



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2017 – 12:49 AM EST

PDB ID : 3N33  
Title : Crystal structure of the N-terminal beta-aminopeptidase BapA in complex with pefabloc SC (AEBSF)  
Authors : Merz, T.; Heck, T.; Geueke, B.; Kohler, H.-P.; Gruetter, M.G.  
Deposited on : 2010-05-19  
Resolution : 1.80 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 : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20028442  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20028442

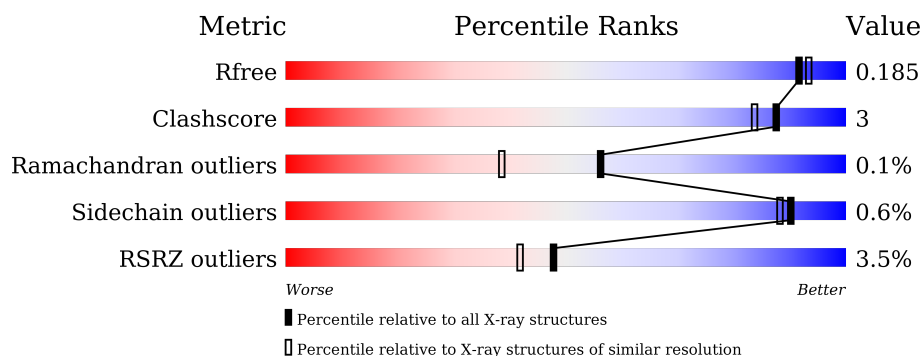
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	4533 (1.80-1.80)
Clashscore	102246	5383 (1.80-1.80)
Ramachandran outliers	100387	5320 (1.80-1.80)
Sidechain outliers	100360	5319 (1.80-1.80)
RSRZ outliers	91569	4547 (1.80-1.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	373	<div> <div>2%</div> <div>92%</div> <div>6%</div> <div>.</div> </div>
1	B	373	<div> <div>4%</div> <div>94%</div> <div>.</div> <div>.</div> </div>
1	C	373	<div> <div>4%</div> <div>91%</div> <div>7%</div> <div>.</div> </div>
1	D	373	<div> <div>4%</div> <div>93%</div> <div>5%</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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	EPE	B	375	-	-	-	X
4	AES	B	377	-	-	-	X
5	SO4	A	379	-	-	-	X
5	SO4	A	381	-	-	-	X
5	SO4	A	382	-	-	-	X
5	SO4	B	379	-	-	-	X
5	SO4	B	380	-	-	-	X
5	SO4	C	378	-	-	-	X
5	SO4	C	379	-	-	-	X
5	SO4	C	380	-	-	-	X
5	SO4	C	381	-	-	-	X
5	SO4	D	379	-	-	-	X

## 2 Entry composition [i](#)

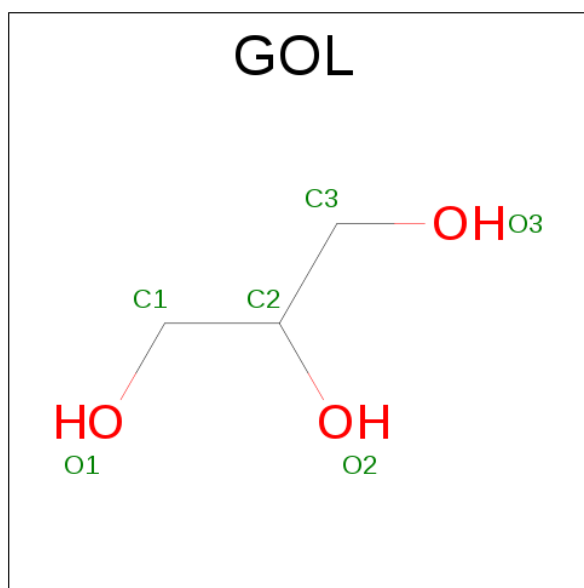
There are 6 unique types of molecules in this entry. The entry contains 12211 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Beta-peptidyl aminopeptidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	367	Total	C	N	O	S	0	3	0
			2681	1678	488	504	11			
1	B	367	Total	C	N	O	S	0	2	0
			2676	1674	488	504	10			
1	C	367	Total	C	N	O	S	0	2	0
			2673	1673	487	503	10			
1	D	367	Total	C	N	O	S	0	3	0
			2678	1677	487	503	11			

