



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 5, 2017 – 02:52 AM EDT

PDB ID : 4X90  
Title : Crystal structure of Lysosomal Phospholipase A2  
Authors : Glukhova, A.; Tesmer, J.J.G.  
Deposited on : unknown  
Resolution : 1.84 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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20029824  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20029824

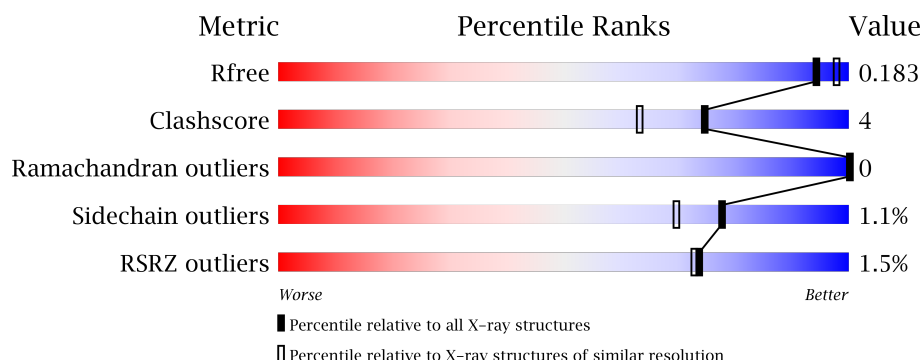
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.84 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	2964 (1.86-1.82)
Clashscore	112137	3197 (1.86-1.82)
Ramachandran outliers	110173	3164 (1.86-1.82)
Sidechain outliers	110143	3165 (1.86-1.82)
RSRZ outliers	101464	2973 (1.86-1.82)

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	380	<div> <div>0.1%</div> <div>92%</div> <div>6%</div> <div>..</div> </div>
1	B	380	<div> <div>3%</div> <div>95%</div> <div>..</div> </div>
1	C	380	<div> <div>2%</div> <div>95%</div> <div>..</div> </div>
1	D	380	<div> <div>0.1%</div> <div>93%</div> <div>6%</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
2	NAG	A	402	-	-	-	X
2	NAG	B	402	-	-	-	X
2	NAG	B	403[B]	-	-	-	X
2	NAG	B	404	-	-	-	X
2	NAG	C	402	-	-	-	X
2	NAG	C	403[A]	-	-	-	X
2	NAG	D	403	-	-	-	X
2	NAG	D	404[A]	-	-	-	X
3	EPE	A	405	-	-	-	X
3	EPE	B	405	-	-	-	X
3	EPE	C	405	-	-	-	X
3	EPE	D	406	-	-	-	X
5	PO4	A	407	-	-	-	X
5	PO4	D	408	-	-	X	-
6	MPD	A	409	-	-	-	X
6	MPD	A	411	-	-	-	X
6	MPD	B	408	-	-	-	X
6	MPD	B	409	-	-	-	X
6	MPD	C	408	-	-	-	X
6	MPD	C	409	-	-	-	X
6	MPD	D	401	-	-	-	X
6	MPD	D	409	-	-	-	X
6	MPD	D	410	-	-	-	X

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 14133 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 Group XV phospholipase A2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	376	Total	C	N	O	S	0	19	0
			3158	2040	529	573	16			
1	B	376	Total	C	N	O	S	0	18	0
			3142	2034	526	566	16			
1	C	376	Total	C	N	O	S	0	16	0
			3133	2026	526	565	16			
1	D	376	Total	C	N	O	S	0	19	0
			3159	2039	529	575	16			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	cloning artifact	UNP Q8NCC3
B	0	GLY	-	cloning artifact	UNP Q8NCC3
C	0	GLY	-	cloning artifact	UNP Q8NCC3
D	0	GLY	-	cloning artifact	UNP Q8NCC3

- Molecule 2 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



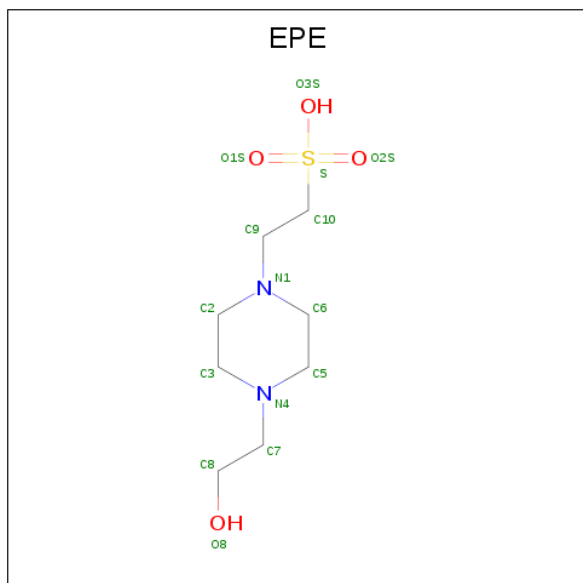
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	1
			28	16	2	10		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	1
			28	16	2	10		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	1
			28	16	2	10		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	D	1	Total	C	N	O	0	0
			14	8	1	5		
2	D	1	Total	C	N	O	0	0
			14	8	1	5		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	D	1	Total	C	N	O	0	1
			28	16	2	10		
2	D	1	Total	C	N	O	0	0
			14	8	1	5		

