



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 12, 2024 – 05:04 PM EDT

PDB ID : 1JAD  
Title : C-terminal Domain of Turkey PLC-beta  
Authors : Singer, A.U.; Waldo, G.L.; Harden, T.K.; Sondek, J.  
Deposited on : 2001-05-30  
Resolution : 2.40 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>.

---

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

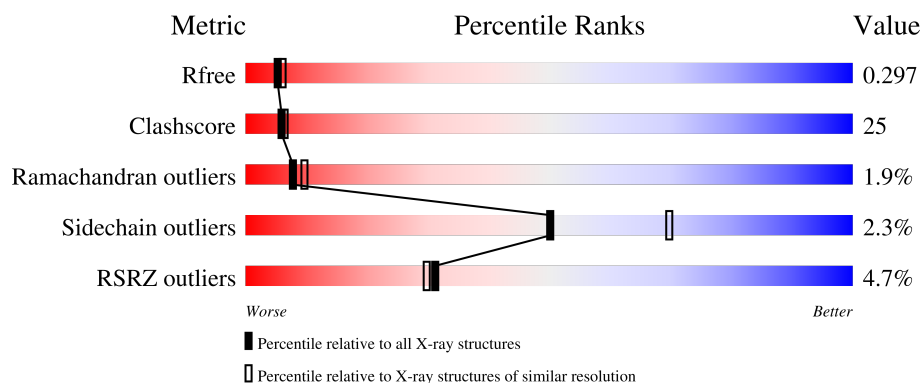
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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))
$R_{free}$	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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	A	251	<div> <div>3%</div> <div>57%</div> <div>35%</div> <div>.</div> <div>.</div> </div>
1	B	251	<div> <div>6%</div> <div>54%</div> <div>40%</div> <div>.</div> <div>.</div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4154 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 phospholipase C beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	242	Total 2003	C 1253	N 356	O 387	Se 7	0	0	0
1	B	242	Total 2003	C 1253	N 356	O 387	Se 7	0	0	0

There are 86 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	cloning artifact	UNP Q91086
A	-1	ALA	-	cloning artifact	UNP Q91086
A	0	MSE	-	cloning artifact	UNP Q91086
A	4	MSE	MET	modified residue	UNP Q91086
A	24	MSE	MET	modified residue	UNP Q91086
A	?	-	LYS	DELETION	UNP Q91086
A	?	-	LYS	DELETION	UNP Q91086
A	?	-	ARG	DELETION	UNP Q91086
A	?	-	SER	DELETION	UNP Q91086
A	?	-	MET	DELETION	UNP Q91086
A	?	-	HIS	DELETION	UNP Q91086
A	?	-	SER	DELETION	UNP Q91086
A	?	-	ARG	DELETION	UNP Q91086
A	?	-	LYS	DELETION	UNP Q91086
A	?	-	THR	DELETION	UNP Q91086
A	?	-	GLN	DELETION	UNP Q91086
A	?	-	LYS	DELETION	UNP Q91086
A	?	-	LYS	DELETION	UNP Q91086
A	?	-	ARG	DELETION	UNP Q91086
A	?	-	SER	DELETION	UNP Q91086
A	?	-	LEU	DELETION	UNP Q91086
A	?	-	THR	DELETION	UNP Q91086
A	?	-	THR	DELETION	UNP Q91086
A	?	-	GLY	DELETION	UNP Q91086
A	?	-	ASP	DELETION	UNP Q91086