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



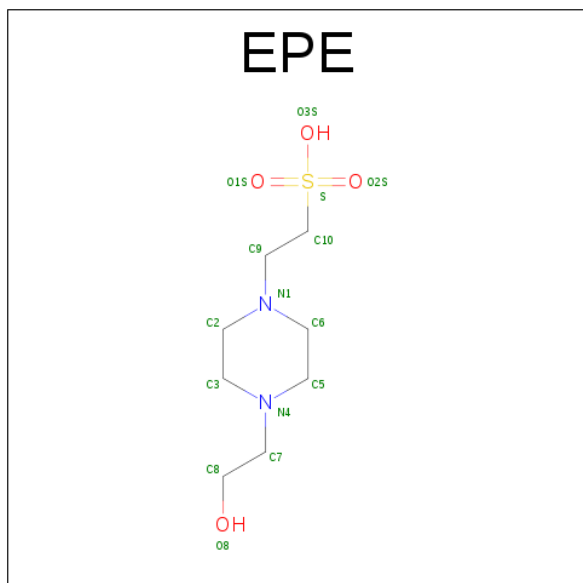
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		

*Continued on next page...*

Continued from previous page...

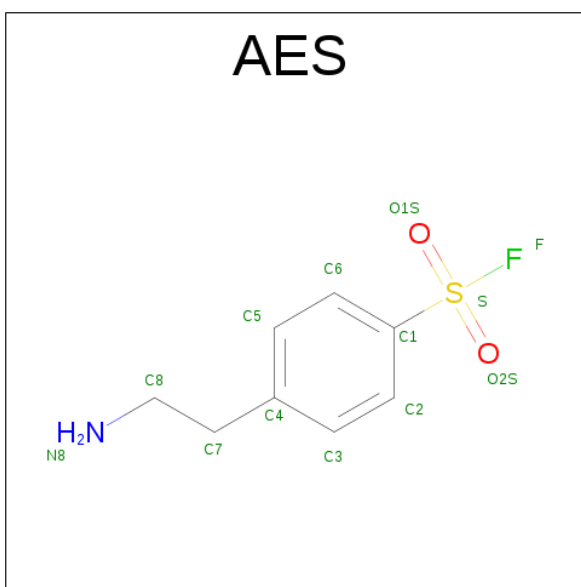
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	1	Total	C	O	0	0
			6	3	3		
2	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 3 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula:  $C_8H_{18}N_2O_4S$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
3	B	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

- Molecule 4 is 4-(2-AMINOETHYL)BENZENESULFONYL FLUORIDE (three-letter code: AES) (formula:  $C_8H_{10}FNO_2S$ ).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total 13	C 8	F 1	N 1	O 2	S 1	0	0
4	A	1	Total 13	C 8	F 1	N 1	O 2	S 1	0	0
4	B	1	Total 13	C 8	F 1	N 1	O 2	S 1	0	0
4	B	1	Total 13	C 8	F 1	N 1	O 2	S 1	0	0
4	C	1	Total 13	C 8	F 1	N 1	O 2	S 1	0	0
4	C	1	Total 13	C 8	F 1	N 1	O 2	S 1	0	0
4	D	1	Total 13	C 8	F 1	N 1	O 2	S 1	0	0
4	D	1	Total 13	C 8	F 1	N 1	O 2	S 1	0	0

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

*Continued on next page...*

*Continued from previous page...*

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

- Molecule 6 is water.

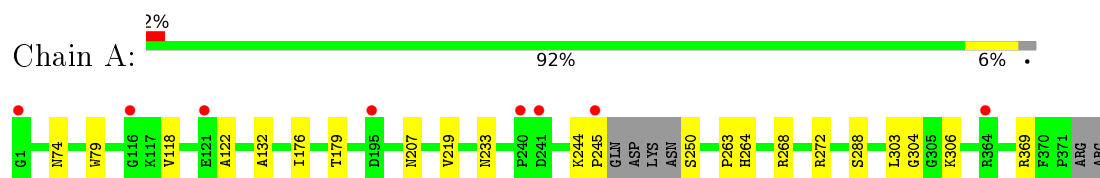
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	308	Total	O	0	0
			308	308		
6	B	322	Total	O	0	0
			322	322		
6	C	326	Total	O	0	0
			326	326		
6	D	309	Total	O	0	0
			309	309		