- 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		
3	C	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
3	D	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total 1 Cl	0	0
			1		
4	A	1	Total 1 Cl	0	0
			1		
4	D	1	Total 1 Cl	0	0
			1		

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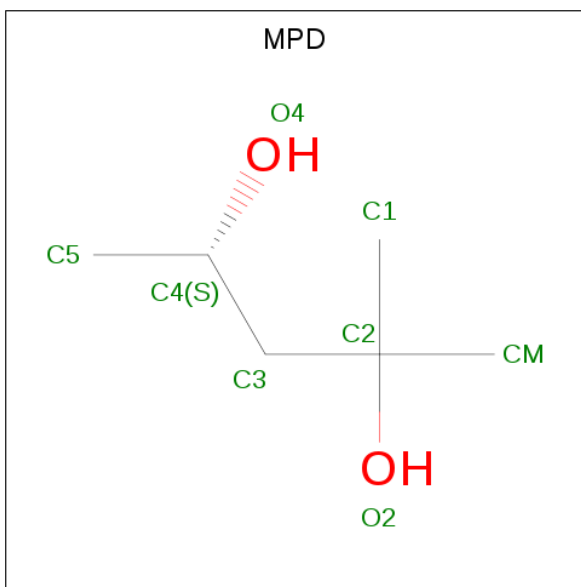
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	1	Total	Cl	0	0
			1	1		

- Molecule 5 is PHOSPHATE ION (three-letter code: PO4) (formula:  $O_4P$ ).



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

- Molecule 6 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula:  $C_6H_{14}O_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			8	6	2		
6	A	1	Total	C	O	0	0
			8	6	2		
6	A	1	Total	C	O	0	0
			8	6	2		
6	A	1	Total	C	O	0	0
			8	6	2		
6	A	1	Total	C	O	0	0
			8	6	2		
6	B	1	Total	C	O	0	0
			8	6	2		
6	B	1	Total	C	O	0	0
			8	6	2		
6	C	1	Total	C	O	0	0
			8	6	2		
6	C	1	Total	C	O	0	0
			8	6	2		
6	D	1	Total	C	O	0	0
			8	6	2		
6	D	1	Total	C	O	0	0
			8	6	2		
6	D	1	Total	C	O	0	0
			8	6	2		
6	D	1	Total	C	O	0	0
			8	6	2		



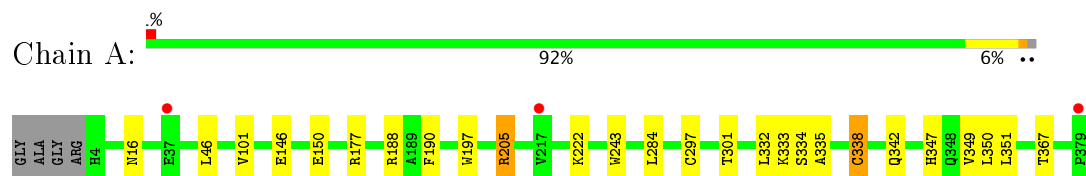
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	280	Total 280	O 280	0	0
7	B	235	Total 235	O 235	0	0
7	C	274	Total 274	O 274	0	0
7	D	276	Total 276	O 276	0	0

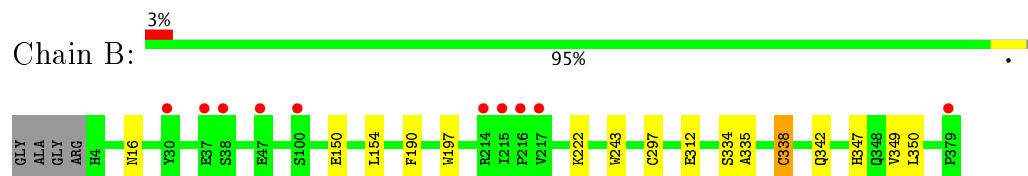
### 3 Residue-property plots [i](#)

