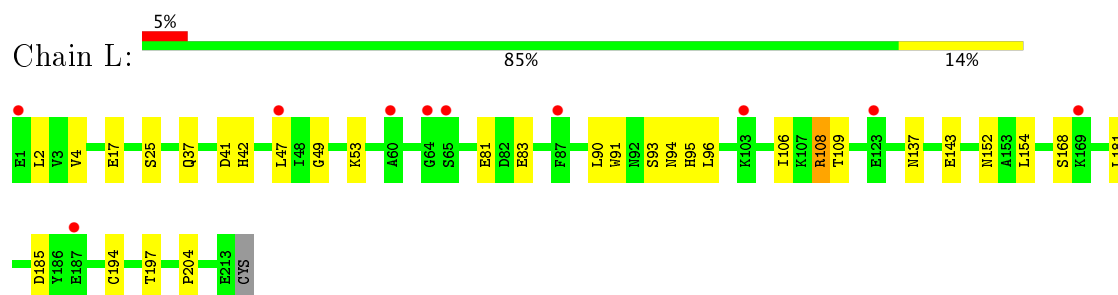
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	J	35	Total 35	O 35	0	0
6	K	16	Total 16	O 16	0	0
6	M	14	Total 14	O 14	0	0
6	N	7	Total 7	O 7	0	0
6	O	16	Total 16	O 16	0	0
6	P	4	Total 4	O 4	0	0



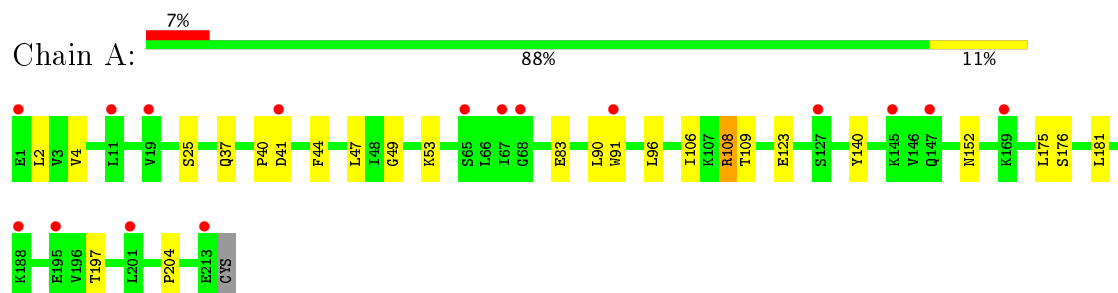
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

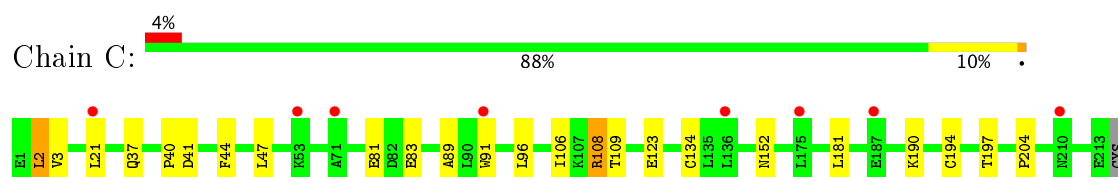
- Molecule 1: CATALYTIC ANTIBODY FAB 34E4 LIGHT CHAIN, Uncharacterized protein



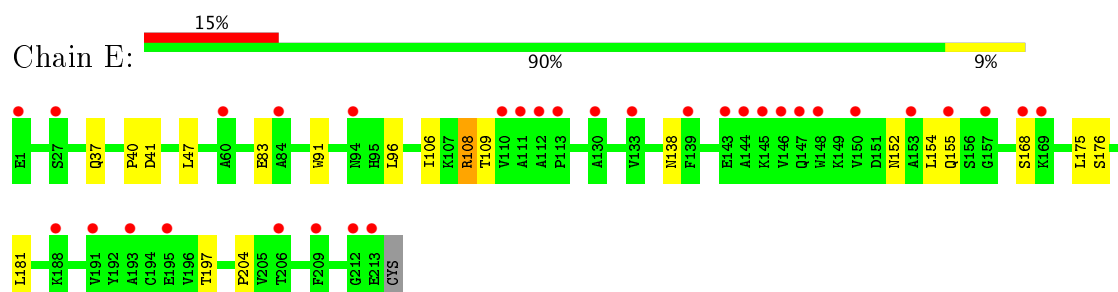
- Molecule 1: CATALYTIC ANTIBODY FAB 34E4 LIGHT CHAIN, Uncharacterized protein



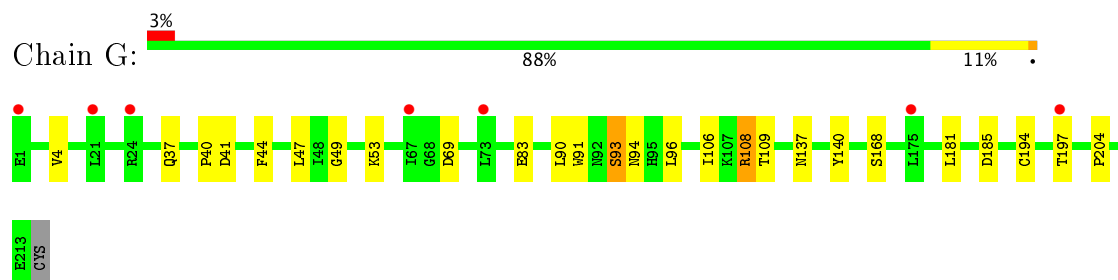
- Molecule 1: CATALYTIC ANTIBODY FAB 34E4 LIGHT CHAIN, Uncharacterized protein



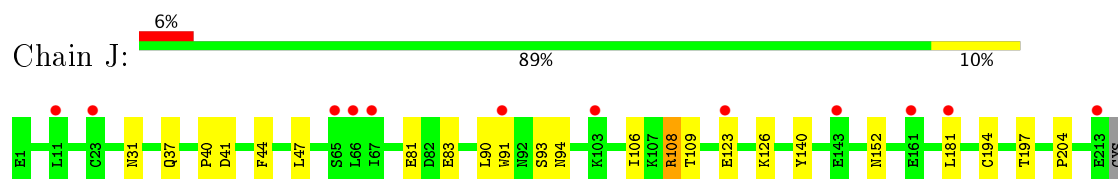
- Molecule 1: CATALYTIC ANTIBODY FAB 34E4 LIGHT CHAIN, Uncharacterized protein



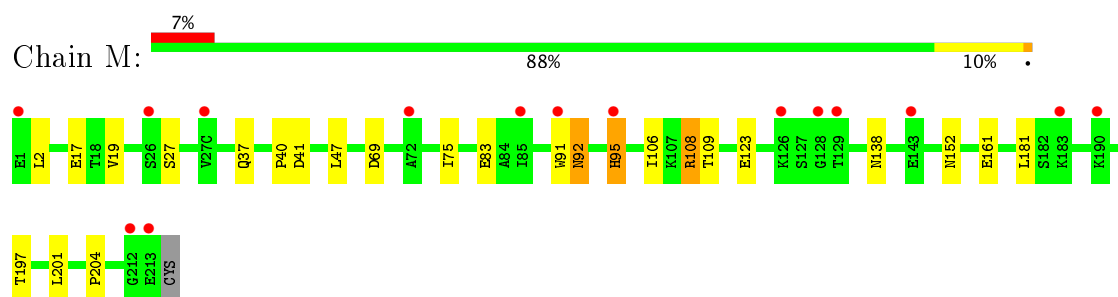
- Molecule 1: CATALYTIC ANTIBODY FAB 34E4 LIGHT CHAIN,Uncharacterized protein



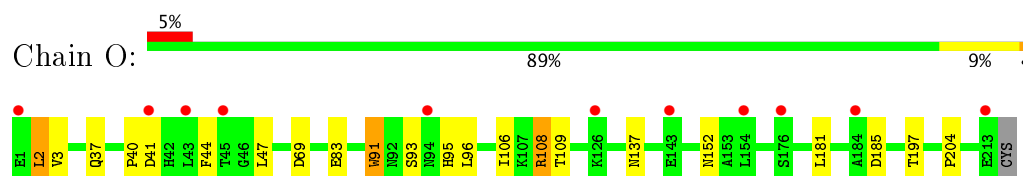
- Molecule 1: CATALYTIC ANTIBODY FAB 34E4 LIGHT CHAIN,Uncharacterized protein