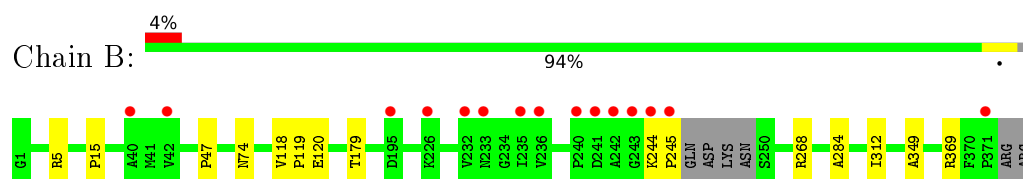
### 3 Residue-property plots [i](#)

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

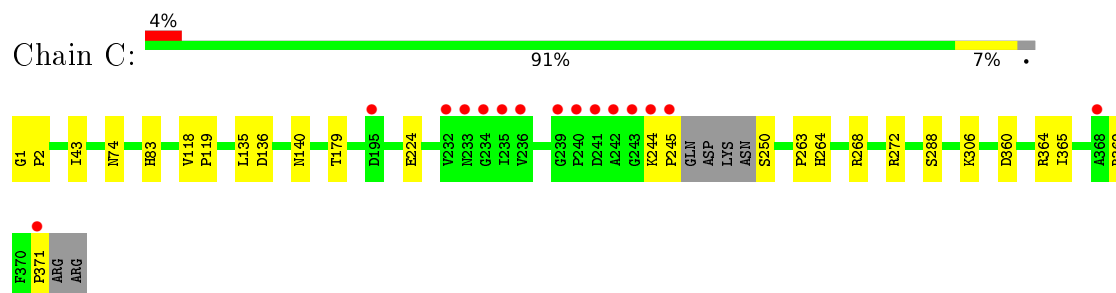
- Molecule 1: Beta-peptidyl aminopeptidase



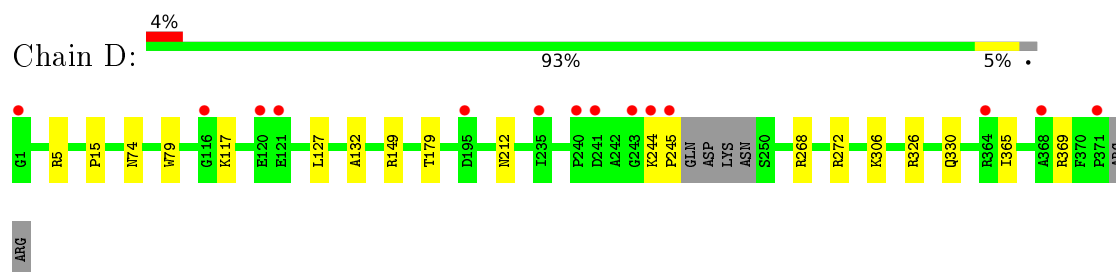
- Molecule 1: Beta-peptidyl aminopeptidase



- Molecule 1: Beta-peptidyl aminopeptidase



- Molecule 1: Beta-peptidyl aminopeptidase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	87.40 Å   96.85 Å   101.30 Å 90.00°   108.38°   90.00°	Depositor
Resolution (Å)	48.07 – 1.80 48.42 – 1.80	Depositor EDS
% Data completeness (in resolution range)	97.7 (48.07-1.80) 97.7 (48.42-1.80)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	0.01	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.93 (at 1.79 Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.1_357)	Depositor
R, $R_{free}$	0.160   ,   0.191 0.153   ,   0.185	Depositor DCC
$R_{free}$ test set	1447 reflections (1.00%)	DCC
Wilson B-factor (Å <sup>2</sup> )	17.8	Xtriage
Anisotropy	0.409	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 53.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	12211	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.31% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, AES, EPE, 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	0.35	0/2734	0.52	0/3711
1	B	0.36	0/2726	0.52	0/3701
1	C	0.34	0/2726	0.52	0/3701
1	D	0.36	0/2734	0.53	0/3711
All	All	0.35	0/10920	0.52	0/14824

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 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	2681	0	2706	19	0
1	B	2676	0	2697	12	0
1	C	2673	0	2698	23	0
1	D	2678	0	2707	16	0
2	A	6	0	8	0	0
2	B	6	0	8	0	0
2	C	6	0	8	0	0
2	D	6	0	8	0	0
3	A	15	0	17	5	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	15	0	17	0	0
4	A	26	0	20	0	0
4	B	26	0	20	2	0
4	C	26	0	20	0	0
4	D	26	0	20	1	0
5	A	25	0	0	0	0
5	B	15	0	0	0	0
5	C	25	0	0	0	0
5	D	15	0	0	0	0
6	A	308	0	0	0	0
6	B	322	0	0	0	0
6	C	326	0	0	2	0
6	D	309	0	0	2	0
All	All	12211	0	10954	56	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 3.

