



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:43 AM GMT

PDB ID : 2ID2  
Title : GAPN T244S mutant X-ray structure at 2.5 Å  
Authors : Pailot, A.; D'Ambrosio, K.; Corbier, C.; Talfournier, F.; Branlant, G.  
Deposited on : 2006-09-14  
Resolution : 2.50 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.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
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) : trunk26865

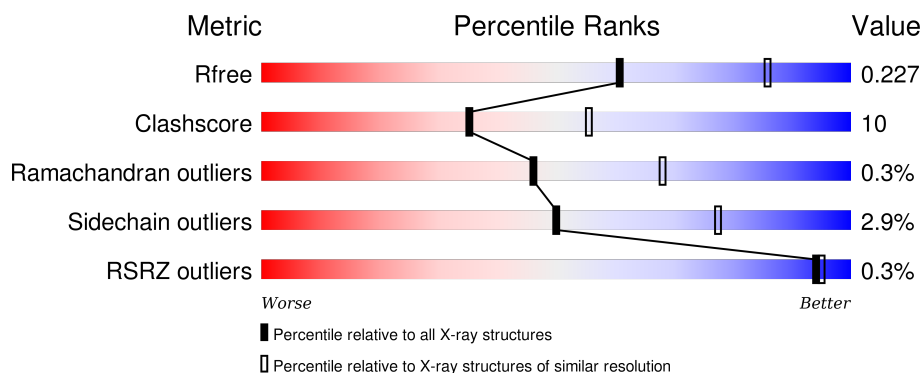
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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	475	<div> <div>80%</div> <div>19%</div> <div>.</div> </div>
1	B	475	<div> <div>79%</div> <div>19%</div> <div>.</div> </div>
1	C	475	<div> <div>80%</div> <div>19%</div> <div>.</div> </div>
1	D	475	<div> <div>81%</div> <div>17%</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	D	2007	-	-	X	-

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 15702 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 NADP-dependent glyceraldehyde-3-phosphate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	473	Total	C	N	O	S	0	0	0
			3588	2281	599	697	11			
1	B	473	Total	C	N	O	S	0	0	0
			3588	2281	599	697	11			
1	C	474	Total	C	N	O	S	0	0	0
			3595	2285	600	699	11			
1	D	474	Total	C	N	O	S	0	0	0
			3595	2285	600	699	11			

There are 16 discrepancies between the modelled and reference sequences:

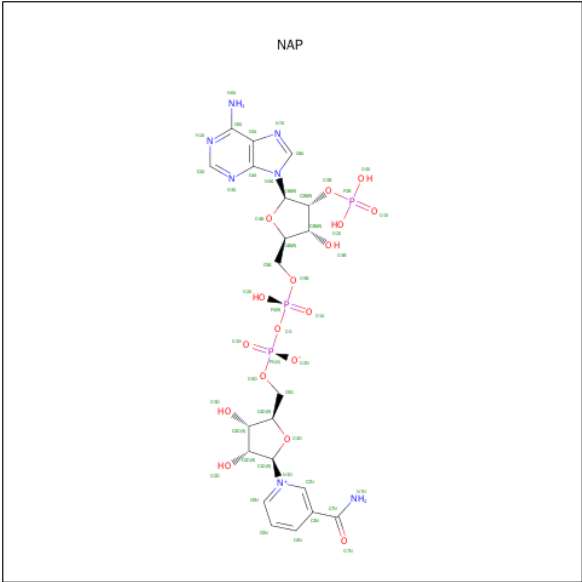
Chain	Residue	Modelled	Actual	Comment	Reference
A	58	ALA	SER	SEE REMARK 999	UNP Q59931
A	85	ILE	VAL	SEE REMARK 999	UNP Q59931
A	229	SER	THR	ENGINEERED	UNP Q59931
A	347	THR	ALA	SEE REMARK 999	UNP Q59931
B	58	ALA	SER	SEE REMARK 999	UNP Q59931
B	85	ILE	VAL	SEE REMARK 999	UNP Q59931
B	229	SER	THR	ENGINEERED	UNP Q59931
B	347	THR	ALA	SEE REMARK 999	UNP Q59931
C	58	ALA	SER	SEE REMARK 999	UNP Q59931
C	85	ILE	VAL	SEE REMARK 999	UNP Q59931
C	229	SER	THR	ENGINEERED	UNP Q59931
C	347	THR	ALA	SEE REMARK 999	UNP Q59931
D	58	ALA	SER	SEE REMARK 999	UNP Q59931
D	85	ILE	VAL	SEE REMARK 999	UNP Q59931
D	229	SER	THR	ENGINEERED	UNP Q59931
D	347	THR	ALA	SEE REMARK 999	UNP Q59931

- 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		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: C<sub>21</sub>H<sub>28</sub>N<sub>7</sub>O<sub>17</sub>P<sub>3</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	D	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

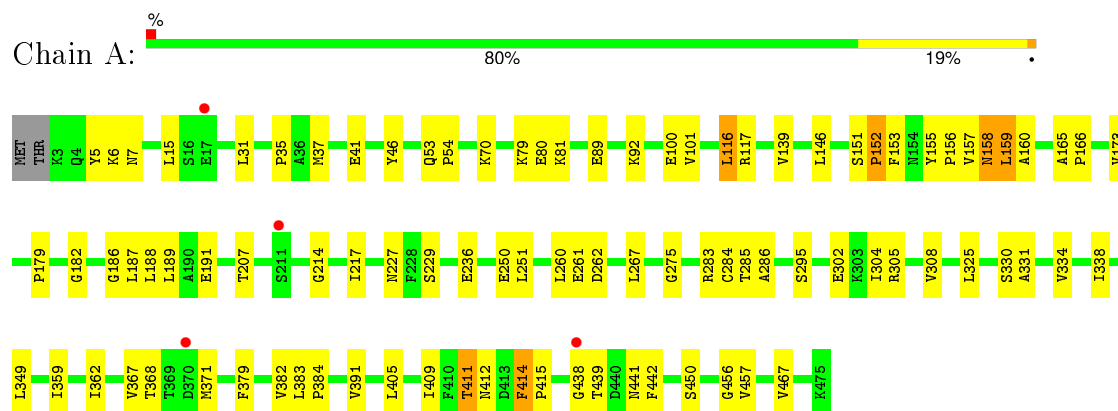
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	250	Total	O	0	0
			250	250		
4	B	243	Total	O	0	0
			243	243		
4	C	309	Total	O	0	0
			309	309		
4	D	307	Total	O	0	0
			307	307		