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	VAL	DELETION	UNP Q91086
A	?	-	GLY	DELETION	UNP Q91086
A	?	-	THR	DELETION	UNP Q91086
A	?	-	CYS	DELETION	UNP Q91086
A	?	-	MET	DELETION	UNP Q91086
A	?	-	GLN	DELETION	UNP Q91086
A	?	-	PRO	DELETION	UNP Q91086
A	?	-	VAL	DELETION	UNP Q91086
A	?	-	GLU	DELETION	UNP Q91086
A	?	-	MET	DELETION	UNP Q91086
A	?	-	ALA	DELETION	UNP Q91086
A	?	-	GLU	DELETION	UNP Q91086
A	?	-	LYS	DELETION	UNP Q91086
A	82	MSE	MET	modified residue	UNP Q91086
A	151	MSE	MET	modified residue	UNP Q91086
A	152	MSE	MET	modified residue	UNP Q91086
A	234	MSE	MET	modified residue	UNP Q91086
A	239	MSE	MET	modified residue	UNP Q91086
B	279	GLY	-	cloning artifact	UNP Q91086
B	280	ALA	-	cloning artifact	UNP Q91086
B	281	MSE	-	cloning artifact	UNP Q91086
B	285	MSE	MET	modified residue	UNP Q91086
B	305	MSE	MET	modified residue	UNP Q91086
B	?	-	LYS	DELETION	UNP Q91086
B	?	-	LYS	DELETION	UNP Q91086
B	?	-	ARG	DELETION	UNP Q91086
B	?	-	SER	DELETION	UNP Q91086
B	?	-	MET	DELETION	UNP Q91086
B	?	-	HIS	DELETION	UNP Q91086
B	?	-	SER	DELETION	UNP Q91086
B	?	-	ARG	DELETION	UNP Q91086
B	?	-	LYS	DELETION	UNP Q91086
B	?	-	THR	DELETION	UNP Q91086
B	?	-	GLN	DELETION	UNP Q91086
B	?	-	LYS	DELETION	UNP Q91086
B	?	-	LYS	DELETION	UNP Q91086
B	?	-	ARG	DELETION	UNP Q91086
B	?	-	SER	DELETION	UNP Q91086
B	?	-	LEU	DELETION	UNP Q91086
B	?	-	THR	DELETION	UNP Q91086
B	?	-	THR	DELETION	UNP Q91086
B	?	-	GLY	DELETION	UNP Q91086

*Continued on next page...*

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	ASP	DELETION	UNP Q91086
B	?	-	VAL	DELETION	UNP Q91086
B	?	-	GLY	DELETION	UNP Q91086
B	?	-	THR	DELETION	UNP Q91086
B	?	-	CYS	DELETION	UNP Q91086
B	?	-	MET	DELETION	UNP Q91086
B	?	-	GLN	DELETION	UNP Q91086
B	?	-	PRO	DELETION	UNP Q91086
B	?	-	VAL	DELETION	UNP Q91086
B	?	-	GLU	DELETION	UNP Q91086
B	?	-	MET	DELETION	UNP Q91086
B	?	-	ALA	DELETION	UNP Q91086
B	?	-	GLU	DELETION	UNP Q91086
B	?	-	LYS	DELETION	UNP Q91086
B	363	MSE	MET	modified residue	UNP Q91086
B	432	MSE	MET	modified residue	UNP Q91086
B	433	MSE	MET	modified residue	UNP Q91086
B	515	MSE	MET	modified residue	UNP Q91086
B	520	MSE	MET	modified residue	UNP Q91086

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



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

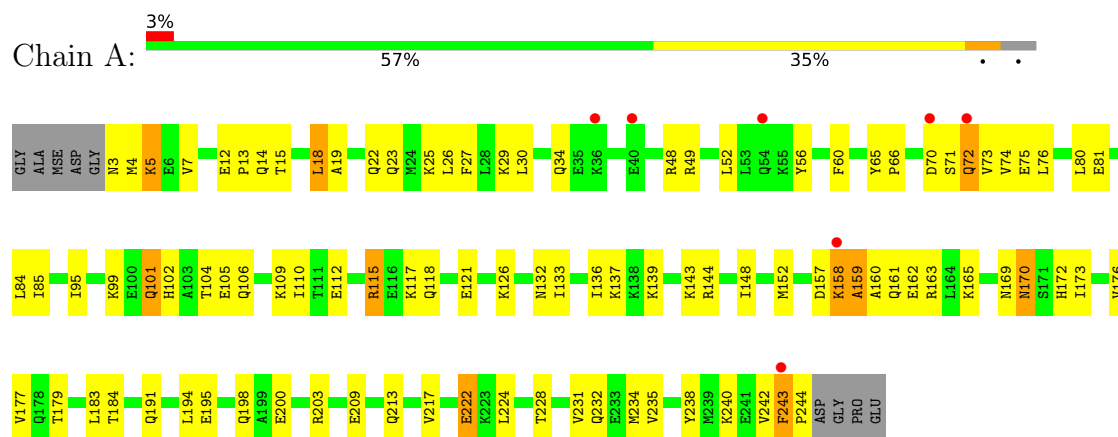
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	70	Total 70	O 70	0	0
3	B	73	Total 73	O 73	0	0