All (56) 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:120:GLU:HG2	4:B:377:AES:H71	1.51	0.91
1:A:268:ARG:HH21	1:D:74:ASN:HD21	1.20	0.88
1:B:74:ASN:HD21	1:C:268:ARG:HH21	1.24	0.85
1:B:268:ARG:HH21	1:C:74:ASN:HD21	1.20	0.84
1:A:74:ASN:HD21	1:D:268:ARG:HH21	1.24	0.83
1:A:303:LEU:HG	3:A:375:EPE:H22	1.68	0.75
1:A:304:GLY:HA3	3:A:375:EPE:H21	1.71	0.73
1:C:365:ILE:O	1:C:369[B]:ARG:HG2	1.91	0.71
1:A:250:SER:N	1:A:288:SER:HG	1.93	0.66
1:C:250:SER:N	1:C:288:SER:HG	1.95	0.65
1:D:326[B]:ARG:CZ	1:D:330:GLN:HE22	2.12	0.62
1:A:303:LEU:HD23	3:A:375:EPE:H52	1.84	0.58
1:C:306:LYS:HD3	6:C:1162:HOH:O	2.02	0.58
1:A:118:VAL:CG1	1:A:122:ALA:HB3	2.36	0.56
1:A:264:HIS:CE1	1:C:263:PRO:HG2	2.41	0.56
1:A:303:LEU:HG	3:A:375:EPE:H101	1.88	0.55
1:C:244:LYS:HB3	1:C:245:PRO:HD2	1.88	0.55
1:C:83:HIS:HE1	1:D:79:TRP:O	1.91	0.53
1:A:263:PRO:HG2	1:C:264:HIS:CE1	2.43	0.53
1:B:369[B]:ARG:NH2	1:C:369[B]:ARG:NH1	2.56	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:360:ASP:O	1:C:364[B]:ARG:HG3	2.09	0.52
1:A:303:LEU:CD2	3:A:375:EPE:H52	2.41	0.50
1:B:120:GLU:HG2	4:B:377:AES:C7	2.33	0.50
1:C:306:LYS:NZ	1:C:306:LYS:HB2	2.27	0.50
1:C:369[B]:ARG:HD3	6:C:1231:HOH:O	2.12	0.49
1:B:244:LYS:HB3	1:B:245:PRO:HD2	1.95	0.49
1:D:5:ARG:NH2	1:D:15:PRO:HG3	2.28	0.48
1:C:43:ILE:HD11	4:D:376:AES:H72	1.95	0.48
1:A:219:VAL:HG22	1:A:369[B]:ARG:HE	1.78	0.48
1:A:79:TRP:CG	1:A:132:ALA:HB2	2.49	0.47
1:B:5:ARG:NH2	1:B:15:PRO:HG3	2.30	0.47
1:B:74:ASN:ND2	1:C:272:ARG:HH12	2.13	0.46
1:A:74:ASN:ND2	1:D:272:ARG:HH12	2.14	0.45
1:D:212:ASN:ND2	6:D:796:HOH:O	2.42	0.45
1:B:118:VAL:HG13	1:B:119:PRO:HD2	1.98	0.45
1:B:312:ILE:HG22	1:D:306:LYS:HE3	1.98	0.45
1:D:326[B]:ARG:CZ	1:D:330:GLN:NE2	2.80	0.44
1:A:272:ARG:HH12	1:D:74:ASN:ND2	2.16	0.43
1:C:118:VAL:HG12	1:C:119:PRO:O	2.18	0.43
1:C:135:LEU:HD13	1:D:127:LEU:HD13	2.00	0.43
1:D:365:ILE:HG23	1:D:369[A]:ARG:HH21	1.84	0.43
1:B:47:PRO:HG2	1:B:349:ALA:HA	2.00	0.42
1:C:118:VAL:HG13	1:C:119:PRO:HD2	2.01	0.42
1:A:79:TRP:CD2	1:A:132:ALA:HB2	2.54	0.42
1:C:224:GLU:HG3	1:C:369[B]:ARG:HH21	1.85	0.41
1:A:244:LYS:HB3	1:A:245:PRO:HD2	2.02	0.41
1:A:306:LYS:HB2	1:A:306:LYS:HE3	1.88	0.41
1:C:136:ASP:O	1:C:140:ASN:HB3	2.21	0.41
1:A:176:ILE:O	1:A:207:ASN:HA	2.21	0.41
1:D:244:LYS:HB3	1:D:245:PRO:HD2	2.03	0.41
1:C:1:GLY:HA2	1:C:2:PRO:HD3	1.95	0.40
1:D:79:TRP:CD2	1:D:132:ALA:HB2	2.56	0.40
1:D:79:TRP:CG	1:D:132:ALA:HB2	2.56	0.40
1:B:369[B]:ARG:HH21	1:C:369[B]:ARG:NH1	2.18	0.40
1:D:117:LYS:HG2	6:D:874:HOH:O	2.22	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	366/373 (98%)	361 (99%)	5 (1%)	0	100	100
1	B	365/373 (98%)	361 (99%)	3 (1%)	1 (0%)	46	29
1	C	365/373 (98%)	360 (99%)	5 (1%)	0	100	100
1	D	366/373 (98%)	360 (98%)	6 (2%)	0	100	100
All	All	1462/1492 (98%)	1442 (99%)	19 (1%)	1 (0%)	56	38