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

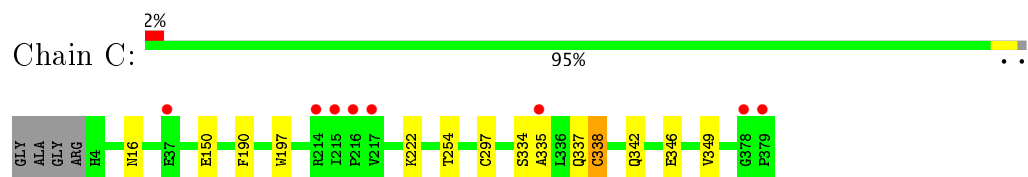
- Molecule 1: Group XV phospholipase A2



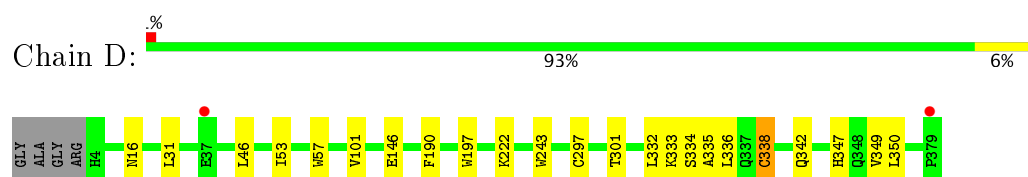
- Molecule 1: Group XV phospholipase A2



- Molecule 1: Group XV phospholipase A2



- Molecule 1: Group XV phospholipase A2



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	62.81Å 91.15Å 100.27Å 78.13° 88.46° 88.50°	Depositor
Resolution (Å)	30.00 – 1.84 30.08 – 1.84	Depositor EDS
% Data completeness (in resolution range)	96.8 (30.00-1.84) 90.8 (30.08-1.84)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.92 (at 1.84Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, $R_{free}$	0.154 , 0.173 0.165 , 0.183	Depositor DCC
$R_{free}$ test set	9227 reflections (5.30%)	DCC
Wilson B-factor (Å <sup>2</sup> )	21.4	Xtriage
Anisotropy	0.439	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 57.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.199 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	14133	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.78% 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: PO4, MPD, EPE, NAG, CL

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	0.56	2/3270 (0.1%)	0.72	3/4457 (0.1%)
1	B	0.52	0/3260	0.69	0/4444
1	C	0.55	0/3245	0.70	0/4423
1	D	0.55	2/3271 (0.1%)	0.69	0/4458
All	All	0.54	4/13046 (0.0%)	0.70	3/17782 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	338[A]	CYS	CB-SG	-5.23	1.73	1.81
1	D	338[B]	CYS	CB-SG	-5.23	1.73	1.81
1	A	338[A]	CYS	CB-SG	-5.18	1.73	1.81
1	A	338[B]	CYS	CB-SG	-5.18	1.73	1.81

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	205	ARG	NE-CZ-NH2	-7.42	116.59	120.30
1	A	205	ARG	NE-CZ-NH1	6.51	123.55	120.30
1	A	188	ARG	NE-CZ-NH2	-5.36	117.62	120.30

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	3158	0	3085	26	0
1	B	3142	0	3089	17	0
1	C	3133	0	3069	16	0
1	D	3159	0	3080	23	0
2	A	70	0	65	3	0
2	B	70	0	65	2	0
2	C	70	0	65	2	0
2	D	70	0	65	2	0
3	A	15	0	18	0	0
3	B	15	0	17	0	0
3	C	15	0	18	0	0
3	D	15	0	18	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	5	0	0	0	0
5	B	5	0	0	0	0
5	C	5	0	0	0	0
5	D	5	0	0	2	0
6	A	40	0	70	4	0
6	B	16	0	28	1	0
6	C	16	0	28	2	0
6	D	40	0	70	1	0
7	A	280	0	0	18	1
7	B	235	0	0	14	0
7	C	274	0	0	12	2
7	D	276	0	0	12	0
All	All	14133	0	12850	97	2

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 4.