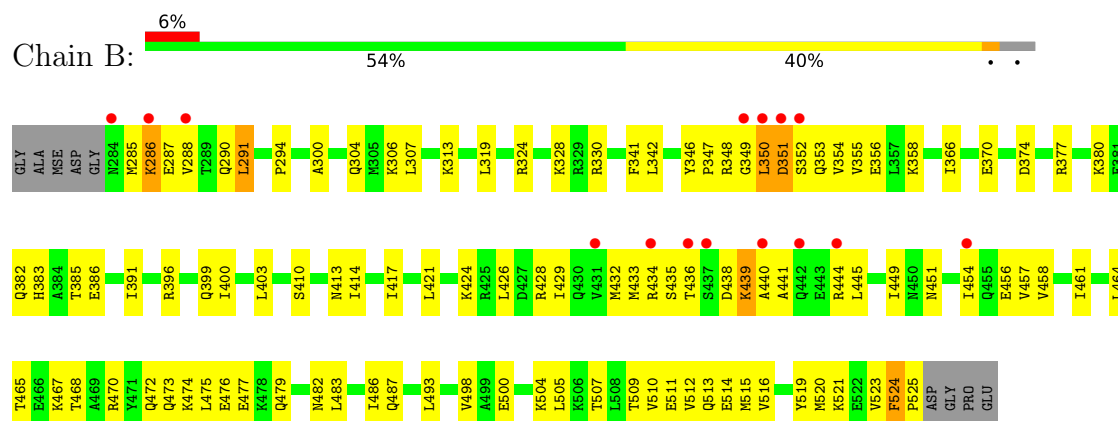
### 3 Residue-property plots

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: phospholipase C beta



- Molecule 1: phospholipase C beta



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	39.11Å 51.93Å 79.35Å 101.07° 96.96° 100.70°	Depositor
Resolution (Å)	30.00 – 2.40 28.07 – 2.10	Depositor EDS
% Data completeness (in resolution range)	90.3 (30.00-2.40) 80.7 (28.07-2.10)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	6.04 (at 2.10Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.254 , 0.295 0.257 , 0.297	Depositor DCC
$R_{free}$ test set	1063 reflections (3.82%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	20.0	Xtriage
Anisotropy	0.472	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 52.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	4154	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 16.26% 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: SO4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.43	0/2013	0.59	0/2672
1	B	0.47	0/2013	0.64	1/2672 (0.0%)
All	All	0.45	0/4026	0.61	1/5344 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	350	LEU	CA-CB-CG	5.09	127.01	115.30

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	2003	0	2098	109	0
1	B	2003	0	2098	105	0
2	A	5	0	0	0	0
3	A	70	0	0	4	0
3	B	73	0	0	6	0
All	All	4154	0	4196	205	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 25.