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	284	ALA

### 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	274/277 (99%)	272 (99%)	2 (1%)	88	86
1	B	273/277 (99%)	272 (100%)	1 (0%)	93	92
1	C	273/277 (99%)	272 (100%)	1 (0%)	93	92
1	D	274/277 (99%)	272 (99%)	2 (1%)	88	86
All	All	1094/1108 (99%)	1088 (100%)	6 (0%)	90	91

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	179	THR
1	A	233	ASN
1	B	179	THR
1	C	179	THR
1	D	149	ARG
1	D	179	THR

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

Mol	Chain	Res	Type
1	A	74	ASN
1	A	212	ASN
1	A	220	GLN
1	B	74	ASN
1	B	212	ASN
1	C	74	ASN
1	C	83	HIS
1	C	220	GLN
1	D	74	ASN
1	D	212	ASN
1	D	220	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](#)

30 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	GOL	A	374	-	5,5,5	0.24	0	5,5,5	0.15	0
3	EPE	A	375	-	15,15,15	3.41	5 (33%)	19,20,20	2.15	5 (26%)
4	AES	A	376	-	13,13,13	1.92	3 (23%)	18,18,18	1.30	3 (16%)
4	AES	A	377	-	13,13,13	1.90	4 (30%)	18,18,18	1.33	3 (16%)
5	SO4	A	378	-	4,4,4	0.26	0	6,6,6	0.13	0
5	SO4	A	379	-	4,4,4	0.27	0	6,6,6	0.27	0
5	SO4	A	380	-	4,4,4	0.45	0	6,6,6	0.16	0
5	SO4	A	381	-	4,4,4	0.24	0	6,6,6	0.19	0
5	SO4	A	382	-	4,4,4	0.43	0	6,6,6	0.21	0
2	GOL	B	374	-	5,5,5	0.36	0	5,5,5	0.22	0
3	EPE	B	375	-	15,15,15	3.39	5 (33%)	19,20,20	2.36	6 (31%)
4	AES	B	376	-	13,13,13	1.89	3 (23%)	18,18,18	1.54	3 (16%)
4	AES	B	377	-	13,13,13	1.94	4 (30%)	18,18,18	1.52	3 (16%)
5	SO4	B	378	-	4,4,4	0.25	0	6,6,6	0.08	0
5	SO4	B	379	-	4,4,4	0.42	0	6,6,6	0.14	0
5	SO4	B	380	-	4,4,4	0.44	0	6,6,6	0.33	0
2	GOL	C	374	-	5,5,5	0.36	0	5,5,5	0.12	0
4	AES	C	375	-	13,13,13	1.95	4 (30%)	18,18,18	1.44	3 (16%)
4	AES	C	376	-	13,13,13	1.87	4 (30%)	18,18,18	1.53	3 (16%)
5	SO4	C	377	-	4,4,4	0.30	0	6,6,6	0.12	0
5	SO4	C	378	-	4,4,4	0.27	0	6,6,6	0.14	0
5	SO4	C	379	-	4,4,4	0.42	0	6,6,6	0.19	0
5	SO4	C	380	-	4,4,4	0.23	0	6,6,6	0.15	0
5	SO4	C	381	-	4,4,4	0.53	0	6,6,6	0.19	0
2	GOL	D	374	-	5,5,5	0.41	0	5,5,5	0.29	0
4	AES	D	375	-	13,13,13	1.95	4 (30%)	18,18,18	1.50	3 (16%)
4	AES	D	376	-	13,13,13	1.99	4 (30%)	18,18,18	1.41	4 (22%)
5	SO4	D	377	-	4,4,4	0.27	0	6,6,6	0.07	0
5	SO4	D	378	-	4,4,4	0.43	0	6,6,6	0.20	0
5	SO4	D	379	-	4,4,4	0.46	0	6,6,6	0.30	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	GOL	A	374	-	-	0/4/4/4	0/0/0/0
3	EPE	A	375	-	-	0/9/19/19	0/1/1/1
4	AES	A	376	-	-	0/9/9/9	0/1/1/1