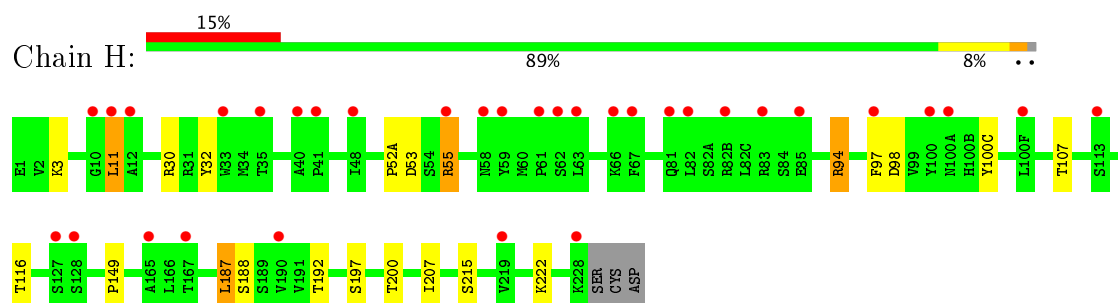
- Molecule 1: CATALYTIC ANTIBODY FAB 34E4 LIGHT CHAIN,Uncharacterized protein




- Molecule 1: CATALYTIC ANTIBODY FAB 34E4 LIGHT CHAIN,Uncharacterized protein

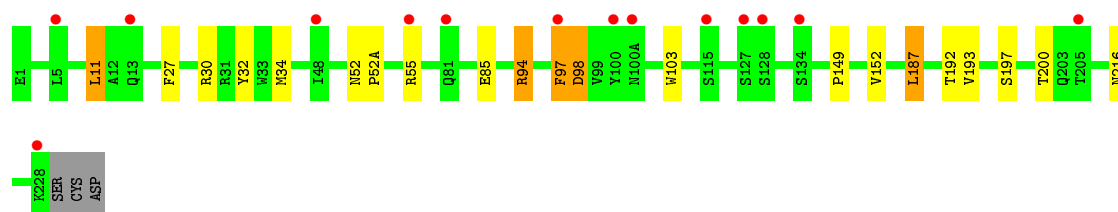


- Molecule 2: CATALYTIC ANTIBODY FAB 34E4 HEAVY CHAIN,Uncharacterized protein




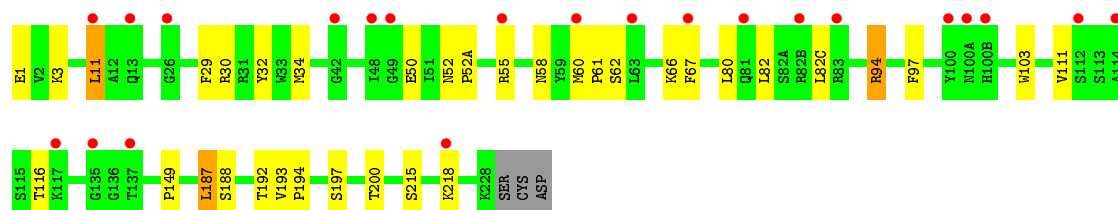
- Molecule 2: CATALYTIC ANTIBODY FAB 34E4 HEAVY CHAIN,Uncharacterized protein

Chain B: 




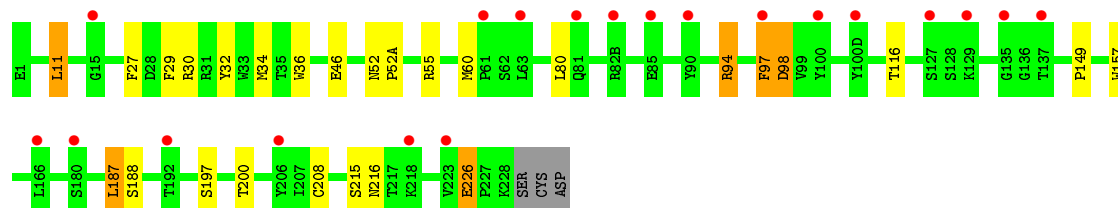
- Molecule 2: CATALYTIC ANTIBODY FAB 34E4 HEAVY CHAIN,Uncharacterized protein

Chain D: 




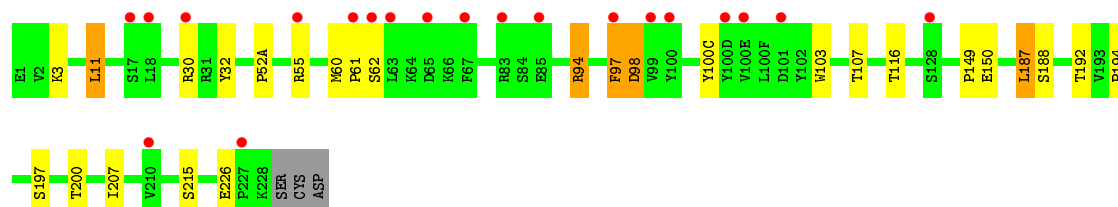
- Molecule 2: CATALYTIC ANTIBODY FAB 34E4 HEAVY CHAIN,Uncharacterized protein

Chain F: 




- Molecule 2: CATALYTIC ANTIBODY FAB 34E4 HEAVY CHAIN,Uncharacterized protein

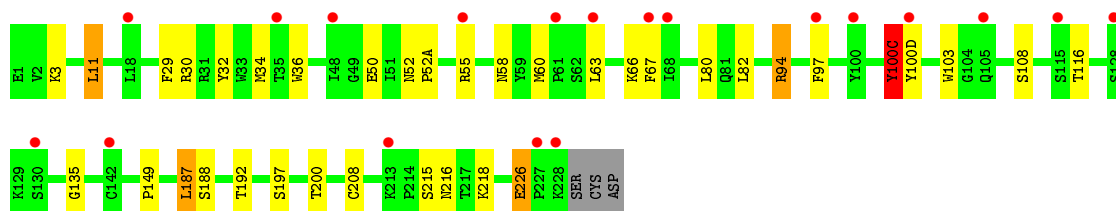
Chain I: 



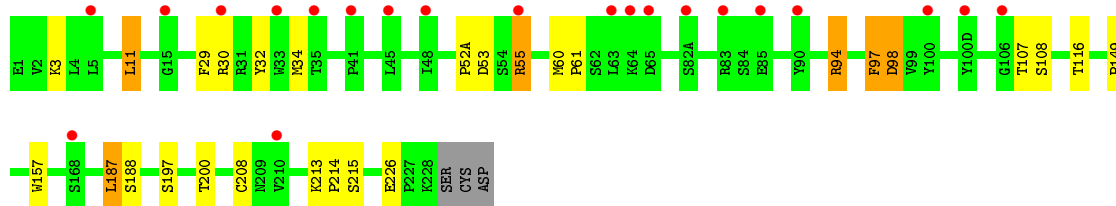
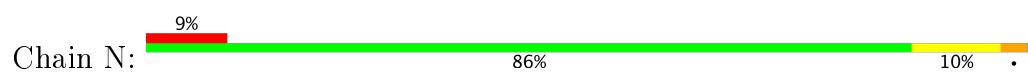
- Molecule 2: CATALYTIC ANTIBODY FAB 34E4 HEAVY CHAIN,Uncharacterized protein

Chain K: 

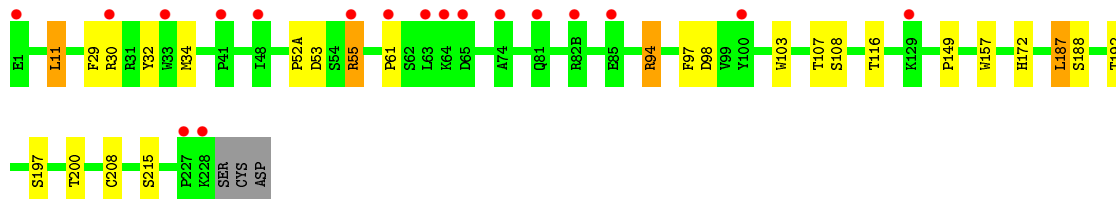
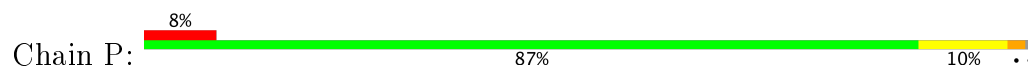