All (205) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:7:VAL:HB	1:A:136:ILE:HD11	1.26	1.13
1:A:184:THR:HG21	1:B:498:VAL:HG21	1.38	1.04
1:A:243:PHE:HB2	1:A:244:PRO:HD3	1.50	0.92
1:B:352:SER:O	1:B:355:VAL:HG12	1.71	0.91
1:B:413:ASN:O	1:B:417:ILE:HG12	1.71	0.90
1:B:350:LEU:O	1:B:350:LEU:HD23	1.73	0.87
1:A:115:ARG:HG3	3:B:5064:HOH:O	1.76	0.85
1:A:7:VAL:HB	1:A:136:ILE:CD1	2.06	0.84
1:A:5:LYS:H	1:A:5:LYS:HD3	1.41	0.83
1:B:509:THR:O	1:B:513:GLN:HG2	1.80	0.81
1:B:353:GLN:HA	1:B:356:GLU:HG2	1.63	0.78
1:A:4:MSE:HE2	1:A:4:MSE:HA	1.66	0.76
1:B:353:GLN:HA	1:B:356:GLU:CG	2.14	0.76
1:B:441:ALA:O	1:B:444:ARG:HG2	1.88	0.74
1:B:358:LYS:HG3	1:B:520:MSE:HE3	1.70	0.73
1:B:285:MSE:HE3	1:B:285:MSE:HA	1.69	0.73
1:B:417:ILE:O	1:B:421:LEU:HG	1.88	0.73
1:A:109:LYS:O	1:A:112:GLU:HB3	1.89	0.72
1:B:396:ARG:O	1:B:400:ILE:HG12	1.89	0.71
1:A:52:LEU:HD23	1:A:84:LEU:HD23	1.71	0.70
1:A:160:ALA:HA	1:A:163:ARG:HH21	1.58	0.69
1:A:160:ALA:CA	1:A:163:ARG:HH21	2.04	0.69
1:B:288:VAL:HG13	1:B:417:ILE:HD12	1.73	0.69
1:B:421:LEU:HD22	1:B:456:GLU:OE2	1.93	0.68
1:A:5:LYS:H	1:A:5:LYS:CD	2.08	0.67
1:B:403:LEU:HD23	1:B:475:LEU:HD23	1.76	0.67
1:B:348:ARG:O	1:B:351:ASP:HB2	1.94	0.67
1:A:18:LEU:HD22	1:A:22:GLN:OE1	1.95	0.67
1:A:5:LYS:HD3	1:A:5:LYS:N	2.09	0.66
1:B:439:LYS:O	1:B:439:LYS:HD3	1.96	0.66
1:A:158:LYS:O	1:A:162:GLU:HG2	1.95	0.66
1:B:288:VAL:HG13	1:B:417:ILE:CD1	2.26	0.66
1:A:160:ALA:HA	1:A:163:ARG:NH2	2.12	0.65
1:A:71:SER:OG	1:A:73:VAL:HG12	1.96	0.64
1:B:470:ARG:O	1:B:474:LYS:HG3	1.97	0.64
1:A:177:VAL:HG22	1:B:505:LEU:HD12	1.79	0.64
1:B:475:LEU:O	1:B:479:GLN:HG3	1.98	0.63
1:B:524:PHE:HB2	1:B:525:PRO:CD	2.28	0.63