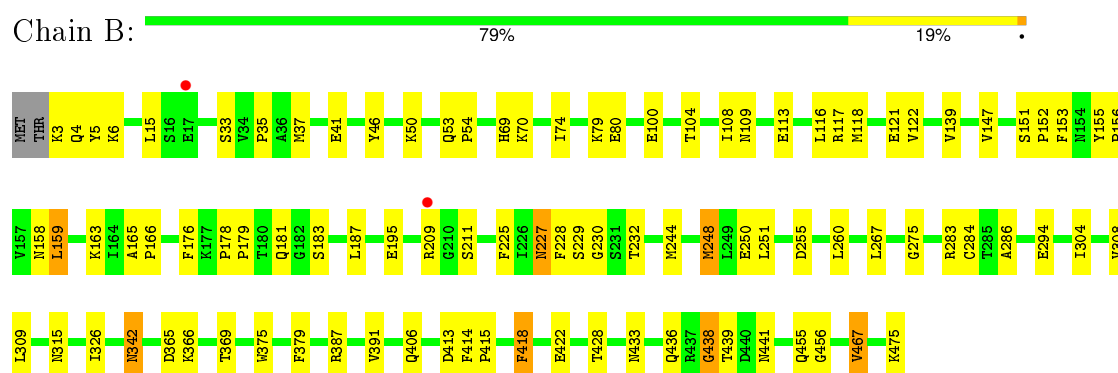
### 3 Residue-property plots

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

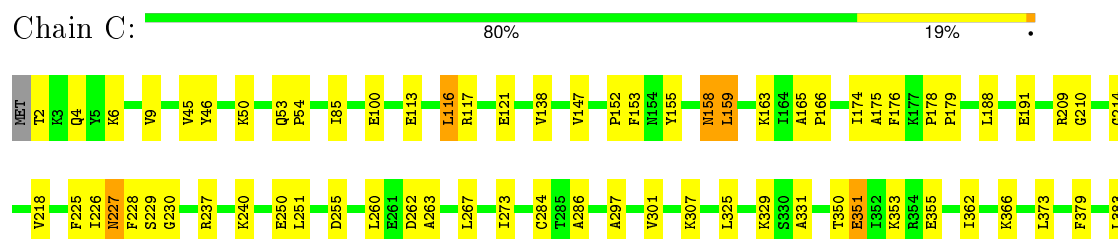
- Molecule 1: NADP-dependent glyceraldehyde-3-phosphate dehydrogenase



- Molecule 1: NADP-dependent glyceraldehyde-3-phosphate dehydrogenase



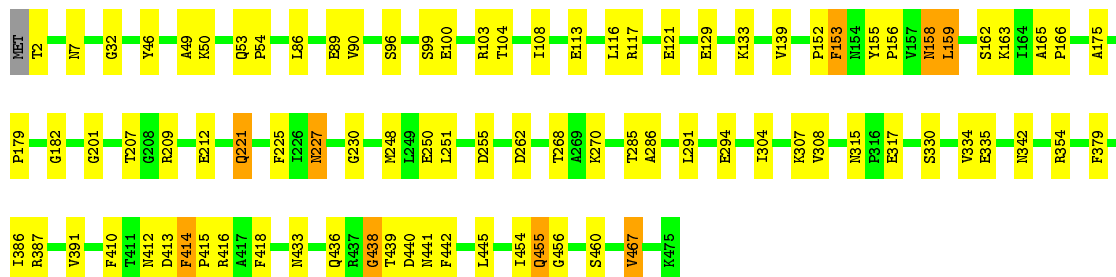
- Molecule 1: NADP-dependent glyceraldehyde-3-phosphate dehydrogenase





- Molecule 1: NADP-dependent glyceraldehyde-3-phosphate dehydrogenase

Chain D: 81% 17%





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 2 <sub>1</sub> 2 <sub>1</sub> 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	143.70 Å   154.40 Å   115.00 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	20.00 – 2.50 19.98 – 2.50	Depositor EDS
% Data completeness (in resolution range)	88.2 (20.00-2.50) 88.2 (19.98-2.50)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.70 (at 2.50 Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.176   ,   0.227 0.176   ,   0.227	Depositor DCC
$R_{free}$ test set	7903 reflections (10.09%)	DCC
Wilson B-factor (Å <sup>2</sup> )	24.8	Xtriage
Anisotropy	0.256	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 52.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 78327 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	15702	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 36.46 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 4.9779e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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, 0.375 respectively for untwinned datasets, and 0.333, 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: NAP, 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	0.31	0/3646	0.59	1/4930 (0.0%)
1	B	0.31	0/3646	0.58	1/4930 (0.0%)
1	C	0.33	0/3653	0.60	1/4940 (0.0%)
1	D	0.33	0/3653	0.60	2/4940 (0.0%)
All	All	0.32	0/14598	0.60	5/19740 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	456	GLY	N-CA-C	-6.49	96.87	113.10
1	A	456	GLY	N-CA-C	-6.35	97.23	113.10
1	C	456	GLY	N-CA-C	-6.06	97.95	113.10
1	B	456	GLY	N-CA-C	-5.83	98.52	113.10
1	D	175	ALA	N-CA-C	-5.10	97.24	111.00