- Molecule 2: CATALYTIC ANTIBODY FAB 34E4 HEAVY CHAIN,Uncharacterized protein



- Molecule 2: CATALYTIC ANTIBODY FAB 34E4 HEAVY CHAIN,Uncharacterized protein



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	81.07Å 106.30Å 116.11Å 89.89° 90.04° 89.48°	Depositor
Resolution (Å)	41.67 – 2.60 41.68 – 2.60	Depositor EDS
% Data completeness (in resolution range)	94.5 (41.67-2.60) 94.2 (41.68-2.60)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.99 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.221 , 0.244 0.263 , 0.282	Depositor DCC
$R_{free}$ test set	5640 reflections (5.02%)	DCC
Wilson B-factor (Å <sup>2</sup> )	54.3	Xtriage
Anisotropy	0.039	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 21.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.098 for h,-k,-l 0.099 for -h,k,-l 0.417 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	27118	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.39% 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 ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, B3P, CD

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	0.58	0/1660	0.63	0/2258
1	C	0.67	2/1660 (0.1%)	0.67	0/2258
1	E	0.56	0/1660	0.63	0/2258
1	G	0.67	1/1660 (0.1%)	0.66	0/2258
1	J	0.65	1/1660 (0.1%)	0.68	0/2258
1	L	0.64	1/1660 (0.1%)	0.66	0/2258
1	M	0.65	2/1660 (0.1%)	0.63	0/2258
1	O	0.58	0/1660	0.63	0/2258
2	B	0.59	0/1762	0.62	0/2397
2	D	0.61	0/1762	0.64	0/2397
2	F	0.61	2/1762 (0.1%)	0.62	0/2397
2	H	0.57	0/1762	0.61	0/2397
2	I	0.58	0/1762	0.61	0/2397
2	K	0.85	5/1762 (0.3%)	0.79	6/2397 (0.3%)
2	N	0.58	0/1762	0.60	0/2397
2	P	0.56	0/1762	0.60	0/2397
All	All	0.63	14/27376 (0.1%)	0.64	6/37240 (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
2	K	0	1

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	K	100(C)	TYR	CG-CD1	16.09	1.60	1.39
2	K	100(C)	TYR	CE2-CZ	12.44	1.54	1.38

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	M	138	ASN	CG-ND2	-8.65	1.11	1.32
1	G	194	CYS	CB-SG	-8.56	1.67	1.82
1	C	194	CYS	CB-SG	-8.03	1.68	1.82
2	K	226	GLU	CG-CD	7.62	1.63	1.51
1	J	194	CYS	CB-SG	-7.33	1.69	1.82
1	L	194	CYS	CB-SG	-7.02	1.70	1.82
1	M	138	ASN	CG-OD1	-6.78	1.09	1.24
2	F	226	GLU	CG-CD	6.53	1.61	1.51
2	K	226	GLU	CB-CG	6.34	1.64	1.52
2	F	226	GLU	CB-CG	6.15	1.63	1.52
2	K	208	CYS	CB-SG	-5.32	1.73	1.81
1	C	134	CYS	CB-SG	-5.29	1.73	1.81

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	100(C)	TYR	CG-CD1-CE1	-13.78	110.28	121.30
2	K	100(C)	TYR	CB-CG-CD1	-8.45	115.93	121.00
2	K	100(C)	TYR	CZ-CE2-CD2	-8.25	112.38	119.80
2	K	100(C)	TYR	CG-CD2-CE2	-7.42	115.37	121.30
2	K	100(C)	TYR	CB-CG-CD2	-7.06	116.77	121.00
2	K	100(C)	TYR	CD1-CG-CD2	6.30	124.83	117.90

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	K	100(C)	TYR	Sidechain

## 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	1628	0	1590	16	0
1	C	1628	0	1588	13	0
1	E	1628	0	1589	12	0
1	G	1628	0	1589	14	2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	J	1628	0	1588	13	0
1	L	1628	0	1589	16	1
1	M	1628	0	1590	18	0
1	O	1628	0	1590	15	0
2	B	1718	0	1693	20	0
2	D	1718	0	1693	28	0
2	F	1718	0	1693	17	0
2	H	1718	0	1693	14	0
2	I	1718	0	1693	18	0
2	K	1718	0	1693	30	0
2	N	1718	0	1693	20	0
2	P	1718	0	1693	15	0
3	A	2	0	0	0	0
3	B	1	0	0	0	0
3	C	3	0	0	0	0
3	D	2	0	0	0	1
3	E	2	0	0	0	0
3	G	4	0	0	0	0
3	J	3	0	0	0	0
3	K	1	0	0	0	2
3	L	3	0	0	0	0
3	M	1	0	0	0	0
3	O	1	0	0	0	0
4	A	6	0	8	0	0
4	E	6	0	8	1	0
5	M	19	0	26	2	0
5	O	19	0	24	4	1
6	A	16	0	0	1	0
6	B	14	0	0	3	0
6	C	35	0	0	3	2
6	D	16	0	0	3	0
6	E	13	0	0	2	1
6	F	10	0	0	0	0
6	G	27	0	0	0	2
6	H	13	0	0	1	0
6	I	15	0	0	1	0
6	J	35	0	0	3	1
6	K	16	0	0	1	0
6	L	26	0	0	4	1
6	M	14	0	0	4	0
6	N	7	0	0	1	0
6	O	16	0	0	2	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	P	4	0	0	0	0
All	All	27118	0	26323	257	7

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 5.

All (257) 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:M:69:ASP:OD2	5:M:501:B3P:O3	1.75	1.05
5:O:502:B3P:O1	5:O:502:B3P:O3	1.53	1.04
1:J:81:GLU:HG3	6:J:332:HOH:O	1.64	0.95
1:L:143:GLU:HG3	6:L:343:HOH:O	1.68	0.91
1:L:81:GLU:HG3	6:L:335:HOH:O	1.69	0.89
2:P:32:TYR:CD2	2:P:94:ARG:HD2	2.15	0.81
1:C:81:GLU:HG3	6:C:329:HOH:O	1.82	0.79
1:L:4:VAL:HG22	1:L:90:LEU:HD12	1.66	0.76
2:N:32:TYR:CD2	2:N:94:ARG:HD2	2.22	0.75
2:I:11:LEU:HD12	2:I:149:PRO:HG3	1.71	0.72
2:H:11:LEU:HD12	2:H:149:PRO:HG3	1.70	0.71
1:A:108:ARG:HD3	1:A:109:THR:O	1.91	0.71
2:K:11:LEU:HD12	2:K:149:PRO:HG3	1.72	0.71
2:K:226:GLU:OE2	2:N:226:GLU:OE2	2.08	0.71
2:B:32:TYR:CD2	2:B:94:ARG:HD2	2.26	0.71
2:N:11:LEU:HD12	2:N:149:PRO:HG3	1.71	0.70
1:J:126:LYS:HE2	6:J:350:HOH:O	1.90	0.70
1:C:190:LYS:NZ	6:C:344:HOH:O	2.25	0.70
2:P:11:LEU:HD12	2:P:149:PRO:HG3	1.72	0.70
1:G:93:SER:OG	1:G:94:ASN:N	2.24	0.69
1:G:197:THR:HG22	1:G:204:PRO:HG3	1.76	0.68
1:L:197:THR:HG22	1:L:204:PRO:HG3	1.76	0.68
2:F:32:TYR:CD2	2:F:94:ARG:HD2	2.28	0.67
1:M:17:GLU:OE1	6:M:513:HOH:O	2.13	0.66
1:C:197:THR:HG22	1:C:204:PRO:HG3	1.78	0.65
2:D:1:GLU:OE2	6:D:313:HOH:O	2.14	0.65
1:M:83:GLU:HG3	1:M:106:ILE:HG12	1.77	0.65
1:A:197:THR:HG22	1:A:204:PRO:HG3	1.78	0.65
1:O:197:THR:HG22	1:O:204:PRO:HG3	1.77	0.65
1:O:83:GLU:HG3	1:O:106:ILE:HG12	1.79	0.65
1:E:197:THR:HG22	1:E:204:PRO:HG3	1.77	0.64
1:M:197:THR:HG22	1:M:204:PRO:HG3	1.78	0.64