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:26:LEU:H	1:A:26:LEU:HD12	1.64	0.62
1:B:521:LYS:O	1:B:525:PRO:HG2	1.98	0.62
1:B:432:MSE:O	1:B:436:THR:HG22	2.00	0.62
1:A:60:PHE:HE2	1:A:76:LEU:HB2	1.64	0.61
1:A:194:LEU:HD21	1:A:198:GLN:OE1	2.01	0.60
1:A:194:LEU:C	1:A:194:LEU:HD23	2.23	0.60
1:A:101:GLN:O	1:A:105:GLU:HG3	2.02	0.59
1:A:191:GLN:O	1:A:195:GLU:HG3	2.02	0.59
1:A:224:LEU:O	1:B:454:ILE:HD11	2.02	0.59
1:A:132:ASN:O	1:A:136:ILE:HG12	2.03	0.59
1:B:291:LEU:HD13	1:B:468:THR:HA	1.85	0.59
1:B:313:LYS:HE3	3:B:5319:HOH:O	2.03	0.59
1:A:117:LYS:O	1:A:121:GLU:HG3	2.02	0.58
1:A:203:ARG:HH11	1:A:203:ARG:HB2	1.68	0.58
1:B:352:SER:C	1:B:354:VAL:H	2.06	0.58
1:B:429:ILE:HD13	1:B:449:ILE:HD12	1.86	0.58
1:B:464:LEU:C	1:B:464:LEU:HD23	2.24	0.58
1:B:306:LYS:NZ	1:B:306:LYS:HB2	2.19	0.58
1:A:72:GLN:HA	1:A:75:GLU:HG3	1.85	0.57
1:A:170:ASN:HD22	1:A:170:ASN:C	2.05	0.57
1:B:473:GLN:O	1:B:477:GLU:HG3	2.04	0.57
1:A:173:ILE:O	1:A:176:VAL:HG22	2.05	0.57
1:A:231:VAL:O	1:A:235:VAL:HG23	2.05	0.56
1:B:421:LEU:HD13	1:B:457:VAL:HG12	1.86	0.56
1:B:464:LEU:HD23	1:B:464:LEU:O	2.05	0.56
1:B:300:ALA:O	1:B:304:GLN:HG2	2.06	0.56
1:A:217:VAL:HG21	1:B:465:THR:HG21	1.86	0.55
1:B:524:PHE:HB2	1:B:525:PRO:HD2	1.89	0.55
1:B:438:ASP:O	1:B:440:ALA:N	2.39	0.55
1:B:472:GLN:O	1:B:476:GLU:HG3	2.06	0.55
1:A:228:THR:O	1:A:232:GLN:HG3	2.07	0.55
1:B:291:LEU:HD12	1:B:467:LYS:HG2	1.89	0.55
1:A:224:LEU:HD23	1:B:458:VAL:CG2	2.36	0.55
1:B:374:ASP:O	1:B:377:ARG:HB3	2.07	0.54
1:B:516:VAL:O	1:B:520:MSE:HG2	2.06	0.54
1:A:148:ILE:HD12	1:A:165:LYS:HG2	1.88	0.54
1:A:170:ASN:C	1:A:170:ASN:ND2	2.61	0.54
1:A:26:LEU:O	1:A:29:LYS:HG2	2.07	0.54
1:A:118:GLN:HA	1:A:121:GLU:OE1	2.07	0.54
1:B:307:LEU:HD12	1:B:307:LEU:N	2.22	0.54
1:A:144:ARG:NH1	1:A:169:ASN:OD1	2.41	0.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:285:MSE:CG	1:B:288:VAL:HG23	2.38	0.53
1:A:115:ARG:HG2	1:A:115:ARG:HH11	1.72	0.53
1:A:126:LYS:NZ	1:B:385:THR:OG1	2.38	0.53
1:B:290:GLN:CD	1:B:291:LEU:N	2.63	0.53
1:B:358:LYS:CG	1:B:520:MSE:HE3	2.39	0.52
1:B:358:LYS:HG3	1:B:520:MSE:CE	2.39	0.52
1:A:26:LEU:H	1:A:26:LEU:CD1	2.22	0.52
1:A:133:ILE:O	1:A:137:LYS:HG3	2.09	0.52
1:B:353:GLN:HA	1:B:356:GLU:HG3	1.90	0.52
1:B:355:VAL:O	1:B:358:LYS:HB3	2.09	0.52
1:B:433:MSE:C	1:B:435:SER:H	2.14	0.52
1:A:85:ILE:HD11	1:A:231:VAL:HG21	1.91	0.51