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	3588	0	3640	77	0
1	B	3588	0	3640	75	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	3595	0	3647	76	0
1	D	3595	0	3647	71	0
2	A	5	0	0	0	0
2	B	10	0	0	0	0
2	C	5	0	0	0	0
2	D	15	0	0	2	0
3	A	48	0	25	3	0
3	B	48	0	25	3	0
3	C	48	0	25	4	0
3	D	48	0	25	4	0
4	A	250	0	0	4	0
4	B	243	0	0	4	0
4	C	309	0	0	5	0
4	D	307	0	0	7	0
All	All	15702	0	14674	288	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 (288) 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:368:THR:H	1:A:371:MET:HE3	1.14	1.08
1:D:152:PRO:HG3	3:D:3004:NAP:H5N	1.57	0.86
1:B:152:PRO:HG3	3:B:3002:NAP:H5N	1.59	0.84
1:D:212:GLU:HA	4:D:3190:HOH:O	1.77	0.84
1:C:152:PRO:HG3	3:C:3003:NAP:H5N	1.58	0.84
1:A:368:THR:N	1:A:371:MET:HE3	1.92	0.83
1:A:152:PRO:HG3	3:A:3001:NAP:H5N	1.60	0.83
1:B:232:THR:HA	1:B:251:LEU:HD13	1.59	0.83
1:B:225:PHE:HZ	1:B:248:MET:HG3	1.45	0.81
1:B:439:THR:HG23	1:B:441:ASN:OD1	1.83	0.78
1:B:155:TYR:HB2	1:B:159:LEU:HD22	1.70	0.73
1:A:414:PHE:HE1	4:A:3248:HOH:O	1.71	0.72
1:B:70:LYS:HA	1:B:70:LYS:HE3	1.72	0.72
1:A:155:TYR:HB2	1:A:159:LEU:HD22	1.72	0.72
1:C:250:GLU:OE2	1:C:455:GLN:HG3	1.90	0.71
1:B:436:GLN:HE21	1:B:438:GLY:HA3	1.55	0.71
1:D:100:GLU:HG3	1:D:158:ASN:HB2	1.70	0.71
1:D:209:ARG:HB2	4:D:3307:HOH:O	1.89	0.71
1:A:439:THR:HG23	1:A:441:ASN:OD1	1.91	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:445:LEU:HD13	1:D:454:ILE:HG12	1.74	0.70
1:B:225:PHE:CZ	1:B:248:MET:HG3	2.28	0.69
1:B:250:GLU:OE2	1:B:455:GLN:HG3	1.92	0.69
1:C:351:GLU:CD	1:C:351:GLU:H	1.96	0.69
1:C:218:VAL:HG13	1:C:226:ILE:HD13	1.74	0.69
1:B:255:ASP:HB2	1:B:286:ALA:O	1.92	0.68
1:C:152:PRO:HD3	1:C:229:SER:HB2	1.76	0.68
1:C:351:GLU:HG3	4:C:3256:HOH:O	1.95	0.67
1:B:309:LEU:HD11	4:B:3008:HOH:O	1.94	0.66
1:D:165:ALA:HB3	1:D:166:PRO:HD3	1.78	0.66
1:D:433:ASN:HB3	4:D:3154:HOH:O	1.97	0.65
1:B:165:ALA:HB3	1:B:166:PRO:HD3	1.79	0.65
1:D:439:THR:CG2	1:D:441:ASN:OD1	2.45	0.64
1:C:436:GLN:NE2	1:C:438:GLY:HA3	2.13	0.64
1:D:251:LEU:O	3:D:3004:NAP:H2N	1.98	0.64
1:D:2:THR:CG2	1:D:32:GLY:HA2	2.28	0.63
1:A:302:GLU:CD	1:A:305:ARG:HH12	2.02	0.63
1:D:53:GLN:HB3	1:D:54:PRO:HD3	1.81	0.63
1:D:270:LYS:HG2	1:D:307:LYS:HE3	1.81	0.63
1:D:317:GLU:HB2	2:D:2007:SO4:O4	1.99	0.62
1:B:439:THR:CG2	1:B:441:ASN:OD1	2.47	0.62
1:B:100:GLU:HG3	1:B:158:ASN:HB2	1.80	0.62
1:C:147:VAL:HG22	1:C:225:PHE:HB3	1.81	0.62
1:C:116:LEU:HD12	1:C:117:ARG:HG3	1.83	0.60
1:C:286:ALA:HA	4:C:3021:HOH:O	2.02	0.60
1:B:3:LYS:HG3	4:B:3037:HOH:O	2.01	0.60
1:C:325:LEU:HD12	1:C:331:ALA:HA	1.83	0.60
1:A:285:THR:HG22	4:A:3203:HOH:O	2.02	0.60
1:D:439:THR:HG22	1:D:441:ASN:OD1	2.02	0.59
1:A:275:GLY:HA2	1:A:283:ARG:HH22	1.68	0.59
1:C:439:THR:CG2	1:C:441:ASN:OD1	2.51	0.59
1:A:100:GLU:HG3	1:A:158:ASN:HB2	1.85	0.58
1:A:305:ARG:NH1	1:A:305:ARG:HB3	2.18	0.58
1:B:251:LEU:O	3:B:3002:NAP:H2N	2.03	0.58
1:B:153:PHE:HA	1:B:179:PRO:HG3	1.86	0.58
1:A:251:LEU:O	3:A:3001:NAP:H2N	2.04	0.58
1:D:225:PHE:HZ	1:D:248:MET:HG3	1.69	0.57
1:C:353:LYS:HE2	1:C:355:GLU:OE1	2.05	0.57
1:D:46:TYR:O	1:D:50:LYS:HG2	2.04	0.57
1:D:163:LYS:HE3	1:D:227:ASN:ND2	2.20	0.56
1:C:188:LEU:O	1:C:191:GLU:HB2	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:6:LYS:HG2	1:A:15:LEU:HG	1.87	0.56
1:C:436:GLN:HE21	1:C:438:GLY:HA3	1.70	0.56
1:B:79:LYS:HE2	1:B:80:GLU:OE2	2.04	0.56
