



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 08:19 am GMT

PDB ID : 2PVS  
Title : Structure of human pancreatic lipase related protein 2 mutant N336Q  
Authors : Spinelli, S.; Eydoux, C.; Carriere, F.; Cambillau, C.  
Deposited on : 2007-05-10  
Resolution : 3.00 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 : trunk28620  
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) : recalc28949

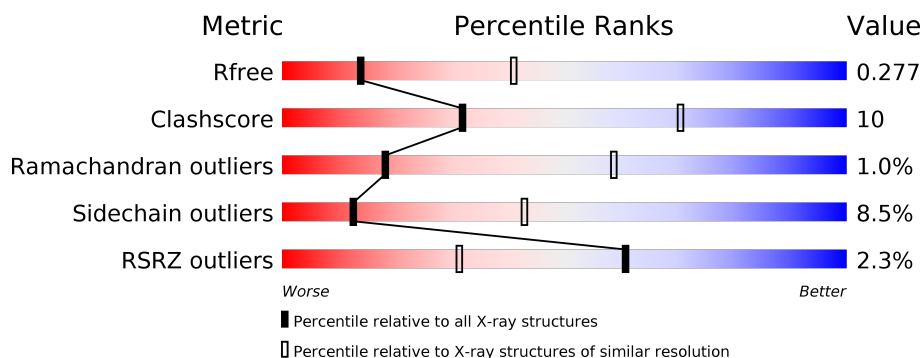
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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	1692 (3.00-3.00)
Clashscore	112137	2037 (3.00-3.00)
Ramachandran outliers	110173	1973 (3.00-3.00)
Sidechain outliers	110143	1976 (3.00-3.00)
RSRZ outliers	101464	1716 (3.00-3.00)

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	452	<div> <div>2%</div> <div> <div></div> <div>70%</div> <div>23%</div> <div>• •</div> </div> </div>
1	B	452	<div> <div>2%</div> <div> <div></div> <div>77%</div> <div>19%</div> <div>• •</div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	B	452	-	-	X	-

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 6977 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 Pancreatic lipase-related protein 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	435	Total	C	N	O	S	0	0	0
			3393	2144	570	658	21			
1	B	445	Total	C	N	O	S	0	1	0
			3475	2197	586	671	21			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	334	GLN	ASN	ENGINEERED	UNP P54317
B	334	GLN	ASN	ENGINEERED	UNP P54317

- 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			

*Continued on next page...*

*Continued from previous page...*

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

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Ca	0	0
			1	1		
3	A	1	Total	Ca	0	0
			1	1		

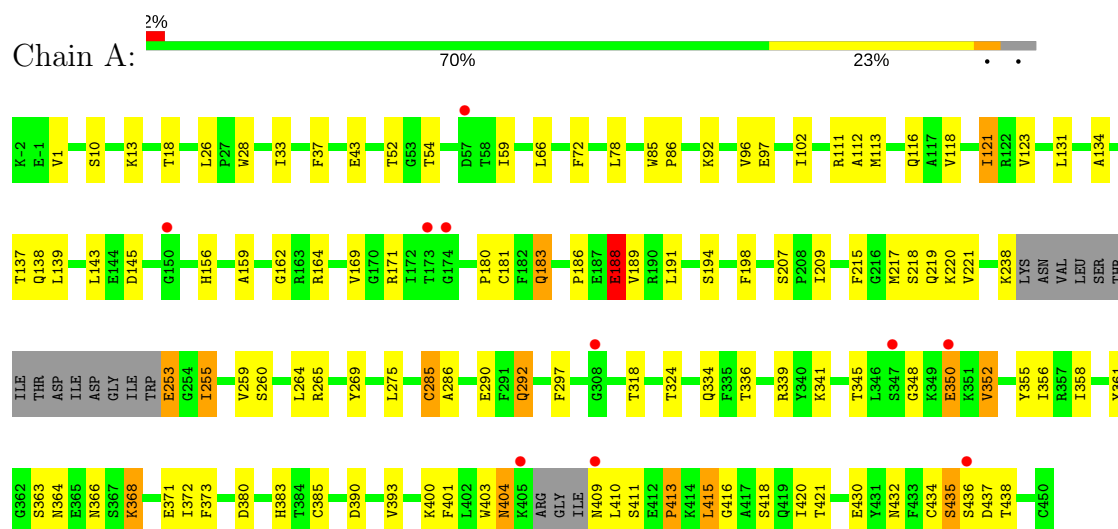
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	30	Total	O	0	0
			30	30		
4	B	37	Total	O	0	0
			37	37		