1:B:286:LYS:HD3	1:B:287:GLU:N	2.25	0.51
1:B:426:LEU:H	1:B:426:LEU:HD22	1.75	0.51
1:A:26:LEU:HD12	1:A:26:LEU:N	2.25	0.51
1:B:349:GLY:O	1:B:350:LEU:HB3	2.11	0.51
1:A:18:LEU:O	1:A:22:GLN:HG3	2.09	0.51
1:A:49:ARG:HD2	1:A:234:MSE:HE2	1.93	0.51
1:A:224:LEU:HD23	1:B:458:VAL:HG23	1.92	0.50
1:B:483:LEU:O	1:B:487:GLN:HG3	2.11	0.50
1:B:421:LEU:CD1	1:B:457:VAL:HG12	2.42	0.50
1:A:102:HIS:O	1:A:106:GLN:HG3	2.12	0.50
1:A:139:LYS:O	1:A:143:LYS:HG2	2.11	0.50
1:B:307:LEU:HD12	1:B:307:LEU:H	1.77	0.50
1:A:152:MSE:HE1	1:A:161:GLN:NE2	2.26	0.49
1:A:179:THR:O	1:A:183:LEU:HD13	2.10	0.49
1:A:85:ILE:CD1	1:A:231:VAL:HG21	2.42	0.49
1:A:81:GLU:O	1:A:85:ILE:HG12	2.12	0.49
1:B:399:GLN:HG2	1:B:479:GLN:CD	2.33	0.49
1:B:285:MSE:HG2	1:B:288:VAL:HG23	1.94	0.49
1:A:27:PHE:CE1	1:A:110:ILE:HG13	2.48	0.49
3:A:5043:HOH:O	1:B:370:GLU:HB3	2.12	0.49
1:A:144:ARG:HD3	1:A:172:HIS:CG	2.47	0.49
1:A:231:VAL:HG23	1:A:232:GLN:N	2.28	0.48
1:A:3:ASN:N	1:A:5:LYS:HZ3	2.12	0.48
1:A:14:GLN:O	1:A:14:GLN:HG3	2.13	0.48
1:A:235:VAL:O	1:A:238:TYR:HB3	2.12	0.48
1:B:413:ASN:C	1:B:417:ILE:HG12	2.32	0.48
1:B:285:MSE:HG3	1:B:287:GLU:HG2	1.97	0.47
1:B:519:TYR:O	1:B:523:VAL:HG23	2.14	0.47
1:B:342:LEU:HA	3:B:5389:HOH:O	2.14	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:510:VAL:O	1:B:514:GLU:HG3	2.14	0.47
1:B:330:ARG:HD2	1:B:515:MSE:HE2	1.97	0.47
1:B:366:ILE:O	1:B:370:GLU:HG3	2.14	0.47
1:B:424:LYS:O	1:B:428:ARG:HG3	2.15	0.47
1:B:500:GLU:O	1:B:504:LYS:HG2	2.14	0.47
1:A:27:PHE:CD1	1:A:110:ILE:HG13	2.50	0.47
1:A:56:TYR:CG	1:A:80:LEU:HD13	2.50	0.46
1:A:72:GLN:N	1:A:72:GLN:NE2	2.63	0.46
1:A:200:GLU:HA	1:A:203:ARG:NH1	2.30	0.46
1:A:72:GLN:HA	1:A:75:GLU:CG	2.44	0.46
1:A:179:THR:HG21	3:A:5052:HOH:O	2.16	0.46
1:B:403:LEU:CD2	1:B:475:LEU:HD23	2.45	0.46
1:A:34:GLN:NE2	1:A:105:GLU:HB2	2.31	0.46
1:B:288:VAL:HG13	1:B:417:ILE:CG1	2.45	0.46
1:A:243:PHE:HB2	1:A:244:PRO:CD	2.34	0.46
1:A:73:VAL:HG13	1:A:74:VAL:N	2.31	0.45
1:A:137:LYS:HE2	3:B:5161:HOH:O	2.16	0.45
1:B:346:TYR:HA	1:B:347:PRO:HD3	1.73	0.45
1:A:25:LYS:NZ	1:A:25:LYS:HB3	2.31	0.45
1:A:48:ARG:O	1:A:48:ARG:HD2	2.16	0.45
1:A:72:GLN:CD	1:A:72:GLN:H	2.20	0.45
1:B:351:ASP:C	1:B:353:GLN:H	2.19	0.45
1:A:84:LEU:HD13	1:A:234:MSE:CE	2.46	0.45
1:A:152:MSE:HE1	1:A:161:GLN:HE22	1.82	0.45
1:A:177:VAL:CG2	1:B:505:LEU:HD12	2.44	0.45
1:B:505:LEU:HD23	1:B:505:LEU:HA	1.79	0.45