All (97) 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:D:335[B]:ALA:CB	7:D:717:HOH:O	1.83	1.25
2:A:403[B]:NAG:H62	7:A:503:HOH:O	1.05	1.20
1:B:335[B]:ALA:CB	7:B:735:HOH:O	1.96	1.13
1:B:297[A]:CYS:SG	1:B:338[A]:CYS:SG	2.40	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:335[B]:ALA:HB1	7:D:717:HOH:O	1.46	1.10
1:B:335[B]:ALA:HA	7:B:735:HOH:O	1.52	1.09
1:D:335[B]:ALA:CA	7:D:717:HOH:O	1.98	1.06
2:D:404[A]:NAG:H62	7:D:502:HOH:O	0.88	1.05
1:D:347[B]:HIS:HD2	5:D:408:PO4:O4	1.39	1.04
1:A:335[B]:ALA:CB	7:A:703:HOH:O	2.05	1.03
1:C:297[B]:CYS:SG	7:C:737:HOH:O	2.18	0.99
1:C:335[B]:ALA:HA	7:C:773:HOH:O	1.63	0.98
1:D:335[B]:ALA:HA	7:D:717:HOH:O	1.59	0.98
1:C:334[B]:SER:CB	7:C:774:HOH:O	2.11	0.97
1:B:335[B]:ALA:CA	7:B:735:HOH:O	2.05	0.96
1:B:334[B]:SER:CB	7:B:697:HOH:O	2.14	0.96
1:C:335[B]:ALA:CB	7:C:773:HOH:O	2.13	0.94
1:D:297[B]:CYS:SG	7:D:657:HOH:O	2.23	0.94
2:B:403[B]:NAG:N2	7:B:501:HOH:O	1.96	0.94
1:C:335[B]:ALA:CA	7:C:773:HOH:O	2.15	0.92
2:B:402:NAG:H83	7:B:518:HOH:O	1.70	0.90
2:A:402:NAG:H83	7:A:515:HOH:O	1.74	0.86
1:A:335[B]:ALA:HA	7:A:703:HOH:O	1.72	0.86
1:A:146[A]:GLU:CD	7:A:780:HOH:O	2.12	0.86
1:D:334[B]:SER:HB3	7:D:637:HOH:O	1.76	0.84
1:D:347[B]:HIS:CD2	5:D:408:PO4:O4	2.30	0.83
1:D:297[A]:CYS:SG	1:D:338[A]:CYS:SG	2.44	0.82
1:A:146[A]:GLU:OE2	7:A:780:HOH:O	1.96	0.82
2:A:403[B]:NAG:C6	7:A:503:HOH:O	1.81	0.82
1:C:335[B]:ALA:HB1	7:C:773:HOH:O	1.78	0.81
1:A:197[B]:TRP:HB2	1:A:334[B]:SER:O	1.80	0.80
1:C:334[B]:SER:HB2	7:C:774:HOH:O	1.78	0.78
1:B:297[B]:CYS:SG	1:B:338[B]:CYS:SG	2.39	0.77
1:B:334[B]:SER:HB2	7:B:697:HOH:O	1.83	0.76
6:B:408:MPD:HM2	6:B:409:MPD:H13	1.67	0.75
1:A:297[A]:CYS:SG	1:A:338[A]:CYS:SG	2.45	0.74
1:A:297[B]:CYS:SG	7:A:702:HOH:O	2.47	0.73
1:A:335[B]:ALA:CA	7:A:703:HOH:O	2.26	0.72
1:D:334[B]:SER:CB	7:D:637:HOH:O	2.35	0.72
1:A:334[B]:SER:HB3	7:A:631:HOH:O	1.92	0.70
1:C:334[B]:SER:HB3	7:C:774:HOH:O	1.78	0.70
2:C:403[A]:NAG:N2	7:C:501:HOH:O	2.25	0.69
1:B:335[B]:ALA:HB1	7:B:735:HOH:O	1.73	0.69
1:A:338[B]:CYS:HB2	1:A:351:LEU:HD11	1.76	0.68
1:D:197[B]:TRP:HB2	1:D:334[B]:SER:O	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:C:408:MPD:HM2	6:C:409:MPD:H13	1.76	0.66
6:A:409:MPD:O4	6:A:409:MPD:HM1	1.95	0.66
6:A:408:MPD:HM2	6:A:409:MPD:HM3	1.81	0.62
1:C:297[A]:CYS:SG	1:C:338[A]:CYS:HB3	2.40	0.62
1:B:334[B]:SER:HB3	7:B:697:HOH:O	1.84	0.60
2:D:404[A]:NAG:C6	7:D:502:HOH:O	1.73	0.60
6:C:409:MPD:O4	6:C:409:MPD:H11	2.04	0.58
1:C:297[A]:CYS:SG	1:C:338[A]:CYS:CB	2.92	0.58
1:D:146[B]:GLU:HG3	7:D:748:HOH:O	2.03	0.57
1:A:46:LEU:HD11	1:A:101:VAL:HG11	1.86	0.57
1:D:46:LEU:HD11	1:D:101:VAL:HG11	1.87	0.56
1:D:297[A]:CYS:SG	7:D:657:HOH:O	2.58	0.55
1:A:150[A]:GLU:HG3	7:A:780:HOH:O	2.06	0.55
1:D:57:TRP:HH2	6:D:412:MPD:H53	1.72	0.55
1:A:335[B]:ALA:O	1:A:338[B]:CYS:SG	2.66	0.54
1:A:146[B]:GLU:HG2	7:A:733:HOH:O	2.08	0.54
1:A:335[B]:ALA:HB1	7:A:703:HOH:O	1.88	0.53
6:A:411:MPD:H52	6:A:411:MPD:HM2	1.89	0.53
1:A:177:ARG:NH2	1:A:284:LEU:O	2.42	0.52
1:B:197[B]:TRP:HB2	1:B:334[B]:SER:O	2.11	0.51
1:D:146[B]:GLU:HG2	7:D:739:HOH:O	2.10	0.50
1:D:342:GLN:HG2	1:D:349:VAL:HB	1.94	0.50
1:B:350[A]:LEU:HD22	1:B:350[A]:LEU:N	2.28	0.49
1:A:342:GLN:HG2	1:A:349:VAL:HB	1.95	0.49
1:B:342:GLN:HG2	1:B:349:VAL:HB	1.95	0.47
1:A:205:ARG:NH2	7:A:651:HOH:O	2.48	0.47
1:C:150[B]:GLU:HG3	7:C:610:HOH:O	2.13	0.47
6:A:409:MPD:CM	6:A:409:MPD:O4	2.64	0.46
1:D:350[A]:LEU:HD23	1:D:350[A]:LEU:N	2.31	0.46
1:A:350[A]:LEU:HD22	1:A:350[A]:LEU:N	2.30	0.46
1:C:197[B]:TRP:HB2	1:C:334[B]:SER:O	2.17	0.45
1:A:243[B]:TRP:NE1	1:A:333:LYS:HD2	2.32	0.45
1:D:243[B]:TRP:NE1	1:D:333:LYS:HD2	2.32	0.45
1:A:335[B]:ALA:HB2	7:A:703:HOH:O	1.94	0.44
1:C:342:GLN:HG2	1:C:349:VAL:HB	1.98	0.44
1:D:31:LEU:HD13	1:D:53:ILE:HD12	1.99	0.44
1:A:347[B]:HIS:HE1	7:A:519:HOH:O	2.01	0.44
1:A:243[B]:TRP:CD1	1:A:333:LYS:HD2	2.53	0.43
1:C:254:THR:C	2:C:403[A]:NAG:H82	2.38	0.43
1:A:301:THR:HG22	1:A:332:LEU:HD13	2.02	0.42
1:B:150[B]:GLU:HG3	7:B:572:HOH:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:301:THR:HG22	1:D:332:LEU:HD13	2.02	0.42
1:B:243[B]:TRP:HD1	7:B:553:HOH:O	2.03	0.42
1:B:154:LEU:HG	7:B:714:HOH:O	2.20	0.41
1:A:350[A]:LEU:HD13	7:A:745:HOH:O	2.21	0.41
1:D:336[B]:LEU:HD23	1:D:336[B]:LEU:HA	1.87	0.41
1:C:346:GLU:HG3	7:C:531:HOH:O	2.21	0.41
1:A:367[A]:THR:HG23	7:A:761:HOH:O	2.20	0.41
1:B:312:GLU:HG2	7:B:527:HOH:O	2.20	0.40
1:B:347[B]:HIS:HE1	7:B:631:HOH:O	2.03	0.40
1:C:337[B]:GLN:HB2	7:C:684:HOH:O	2.21	0.40
1:D:31:LEU:HD13	1:D:53:ILE:CD1	2.50	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:528:HOH:O	7:C:534:HOH:O[1_556]	2.02	0.18
7:C:533:HOH:O	7:C:537:HOH:O[1_655]	2.08	0.12