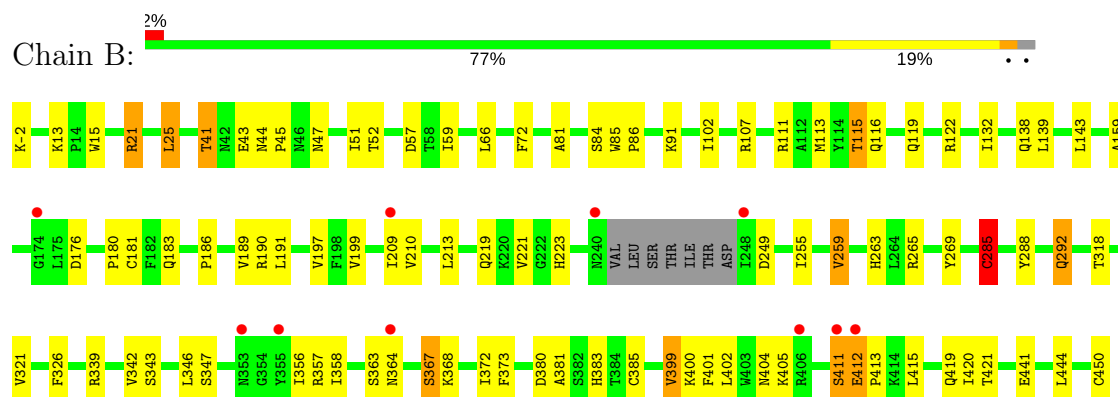
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: Pancreatic lipase-related protein 2



#### • Molecule 1: Pancreatic lipase-related protein 2



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 41 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	216.18Å 216.18Å 123.67Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.18 – 3.00 34.18 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.2 (34.18-3.00) 99.3 (34.18-2.70)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	0.12	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.98 (at 2.68Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.190 , 0.249 0.223 , 0.277	Depositor DCC
$R_{free}$ test set	1476 reflections (5.05%)	DCC
Wilson B-factor (Å <sup>2</sup> )	62.7	Xtriage
Anisotropy	0.432	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 48.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	6977	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.03% 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: CA, 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	0.60	1/3476 (0.0%)	0.67	0/4703
1	B	0.97	2/3572 (0.1%)	0.84	2/4833 (0.0%)
All	All	0.81	3/7048 (0.0%)	0.76	2/9536 (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	A	0	2
1	B	0	1
All	All	0	3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	111[A]	ARG	CG-CD	-32.26	0.71	1.51
1	B	111[B]	ARG	CG-CD	-32.26	0.71	1.51
1	A	188	GLU	CG-CD	6.21	1.61	1.51

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	111[A]	ARG	CG-CD-NE	22.84	159.77	111.80
1	B	111[B]	ARG	CG-CD-NE	22.84	159.77	111.80

There are no chirality outliers.

All (3) planarity outliers are listed below:



Mol	Chain	Res	Type	Group
1	A	409	ASN	Peptide
1	A	410	LEU	Peptide
1	B	412	GLU	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	A	3393	0	3237	72	0
1	B	3475	0	3319	65	0
2	A	25	0	0	0	0
2	B	15	0	0	2	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	30	0	0	3	0
4	B	37	0	0	2	0
All	All	6977	0	6556	134	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 (134) 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:B:25:LEU:HD21	1:B:115:THR:HG22	1.40	1.02
1:A:255:ILE:HG22	1:A:255:ILE:O	1.67	0.93
1:B:25:LEU:HD21	1:B:115:THR:CG2	2.07	0.83
1:B:209:ILE:HG22	1:B:210:VAL:HG23	1.63	0.79
1:B:25:LEU:CD2	1:B:115:THR:HG22	2.14	0.77
1:A:255:ILE:CG2	1:A:255:ILE:O	2.35	0.75
1:A:350:GLU:OE2	1:A:352:VAL:HG12	1.88	0.74
1:B:25:LEU:CD2	1:B:115:THR:CG2	2.66	0.73
1:B:199:VAL:H	1:B:223:HIS:HD2	1.38	0.69
1:A:66:LEU:CD2	1:A:139:LEU:HD22	2.23	0.68
1:B:358:ILE:HD11	1:B:420:ILE:HD13	1.74	0.68
1:B:41:THR:HG22	1:B:43:GLU:H	1.60	0.67
1:A:358:ILE:HD12	1:A:372:ILE:CD1	2.26	0.66