4	AES	A	377	-	-	0/9/9/9	0/1/1/1
5	SO4	A	378	-	-	0/0/0/0	0/0/0/0
5	SO4	A	379	-	-	0/0/0/0	0/0/0/0
5	SO4	A	380	-	-	0/0/0/0	0/0/0/0
5	SO4	A	381	-	-	0/0/0/0	0/0/0/0
5	SO4	A	382	-	-	0/0/0/0	0/0/0/0
2	GOL	B	374	-	-	0/4/4/4	0/0/0/0
3	EPE	B	375	-	-	0/9/19/19	0/1/1/1
4	AES	B	376	-	-	0/9/9/9	0/1/1/1
4	AES	B	377	-	-	0/9/9/9	0/1/1/1
5	SO4	B	378	-	-	0/0/0/0	0/0/0/0
5	SO4	B	379	-	-	0/0/0/0	0/0/0/0
5	SO4	B	380	-	-	0/0/0/0	0/0/0/0
2	GOL	C	374	-	-	0/4/4/4	0/0/0/0
4	AES	C	375	-	-	0/9/9/9	0/1/1/1
4	AES	C	376	-	-	0/9/9/9	0/1/1/1
5	SO4	C	377	-	-	0/0/0/0	0/0/0/0
5	SO4	C	378	-	-	0/0/0/0	0/0/0/0
5	SO4	C	379	-	-	0/0/0/0	0/0/0/0
5	SO4	C	380	-	-	0/0/0/0	0/0/0/0
5	SO4	C	381	-	-	0/0/0/0	0/0/0/0
2	GOL	D	374	-	-	0/4/4/4	0/0/0/0
4	AES	D	375	-	-	0/9/9/9	0/1/1/1
4	AES	D	376	-	-	0/9/9/9	0/1/1/1
5	SO4	D	377	-	-	0/0/0/0	0/0/0/0
5	SO4	D	378	-	-	0/0/0/0	0/0/0/0
5	SO4	D	379	-	-	0/0/0/0	0/0/0/0

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	375	EPE	O8-C8	-4.31	1.18	1.42
3	B	375	EPE	O8-C8	-4.25	1.19	1.42
4	A	377	AES	O2S-S	2.09	1.46	1.42
4	C	376	AES	O2S-S	2.09	1.46	1.42
4	C	375	AES	O2S-S	2.10	1.46	1.42
4	A	377	AES	O1S-S	2.11	1.46	1.42
4	B	377	AES	O2S-S	2.16	1.46	1.42
4	B	376	AES	O1S-S	2.18	1.46	1.42
4	D	376	AES	O2S-S	2.21	1.47	1.42

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	376	AES	O1S-S	2.27	1.47	1.42
4	A	376	AES	O1S-S	2.28	1.47	1.42
4	A	377	AES	C5-C6	2.30	1.43	1.38
4	D	375	AES	O2S-S	2.30	1.47	1.42
4	C	376	AES	C5-C6	2.31	1.43	1.38
4	A	376	AES	C5-C6	2.32	1.43	1.38
4	C	375	AES	O1S-S	2.34	1.47	1.42
4	D	376	AES	O1S-S	2.37	1.47	1.42
4	D	375	AES	O1S-S	2.39	1.47	1.42
4	B	377	AES	O1S-S	2.43	1.47	1.42
4	B	377	AES	C5-C6	2.48	1.43	1.38
4	C	375	AES	C5-C6	2.52	1.43	1.38
4	B	376	AES	C5-C6	2.60	1.43	1.38
4	D	375	AES	C5-C6	2.64	1.44	1.38
4	D	376	AES	C5-C6	2.65	1.44	1.38
3	B	375	EPE	C10-S	3.80	1.83	1.77
3	A	375	EPE	C10-S	3.97	1.83	1.77
4	B	376	AES	C2-C3	4.57	1.47	1.38
4	D	375	AES	C2-C3	4.70	1.48	1.38
4	C	375	AES	C2-C3	4.76	1.48	1.38
4	C	376	AES	C2-C3	4.78	1.48	1.38
4	B	377	AES	C2-C3	4.80	1.48	1.38
4	D	376	AES	C2-C3	4.90	1.48	1.38
4	A	376	AES	C2-C3	5.01	1.48	1.38
4	A	377	AES	C2-C3	5.04	1.48	1.38
3	A	375	EPE	O3S-S	5.38	1.65	1.47
3	B	375	EPE	O3S-S	5.40	1.65	1.47
3	A	375	EPE	O1S-S	6.96	1.65	1.45
3	B	375	EPE	O1S-S	6.99	1.65	1.45
3	B	375	EPE	O2S-S	7.25	1.66	1.45
3	A	375	EPE	O2S-S	7.31	1.66	1.45