## 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	393/380 (103%)	383 (98%)	10 (2%)	0	100	100
1	B	392/380 (103%)	385 (98%)	7 (2%)	0	100	100
1	C	390/380 (103%)	383 (98%)	7 (2%)	0	100	100
1	D	393/380 (103%)	385 (98%)	8 (2%)	0	100	100
All	All	1568/1520 (103%)	1536 (98%)	32 (2%)	0	100	100

There are no Ramachandran outliers to report.



### 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	345/329 (105%)	342 (99%)	3 (1%)	82	76
1	B	344/329 (105%)	339 (98%)	5 (2%)	70	57
1	C	342/329 (104%)	337 (98%)	5 (2%)	70	57
1	D	345/329 (105%)	342 (99%)	3 (1%)	82	76
All	All	1376/1316 (105%)	1360 (99%)	16 (1%)	78	67

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	ASN
1	A	190	PHE
1	A	222	LYS
1	B	16	ASN
1	B	190	PHE
1	B	222	LYS
1	B	338[A]	CYS
1	B	338[B]	CYS
1	C	16	ASN
1	C	190	PHE
1	C	222	LYS
1	C	338[A]	CYS
1	C	338[B]	CYS
1	D	16	ASN
1	D	190	PHE
1	D	222	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	226	GLN
1	D	226	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 ⓘ