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:11:LEU:HD12	2:B:149:PRO:HG3	1.80	0.64
1:J:197:THR:HG22	1:J:204:PRO:HG3	1.80	0.63
5:O:502:B3P:H62	5:O:502:B3P:H112	1.81	0.63
2:F:11:LEU:HD12	2:F:149:PRO:HG3	1.80	0.63
1:O:108:ARG:HD3	1:O:109:THR:O	1.98	0.63
2:K:67:PHE:CZ	2:K:82:LEU:HD22	2.33	0.63
2:D:67:PHE:HD2	2:D:80:LEU:HD11	1.65	0.62
1:G:4:VAL:HG22	1:G:90:LEU:HD12	1.82	0.61
2:D:67:PHE:CE2	2:D:82:LEU:CD2	2.84	0.61
1:O:185:ASP:OD2	6:O:512:HOH:O	2.16	0.61
2:B:152:VAL:CG2	2:B:187:LEU:CD2	2.78	0.61
1:G:108:ARG:HD3	1:G:109:THR:O	2.01	0.60
1:M:123:GLU:HG3	6:M:512:HOH:O	2.02	0.60
5:M:501:B3P:O2	5:M:501:B3P:O3	2.18	0.59
2:D:67:PHE:CZ	2:D:82:LEU:HD22	2.37	0.59
2:I:32:TYR:CD2	2:I:94:ARG:HD2	2.38	0.59
2:K:32:TYR:CD1	2:K:94:ARG:HD2	2.37	0.59
2:H:53:ASP:CG	2:H:55:ARG:HD2	2.22	0.59
1:M:201:LEU:O	6:M:509:HOH:O	2.17	0.59
1:L:17:GLU:OE1	6:L:347:HOH:O	2.17	0.59
2:D:11:LEU:HD12	2:D:149:PRO:HG3	1.85	0.58
2:K:226:GLU:OE1	2:N:226:GLU:OE2	2.22	0.58
4:E:403:GOL:H2	6:E:406:HOH:O	2.04	0.58
2:H:32:TYR:CD2	2:H:94:ARG:HD2	2.39	0.58
2:K:100(C):TYR:C	2:K:100(C):TYR:CD1	2.78	0.57
2:D:32:TYR:CD1	2:D:94:ARG:HD2	2.40	0.57
2:B:152:VAL:HG21	2:B:187:LEU:CD2	2.34	0.57
6:O:516:HOH:O	2:P:172:HIS:NE2	2.32	0.57
1:M:108:ARG:HD3	1:M:109:THR:O	2.04	0.57
1:C:123:GLU:HG3	6:C:337:HOH:O	2.04	0.56
2:D:29:PHE:HE1	2:D:34:MET:HE3	1.70	0.56
2:K:226:GLU:CD	2:N:226:GLU:OE2	2.44	0.56
2:D:29:PHE:CE1	2:D:34:MET:HE3	2.41	0.56
1:L:108:ARG:HD3	1:L:109:THR:O	2.04	0.56
1:O:95:HIS:CD2	2:P:61:PRO:HD3	2.40	0.55
1:A:40:PRO:O	1:A:41:ASP:HB2	2.06	0.55
1:J:108:ARG:HD3	1:J:109:THR:O	2.07	0.55
2:B:152:VAL:CG2	2:B:187:LEU:HD21	2.36	0.55
2:K:60:MET:HB3	2:K:63:LEU:HD12	1.89	0.55
2:N:55:ARG:NH2	6:N:238:HOH:O	2.26	0.55
2:B:11:LEU:CD2	6:B:313:HOH:O	2.55	0.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:138:ASN:ND2	6:E:410:HOH:O	2.40	0.54
1:O:91:TRP:CD2	1:O:96:LEU:HD13	2.43	0.54
1:E:108:ARG:HD3	1:E:109:THR:O	2.07	0.54
1:L:37:GLN:HB2	1:L:47:LEU:HD11	1.90	0.54
1:M:161:GLU:HB2	6:M:511:HOH:O	2.07	0.54
1:G:137:ASN:ND2	2:I:192:THR:HG21	2.23	0.53
2:D:218:LYS:NZ	2:I:207:ILE:HD12	2.23	0.53
2:H:207:ILE:HD12	2:K:218:LYS:NZ	2.23	0.53
2:P:187:LEU:HD12	2:P:188:SER:N	2.22	0.53
1:J:40:PRO:O	1:J:41:ASP:HB2	2.09	0.53
1:L:42:HIS:CE1	6:L:346:HOH:O	2.61	0.53
1:G:91:TRP:CE2	1:G:96:LEU:HD13	2.44	0.52
2:K:100(C):TYR:HD1	2:K:100(C):TYR:C	2.12	0.52
2:F:187:LEU:HD12	2:F:188:SER:N	2.25	0.52
1:E:83:GLU:OE1	1:E:168:SER:HA	2.10	0.52
2:K:29:PHE:CE1	2:K:34:MET:HE3	2.44	0.52
1:O:69:ASP:OD2	5:O:502:B3P:O1	2.28	0.52
1:A:123:GLU:HG3	6:A:415:HOH:O	2.08	0.51
2:B:216:ASN:ND2	1:J:123:GLU:HG2	2.25	0.51
2:N:97:PHE:O	2:N:98:ASP:HB2	2.11	0.51
1:G:37:GLN:HB2	1:G:47:LEU:HD11	1.93	0.51
1:L:83:GLU:HG3	1:L:106:ILE:HG12	1.93	0.51
2:I:150:GLU:OE2	6:I:241:HOH:O	2.19	0.51
2:K:50:GLU:HG2	2:K:58:ASN:HB2	1.93	0.51
2:H:187:LEU:HD12	2:H:188:SER:N	2.26	0.50
1:A:175:LEU:HD23	1:A:175:LEU:C	2.31	0.50
1:C:2:LEU:HD23	1:C:3:VAL:N	2.27	0.50
1:L:91:TRP:CE2	1:L:96:LEU:HD13	2.46	0.50
1:E:40:PRO:O	1:E:41:ASP:HB2	2.12	0.50
1:A:108:ARG:HD2	1:A:140:TYR:HB3	1.94	0.49
2:B:27:PHE:HZ	2:B:34:MET:HE1	1.77	0.49
1:J:83:GLU:HG3	1:J:106:ILE:HG12	1.95	0.49
1:J:37:GLN:HB2	1:J:47:LEU:HD11	1.94	0.49
1:E:83:GLU:HG3	1:E:106:ILE:HG12	1.95	0.49
2:K:29:PHE:HE1	2:K:34:MET:HE3	1.78	0.49
5:O:502:B3P:C6	5:O:502:B3P:H112	2.43	0.49
1:O:83:GLU:HG3	1:O:106:ILE:CG1	2.43	0.49
1:M:83:GLU:OE2	1:M:106:ILE:HB	2.12	0.49
1:M:83:GLU:HG3	1:M:106:ILE:CG1	2.41	0.49
2:D:67:PHE:CE2	2:D:82:LEU:HD22	2.47	0.49
1:C:108:ARG:HD3	1:C:109:THR:O	2.12	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:40:PRO:O	1:G:41:ASP:HB2	2.13	0.48
1:G:91:TRP:CD2	1:G:96:LEU:HD13	2.48	0.48
2:N:187:LEU:HD12	2:N:188:SER:N	2.28	0.48
1:J:44:PHE:HB2	2:K:103:TRP:CG	2.47	0.48
1:A:83:GLU:HG3	1:A:106:ILE:HG12	1.94	0.48
2:B:152:VAL:HG21	2:B:187:LEU:HD23	1.96	0.48
2:F:226:GLU:OE1	2:I:226:GLU:OE2	2.31	0.48
2:B:97:PHE:O	2:B:98:ASP:HB2	2.13	0.48
2:K:67:PHE:CE1	2:K:82:LEU:HD22	2.49	0.48
1:L:2:LEU:HD11	1:L:25:SER:OG	2.13	0.48
1:A:123:GLU:HG2	2:K:216:ASN:ND2	2.28	0.48
2:D:197:SER:O	2:D:200:THR:HB	2.14	0.48
2:K:187:LEU:HD12	2:K:188:SER:N	2.29	0.48
2:P:116:THR:HG22	2:P:215:SER:HB3	1.96	0.48
2:K:197:SER:O	2:K:200:THR:HB	2.14	0.47
2:D:30:ARG:O	2:D:52(A):PRO:HB3	2.13	0.47
1:E:91:TRP:CE2	1:E:96:LEU:HD13	2.49	0.47
1:A:91:TRP:CE2	1:A:96:LEU:HD13	2.49	0.47
1:C:40:PRO:O	1:C:41:ASP:HB2	2.14	0.47
2:B:193:VAL:HA	2:N:3:LYS:HE2	1.96	0.47
1:O:2:LEU:HD12	1:O:3:VAL:N	2.30	0.47
2:D:67:PHE:CD2	2:D:80:LEU:HD11	2.46	0.46
1:G:49:GLY:O	1:G:53:LYS:HB2	2.16	0.46
2:B:152:VAL:HG21	2:B:187:LEU:HD21	1.95	0.46
1:C:44:PHE:HB2	2:D:103:TRP:CG	2.50	0.46
1:L:4:VAL:HG22	1:L:90:LEU:CD1	2.43	0.46
2:B:30:ARG:O	2:B:52(A):PRO:HB3	2.16	0.46
1:J:31:ASN:HB3	1:J:90:LEU:HD22	1.98	0.46
1:O:91:TRP:CE2	1:O:96:LEU:HD13	2.51	0.46
1:A:175:LEU:HD23	1:A:176:SER:N	2.30	0.46
2:P:29:PHE:HE1	2:P:34:MET:HE3	1.81	0.46
1:G:83:GLU:OE1	1:G:168:SER:HA	2.16	0.46
2:P:29:PHE:CE1	2:P:34:MET:HE3	2.52	0.45
1:A:37:GLN:HB2	1:A:47:LEU:HD11	1.99	0.45
1:L:93:SER:OG	1:L:94:ASN:N	2.41	0.45
2:B:197:SER:O	2:B:200:THR:HB	2.17	0.45
2:K:66:LYS:HG3	2:K:67:PHE:HD1	1.81	0.45
2:N:197:SER:O	2:N:200:THR:HB	2.17	0.45
2:B:11:LEU:HD21	6:B:313:HOH:O	2.17	0.45
1:E:37:GLN:HB2	1:E:47:LEU:HD11	1.98	0.44
2:K:135:GLY:HA2	6:K:318:HOH:O	2.17	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:92:ASN:HD22	1:M:92:ASN:C	2.20	0.44
1:O:40:PRO:O	1:O:41:ASP:HB2	2.17	0.44
1:A:49:GLY:O	1:A:53:LYS:HB2	2.17	0.44
2:H:197:SER:O	2:H:200:THR:HB	2.17	0.44
2:P:197:SER:O	2:P:200:THR:HB	2.17	0.44
1:J:93:SER:HB3	6:J:335:HOH:O	2.18	0.44
2:D:193:VAL:HA	2:I:3:LYS:HE2	2.00	0.44
2:H:98:ASP:HB3	2:H:100(C):TYR:HB3	2.00	0.44
1:E:175:LEU:HD23	1:E:175:LEU:C	2.38	0.44
2:I:187:LEU:HD12	2:I:188:SER:N	2.32	0.44
1:C:37:GLN:HB2	1:C:47:LEU:HD11	1.98	0.44
2:D:11:LEU:CD2	6:D:323:HOH:O	2.65	0.44
2:N:116:THR:HG22	2:N:215:SER:HB3	1.99	0.44
2:K:30:ARG:O	2:K:52(A):PRO:HB3	2.17	0.44
2:F:30:ARG:O	2:F:52(A):PRO:HB3	2.17	0.44
1:G:83:GLU:HG3	1:G:106:ILE:HG12	2.00	0.44
1:M:2:LEU:HD13	1:M:27:SER:OG	2.18	0.44
2:K:66:LYS:HG3	2:K:67:PHE:CD1	2.52	0.43
2:P:187:LEU:HD12	2:P:187:LEU:C	2.38	0.43
2:F:116:THR:HG22	2:F:215:SER:HB3	1.99	0.43
1:C:83:GLU:HG3	1:C:106:ILE:HG12	1.99	0.43
2:D:29:PHE:CE1	2:D:34:MET:CE	3.02	0.43
2:D:50:GLU:HG2	2:D:58:ASN:HB2	1.99	0.43
1:E:175:LEU:HD23	1:E:176:SER:N	2.34	0.43
2:N:53:ASP:CG	2:N:55:ARG:HD2	2.39	0.43
2:H:222:LYS:HE2	6:H:236:HOH:O	2.18	0.43
2:I:60:MET:O	2:I:62:SER:N	2.52	0.43
1:O:83:GLU:OE2	1:O:106:ILE:HB	2.19	0.43
2:F:27:PHE:HZ	2:F:34:MET:HE1	1.84	0.43
2:D:82(C):LEU:HB3	2:D:111:VAL:HG21	2.01	0.43
2:F:187:LEU:HD12	2:F:187:LEU:C	2.39	0.43
2:H:116:THR:HG22	2:H:215:SER:HB3	2.00	0.43
2:N:157:TRP:CH2	2:N:208:CYS:HB3	2.54	0.43
1:C:21:LEU:HD12	1:C:21:LEU:N	2.34	0.43
2:H:30:ARG:O	2:H:52(A):PRO:HB3	2.18	0.43
1:L:137:ASN:ND2	2:H:192:THR:HG21	2.33	0.43
2:D:187:LEU:HD12	2:D:188:SER:N	2.34	0.42
1:M:2:LEU:CD1	1:M:27:SER:OG	2.67	0.42
2:P:157:TRP:CH2	2:P:208:CYS:HB3	2.53	0.42
2:D:60:MET:O	2:D:61:PRO:C	2.57	0.42
1:C:123:GLU:HG2	2:F:216:ASN:ND2	2.34	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:192:THR:O	2:K:3:LYS:HE2	2.18	0.42
2:P:53:ASP:CG	2:P:55:ARG:HD2	2.39	0.42
2:D:11:LEU:HD21	6:D:323:HOH:O	2.19	0.42
2:D:116:THR:HG22	2:D:215:SER:HB3	2.01	0.42
1:M:95:HIS:CD2	2:N:61:PRO:HD3	2.54	0.42
2:F:29:PHE:CE1	2:F:34:MET:HE3	2.55	0.42
2:D:194:PRO:HD3	2:I:3:LYS:HE3	2.00	0.42
2:D:52:ASN:HB2	2:D:52(A):PRO:HD2	2.01	0.42
1:E:154:LEU:HD12	1:E:155:GLN:H	1.85	0.42
2:K:100(C):TYR:HD1	2:K:100(D):TYR:N	2.17	0.42
2:K:50:GLU:OE2	2:K:58:ASN:ND2	2.46	0.42
1:M:19:VAL:HG12	1:M:75:ILE:HB	2.01	0.42
2:I:116:THR:HG22	2:I:215:SER:HB3	2.00	0.42
2:D:192:THR:O	2:I:3:LYS:HE2	2.19	0.42
2:K:11:LEU:HD12	2:K:149:PRO:CG	2.47	0.42
2:K:52:ASN:HB2	2:K:52(A):PRO:HD2	2.00	0.42
2:B:192:THR:O	2:N:3:LYS:HE2	2.20	0.42
2:F:52:ASN:HB2	2:F:52(A):PRO:HD2	2.02	0.42
1:L:49:GLY:O	1:L:53:LYS:HB2	2.20	0.42
2:N:187:LEU:C	2:N:187:LEU:HD12	2.40	0.42
2:N:29:PHE:HE1	2:N:34:MET:HE3	1.85	0.42
2:N:29:PHE:CE1	2:N:34:MET:HE3	2.55	0.42
2:H:187:LEU:C	2:H:187:LEU:HD12	2.40	0.42
1:L:83:GLU:OE1	1:L:168:SER:HA	2.19	0.42
1:G:108:ARG:HD2	1:G:140:TYR:HB3	2.01	0.41
2:B:52:ASN:HB2	2:B:52(A):PRO:HD2	2.01	0.41
2:B:85:GLU:HG3	6:B:307:HOH:O	2.19	0.41
2:F:97:PHE:O	2:F:98:ASP:HB2	2.21	0.41
1:M:92:ASN:ND2	1:M:92:ASN:C	2.73	0.41
1:G:44:PHE:HB2	2:I:103:TRP:CG	2.56	0.41
1:M:37:GLN:HB2	1:M:47:LEU:HD11	2.01	0.41
1:E:197:THR:CG2	1:E:204:PRO:HG3	2.49	0.41
1:A:4:VAL:HG22	1:A:90:LEU:HD12	2.02	0.41
2:F:36:TRP:CE2	2:F:80:LEU:HB2	2.55	0.41
1:O:44:PHE:HB2	2:P:103:TRP:CG	2.56	0.41
2:P:30:ARG:O	2:P:52(A):PRO:HB3	2.21	0.41
2:N:30:ARG:O	2:N:52(A):PRO:HB3	2.20	0.41
1:A:44:PHE:HB2	2:B:103:TRP:CG	2.56	0.41
2:B:27:PHE:CZ	2:B:34:MET:HE1	2.55	0.41
2:I:97:PHE:O	2:I:98:ASP:HB2	2.21	0.41
2:K:116:THR:HG22	2:K:215:SER:HB3	2.01	0.41