1:A:275:GLY:O	1:A:286:ALA:HB1	2.06	0.55
1:A:305:ARG:HG3	1:A:349:LEU:HB3	1.87	0.55
1:A:285:THR:O	1:A:285:THR:HG23	2.07	0.54
1:D:285:THR:O	1:D:285:THR:HG23	2.06	0.54
1:B:436:GLN:C	1:B:438:GLY:H	2.10	0.54
1:C:251:LEU:O	3:C:3003:NAP:H2N	2.07	0.54
1:C:406:GLN:HG2	1:C:428:THR:HB	1.90	0.54
1:C:209:ARG:NE	4:C:3309:HOH:O	2.23	0.53
1:B:100:GLU:CG	1:B:158:ASN:HB2	2.38	0.53
1:D:155:TYR:HB2	1:D:159:LEU:HD22	1.91	0.53
1:D:436:GLN:NE2	1:D:438:GLY:HA3	2.23	0.53
1:A:267:LEU:C	1:A:267:LEU:HD23	2.30	0.53
1:C:53:GLN:HB3	1:C:54:PRO:HD3	1.91	0.52
1:A:439:THR:CG2	1:A:441:ASN:OD1	2.56	0.52
1:B:181:GLN:HG2	1:B:326:ILE:HD11	1.90	0.52
1:A:153:PHE:O	1:A:156:PRO:HD3	2.09	0.52
1:A:330:SER:O	1:A:334:VAL:HG23	2.10	0.52
1:B:153:PHE:O	1:B:156:PRO:HD3	2.10	0.52
1:D:116:LEU:HD12	1:D:116:LEU:C	2.30	0.52
1:B:475:LYS:NZ	4:B:3217:HOH:O	2.43	0.52
1:A:286:ALA:HA	4:A:3074:HOH:O	2.11	0.51
1:D:153:PHE:O	1:D:156:PRO:HD3	2.10	0.51
1:B:406:GLN:HG2	1:B:428:THR:HB	1.93	0.51
1:A:100:GLU:CG	1:A:158:ASN:HB2	2.40	0.51
1:B:275:GLY:O	1:B:286:ALA:HB1	2.11	0.51
1:A:80:GLU:H	1:A:80:GLU:CD	2.14	0.51
1:A:325:LEU:HD11	1:A:359:ILE:HD12	1.93	0.51
1:D:162:SER:O	1:D:166:PRO:HG2	2.11	0.51
1:D:100:GLU:CG	1:D:158:ASN:HB2	2.40	0.51
1:C:439:THR:HG22	1:C:441:ASN:OD1	2.10	0.51
1:D:438:GLY:O	1:D:439:THR:HB	2.11	0.50
1:D:139:VAL:HG12	1:D:467:VAL:HG22	1.94	0.50
1:D:153:PHE:HA	1:D:179:PRO:HG3	1.93	0.50
1:C:445:LEU:HD23	1:C:445:LEU:H	1.76	0.50
1:C:445:LEU:N	1:C:445:LEU:HD23	2.26	0.50
1:C:228:PHE:CZ	1:C:230:GLY:HA3	2.46	0.50
1:C:46:TYR:O	1:C:50:LYS:HG2	2.12	0.50
1:C:366:LYS:HE3	4:C:3183:HOH:O	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:163:LYS:HE3	1:C:227:ASN:ND2	2.26	0.50
1:A:362:ILE:HG23	1:A:382:VAL:HG23	1.93	0.50
1:A:5:TYR:O	1:A:35:PRO:HD3	2.11	0.50
1:A:409:ILE:HG22	1:A:411:THR:HG22	1.92	0.50
1:D:436:GLN:HE21	1:D:438:GLY:HA3	1.76	0.50
1:A:304:ILE:O	1:A:308:VAL:HG23	2.11	0.50
1:D:221:GLN:HG3	4:D:3027:HOH:O	2.12	0.50
1:B:436:GLN:C	1:B:438:GLY:N	2.65	0.50
1:C:472:PHE:CG	1:D:414:PHE:HZ	2.30	0.50
1:B:250:GLU:HB3	3:B:3002:NAP:C7N	2.41	0.49
1:A:261:GLU:HG2	1:A:295:SER:OG	2.12	0.49
1:D:439:THR:HG23	1:D:441:ASN:OD1	2.12	0.49
1:A:415:PRO:HB3	1:C:475:LYS:HG2	1.94	0.49
1:C:273:ILE:HG13	1:C:307:LYS:HB2	1.94	0.49
1:A:6:LYS:HG2	1:A:15:LEU:CD2	2.43	0.49
1:C:250:GLU:HB3	3:C:3003:NAP:C7N	2.42	0.49
1:D:330:SER:O	1:D:334:VAL:HG23	2.13	0.49
1:D:255:ASP:HB2	1:D:286:ALA:O	2.12	0.49
1:B:209:ARG:C	1:B:211:SER:H	2.16	0.49
1:B:418:PHE:O	1:B:422:GLU:HG3	2.13	0.49
1:C:100:GLU:CG	1:C:158:ASN:HB2	2.42	0.49
1:C:439:THR:HG23	1:C:441:ASN:OD1	2.12	0.49
1:D:391:VAL:HG21	1:D:416:ARG:NH2	2.28	0.49
1:B:260:LEU:HD22	1:B:391:VAL:HG22	1.93	0.49
1:D:103:ARG:HD2	1:D:440:ASP:OD2	2.12	0.49
1:B:37:MET:HA	1:B:41:GLU:OE2	2.13	0.49
1:B:6:LYS:HG2	1:B:15:LEU:CD2	2.43	0.49
1:A:165:ALA:HB3	1:A:166:PRO:HD3	1.95	0.49
1:B:121:GLU:HA	1:C:121:GLU:HA	1.95	0.48
1:D:152:PRO:HG3	1:D:159:LEU:HD23	1.95	0.48
1:D:414:PHE:HD1	4:D:3215:HOH:O	1.97	0.48
1:D:139:VAL:HG12	1:D:467:VAL:CG2	2.43	0.48
1:A:7:ASN:OD1	1:A:207:THR:HG23	2.12	0.48
1:B:4:GLN:HG2	1:B:33:SER:OG	2.13	0.48
1:A:415:PRO:CB	1:C:475:LYS:HG2	2.44	0.48
1:C:404:GLY:O	1:C:426:VAL:HA	2.14	0.48
1:C:116:LEU:C	1:C:116:LEU:HD12	2.34	0.48
1:D:248:MET:HE1	1:D:460:SER:HA	1.95	0.47
1:A:117:ARG:HH11	1:A:117:ARG:HG3	1.79	0.47