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:367:SER:OG	1:B:368:LYS:O	2.13	0.66
1:B:180:PRO:O	1:B:181:CYS:HB2	1.96	0.65
1:B:221:VAL:O	1:B:221:VAL:CG1	2.43	0.65
1:B:285:CYS:HB3	1:B:326:PHE:HD1	1.61	0.65
1:B:221:VAL:O	1:B:221:VAL:HG12	1.98	0.64
1:A:118:VAL:O	1:A:121:ILE:HG22	1.97	0.63
1:A:411:SER:O	1:A:413:PRO:HD3	2.00	0.62
1:A:96:VAL:HG23	1:A:97:GLU:HG2	1.81	0.62
1:A:1:VAL:HG13	1:A:26:LEU:HD13	1.82	0.62
1:B:346:LEU:HD12	1:B:381:ALA:HB3	1.81	0.62
1:A:348:GLY:HA2	1:A:438:THR:HG21	1.81	0.61
1:B:356:ILE:HD12	1:B:401:PHE:CZ	2.35	0.61
1:A:356:ILE:HD12	1:A:401:PHE:CE1	2.35	0.60
1:B:199:VAL:H	1:B:223:HIS:CD2	2.19	0.59
1:B:15:TRP:CE3	1:B:122:ARG:HD3	2.37	0.59
1:A:66:LEU:HD21	1:A:139:LEU:HD22	1.84	0.59
1:A:434:CYS:O	1:A:435:SER:HB2	2.03	0.58
1:B:358:ILE:CD1	1:B:420:ILE:HD13	2.34	0.57
1:B:41:THR:HG22	1:B:43:GLU:N	2.20	0.57
1:B:405:LYS:NZ	1:B:411:SER:HA	2.21	0.56
1:A:180:PRO:O	1:A:181:CYS:HB2	2.05	0.55
1:A:118:VAL:O	1:A:121:ILE:CG2	2.55	0.55
1:B:399:VAL:HG11	1:B:420:ILE:HG21	1.88	0.55
1:A:159:ALA:HB2	1:A:191:LEU:HD13	1.88	0.55
1:A:121:ILE:HD11	1:A:156:HIS:HB2	1.87	0.55
1:A:66:LEU:HD22	1:A:139:LEU:HD22	1.88	0.54
1:B:265:ARG:HG2	1:B:269:TYR:CZ	2.42	0.54
1:B:132:ILE:CG2	1:B:143:LEU:HD22	2.38	0.53
1:A:434:CYS:O	1:A:435:SER:CB	2.57	0.53
1:A:72:PHE:HA	1:A:102:ILE:O	2.09	0.53
1:A:215:PHE:HE1	1:B:255:ILE:HD13	1.73	0.52
1:A:358:ILE:HD12	1:A:372:ILE:HD11	1.90	0.52
1:A:436:SER:C	1:A:437:ASP:CG	2.68	0.52
1:B:356:ILE:HG22	1:B:372:ILE:HB	1.92	0.52
1:B:356:ILE:HD12	1:B:401:PHE:CE1	2.45	0.52
1:A:259:VAL:HG22	1:A:259:VAL:O	2.10	0.52
1:A:421:THR:HG23	1:A:432:ASN:OD1	2.09	0.52
1:A:436:SER:O	1:A:437:ASP:OD1	2.27	0.51
1:B:132:ILE:HG22	1:B:143:LEU:HD22	1.91	0.51
1:B:66:LEU:HD21	1:B:139:LEU:HD13	1.93	0.51
1:A:188:GLU:HG2	4:A:522:HOH:O	2.12	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:358:ILE:CD1	1:A:420:ILE:HD13	2.42	0.50
1:A:92:LYS:CD	1:A:275:LEU:HD11	2.41	0.50
1:A:186:PRO:O	1:A:189:VAL:HG22	2.11	0.50
1:A:28:TRP:CH2	1:A:112:ALA:HB2	2.47	0.50
1:A:265:ARG:HG2	1:A:269:TYR:CZ	2.47	0.49
1:A:183:GLN:NE2	1:A:219:GLN:H	2.09	0.49
1:B:72:PHE:HA	1:B:102:ILE:O	2.12	0.49
1:A:92:LYS:HD3	1:A:275:LEU:HD11	1.95	0.48
1:B:66:LEU:HD21	1:B:139:LEU:CD1	2.44	0.48
1:A:400:LYS:NZ	4:A:514:HOH:O	2.47	0.47
1:B:223:HIS:HA	1:B:321:VAL:HA	1.96	0.47
1:A:215:PHE:CE1	1:B:255:ILE:HD13	2.49	0.47
1:A:217:MET:HE1	1:A:221:VAL:HG11	1.97	0.47
1:A:171:ARG:HA	1:A:198:PHE:O	2.15	0.47
1:A:78:LEU:HD23	1:A:111:ARG:HA	1.97	0.47
1:B:176:ASP:OD2	1:B:263:HIS:ND1	2.43	0.47
1:A:253:GLU:HG3	1:A:255:ILE:HG13	1.97	0.47
1:B:13:LYS:NZ	4:B:517:HOH:O	2.48	0.46
1:A:292:GLN:NE2	4:A:504:HOH:O	2.48	0.46
1:A:416:GLY:HA3	1:A:438:THR:HA	1.98	0.46
1:A:285:CYS:O	1:A:324:THR:HG22	2.15	0.46