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:40:PRO:O	1:M:41:ASP:HB2	2.21	0.41
2:I:98:ASP:HB3	2:I:100(C):TYR:HB3	2.02	0.41
1:J:108:ARG:HD2	1:J:140:TYR:HB3	2.02	0.41
2:F:157:TRP:CH2	2:F:208:CYS:HB3	2.56	0.40
1:J:108:ARG:HD2	1:J:140:TYR:CB	2.51	0.40
1:A:2:LEU:HD11	1:A:25:SER:OG	2.22	0.40
1:C:89:ALA:HB1	1:C:96:LEU:HD11	2.03	0.40
2:D:29:PHE:CD1	2:D:34:MET:HE2	2.57	0.40
2:I:197:SER:O	2:I:200:THR:HB	2.21	0.40
1:O:137:ASN:ND2	2:P:192:THR:HG21	2.35	0.40
1:O:37:GLN:HB2	1:O:47:LEU:HD11	2.03	0.40
2:D:3:LYS:HE3	2:I:194:PRO:HD3	2.03	0.40
2:N:213:LYS:N	2:N:214:PRO:CD	2.84	0.40
2:F:197:SER:O	2:F:200:THR:HB	2.20	0.40
2:F:29:PHE:HE1	2:F:34:MET:HE3	1.86	0.40
2:I:30:ARG:O	2:I:52(A):PRO:HB3	2.21	0.40
2:K:36:TRP:CE2	2:K:80:LEU:HB2	2.57	0.40
1:A:197:THR:CG2	1:A:204:PRO:HG3	2.51	0.40
2:F:46:GLU:OE2	2:F:60:MET:HE1	2.21	0.40
2:H:3:LYS:HE2	2:K:192:THR:O	2.22	0.40