1:A:158:LYS:NZ	1:B:350:LEU:HD12	2.32	0.44
1:B:324:ARG:O	1:B:328:LYS:HG2	2.17	0.44
1:B:457:VAL:HG23	1:B:458:VAL:N	2.33	0.44
1:A:18:LEU:HD22	1:A:22:GLN:CD	2.38	0.44
1:A:95:ILE:O	1:A:99:LYS:HG2	2.18	0.43
1:B:341:PHE:CZ	1:B:520:MSE:HE1	2.53	0.43
1:A:12:GLU:H	1:A:12:GLU:CD	2.21	0.43
1:A:12:GLU:HA	1:A:13:PRO:HD3	1.85	0.43
1:B:433:MSE:C	1:B:435:SER:N	2.72	0.43
1:A:84:LEU:HD13	1:A:234:MSE:HE1	2.00	0.43
1:A:194:LEU:HD23	1:A:194:LEU:O	2.18	0.43
1:B:382:GLN:O	1:B:386:GLU:HG3	2.19	0.43
1:B:383:HIS:HD2	3:B:5341:HOH:O	2.01	0.43
1:B:433:MSE:O	1:B:435:SER:N	2.51	0.43
1:A:19:ALA:O	1:A:23:GLN:HG2	2.19	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:52:LEU:HD23	1:A:84:LEU:CD2	2.45	0.43
1:A:70:ASP:O	1:A:72:GLN:NE2	2.51	0.43
1:A:209:GLU:O	1:A:213:GLN:HG3	2.18	0.43
1:B:482:ASN:O	1:B:486:ILE:HG13	2.18	0.43
1:B:512:VAL:O	1:B:516:VAL:HG23	2.18	0.43
1:B:396:ARG:HH11	1:B:396:ARG:HG2	1.83	0.42
1:B:507:THR:O	1:B:511:GLU:HG3	2.18	0.42
1:B:307:LEU:H	1:B:307:LEU:CD1	2.32	0.42
1:A:15:THR:HA	1:A:121:GLU:OE2	2.18	0.42
1:A:158:LYS:O	1:A:160:ALA:N	2.52	0.42
1:B:306:LYS:HB2	1:B:306:LYS:HZ3	1.83	0.42
1:B:458:VAL:O	1:B:461:ILE:HG22	2.18	0.42
1:B:473:GLN:HG2	1:B:477:GLU:OE2	2.19	0.42
1:A:222:GLU:OE1	1:A:222:GLU:C	2.57	0.42
1:A:143:LYS:HD2	3:A:5090:HOH:O	2.19	0.42
1:A:170:ASN:ND2	1:A:170:ASN:O	2.48	0.42
1:B:386:GLU:HA	3:B:5188:HOH:O	2.20	0.42
1:B:441:ALA:O	1:B:445:LEU:HG	2.20	0.42
1:B:513:GLN:HA	1:B:513:GLN:HE21	1.84	0.42
1:B:319:LEU:HD13	1:B:380:LYS:HE2	2.00	0.42
1:A:29:LYS:HG3	1:A:30:LEU:N	2.34	0.42
1:B:449:ILE:C	1:B:451:ASN:H	2.23	0.42
1:A:30:LEU:O	1:A:34:GLN:HG3	2.20	0.41
1:A:176:VAL:HG23	1:A:177:VAL:N	2.36	0.41
1:B:288:VAL:HG13	1:B:417:ILE:HG13	2.01	0.41
1:A:160:ALA:N	1:A:163:ARG:HH21	2.18	0.41
1:B:350:LEU:O	1:B:352:SER:N	2.54	0.41
1:B:429:ILE:HD13	1:B:449:ILE:CD1	2.50	0.41
1:A:104:THR:HG23	3:A:5244:HOH:O	2.20	0.41
1:A:158:LYS:O	1:A:159:ALA:C	2.57	0.41
1:A:71:SER:O	1:A:75:GLU:HG2	2.21	0.41
1:A:102:HIS:HA	1:A:105:GLU:OE1	2.21	0.41
1:B:350:LEU:C	1:B:352:SER:H	2.24	0.41
1:B:410:SER:O	1:B:414:ILE:HG13	2.20	0.41
1:B:444:ARG:HE	1:B:445:LEU:HD21	1.85	0.41
1:A:18:LEU:HD22	1:A:22:GLN:HG3	2.03	0.41
1:A:109:LYS:HD2	1:A:109:LYS:HA	1.89	0.41
1:A:157:ASP:O	1:A:160:ALA:HB3	2.20	0.41
1:A:172:HIS:O	1:A:176:VAL:HG13	2.21	0.41
1:A:240:LYS:HA	1:A:244:PRO:HD2	2.02	0.41
1:A:238:TYR:O	1:A:242:VAL:HG23	2.21	0.40