1:B:304:ILE:O	1:B:308:VAL:HG23	2.14	0.47
1:B:176:PHE:CZ	1:B:178:PRO:HB3	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:152:PRO:HD3	1:B:229:SER:HB2	1.96	0.47
1:A:236:GLU:HG2	1:B:244:MET:SD	2.55	0.47
1:A:92:LYS:NZ	1:A:100:GLU:OE1	2.45	0.47
1:C:273:ILE:HG13	1:C:307:LYS:CB	2.45	0.47
1:B:183:SER:O	1:B:187:LEU:HG	2.14	0.47
1:A:405:LEU:HD13	1:A:450:SER:HB3	1.95	0.47
1:D:335:GLU:OE1	1:D:354:ARG:NH1	2.43	0.47
1:B:5:TYR:O	1:B:35:PRO:HD3	2.14	0.47
1:A:152:PRO:HG3	1:A:159:LEU:HD23	1.97	0.47
1:B:3:LYS:HG2	1:B:4:GLN:HG3	1.97	0.47
1:C:116:LEU:HD12	1:C:117:ARG:N	2.30	0.47
1:A:188:LEU:O	1:A:191:GLU:HB2	2.15	0.47
1:B:53:GLN:HB3	1:B:54:PRO:HD3	1.97	0.47
1:C:2:THR:O	1:C:4:GLN:HG3	2.15	0.47
4:A:3093:HOH:O	1:D:414:PHE:HB2	2.15	0.46
1:B:365:ASP:O	1:B:366:LYS:HB2	2.15	0.46
1:B:46:TYR:O	1:B:50:LYS:HG2	2.15	0.46
1:C:165:ALA:HB3	1:C:166:PRO:HD3	1.98	0.46
1:A:117:ARG:NH2	1:C:113:GLU:HB2	2.29	0.46
1:A:37:MET:HA	1:A:41:GLU:OE2	2.16	0.46
1:B:342:ASN:HA	1:B:342:ASN:HD22	1.61	0.46
1:B:163:LYS:HE3	1:B:227:ASN:ND2	2.31	0.46
1:A:260:LEU:CD2	1:A:391:VAL:HG22	2.46	0.46
1:A:116:LEU:C	1:A:116:LEU:HD12	2.37	0.46
1:D:89:GLU:CD	1:D:182:GLY:HA2	2.36	0.46
1:D:262:ASP:O	1:D:412:ASN:ND2	2.45	0.46
1:A:367:VAL:HG21	1:A:384:PRO:CB	2.46	0.45
1:C:373:LEU:HG	1:C:384:PRO:HB3	1.98	0.45
1:A:79:LYS:HA	1:A:101:VAL:HG11	1.98	0.45
1:A:46:TYR:CD1	1:A:146:LEU:HD21	2.51	0.45
1:D:304:ILE:O	1:D:308:VAL:HG23	2.17	0.45
1:B:151:SER:HB2	1:B:152:PRO:HD2	1.97	0.45
1:A:383:LEU:HD12	1:A:384:PRO:HD2	1.98	0.45
1:A:302:GLU:OE1	1:A:305:ARG:NH1	2.50	0.45
1:A:146:LEU:HA	1:A:173:VAL:HG23	1.98	0.45
1:B:267:LEU:HD23	1:B:267:LEU:C	2.37	0.45
1:A:116:LEU:HD12	1:A:117:ARG:HG3	1.99	0.45
1:C:433:ASN:HB3	4:C:3182:HOH:O	2.15	0.45
1:B:139:VAL:HG12	1:B:467:VAL:HG22	1.98	0.44
1:B:74:ILE:HD13	1:B:195:GLU:HB3	1.99	0.44
1:B:286:ALA:HA	4:B:3028:HOH:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:433:ASN:HB2	4:D:3242:HOH:O	2.18	0.44
1:C:267:LEU:HD23	1:C:267:LEU:C	2.37	0.44
1:B:122:VAL:HG21	1:C:138:VAL:HG13	1.99	0.44
1:C:159:LEU:HD12	1:C:159:LEU:HA	1.74	0.44
1:D:445:LEU:N	1:D:445:LEU:HD23	2.33	0.44
1:B:69:HIS:ND1	1:B:109:ASN:ND2	2.64	0.44
1:D:209:ARG:HA	1:D:209:ARG:HD2	1.79	0.44
1:D:315:ASN:HB3	2:D:2007:SO4:O4	2.17	0.44
1:B:209:ARG:HG3	1:B:211:SER:H	1.82	0.44
1:C:174:ILE:CG2	1:C:175:ALA:N	2.80	0.44
1:B:117:ARG:NH2	1:D:113:GLU:HB2	2.31	0.44
1:B:438:GLY:O	1:B:439:THR:HB	2.18	0.44
1:D:455:GLN:HE21	1:D:455:GLN:HB3	1.65	0.44
1:C:329:LYS:HB3	1:C:329:LYS:HE2	1.85	0.44
1:C:155:TYR:HB2	1:C:159:LEU:HD22	2.00	0.44
1:D:294:GLU:OE2	1:D:387:ARG:HD3	2.17	0.44
1:B:294:GLU:OE2	1:B:387:ARG:HD3	2.18	0.44
1:A:70:LYS:HB2	1:A:70:LYS:HE2	1.76	0.44
1:C:6:LYS:N	1:C:6:LYS:HD2	2.33	0.43
1:C:9:VAL:HG13	1:C:45:VAL:HG22	1.98	0.43
1:A:53:GLN:HB3	1:A:54:PRO:HD3	2.00	0.43
1:B:104:THR:O	1:B:108:ILE:HG13	2.17	0.43
1:B:152:PRO:HG3	1:B:159:LEU:HD23	2.00	0.43
1:B:294:GLU:HA	1:B:294:GLU:OE2	2.18	0.43
1:C:116:LEU:HD11	1:C:117:ARG:NH1	2.33	0.43
1:A:158:ASN:HD22	1:A:158:ASN:C	2.21	0.43
1:A:152:PRO:HD3	1:A:229:SER:HB2	2.00	0.43
1:D:86:LEU:O	1:D:90:VAL:HG22	2.17	0.43
1:B:275:GLY:HA2	1:B:283:ARG:NH2	2.34	0.43
1:C:210:GLY:O	1:C:214:GLY:HA3	2.18	0.43
1:C:418:PHE:O	1:C:422:GLU:HG3	2.19	0.43
1:C:438:GLY:O	1:C:439:THR:HB	2.17	0.43
1:A:187:LEU:HD11	1:A:207:THR:HG21	2.01	0.43