Of 46 ligands modelled in this entry, 4 are monoatomic - leaving 42 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	NAG	A	401	1	14,14,15	0.62	0	15,19,21	1.32	1 (6%)
2	NAG	A	402	1	14,14,15	0.67	0	15,19,21	1.70	4 (26%)
2	NAG	A	403[A]	1	14,14,15	0.53	0	15,19,21	0.87	1 (6%)
2	NAG	A	403[B]	1	14,14,15	0.66	0	15,19,21	0.78	0
2	NAG	A	404	1	14,14,15	0.59	0	15,19,21	1.00	0
3	EPE	A	405	-	15,15,15	1.67	1 (6%)	18,20,20	1.18	2 (11%)
5	PO4	A	407	-	4,4,4	0.42	0	6,6,6	0.90	0
6	MPD	A	408	-	7,7,7	0.26	0	9,10,10	0.36	0
6	MPD	A	409	-	7,7,7	0.25	0	9,10,10	0.38	0
6	MPD	A	410	-	7,7,7	0.24	0	9,10,10	0.21	0
6	MPD	A	411	-	7,7,7	0.24	0	9,10,10	0.54	0
6	MPD	A	412	-	7,7,7	0.37	0	9,10,10	0.41	0
2	NAG	B	401	1	14,14,15	0.53	0	15,19,21	0.89	1 (6%)
2	NAG	B	402	1	14,14,15	0.55	0	15,19,21	2.22	5 (33%)
2	NAG	B	403[A]	1	14,14,15	0.67	0	15,19,21	1.59	3 (20%)
2	NAG	B	403[B]	1	14,14,15	0.55	0	15,19,21	1.38	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	NAG	B	404	1	14,14,15	0.68	0	15,19,21	1.43	3 (20%)
3	EPE	B	405	-	15,15,15	1.92	1 (6%)	18,20,20	1.78	3 (16%)
5	PO4	B	407	-	4,4,4	0.73	0	6,6,6	0.51	0
6	MPD	B	408	-	7,7,7	0.23	0	9,10,10	0.44	0
6	MPD	B	409	-	7,7,7	0.28	0	9,10,10	0.51	0
2	NAG	C	401	1	14,14,15	0.35	0	15,19,21	1.79	4 (26%)
2	NAG	C	402	1	14,14,15	0.79	1 (7%)	15,19,21	1.51	4 (26%)
2	NAG	C	403[A]	1	14,14,15	0.60	0	15,19,21	1.38	1 (6%)
2	NAG	C	403[B]	1	14,14,15	0.63	0	15,19,21	1.38	2 (13%)
2	NAG	C	404	1	14,14,15	0.64	0	15,19,21	1.06	2 (13%)
3	EPE	C	405	-	15,15,15	1.61	1 (6%)	18,20,20	1.75	3 (16%)
5	PO4	C	407	-	4,4,4	0.63	0	6,6,6	0.90	0
6	MPD	C	408	-	7,7,7	0.18	0	9,10,10	0.46	0
6	MPD	C	409	-	7,7,7	0.23	0	9,10,10	0.48	0
6	MPD	D	401	-	7,7,7	0.31	0	9,10,10	0.29	0
2	NAG	D	402	1	14,14,15	0.64	0	15,19,21	1.34	2 (13%)
2	NAG	D	403	1	14,14,15	0.53	0	15,19,21	1.14	1 (6%)
2	NAG	D	404[A]	1	14,14,15	0.85	0	15,19,21	1.39	3 (20%)
2	NAG	D	404[B]	1	14,14,15	0.61	0	15,19,21	0.98	1 (6%)
2	NAG	D	405	1	14,14,15	0.46	0	15,19,21	0.85	0
3	EPE	D	406	-	15,15,15	1.85	1 (6%)	18,20,20	1.63	3 (16%)
5	PO4	D	408	-	4,4,4	0.79	0	6,6,6	0.67	0
6	MPD	D	409	-	7,7,7	0.29	0	9,10,10	0.41	0
6	MPD	D	410	-	7,7,7	0.19	0	9,10,10	0.33	0
6	MPD	D	411	-	7,7,7	0.20	0	9,10,10	0.37	0
6	MPD	D	412	-	7,7,7	0.29	0	9,10,10	0.44	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	NAG	A	401	1	-	0/6/23/26	0/1/1/1
2	NAG	A	402	1	-	0/6/23/26	0/1/1/1
2	NAG	A	403[A]	1	-	0/6/23/26	0/1/1/1
2	NAG	A	403[B]	1	-	0/6/23/26	0/1/1/1
2	NAG	A	404	1	-	0/6/23/26	0/1/1/1
3	EPE	A	405	-	-	0/9/19/19	0/1/1/1
5	PO4	A	407	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	MPD	A	408	-	-	0/5/5/5	0/0/0/0
6	MPD	A	409	-	-	0/5/5/5	0/0/0/0
6	MPD	A	410	-	-	0/5/5/5	0/0/0/0
6	MPD	A	411	-	-	0/5/5/5	0/0/0/0
6	MPD	A	412	-	-	0/5/5/5	0/0/0/0
2	NAG	B	401	1	-	0/6/23/26	0/1/1/1
2	NAG	B	402	1	-	0/6/23/26	0/1/1/1
2	NAG	B	403[A]	1	-	0/6/23/26	0/1/1/1
2	NAG	B	403[B]	1	-	0/6/23/26	0/1/1/1
2	NAG	B	404	1	-	0/6/23/26	0/1/1/1
3	EPE	B	405	-	-	0/9/19/19	0/1/1/1
5	PO4	B	407	-	-	0/0/0/0	0/0/0/0
6	MPD	B	408	-	-	0/5/5/5	0/0/0/0
6	MPD	B	409	-	-	0/5/5/5	0/0/0/0
2	NAG	C	401	1	-	0/6/23/26	0/1/1/1
2	NAG	C	402	1	-	0/6/23/26	0/1/1/1
2	NAG	C	403[A]	1	-	0/6/23/26	0/1/1/1
2	NAG	C	403[B]	1	-	0/6/23/26	0/1/1/1
2	NAG	C	404	1	-	0/6/23/26	0/1/1/1
3	EPE	C	405	-	-	0/9/19/19	0/1/1/1
5	PO4	C	407	-	-	0/0/0/0	0/0/0/0
6	MPD	C	408	-	-	0/5/5/5	0/0/0/0
6	MPD	C	409	-	-	0/5/5/5	0/0/0/0
6	MPD	D	401	-	-	0/5/5/5	0/0/0/0
2	NAG	D	402	1	-	0/6/23/26	0/1/1/1
2	NAG	D	403	1	-	0/6/23/26	0/1/1/1
2	NAG	D	404[A]	1	-	0/6/23/26	0/1/1/1
2	NAG	D	404[B]	1	-	0/6/23/26	0/1/1/1
2	NAG	D	405	1	-	0/6/23/26	0/1/1/1
3	EPE	D	406	-	-	0/9/19/19	0/1/1/1
5	PO4	D	408	-	-	0/0/0/0	0/0/0/0
6	MPD	D	409	-	-	0/5/5/5	0/0/0/0
6	MPD	D	410	-	-	0/5/5/5	0/0/0/0
6	MPD	D	411	-	-	0/5/5/5	0/0/0/0
6	MPD	D	412	-	-	0/5/5/5	0/0/0/0