All (7) 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)
6:C:312:HOH:O	6:G:345:HOH:O[1_455]	1.80	0.40
6:C:345:HOH:O	6:E:404:HOH:O[1_565]	2.04	0.16
6:L:326:HOH:O	6:J:329:HOH:O[1_455]	2.05	0.15
3:K:304:CD:CD	6:G:343:HOH:O[1_456]	2.07	0.13
1:G:69:ASP:OD2	5:O:502:B3P:O6[1_565]	2.10	0.10
1:L:185:ASP:OD1	3:D:311:CD:CD[1_455]	2.15	0.05
1:G:185:ASP:OD1	3:K:304:CD:CD[1_654]	2.18	0.02

## 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	213/216 (99%)	206 (97%)	7 (3%)	0	100	100
1	C	213/216 (99%)	206 (97%)	7 (3%)	0	100	100
1	E	213/216 (99%)	206 (97%)	7 (3%)	0	100	100
1	G	213/216 (99%)	207 (97%)	6 (3%)	0	100	100
1	J	213/216 (99%)	204 (96%)	9 (4%)	0	100	100
1	L	213/216 (99%)	210 (99%)	3 (1%)	0	100	100
1	M	213/216 (99%)	208 (98%)	5 (2%)	0	100	100
1	O	213/216 (99%)	206 (97%)	6 (3%)	1 (0%)	32	58
2	B	222/227 (98%)	217 (98%)	4 (2%)	1 (0%)	32	58
2	D	222/227 (98%)	216 (97%)	5 (2%)	1 (0%)	32	58
2	F	222/227 (98%)	216 (97%)	5 (2%)	1 (0%)	32	58
2	H	222/227 (98%)	214 (96%)	8 (4%)	0	100	100
2	I	222/227 (98%)	215 (97%)	5 (2%)	2 (1%)	20	40
2	K	222/227 (98%)	216 (97%)	6 (3%)	0	100	100
2	N	222/227 (98%)	215 (97%)	6 (3%)	1 (0%)	32	58
2	P	222/227 (98%)	216 (97%)	5 (2%)	1 (0%)	32	58
All	All	3480/3544 (98%)	3378 (97%)	94 (3%)	8 (0%)	51	76

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	98	ASP
2	D	66	LYS
2	F	98	ASP
2	I	98	ASP
2	N	98	ASP
2	P	98	ASP
2	I	61	PRO
1	O	93	SER

### 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	182/183 (100%)	179 (98%)	3 (2%)	68	87
1	C	182/183 (100%)	177 (97%)	5 (3%)	50	77
1	E	182/183 (100%)	179 (98%)	3 (2%)	68	87
1	G	182/183 (100%)	179 (98%)	3 (2%)	68	87
1	J	182/183 (100%)	177 (97%)	5 (3%)	50	77
1	L	182/183 (100%)	176 (97%)	6 (3%)	43	70
1	M	182/183 (100%)	176 (97%)	6 (3%)	43	70
1	O	182/183 (100%)	177 (97%)	5 (3%)	50	77
2	B	193/196 (98%)	188 (97%)	5 (3%)	51	78
2	D	193/196 (98%)	187 (97%)	6 (3%)	45	73
2	F	193/196 (98%)	188 (97%)	5 (3%)	51	78
2	H	193/196 (98%)	187 (97%)	6 (3%)	45	73
2	I	193/196 (98%)	187 (97%)	6 (3%)	45	73
2	K	193/196 (98%)	186 (96%)	7 (4%)	40	68
2	N	193/196 (98%)	185 (96%)	8 (4%)	35	63
2	P	193/196 (98%)	186 (96%)	7 (4%)	40	68
All	All	3000/3032 (99%)	2914 (97%)	86 (3%)	48	75

All (86) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	41	ASP
1	L	95	HIS
1	L	108	ARG
1	L	152	ASN
1	L	154	LEU
1	L	181	LEU
2	H	11	LEU
2	H	55	ARG
2	H	94	ARG
2	H	97	PHE
2	H	107	THR
2	H	187	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	108	ARG
1	A	152	ASN
1	A	181	LEU
2	B	11	LEU
2	B	55	ARG
2	B	94	ARG
2	B	97	PHE
2	B	187	LEU
1	C	2	LEU
1	C	91	TRP
1	C	108	ARG
1	C	152	ASN
1	C	181	LEU
2	D	11	LEU
2	D	55	ARG
2	D	62	SER
2	D	94	ARG
2	D	97	PHE
2	D	187	LEU
1	E	108	ARG
1	E	152	ASN
1	E	181	LEU
2	F	11	LEU
2	F	55	ARG
2	F	94	ARG
2	F	97	PHE
2	F	187	LEU
1	G	93	SER
1	G	108	ARG
1	G	181	LEU
2	I	11	LEU
2	I	55	ARG
2	I	94	ARG
2	I	97	PHE
2	I	107	THR
2	I	187	LEU
1	J	91	TRP
1	J	94	ASN
1	J	108	ARG
1	J	152	ASN
1	J	181	LEU
2	K	11	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	K	55	ARG
2	K	94	ARG
2	K	97	PHE
2	K	100(C)	TYR
2	K	108	SER
2	K	187	LEU
1	M	91	TRP
1	M	92	ASN
1	M	95	HIS
1	M	108	ARG
1	M	152	ASN
1	M	181	LEU
2	N	11	LEU
2	N	55	ARG
2	N	60	MET
2	N	94	ARG
2	N	97	PHE
2	N	107	THR
2	N	108	SER
2	N	187	LEU
1	O	2	LEU
1	O	91	TRP
1	O	108	ARG
1	O	152	ASN
1	O	181	LEU
2	P	11	LEU
2	P	55	ARG
2	P	94	ARG
2	P	97	PHE
2	P	107	THR
2	P	108	SER
2	P	187	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	95	HIS
1	L	152	ASN
1	L	199	GLN
1	A	199	GLN
2	B	216	ASN
1	C	199	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	D	216	ASN
1	E	199	GLN
2	F	216	ASN
1	G	95	HIS
1	G	199	GLN
1	J	199	GLN
2	K	216	ASN
1	M	92	ASN
1	M	95	HIS
1	M	199	GLN
1	O	95	HIS
1	O	138	ASN
1	O	152	ASN
1	O	199	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 27 ligands modelled in this entry, 23 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	GOL	A	402	-	5,5,5	0.38	0	5,5,5	0.47	0
4	GOL	E	403	-	5,5,5	0.24	0	5,5,5	0.43	0
5	B3P	M	501	-	18,18,18	1.79	5 (27%)	21,23,23	2.68	5 (23%)
5	B3P	O	502	-	18,18,18	2.42	4 (22%)	21,23,23	2.86	10 (47%)