1:A:350:GLU:OE2	1:A:352:VAL:CG1	2.62	0.45
1:B:342:VAL:HG11	1:B:358:ILE:HD13	1.98	0.45
1:A:13:LYS:HD2	1:A:18:THR:HG22	1.98	0.45
1:B:412:GLU:N	1:B:413:PRO:HD3	2.31	0.45
1:B:25:LEU:CD2	1:B:115:THR:HG23	2.46	0.45
1:A:358:ILE:HD12	1:A:372:ILE:HD12	1.99	0.45
1:B:219:GLN:HG2	1:B:221:VAL:HG23	1.99	0.45
1:B:41:THR:CG2	1:B:43:GLU:H	2.28	0.45
1:A:361:TYR:CD1	1:A:366:ASN:HB3	2.52	0.44
1:B:400:LYS:HB3	1:B:444:LEU:HD22	1.98	0.44
1:B:183:GLN:HE21	1:B:209:ILE:HD12	1.82	0.44
1:A:372:ILE:HG23	1:A:385:CYS:HB3	2.00	0.44
1:A:37:PHE:CG	1:A:131:LEU:HD22	2.53	0.43
1:A:85:TRP:CG	1:A:86:PRO:HD3	2.53	0.43
1:B:51:ILE:HB	1:B:59:ILE:HD13	1.99	0.43
1:B:45:PRO:HD2	2:B:452:SO4:O3	2.19	0.43
1:A:112:ALA:C	1:B:259:VAL:HG21	2.39	0.43
1:A:183:GLN:HE22	1:A:218:SER:N	2.16	0.43
1:A:356:ILE:HD12	1:A:401:PHE:HE1	1.80	0.43
1:A:286:ALA:HB3	1:A:290:GLU:OE1	2.18	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:180:PRO:O	1:B:181:CYS:CB	2.64	0.43
1:B:197:VAL:O	1:B:318:THR:HG21	2.19	0.43
1:A:183:GLN:HE22	1:A:219:GLN:H	1.65	0.43
1:A:220:LYS:HE3	1:A:324:THR:OG1	2.19	0.43
1:A:373:PHE:CD2	1:A:383:HIS:CE1	3.07	0.43
1:B:21:ARG:NH2	1:B:181:CYS:O	2.51	0.43
1:B:84:SER:OG	1:B:85:TRP:N	2.51	0.43
1:A:403:TRP:CD1	1:A:415:LEU:HB3	2.53	0.43
1:B:159:ALA:HB2	1:B:191:LEU:HA	1.99	0.43
1:B:47:ASN:N	2:B:452:SO4:O2	2.48	0.43
1:A:403:TRP:NE1	1:A:415:LEU:HB3	2.34	0.42
1:B:405:LYS:HZ3	1:B:411:SER:HA	1.84	0.42
1:B:15:TRP:CZ3	1:B:122:ARG:HD3	2.55	0.42
1:B:292:GLN:NE2	4:B:504:HOH:O	2.52	0.42
1:A:134:ALA:O	1:A:138:GLN:HB2	2.19	0.42
1:B:191:LEU:HD23	1:B:221:VAL:HG12	2.02	0.42
1:B:347:SER:O	1:B:415:LEU:HD12	2.19	0.42
1:B:285:CYS:HB3	1:B:326:PHE:CD1	2.48	0.42
1:A:260:SER:O	1:A:264:LEU:HG	2.20	0.41
1:A:159:ALA:HB2	1:A:191:LEU:CD1	2.49	0.41
1:A:297:PHE:CE1	1:A:341:LYS:HB2	2.56	0.41
1:A:334:GLN:HB3	1:A:336:THR:HG23	2.02	0.41
1:A:418:SER:HA	1:A:436:SER:HA	2.02	0.41
1:B:186:PRO:O	1:B:189:VAL:HG22	2.21	0.41
1:B:41:THR:HB	1:B:44:ASN:OD1	2.20	0.41
1:A:368:LYS:HE2	1:A:390:ASP:HB2	2.03	0.41
1:A:92:LYS:HD2	1:A:275:LEU:CD1	2.50	0.41
1:B:66:LEU:HD21	1:B:139:LEU:HB3	2.02	0.41
1:A:404:ASN:HD22	1:A:404:ASN:N	2.19	0.41
1:B:190:ARG:NH2	1:B:221:VAL:HG22	2.36	0.41
1:B:342:VAL:CG1	1:B:358:ILE:HD13	2.50	0.41
1:B:288:TYR:O	1:B:292:GLN:HG2	2.21	0.41
1:B:15:TRP:CD2	1:B:122:ARG:NH2	2.88	0.41
1:A:33:ILE:HD12	1:A:123:VAL:HB	2.02	0.40
1:A:162:GLY:HA2	1:A:169:VAL:HG11	2.03	0.40
1:A:356:ILE:HD12	1:A:401:PHE:CZ	2.56	0.40
1:A:43:GLU:OE1	1:A:43:GLU:N	2.54	0.40
1:B:373:PHE:CE2	1:B:383:HIS:CE1	3.10	0.40
1:B:81:ALA:HA	1:B:86:PRO:HG2	2.04	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	429/452 (95%)	394 (92%)	29 (7%)	6 (1%)	13	49
1	B	442/452 (98%)	409 (92%)	30 (7%)	3 (1%)	25	67
All	All	871/904 (96%)	803 (92%)	59 (7%)	9 (1%)	18	59