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	405	EPE	C10-S	-7.16	1.66	1.77
3	D	406	EPE	C10-S	-6.83	1.67	1.77
3	A	405	EPE	C10-S	-6.12	1.68	1.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	405	EPE	C10-S	-5.97	1.68	1.77
2	C	402	NAG	C1-C2	2.38	1.55	1.52

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	NAG	O5-C1-C2	-4.10	105.76	111.47
2	B	402	NAG	O7-C7-C8	-4.08	114.62	122.06
2	B	403[A]	NAG	O5-C1-C2	-3.93	106.01	111.47
2	D	404[A]	NAG	O5-C1-C2	-3.32	106.85	111.47
2	C	401	NAG	C6-C5-C4	-3.22	105.47	113.00
2	D	402	NAG	O5-C1-C2	-3.14	107.10	111.47
2	A	402	NAG	O7-C7-C8	-2.79	116.98	122.06
3	C	405	EPE	O3S-S-O1S	-2.68	105.24	111.37
3	A	405	EPE	O2S-S-C10	-2.57	104.58	106.79
2	D	404[B]	NAG	O5-C1-C2	-2.54	107.93	111.47
2	C	404	NAG	C1-C2-N2	-2.52	106.18	110.49
3	D	406	EPE	O1S-S-C10	-2.44	104.70	106.79
2	C	404	NAG	O5-C1-C2	-2.44	108.08	111.47
2	C	401	NAG	O5-C1-C2	-2.40	108.13	111.47
2	C	402	NAG	O7-C7-C8	-2.28	117.91	122.06
2	D	404[A]	NAG	O4-C4-C3	-2.25	105.45	110.36
2	B	404	NAG	C6-C5-C4	-2.22	107.80	113.00
2	B	404	NAG	C1-C2-N2	-2.20	106.74	110.49
2	B	401	NAG	C1-C2-N2	-2.16	106.79	110.49
2	C	403[B]	NAG	O5-C1-C2	-2.11	108.54	111.47
2	B	402	NAG	O5-C1-C2	-2.06	108.61	111.47
2	D	402	NAG	C1-C2-N2	-2.04	107.00	110.49
2	A	403[A]	NAG	O7-C7-C8	-2.02	118.37	122.06
3	B	405	EPE	O2S-S-C10	2.01	108.52	106.79
2	D	404[A]	NAG	C3-C4-C5	2.02	113.78	110.22
2	C	403[A]	NAG	C1-O5-C5	2.03	114.97	112.17
2	C	402	NAG	C1-C2-N2	2.08	114.05	110.49
2	B	403[A]	NAG	C1-C2-N2	2.12	114.11	110.49
2	C	402	NAG	C2-N2-C7	2.15	126.08	122.94
3	B	405	EPE	O3S-S-C10	2.21	108.78	106.06
3	A	405	EPE	O3S-S-C10	2.25	108.83	106.06
2	C	401	NAG	C3-C4-C5	2.42	114.49	110.22
2	B	403[A]	NAG	C1-O5-C5	2.46	115.55	112.17
2	A	402	NAG	C1-O5-C5	2.50	115.62	112.17
2	A	402	NAG	C2-N2-C7	2.59	126.73	122.94
2	B	404	NAG	C1-O5-C5	2.59	115.74	112.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	406	EPE	O3S-S-C10	2.65	109.31	106.06
2	C	402	NAG	C1-O5-C5	3.04	116.36	112.17
2	D	403	NAG	C1-O5-C5	3.15	116.50	112.17
2	B	402	NAG	C2-N2-C7	3.20	127.61	122.94
2	B	402	NAG	C1-O5-C5	3.27	116.67	112.17
3	C	405	EPE	O2S-S-C10	3.47	109.78	106.79
2	A	402	NAG	C8-C7-N2	3.51	122.45	116.11
2	B	403[B]	NAG	C1-O5-C5	3.75	117.34	112.17
2	C	403[B]	NAG	C1-O5-C5	3.94	117.59	112.17
2	C	401	NAG	C1-O5-C5	4.42	118.26	112.17
3	C	405	EPE	O1S-S-C10	4.47	110.63	106.79
2	B	402	NAG	C8-C7-N2	4.68	124.57	116.11
3	D	406	EPE	O2S-S-C10	4.82	110.94	106.79
3	B	405	EPE	O1S-S-C10	5.82	111.80	106.79

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

15 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	402	NAG	1	0
2	A	403[B]	NAG	2	0
6	A	408	MPD	1	0
6	A	409	MPD	3	0
6	A	411	MPD	1	0
2	B	402	NAG	1	0
2	B	403[B]	NAG	1	0
6	B	408	MPD	1	0
6	B	409	MPD	1	0
2	C	403[A]	NAG	2	0
6	C	408	MPD	1	0
6	C	409	MPD	2	0
2	D	404[A]	NAG	2	0
5	D	408	PO4	2	0
6	D	412	MPD	1	0