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
4	GOL	A	402	-	-	0/4/4/4	0/0/0/0
4	GOL	E	403	-	-	0/4/4/4	0/0/0/0
5	B3P	M	501	-	-	0/28/28/28	0/0/0/0
5	B3P	O	502	-	-	0/28/28/28	0/0/0/0

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	O	502	B3P	C7-C4	-5.87	1.46	1.53
5	O	502	B3P	C11-C8	-5.10	1.47	1.53
5	O	502	B3P	C9-C8	-4.36	1.48	1.53
5	O	502	B3P	C5-C4	-4.01	1.49	1.53
5	M	501	B3P	C11-C8	-3.75	1.49	1.53
5	M	501	B3P	C7-C4	-3.58	1.49	1.53
5	M	501	B3P	C10-C8	-3.31	1.49	1.53
5	M	501	B3P	C5-C4	-3.12	1.50	1.53
5	M	501	B3P	C9-C8	-2.74	1.50	1.53

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	O	502	B3P	O4-C5-C4	-5.50	100.17	111.54
5	O	502	B3P	O1-C9-C8	-4.82	101.58	111.54
5	O	502	B3P	O6-C7-C4	-4.02	103.24	111.54
5	O	502	B3P	O3-C11-C8	-3.95	103.37	111.54
5	O	502	B3P	C11-C8-C9	-3.59	102.69	110.09
5	M	501	B3P	O6-C7-C4	-3.44	104.42	111.54
5	M	501	B3P	O4-C5-C4	-3.36	104.59	111.54
5	O	502	B3P	C7-C4-C5	-2.44	105.07	110.09
5	M	501	B3P	C7-C4-C5	-2.42	105.10	110.09
5	O	502	B3P	C3-C1-C2	-2.02	106.17	114.16

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	O	502	B3P	O5-C6-C4	2.17	116.03	111.54
5	O	502	B3P	C2-N2-C8	4.25	122.29	116.12
5	O	502	B3P	C3-N1-C4	5.67	124.35	116.12
5	M	501	B3P	C3-N1-C4	6.94	126.19	116.12
5	M	501	B3P	C2-N2-C8	7.41	126.87	116.12

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	403	GOL	1	0
5	M	501	B3P	2	0
5	O	502	B3P	4	1

## 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	215/216 (99%)	0.74	16 (7%) 15 11	56, 58, 59, 62	0
1	C	215/216 (99%)	0.64	8 (3%) 42 34	55, 58, 59, 61	0
1	E	215/216 (99%)	1.01	32 (14%) 3 1	56, 58, 59, 63	0
1	G	215/216 (99%)	0.63	7 (3%) 47 39	55, 58, 59, 60	0
1	J	215/216 (99%)	0.62	12 (5%) 25 19	56, 58, 59, 63	0
1	L	215/216 (99%)	0.69	10 (4%) 32 25	55, 58, 59, 60	0
1	M	215/216 (99%)	0.74	15 (6%) 17 12	57, 58, 59, 63	0
1	O	215/216 (99%)	0.61	11 (5%) 29 22	56, 58, 59, 63	0
2	B	224/227 (98%)	0.75	14 (6%) 21 15	56, 58, 59, 66	0
2	D	224/227 (98%)	0.86	22 (9%) 8 5	53, 58, 62, 67	0
2	F	224/227 (98%)	0.87	20 (8%) 10 6	56, 58, 59, 64	0
2	H	224/227 (98%)	0.90	33 (14%) 3 1	56, 58, 60, 67	0
2	I	224/227 (98%)	0.85	20 (8%) 10 6	56, 58, 60, 67	0
2	K	224/227 (98%)	0.79	19 (8%) 11 7	55, 58, 61, 67	0
2	N	224/227 (98%)	0.82	21 (9%) 9 6	55, 58, 59, 66	0
2	P	224/227 (98%)	0.78	18 (8%) 13 9	55, 58, 59, 65	0
All	All	3512/3544 (99%)	0.77	278 (7%) 13 9	53, 58, 59, 67	0

All (278) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1	GLU	6.3
2	P	100	TYR	6.1
2	I	100	TYR	5.9
2	B	100	TYR	5.7
2	K	100	TYR	5.6

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	D	48	ILE	5.5
2	H	100	TYR	5.4
2	H	97	PHE	5.3
2	F	129	LYS	5.3
2	I	65	ASP	5.1
2	D	67	PHE	5.1
2	I	97	PHE	5.0
1	J	67	ILE	4.9
2	I	63	LEU	4.8
1	E	213	GLU	4.8
2	D	63	LEU	4.7
2	D	100	TYR	4.5
2	K	228	LYS	4.5
1	M	129	THR	4.5
1	O	154	LEU	4.5
1	M	212	GLY	4.4
1	G	1	GLU	4.4
2	F	82(B)	ARG	4.4
2	D	100(A)	ASN	4.3
2	P	55	ARG	4.3
1	E	143	GLU	4.3
2	B	128	SER	4.3
2	I	67	PHE	4.2
2	I	62	SER	4.2
2	D	83	ARG	4.2
1	J	143	GLU	4.2
2	H	59	TYR	4.2
1	E	191	VAL	4.1
2	P	65	ASP	4.1
2	B	228	LYS	4.1
1	M	126	LYS	4.0
1	O	213	GLU	3.9
2	K	55	ARG	3.8
1	E	110	VAL	3.8
2	K	67	PHE	3.7
2	D	81	GLN	3.7
1	M	213	GLU	3.7
2	H	10	GLY	3.7
1	M	72	ALA	3.6
1	E	212	GLY	3.6
2	F	206	TYR	3.6
2	I	85	GLU	3.6

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	41	ASP	3.5
2	K	63	LEU	3.5
1	A	145	LYS	3.5
1	E	130	ALA	3.5
2	N	85	GLU	3.5
2	N	100	TYR	3.5
2	I	55	ARG	3.5
1	L	103	LYS	3.5
2	P	1	GLU	3.4
2	F	100	TYR	3.4
1	L	65	SER	3.3
2	N	33	TRP	3.3
2	H	61	PRO	3.3
1	E	188	LYS	3.3
2	H	100(A)	ASN	3.3
2	K	115	SER	3.3
1	E	146	VAL	3.2
2	D	11	LEU	3.2
1	M	1	GLU	3.2
2	B	134	SER	3.2
2	N	35	THR	3.2
1	C	71	ALA	3.2
1	E	113	PRO	3.2
2	N	5	LEU	3.2
1	E	150	VAL	3.2
2	H	62	SER	3.2
2	N	41	PRO	3.2
2	N	64	LYS	3.1
1	A	19	VAL	3.1
2	K	100(D)	TYR	3.1
2	N	63	LEU	3.1
2	P	41	PRO	3.1
1	A	67	ILE	3.1
2	H	82(B)	ARG	3.1
2	N	100(D)	TYR	3.0
2	I	83	ARG	3.0
2	H	128	SER	3.0
2	P	85	GLU	3.0
1	A	127	SER	3.0
2	F	63	LEU	3.0
2	K	61	PRO	3.0
1	J	66	LEU	3.0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	I	18	LEU	3.0
1	E	168	SER	3.0
1	O	43	LEU	3.0
1	E	112	ALA	2.9
2	H	67	PHE	2.9
2	F	180	SER	2.9
2	N	168	SER	2.9
2	P	64	LYS	2.9
2	P	227	PRO	2.9
2	P	30	ARG	2.9
2	K	97	PHE	2.9
2	B	5	LEU	2.9
1	E	153	ALA	2.9
1	E	169	LYS	2.8
2	P	129	LYS	2.8
1	O	94	ASN	2.8
2	F	137	THR	2.8
2	N	83	ARG	2.8
2	N	45	LEU	2.8
2	D	60	MET	2.8
2	N	90	TYR	2.8
1	E	148	TRP	2.8
2	H	83	ARG	2.8
1	A	11	LEU	2.7
2	F	100(D)	TYR	2.7
2	H	82	LEU	2.7
2	H	127	SER	2.7
1	A	195	GLU	2.7
1	O	176	SER	2.7
1	C	21	LEU	2.7
1	G	21	LEU	2.7
2	H	85	GLU	2.7
1	O	45	THR	2.7
2	D	137	THR	2.6
2	F	15	GLY	2.6
2	P	82(B)	ARG	2.6
2	I	99	VAL	2.6
1	E	145	LYS	2.6
2	F	223	VAL	2.6
1	E	206	THR	2.6
1	E	94	ASN	2.6
1	E	27	SER	2.6