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	145	ASP
1	A	364	ASN
1	A	435	SER
1	B	249	ASP
1	B	411	SER
1	A	380	ASP
1	B	285	CYS
1	A	255	ILE
1	A	413	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	373/388 (96%)	341 (91%)	32 (9%)	12	42
1	B	382/388 (98%)	350 (92%)	32 (8%)	13	43
All	All	755/776 (97%)	691 (92%)	64 (8%)	12	43

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	SER
1	A	52	THR
1	A	54	THR
1	A	59	ILE
1	A	113	MET
1	A	116	GLN
1	A	121	ILE
1	A	137	THR
1	A	143	LEU
1	A	164	ARG
1	A	183	GLN
1	A	188	GLU
1	A	194	SER
1	A	207	SER
1	A	209	ILE
1	A	238	LYS
1	A	253	GLU
1	A	285	CYS
1	A	292	GLN
1	A	318	THR
1	A	339	ARG
1	A	345	THR
1	A	350	GLU
1	A	352	VAL
1	A	355	TYR
1	A	363	SER
1	A	368	LYS
1	A	371	GLU
1	A	393	VAL
1	A	404	ASN
1	A	415	LEU
1	A	430	GLU
1	B	-2	LYS
1	B	21	ARG
1	B	25	LEU
1	B	41	THR
1	B	52	THR
1	B	57	ASP
1	B	91	LYS
1	B	107	ARG
1	B	113	MET
1	B	115	THR