## 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	376/380 (98%)	-0.39	3 (0%) 86 86	13, 22, 38, 65	0
1	B	376/380 (98%)	-0.18	10 (2%) 55 52	16, 25, 50, 82	0
1	C	376/380 (98%)	-0.31	8 (2%) 64 62	14, 22, 41, 76	0
1	D	376/380 (98%)	-0.36	2 (0%) 90 90	13, 22, 39, 68	0
All	All	1504/1520 (98%)	-0.31	23 (1%) 74 73	13, 23, 43, 82	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	379	PRO	8.3
1	B	379	PRO	7.4
1	C	379	PRO	7.0
1	A	379	PRO	6.2
1	B	214	ARG	5.4
1	B	216	PRO	5.3
1	C	216	PRO	5.2
1	C	214	ARG	5.2
1	B	217	VAL	4.8
1	B	37	GLU	4.1
1	C	217	VAL	3.8
1	B	30	TYR	3.4
1	B	47	GLU	3.2
1	A	217	VAL	3.0
1	C	37	GLU	2.9
1	B	215	ILE	2.6
1	C	335[A]	ALA	2.5
1	C	215	ILE	2.4
1	D	37	GLU	2.4
1	B	100	SER	2.2
1	C	378	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	38	SER	2.1
1	A	37	GLU	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
5	PO4	A	407	5/5	0.61	0.33	6.82	32,43,44,46	5
6	MPD	B	409	8/8	0.81	0.23	6.06	52,53,54,54	0
6	MPD	A	411	8/8	0.78	0.32	5.86	58,60,63,70	0
3	EPE	D	406	15/15	0.93	0.19	5.49	40,44,58,63	0
6	MPD	C	409	8/8	0.88	0.21	5.25	47,49,51,53	0
2	NAG	B	402	14/15	0.93	0.16	3.86	35,40,44,51	0
6	MPD	D	401	8/8	0.93	0.15	3.68	44,47,49,50	0
3	EPE	A	405	15/15	0.94	0.16	3.51	36,40,53,59	0
2	NAG	C	402	14/15	0.94	0.14	3.34	34,39,42,43	0
2	NAG	C	403[A]	14/15	0.93	0.12	3.29	27,28,30,31	14
2	NAG	B	403[B]	14/15	0.93	0.13	3.21	24,28,29,30	14
6	MPD	A	409	8/8	0.89	0.17	3.21	39,42,43,45	0
6	MPD	D	410	8/8	0.85	0.17	3.10	39,41,41,42	0
2	NAG	A	402	14/15	0.94	0.15	2.98	29,35,38,45	0
6	MPD	C	408	8/8	0.88	0.17	2.87	34,42,47,49	0
6	MPD	B	408	8/8	0.87	0.15	2.68	36,42,51,53	0
2	NAG	D	404[A]	14/15	0.92	0.13	2.24	23,25,27,29	14
3	EPE	C	405	15/15	0.96	0.16	2.19	40,49,60,62	0
2	NAG	D	403	14/15	0.94	0.17	2.16	32,37,39,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	EPE	B	405	15/15	0.91	0.20	2.16	61,66,77,81	0
6	MPD	D	409	8/8	0.84	0.18	2.15	45,47,50,51	0
2	NAG	B	404	14/15	0.94	0.15	2.10	35,40,47,48	0
2	NAG	C	404	14/15	0.94	0.16	1.99	30,34,41,41	0
6	MPD	D	412	8/8	0.92	0.18	1.92	47,50,51,54	0
6	MPD	A	412	8/8	0.93	0.11	1.89	45,47,48,49	0
2	NAG	A	404	14/15	0.94	0.14	1.82	29,34,41,41	0
2	NAG	D	405	14/15	0.93	0.14	1.71	29,34,40,41	0
2	NAG	D	404[B]	14/15	0.92	0.13	1.36	21,22,23,23	14
2	NAG	A	403[B]	14/15	0.94	0.11	1.36	22,24,27,27	14
2	NAG	C	403[B]	14/15	0.93	0.12	1.18	28,29,31,31	14
2	NAG	B	403[A]	14/15	0.93	0.13	0.99	27,30,31,32	14
5	PO4	D	408	5/5	0.96	0.10	0.99	27,30,31,34	5
6	MPD	A	408	8/8	0.89	0.14	0.79	41,43,44,45	0
5	PO4	C	407	5/5	0.94	0.11	0.61	25,29,30,30	5
2	NAG	A	403[A]	14/15	0.94	0.11	0.61	24,25,25,26	14
5	PO4	B	407	5/5	0.92	0.13	0.36	31,33,34,35	5
6	MPD	D	411	8/8	0.91	0.11	-0.12	51,54,55,56	0
6	MPD	A	410	8/8	0.95	0.09	-0.82	53,55,58,58	0
4	CL	D	407	1/1	0.98	0.06	-1.24	47,47,47,47	0
4	CL	A	406	1/1	0.95	0.06	-1.37	41,41,41,41	0
4	CL	C	406	1/1	0.99	0.03	-1.61	32,32,32,32	0
4	CL	B	406	1/1	0.98	0.04	-2.33	40,40,40,40	0
2	NAG	D	402	14/15	0.96	0.17	-	34,39,41,41	0
2	NAG	C	401	14/15	0.93	0.22	-	41,46,50,54	0
2	NAG	A	401	14/15	0.93	0.15	-	37,41,43,45	0
2	NAG	B	401	14/15	0.93	0.20	-	45,51,52,56	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.