1:B:228:PHE:CZ	1:B:230:GLY:HA3	2.54	0.43
1:D:133:LYS:NZ	4:D:3252:HOH:O	2.52	0.43
1:A:159:LEU:HA	1:A:159:LEU:HD12	1.83	0.43
1:A:414:PHE:HB2	1:D:414:PHE:HB2	2.01	0.43
1:D:436:GLN:C	1:D:438:GLY:N	2.69	0.43
1:C:100:GLU:HG3	1:C:158:ASN:HB2	2.00	0.43
1:C:85:ILE:HD12	1:C:188:LEU:HD11	2.01	0.42
1:B:116:LEU:HD12	1:B:116:LEU:C	2.39	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:334:VAL:O	1:A:338:ILE:HG13	2.20	0.42
1:D:49:ALA:HA	1:D:201:GLY:O	2.19	0.42
1:C:297:ALA:O	1:C:301:VAL:HG23	2.20	0.42
1:C:420:ILE:O	1:C:424:LEU:HG	2.19	0.42
1:D:413:ASP:OD1	1:D:415:PRO:HD2	2.20	0.42
1:C:209:ARG:HD2	1:C:209:ARG:HA	1.74	0.42
1:D:96:SER:O	1:D:99:SER:HB2	2.19	0.42
1:C:383:LEU:HD12	1:C:384:PRO:HD2	2.00	0.42
1:C:260:LEU:HD21	1:C:391:VAL:HG22	2.02	0.42
1:A:158:ASN:ND2	1:A:158:ASN:C	2.73	0.42
1:B:209:ARG:HA	1:B:209:ARG:HD2	1.82	0.42
1:C:260:LEU:CD2	1:C:391:VAL:HG22	2.50	0.42
1:D:7:ASN:OD1	1:D:207:THR:HG23	2.19	0.42
1:A:214:GLY:O	1:A:217:ILE:HG12	2.20	0.42
1:B:147:VAL:HG22	1:B:225:PHE:HB3	2.00	0.42
1:C:263:ALA:HB2	1:C:410:PHE:O	2.19	0.42
1:C:152:PRO:HG3	1:C:159:LEU:HD23	2.02	0.42
1:C:228:PHE:HE1	3:C:3003:NAP:O4B	2.03	0.42
1:D:439:THR:O	1:D:442:PHE:HB2	2.19	0.42
1:D:2:THR:HG21	1:D:32:GLY:HA2	1.99	0.41
1:A:305:ARG:HH11	1:A:305:ARG:HB3	1.84	0.41
1:D:104:THR:O	1:D:108:ILE:HG13	2.19	0.41
1:C:472:PHE:CD2	1:D:414:PHE:HZ	2.38	0.41
1:A:157:VAL:O	1:A:160:ALA:HB3	2.20	0.41
1:B:413:ASP:OD1	1:B:415:PRO:HD2	2.20	0.41
1:A:186:GLY:O	1:A:189:LEU:HB3	2.20	0.41
1:C:153:PHE:C	1:C:153:PHE:CD1	2.93	0.41
1:D:250:GLU:HB3	3:D:3004:NAP:C7N	2.51	0.41
1:A:250:GLU:HB3	3:A:3001:NAP:C7N	2.50	0.41
1:B:209:ARG:C	1:B:211:SER:N	2.73	0.41
1:C:153:PHE:HA	1:C:179:PRO:HG3	2.02	0.41
1:B:369:THR:HB	1:B:375:TRP:HZ2	1.85	0.41
1:D:268:THR:HG23	1:D:410:PHE:CD1	2.55	0.41
1:A:302:GLU:CD	1:A:305:ARG:NH1	2.73	0.41
1:D:227:ASN:C	1:D:227:ASN:HD22	2.24	0.41
1:A:367:VAL:HG21	1:A:384:PRO:HB2	2.02	0.41
1:A:139:VAL:HG13	1:A:467:VAL:HG13	2.02	0.41
1:C:255:ASP:HB2	1:C:286:ALA:O	2.21	0.41
1:A:325:LEU:HD12	1:A:331:ALA:HA	2.03	0.41
1:B:116:LEU:HD12	1:B:117:ARG:HG3	2.03	0.41
1:C:176:PHE:CZ	1:C:178:PRO:HB3	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:GLU:CD	1:A:182:GLY:HA2	2.41	0.41
1:A:151:SER:HB2	1:A:152:PRO:HD2	2.02	0.41
1:A:153:PHE:HA	1:A:179:PRO:HG3	2.01	0.41
1:C:262:ASP:O	1:C:412:ASN:ND2	2.54	0.41
1:C:240:LYS:HB3	1:C:240:LYS:HE2	1.84	0.41
1:D:230:GLY:HA3	3:D:3004:NAP:H51A	2.03	0.41
1:A:439:THR:O	1:A:442:PHE:HB2	2.21	0.41
1:B:275:GLY:HA2	1:B:283:ARG:HH22	1.85	0.41
1:B:159:LEU:HD12	1:B:159:LEU:HA	1.88	0.41
1:B:315:ASN:HA	1:B:315:ASN:HD22	1.69	0.41
1:D:129:GLU:O	1:D:129:GLU:HG3	2.20	0.41
1:A:262:ASP:O	1:A:412:ASN:ND2	2.54	0.41
1:D:291:LEU:HD23	1:D:386:ILE:HB	2.03	0.41
1:C:391:VAL:HG21	1:C:416:ARG:NH2	2.36	0.41
1:C:350:THR:HB	1:C:362:ILE:HG13	2.02	0.41
1:A:81:LYS:HB2	1:A:81:LYS:HE3	1.87	0.41
1:D:153:PHE:C	1:D:153:PHE:CD1	2.94	0.40
1:C:351:GLU:OE2	1:C:351:GLU:N	2.54	0.40
1:B:260:LEU:CD2	1:B:391:VAL:HG22	2.51	0.40
1:B:117:ARG:HH11	1:B:117:ARG:HG3	1.86	0.40
1:B:113:GLU:HB2	1:D:117:ARG:NH2	2.35	0.40
1:A:116:LEU:HD12	1:A:117:ARG:N	2.36	0.40
1:A:325:LEU:CD1	1:A:359:ILE:HD12	2.51	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	471/475 (99%)	448 (95%)	21 (4%)	2 (0%)	39	61
1	B	471/475 (99%)	447 (95%)	23 (5%)	1 (0%)	52	75