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	376	AES	O1S-S-C1	-3.97	106.44	110.73
4	B	376	AES	O2S-S-O1S	-3.50	107.80	118.82
4	D	375	AES	O2S-S-O1S	-3.43	108.01	118.82
4	C	375	AES	O2S-S-O1S	-3.22	108.67	118.82
4	B	377	AES	O1S-S-C1	-3.15	107.32	110.73
4	D	376	AES	O2S-S-C1	-2.87	107.62	110.73
4	A	377	AES	O2S-S-O1S	-2.69	110.33	118.82

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	376	AES	O2S-S-O1S	-2.69	110.35	118.82
4	B	377	AES	O2S-S-O1S	-2.68	110.37	118.82
4	D	376	AES	O2S-S-O1S	-2.61	110.59	118.82
4	A	376	AES	O2S-S-O1S	-2.50	110.94	118.82
4	A	377	AES	C8-C7-C4	2.02	117.29	112.83
3	B	375	EPE	O8-C8-C7	2.04	120.66	111.27
3	B	375	EPE	C9-C10-S	2.21	119.84	112.61
4	D	376	AES	F-S-C1	2.23	107.59	102.47
3	A	375	EPE	C9-C10-S	2.26	120.02	112.61
4	A	377	AES	F-S-C1	2.28	107.70	102.47
4	C	375	AES	F-S-C1	2.29	107.73	102.47
4	C	376	AES	F-S-C1	2.36	107.90	102.47
4	A	376	AES	F-S-C1	2.48	108.17	102.47
4	B	377	AES	F-S-C1	2.56	108.36	102.47
4	B	376	AES	F-S-C1	2.58	108.40	102.47
4	A	376	AES	C8-C7-C4	2.64	118.64	112.83
4	D	376	AES	C8-C7-C4	2.75	118.89	112.83
4	D	375	AES	F-S-C1	2.77	108.84	102.47
4	C	375	AES	C8-C7-C4	2.94	119.30	112.83
3	A	375	EPE	O3S-S-C10	2.94	111.11	104.99
4	D	375	AES	C8-C7-C4	3.10	119.66	112.83
3	B	375	EPE	C5-N4-C3	3.57	116.86	108.87
3	A	375	EPE	C6-N1-C2	3.67	117.09	108.87
4	B	376	AES	C8-C7-C4	3.73	121.06	112.83
3	A	375	EPE	O1S-S-C10	3.94	109.65	106.87
3	B	375	EPE	O2S-S-C10	4.15	109.80	106.87
3	B	375	EPE	O1S-S-C10	4.59	110.11	106.87
3	A	375	EPE	C5-N4-C3	4.72	119.43	108.87
3	B	375	EPE	C6-N1-C2	5.64	121.50	108.87

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
3	A	375	EPE	5	0
4	B	377	AES	2	0
4	D	376	AES	1	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	367/373 (98%)	-0.31	8 (2%) 65 60	10, 16, 36, 53	0
1	B	367/373 (98%)	-0.14	15 (4%) 41 35	10, 17, 35, 60	0
1	C	367/373 (98%)	-0.10	15 (4%) 41 35	10, 17, 38, 59	0
1	D	367/373 (98%)	-0.31	14 (3%) 44 38	10, 16, 35, 55	0
All	All	1468/1492 (98%)	-0.22	52 (3%) 48 42	10, 17, 36, 60	0