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	H	55	ARG	2.6
2	K	18	LEU	2.5
2	P	48	ILE	2.5
2	P	61	PRO	2.5
2	H	12	ALA	2.5
1	A	201	LEU	2.5
2	I	17	SER	2.5
2	I	128	SER	2.5
2	F	85	GLU	2.5
2	H	228	LYS	2.5
2	P	63	LEU	2.5
1	C	187	GLU	2.5
2	K	227	PRO	2.5
2	B	13	GLN	2.5
1	O	126	LYS	2.5
2	P	228	LYS	2.5
1	M	85	ILE	2.5
2	H	11	LEU	2.5
2	I	100(E)	VAL	2.5
1	M	183	LYS	2.5
2	N	30	ARG	2.5
1	L	123	GLU	2.4
1	L	187	GLU	2.4
2	B	55	ARG	2.4
1	L	1	GLU	2.4
2	H	63	LEU	2.4
1	A	65	SER	2.4
1	M	26	SER	2.4
2	B	97	PHE	2.4
1	E	144	ALA	2.4
2	H	40	ALA	2.4
2	B	205	THR	2.4
1	J	181	LEU	2.4
2	H	113	SER	2.4
1	O	184	ALA	2.4
2	K	128	SER	2.4
2	N	15	GLY	2.4
1	J	161	GLU	2.4
1	O	143	GLU	2.4
2	D	218	LYS	2.4
2	K	68	ILE	2.4
2	I	210	VAL	2.4

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	M	190	LYS	2.4
2	D	82(B)	ARG	2.4
1	L	60	ALA	2.4
1	J	65	SER	2.4
1	L	64	GLY	2.4
1	M	27(C)	VAL	2.4
1	C	91	TRP	2.4
2	F	218	LYS	2.4
1	J	23	CYS	2.4
2	D	55	ARG	2.4
2	I	101	ASP	2.3
1	A	188	LYS	2.3
2	F	97	PHE	2.3
2	N	82(A)	SER	2.3
2	H	41	PRO	2.3
2	H	35	THR	2.3
1	E	147	GLN	2.3
1	L	87	PHE	2.3
2	N	65	ASP	2.3
1	A	68	GLY	2.3
2	D	135	GLY	2.3
1	A	147	GLN	2.3
2	K	35	THR	2.3
2	K	105	GLN	2.3
1	G	67	ILE	2.3
1	J	123	GLU	2.3
2	B	127	SER	2.3
1	E	1	GLU	2.3
2	D	42	GLY	2.3
2	D	117	LYS	2.3
1	G	73	LEU	2.3
2	F	61	PRO	2.3
1	E	84	ALA	2.3
2	K	142	CYS	2.3
2	K	213	LYS	2.3
1	J	91	TRP	2.2
2	F	127	SER	2.2
2	P	33	TRP	2.2
2	N	55	ARG	2.2
1	E	209	PHE	2.2
2	D	49	GLY	2.2
1	M	95	HIS	2.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	I	30	ARG	2.2
2	I	100(D)	TYR	2.2
2	F	81	GLN	2.2
1	A	169	LYS	2.2
2	H	33	TRP	2.2
1	O	41	ASP	2.2
2	H	190	VAL	2.2
2	H	58	ASN	2.2
1	C	136	LEU	2.2
2	P	81	GLN	2.2
2	N	106	GLY	2.2
2	B	115	SER	2.2
2	N	48	ILE	2.2
1	M	91	TRP	2.2
1	E	139	PHE	2.2
1	O	1	GLU	2.2
1	A	91	TRP	2.2
1	E	111	ALA	2.2
1	E	157	GLY	2.1
1	E	193	ALA	2.1
2	H	66	LYS	2.1
2	H	219	VAL	2.1
1	G	175	LEU	2.1
1	M	128	GLY	2.1
2	I	61	PRO	2.1
1	L	169	LYS	2.1
2	D	114	ALA	2.1
2	P	74	ALA	2.1
1	E	195	GLU	2.1
1	J	213	GLU	2.1
2	D	26	GLY	2.1
1	C	53	LYS	2.1
1	M	143	GLU	2.1
2	H	81	GLN	2.1
1	J	11	LEU	2.1
2	H	165	ALA	2.1
2	B	81	GLN	2.1
1	C	175	LEU	2.1
1	L	47	LEU	2.1
2	H	48	ILE	2.1
1	E	155	GLN	2.1
1	G	24	ARG	2.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	H	100(F)	LEU	2.1
2	D	100(B)	HIS	2.1
2	D	13	GLN	2.1
2	H	167	THR	2.1
2	K	130	SER	2.1
1	E	133	VAL	2.0
2	N	210	VAL	2.0
2	B	100(A)	ASN	2.0
2	B	48	ILE	2.0
2	K	48	ILE	2.0
1	A	213	GLU	2.0
1	J	103	LYS	2.0
2	D	112	SER	2.0
2	F	135	GLY	2.0
2	F	192	THR	2.0
2	F	166	LEU	2.0
2	I	227	PRO	2.0
1	C	210	ASN	2.0
1	E	60	ALA	2.0
2	F	90	TYR	2.0
1	G	197	THR	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
5	B3P	O	502	19/19	0.86	0.31	3.04	48,56,61,61	0

*Continued on next page...*

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	CD	L	319	1/1	0.76	0.28	2.98	98,98,98,98	1
4	GOL	E	403	6/6	0.90	0.27	1.53	41,46,49,49	0
4	GOL	A	402	6/6	0.80	0.26	1.05	66,67,67,67	0
5	B3P	M	501	19/19	0.90	0.25	0.98	55,60,64,66	0
3	CD	J	302	1/1	0.96	0.17	-0.91	97,97,97,97	1
3	CD	L	323	1/1	0.86	0.15	-1.14	93,93,93,93	1
3	CD	C	309	1/1	0.90	0.14	-1.35	94,94,94,94	1
3	CD	E	322	1/1	0.87	0.09	-1.55	105,105,105,105	1
3	CD	G	315	1/1	0.82	0.15	-1.71	97,97,97,97	1
3	CD	K	304	1/1	0.97	0.17	-	84,84,84,84	1
3	CD	G	307	1/1	0.98	0.11	-	75,75,75,75	1
3	CD	E	314	1/1	0.94	0.14	-	79,79,79,79	1
3	CD	M	305	1/1	0.69	0.12	-	95,95,95,95	1
3	CD	A	317	1/1	0.74	0.09	-	90,90,90,90	1
3	CD	L	301	1/1	0.97	0.11	-	76,76,76,76	1
3	CD	D	311	1/1	0.76	0.14	-	84,84,84,84	1
3	CD	J	316	1/1	0.83	0.09	-	86,86,86,86	1
3	CD	O	313	1/1	0.95	0.14	-	83,83,83,83	1
3	CD	C	310	1/1	0.99	0.18	-	48,48,48,48	0
3	CD	J	303	1/1	0.99	0.15	-	52,52,52,52	0
3	CD	A	318	1/1	0.97	0.13	-	96,96,96,96	1
3	CD	G	320	1/1	0.88	0.34	-	105,105,105,105	1
3	CD	D	312	1/1	0.83	0.15	-	86,86,86,86	1
3	CD	C	308	1/1	0.95	0.11	-	76,76,76,76	1
3	CD	G	321	1/1	0.90	0.13	-	93,93,93,93	1
3	CD	B	306	1/1	0.93	0.12	-	92,92,92,92	1

## 6.5 Other polymers [i](#)

There are no such residues in this entry.