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	472/475 (99%)	446 (94%)	24 (5%)	2 (0%)	39	61
1	D	472/475 (99%)	452 (96%)	19 (4%)	1 (0%)	52	75
All	All	1886/1900 (99%)	1793 (95%)	87 (5%)	6 (0%)	46	68

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	438	GLY
1	B	438	GLY
1	C	438	GLY
1	D	438	GLY
1	A	457	VAL
1	C	457	VAL

### 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	377/379 (100%)	367 (97%)	10 (3%)	52	79
1	B	377/379 (100%)	366 (97%)	11 (3%)	50	77
1	C	378/379 (100%)	367 (97%)	11 (3%)	50	77
1	D	378/379 (100%)	366 (97%)	12 (3%)	46	74
All	All	1510/1516 (100%)	1466 (97%)	44 (3%)	50	77

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	LEU
1	A	116	LEU
1	A	152	PRO
1	A	158	ASN
1	A	159	LEU
1	A	227	ASN

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Mol	Chain	Res	Type
1	A	284	CYS
1	A	379	PHE
1	A	411	THR
1	A	414	PHE
1	B	118	MET
1	B	159	LEU
1	B	227	ASN
1	B	248	MET
1	B	284	CYS
1	B	342	ASN
1	B	379	PHE
1	B	414	PHE
1	B	418	PHE
1	B	433	ASN
1	B	467	VAL
1	C	116	LEU
1	C	158	ASN
1	C	159	LEU
1	C	227	ASN
1	C	237	ARG
1	C	284	CYS
1	C	351	GLU
1	C	379	PHE
1	C	414	PHE
1	C	418	PHE
1	C	467	VAL
1	D	121	GLU
1	D	153	PHE
1	D	158	ASN
1	D	159	LEU
1	D	221	GLN
1	D	227	ASN
1	D	342	ASN
1	D	379	PHE
1	D	414	PHE
1	D	418	PHE
1	D	455	GLN
1	D	467	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	109	ASN
1	A	158	ASN
1	A	227	ASN
1	A	315	ASN
1	A	342	ASN
1	A	412	ASN
1	A	430	HIS
1	A	436	GLN
1	A	455	GLN
1	B	109	ASN
1	B	158	ASN
1	B	227	ASN
1	B	315	ASN
1	B	342	ASN
1	B	436	GLN
1	B	455	GLN
1	C	109	ASN
1	C	158	ASN
1	C	227	ASN
1	C	315	ASN
1	C	430	HIS
1	C	455	GLN
1	D	109	ASN
1	D	158	ASN
1	D	227	ASN
1	D	315	ASN
1	D	342	ASN
1	D	423	GLN
1	D	436	GLN
1	D	455	GLN

### 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 ⓘ

11 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	SO4	A	2001	-	4,4,4	3.39	2 (50%)	6,6,6	0.91	0
3	NAP	A	3001	-	42,52,52	1.80	10 (23%)	54,80,80	1.67	10 (18%)
2	SO4	B	2002	-	4,4,4	3.38	2 (50%)	6,6,6	0.95	0
2	SO4	B	2003	-	4,4,4	3.42	2 (50%)	6,6,6	0.94	0
3	NAP	B	3002	-	42,52,52	1.76	8 (19%)	54,80,80	1.69	8 (14%)
2	SO4	C	2004	-	4,4,4	3.39	2 (50%)	6,6,6	0.94	0
3	NAP	C	3003	-	42,52,52	1.74	9 (21%)	54,80,80	1.71	8 (14%)
2	SO4	D	2005	-	4,4,4	3.38	2 (50%)	6,6,6	0.90	0
2	SO4	D	2006	-	4,4,4	3.39	2 (50%)	6,6,6	0.95	0
2	SO4	D	2007	-	4,4,4	3.36	2 (50%)	6,6,6	0.97	0
3	NAP	D	3004	-	42,52,52	1.77	8 (19%)	54,80,80	1.68	8 (14%)

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	2001	-	-	0/0/0/0	0/0/0/0
3	NAP	A	3001	-	-	0/27/67/67	0/5/5/5
2	SO4	B	2002	-	-	0/0/0/0	0/0/0/0
2	SO4	B	2003	-	-	0/0/0/0	0/0/0/0
3	NAP	B	3002	-	-	0/27/67/67	0/5/5/5
2	SO4	C	2004	-	-	0/0/0/0	0/0/0/0
3	NAP	C	3003	-	-	0/27/67/67	0/5/5/5
2	SO4	D	2005	-	-	0/0/0/0	0/0/0/0
2	SO4	D	2006	-	-	0/0/0/0	0/0/0/0
2	SO4	D	2007	-	-	0/0/0/0	0/0/0/0
3	NAP	D	3004	-	-	0/27/67/67	0/5/5/5

All (49) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2003	SO4	O3-S	-4.93	1.29	1.47
2	D	2005	SO4	O3-S	-4.90	1.29	1.47
2	B	2002	SO4	O3-S	-4.87	1.29	1.47
2	D	2006	SO4	O3-S	-4.83	1.30	1.47
2	A	2001	SO4	O3-S	-4.81	1.30	1.47
2	C	2004	SO4	O3-S	-4.77	1.30	1.47
2	D	2007	SO4	O3-S	-4.72	1.30	1.47
3	D	3004	NAP	PA-O1A	-2.78	1.41	1.51
3	C	3003	NAP	PA-O1A	-2.72	1.41	1.51
3	B	3002	NAP	PA-O1A	-2.72	1.41	1.51
3	A	3001	NAP	PA-O1A	-2.66	1.41	1.51
3	C	3003	NAP	C5B-C4B	2.01	1.58	1.51
3	A	3001	NAP	C6N-C5N	2.02	1.43	1.38
3	C	3003	NAP	C4A-N3A	2.11	1.38	1.35
3	A	3001	NAP	C5B-C4B	2.17	1.58	1.51
3	B	3002	NAP	O4B-C4B	2.17	1.50	1.45
3	A	3001	NAP	O4B-C4B	2.26	1.50	1.45
3	D	3004	NAP	O4B-C4B	2.26	1.50	1.45
3	D	3004	NAP	C4A-N3A	2.31	1.39	1.35
3	B	3002	NAP	C4A-N3A	2.41	1.39	1.35
3	A	3001	NAP	C4A-N3A	2.43	1.39	1.35
3	C	3003	NAP	O4B-C4B	2.45	1.50	1.45
3	D	3004	NAP	C6N-N1N	3.25	1.44	1.35
3	C	3003	NAP	C2A-N1A	3.31	1.40	1.33
3	B	3002	NAP	C6N-N1N	3.32	1.44	1.35
3	C	3003	NAP	C6N-N1N	3.32	1.44	1.35
3	A	3001	NAP	C6N-N1N	3.36	1.44	1.35
3	B	3002	NAP	C2A-N1A	3.62	1.40	1.33
3	D	3004	NAP	C2A-N1A	3.67	1.40	1.33
3	A	3001	NAP	C2A-N1A	3.75	1.41	1.33
3	D	3004	NAP	C2A-N3A	3.84	1.39	1.32
3	C	3003	NAP	C2A-N3A	3.86	1.39	1.32
3	B	3002	NAP	C2A-N3A	3.97	1.39	1.32
3	A	3001	NAP	C2A-N3A	3.98	1.39	1.32
3	B	3002	NAP	O4D-C1D	4.47	1.46	1.41
3	D	3004	NAP	C4N-C3N	4.48	1.47	1.39
3	B	3002	NAP	C4N-C3N	4.55	1.47	1.39
2	D	2005	SO4	O1-S	4.61	1.62	1.47
3	C	3003	NAP	O4D-C1D	4.62	1.47	1.41
2	B	2002	SO4	O1-S	4.62	1.63	1.47
3	A	3001	NAP	C4N-C3N	4.63	1.47	1.39
2	B	2003	SO4	O1-S	4.64	1.63	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	3003	NAP	C4N-C3N	4.64	1.47	1.39
2	D	2007	SO4	O1-S	4.64	1.63	1.47
3	A	3001	NAP	O4D-C1D	4.65	1.47	1.41
2	D	2006	SO4	O1-S	4.66	1.63	1.47
3	D	3004	NAP	O4D-C1D	4.67	1.47	1.41
2	A	2001	SO4	O1-S	4.71	1.63	1.47
2	C	2004	SO4	O1-S	4.73	1.63	1.47