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	116	GLN
1	B	119	GLN
1	B	138	GLN
1	B	213	LEU
1	B	259	VAL
1	B	285	CYS
1	B	292	GLN
1	B	339	ARG
1	B	343	SER
1	B	357	ARG
1	B	363	SER
1	B	364	ASN
1	B	367	SER
1	B	380	ASP
1	B	385	CYS
1	B	399	VAL
1	B	402	LEU
1	B	404	ASN
1	B	419	GLN
1	B	421	THR
1	B	441	GLU
1	B	450	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	GLN
1	A	65	GLN
1	A	183	GLN
1	A	292	GLN
1	A	383	HIS
1	A	423	GLN
1	B	116	GLN
1	B	119	GLN
1	B	223	HIS
1	B	292	GLN
1	B	366	ASN
1	B	404	ASN
1	B	419	GLN
1	B	442	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 10 ligands modelled in this entry, 2 are monoatomic - leaving 8 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	$\# Z  > 2$
2	SO4	A	451	-	4,4,4	0.12	0	6,6,6	0.62	0
2	SO4	A	452	-	4,4,4	0.16	0	6,6,6	0.38	0
2	SO4	A	453	-	4,4,4	0.27	0	6,6,6	0.36	0
2	SO4	A	454	-	4,4,4	0.14	0	6,6,6	0.24	0
2	SO4	A	455	-	4,4,4	0.20	0	6,6,6	0.28	0
2	SO4	B	451	-	4,4,4	0.14	0	6,6,6	0.21	0
2	SO4	B	452	-	4,4,4	0.16	0	6,6,6	0.45	0
2	SO4	B	453	-	4,4,4	0.22	0	6,6,6	0.27	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SO4	A	451	-	-	0/0/0/0	0/0/0/0
2	SO4	A	452	-	-	0/0/0/0	0/0/0/0

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SO4	A	453	-	-	0/0/0/0	0/0/0/0
2	SO4	A	454	-	-	0/0/0/0	0/0/0/0
2	SO4	A	455	-	-	0/0/0/0	0/0/0/0
2	SO4	B	451	-	-	0/0/0/0	0/0/0/0
2	SO4	B	452	-	-	0/0/0/0	0/0/0/0
2	SO4	B	453	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	452	SO4	2	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	435/452 (96%)	-0.08	10 (2%) 61 31	42, 58, 75, 85	8 (1%)
1	B	445/452 (98%)	-0.02	10 (2%) 62 33	38, 58, 77, 89	10 (2%)
All	All	880/904 (97%)	-0.05	20 (2%) 61 31	38, 58, 76, 89	18 (2%)

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	240	ASN	4.9
1	A	150	GLY	3.1
1	A	409	ASN	3.0
1	A	174	GLY	2.9
1	A	173	THR	2.8
1	A	347	SER	2.7
1	B	248	ILE	2.5
1	B	406	ARG	2.5
1	B	411	SER	2.4
1	B	209	ILE	2.4
1	A	436	SER	2.3
1	A	350	GLU	2.3
1	B	355	TYR	2.3
1	B	412	GLU	2.2
1	B	353	ASN	2.2
1	B	364	ASN	2.1
1	A	57	ASP	2.1
1	A	308	GLY	2.0
1	B	174	GLY	2.0
1	A	405	LYS	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
3	CA	A	502	1/1	0.96	0.22	0.21	50,50,50,50	0
2	SO4	A	455	5/5	0.86	0.21	-0.27	110,111,112,112	0
2	SO4	B	453	5/5	0.88	0.20	-0.57	101,102,103,103	0
2	SO4	A	453	5/5	0.97	0.15	-1.25	56,57,58,58	0
3	CA	B	501	1/1	0.97	0.14	-1.54	43,43,43,43	0
2	SO4	B	451	5/5	0.98	0.12	-2.00	69,69,70,71	0
2	SO4	A	451	5/5	0.97	0.10	-2.67	61,63,63,64	0
2	SO4	A	454	5/5	0.98	0.18	-	72,72,72,73	0
2	SO4	A	452	5/5	0.98	0.10	-	47,48,49,49	5
2	SO4	B	452	5/5	0.94	0.20	-	70,72,73,73	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.