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:65:TYR:HA	1:A:66:PRO:HD2	1.86	0.40
1:A:194:LEU:CD2	1:A:198:GLN:OE1	2.68	0.40
1:B:350:LEU:O	1:B:350:LEU:CD2	2.55	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	A	240/251 (96%)	230 (96%)	7 (3%)	3 (1%)	12	17
1	B	240/251 (96%)	216 (90%)	18 (8%)	6 (2%)	5	6
All	All	480/502 (96%)	446 (93%)	25 (5%)	9 (2%)	8	10

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	439	LYS
1	B	524	PHE
1	A	158	LYS
1	B	351	ASP
1	B	434	ARG
1	A	159	ALA
1	B	291	LEU
1	A	243	PHE
1	B	294	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	222/219 (101%)	215 (97%)	7 (3%)	39	59
1	B	222/219 (101%)	219 (99%)	3 (1%)	67	82
All	All	444/438 (101%)	434 (98%)	10 (2%)	50	70

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	LYS
1	A	18	LEU
1	A	72	GLN
1	A	101	GLN
1	A	115	ARG
1	A	170	ASN
1	A	222	GLU
1	B	286	LYS
1	B	391	ILE
1	B	493	LEU

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

Mol	Chain	Res	Type
1	A	3	ASN
1	A	72	GLN
1	A	106	GLN
1	A	118	GLN
1	A	161	GLN
1	A	170	ASN
1	A	172	HIS
1	A	174	GLN
1	A	191	GLN
1	A	198	GLN
1	A	211	GLN
1	B	315	GLN
1	B	383	HIS
1	B	387	GLN
1	B	413	ASN
1	B	455	GLN
1	B	479	GLN

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	B	494	GLN
1	B	495	GLN
1	B	513	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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

1 ligand is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	SO4	A	4001	-	4,4,4	0.32	0	6,6,6	0.12	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

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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	235/251 (93%)	0.05	7 (2%) 50 49	12, 41, 69, 92	0
1	B	235/251 (93%)	-0.02	15 (6%) 19 18	7, 38, 83, 98	0
All	All	470/502 (93%)	0.01	22 (4%) 31 30	7, 39, 79, 98	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	288	VAL	7.8
1	B	284	ASN	5.9
1	A	72	GLN	4.4
1	B	350	LEU	3.6
1	A	243	PHE	3.3
1	B	349	GLY	3.2
1	B	440	ALA	3.2
1	B	442	GLN	3.0
1	A	54	GLN	2.9
1	B	286	LYS	2.9
1	A	40	GLU	2.7
1	A	70	ASP	2.6
1	A	36	LYS	2.5
1	B	352	SER	2.4
1	B	454	ILE	2.4
1	B	434	ARG	2.4
1	B	437	SER	2.3
1	B	351	ASP	2.3
1	B	436	THR	2.2
1	A	158	LYS	2.1
1	B	444	ARG	2.1
1	B	431	VAL	2.1

## 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 monosaccharides 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( $\text{\AA}^2$ )	Q<0.9
2	SO4	A	4001	5/5	0.96	0.13	51,52,52,52	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.