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	3002	NAP	N3A-C2A-N1A	-7.69	123.01	128.89
3	C	3003	NAP	N3A-C2A-N1A	-7.63	123.05	128.89
3	A	3001	NAP	N3A-C2A-N1A	-7.61	123.07	128.89
3	D	3004	NAP	N3A-C2A-N1A	-7.55	123.11	128.89
3	B	3002	NAP	C1B-N9A-C4A	-3.31	121.95	126.94
3	C	3003	NAP	O7N-C7N-C3N	-3.29	116.00	119.59
3	D	3004	NAP	C1B-N9A-C4A	-3.19	122.13	126.94
3	C	3003	NAP	O4B-C1B-C2B	-3.08	101.02	106.60
3	B	3002	NAP	O4B-C1B-C2B	-3.08	101.03	106.60
3	D	3004	NAP	O4B-C1B-C2B	-3.06	101.07	106.60
3	A	3001	NAP	C1B-N9A-C4A	-3.06	122.33	126.94
3	D	3004	NAP	O7N-C7N-C3N	-3.05	116.26	119.59
3	C	3003	NAP	C1B-N9A-C4A	-3.04	122.36	126.94
3	B	3002	NAP	O7N-C7N-C3N	-2.93	116.39	119.59
3	A	3001	NAP	O7N-C7N-C3N	-2.87	116.45	119.59
3	A	3001	NAP	O4B-C1B-C2B	-2.61	101.89	106.60
3	C	3003	NAP	O3B-C3B-C4B	-2.18	104.52	111.05
3	A	3001	NAP	O3B-C3B-C4B	-2.14	104.63	111.05
3	D	3004	NAP	O3B-C3B-C4B	-2.13	104.66	111.05
3	B	3002	NAP	O3B-C3B-C4B	-2.05	104.91	111.05
3	A	3001	NAP	O4D-C1D-N1N	-2.02	105.91	108.13
3	A	3001	NAP	C4B-O4B-C1B	2.21	112.14	109.72
3	C	3003	NAP	O3X-P2B-O2X	2.23	115.86	107.38
3	A	3001	NAP	O3X-P2B-O2X	2.26	116.00	107.38
3	D	3004	NAP	O3X-P2B-O2X	2.28	116.04	107.38
3	B	3002	NAP	O3X-P2B-O2X	2.28	116.06	107.38
3	D	3004	NAP	C2N-C3N-C4N	2.72	121.32	118.29
3	C	3003	NAP	C2N-C3N-C4N	2.79	121.40	118.29
3	B	3002	NAP	C2N-C3N-C4N	2.86	121.47	118.29
3	A	3001	NAP	C2N-C3N-C4N	2.90	121.52	118.29
3	B	3002	NAP	C3N-C7N-N7N	3.06	121.17	117.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	3001	NAP	C3N-C7N-N7N	3.09	121.20	117.82
3	D	3004	NAP	C3N-C7N-N7N	3.23	121.35	117.82
3	C	3003	NAP	C3N-C7N-N7N	3.41	121.55	117.82

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	3001	NAP	3	0
3	B	3002	NAP	3	0
3	C	3003	NAP	4	0
2	D	2007	SO4	2	0
3	D	3004	NAP	4	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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	473/475 (99%)	-0.43	4 (0%) 87 89	12, 24, 40, 59	0
1	B	473/475 (99%)	-0.46	2 (0%) 93 93	15, 28, 41, 58	0
1	C	474/475 (99%)	-0.60	0 100 100	10, 19, 31, 44	0
1	D	474/475 (99%)	-0.62	0 100 100	11, 20, 32, 54	0
All	All	1894/1900 (99%)	-0.53	6 (0%) 94 95	10, 23, 37, 59	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	438	GLY	3.8
1	A	17	GLU	3.2
1	B	17	GLU	3.1
1	A	211	SER	2.6
1	B	209	ARG	2.3
1	A	370	ASP	2.3

### 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	NAP	B	3002	48/48	0.93	0.18	1.10	32,35,41,41	48
3	NAP	A	3001	48/48	0.94	0.15	0.63	30,34,39,40	48
3	NAP	C	3003	48/48	0.96	0.13	0.53	13,24,32,32	48
3	NAP	D	3004	48/48	0.95	0.14	0.46	21,27,35,37	48
2	SO4	D	2005	5/5	0.97	0.17	0.46	43,43,45,45	0
2	SO4	B	2002	5/5	0.96	0.15	0.33	48,48,51,51	0
2	SO4	A	2001	5/5	0.97	0.15	-0.05	40,43,43,44	0
2	SO4	D	2007	5/5	0.99	0.11	-0.92	39,39,40,41	0
2	SO4	C	2004	5/5	0.97	0.11	-0.94	28,31,33,35	0
2	SO4	B	2003	5/5	0.98	0.12	-	20,20,20,21	5
2	SO4	D	2006	5/5	0.98	0.18	-	31,32,33,34	5

## 6.5 Other polymers [i](#)

There are no such residues in this entry.