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	195	ASP	6.7
1	C	235	ILE	5.1
1	C	245	PRO	5.1
1	C	244	LYS	4.5
1	B	233	ASN	4.3
1	B	244	LYS	4.3
1	B	245	PRO	4.1
1	C	240	PRO	4.0
1	A	240	PRO	3.9
1	C	233	ASN	3.8
1	A	195	ASP	3.8
1	D	195	ASP	3.7
1	B	240	PRO	3.6
1	B	235	ILE	3.4
1	D	240	PRO	3.3
1	D	241	ASP	3.2
1	C	236	VAL	3.2
1	A	245	PRO	3.1
1	B	242	ALA	3.1
1	B	232	VAL	3.0
1	D	364	ARG	2.9

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	C	371	PRO	2.9
1	C	242	ALA	2.9
1	D	116	GLY	2.9
1	D	1	GLY	2.8
1	B	243	GLY	2.7
1	C	234	GLY	2.7
1	C	243	GLY	2.7
1	B	371	PRO	2.7
1	D	245	PRO	2.5
1	A	364	ARG	2.5
1	C	239	GLY	2.5
1	C	241	ASP	2.5
1	D	244	LYS	2.5
1	C	195	ASP	2.5
1	A	116	GLY	2.4
1	A	241	ASP	2.4
1	A	121	GLU	2.3
1	B	226	LYS	2.3
1	B	42	VAL	2.3
1	B	40	ALA	2.3
1	D	371	PRO	2.2
1	C	368	ALA	2.2
1	B	241	ASP	2.2
1	D	243	GLY	2.2
1	D	368	ALA	2.2
1	A	1	GLY	2.1
1	B	236	VAL	2.1
1	C	232	VAL	2.1
1	D	121	GLU	2.1
1	D	120	GLU	2.0
1	D	235	ILE	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

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	SO4	C	380	5/5	0.89	0.13	8.27	24,27,29,30	5
5	SO4	A	381	5/5	0.93	0.14	6.99	26,30,31,32	5
5	SO4	C	378	5/5	0.93	0.13	6.02	27,32,36,39	5
5	SO4	C	379	5/5	0.98	0.12	3.91	16,20,26,27	5
5	SO4	A	379	5/5	0.90	0.20	3.50	33,33,37,40	5
5	SO4	B	380	5/5	0.97	0.12	3.47	16,18,25,26	5
5	SO4	C	381	5/5	0.97	0.13	2.96	14,17,26,26	5
5	SO4	D	379	5/5	0.98	0.14	2.90	11,14,23,26	5
5	SO4	B	379	5/5	0.98	0.12	2.37	15,21,25,27	5
3	EPE	B	375	15/15	0.83	0.20	2.23	32,37,42,44	15
5	SO4	A	382	5/5	0.98	0.13	2.22	12,14,22,26	5
4	AES	B	377	13/13	0.96	0.14	2.05	24,30,43,50	0
3	EPE	A	375	15/15	0.84	0.24	1.92	33,38,45,52	15
5	SO4	A	380	5/5	0.99	0.11	1.72	15,19,22,26	5
2	GOL	B	374	6/6	0.95	0.11	1.62	13,14,16,17	0
5	SO4	D	378	5/5	0.99	0.10	0.99	17,19,23,25	5
4	AES	D	376	13/13	0.97	0.17	0.75	28,32,46,47	0
4	AES	B	376	13/13	0.95	0.10	0.75	16,18,31,32	0
4	AES	C	375	13/13	0.95	0.11	0.72	16,21,31,34	0
5	SO4	A	378	5/5	0.93	0.10	0.47	33,34,34,35	5
4	AES	A	377	13/13	0.93	0.16	0.41	24,26,43,50	13
4	AES	C	376	13/13	0.96	0.10	0.34	19,25,36,41	13
2	GOL	D	374	6/6	0.95	0.08	0.07	15,16,18,19	0
5	SO4	B	378	5/5	0.94	0.14	-0.04	32,36,38,38	5
5	SO4	D	377	5/5	0.96	0.08	-0.13	34,37,38,38	5
4	AES	D	375	13/13	0.95	0.09	-0.15	15,17,31,38	0
5	SO4	C	377	5/5	0.94	0.13	-0.31	34,38,42,43	5
4	AES	A	376	13/13	0.96	0.09	-0.45	14,18,29,34	0
2	GOL	C	374	6/6	0.97	0.07	-0.77	14,15,16,16	0
2	GOL	A	374	6/6	0.97	0.06	-1.66	16,17,18,20	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.