



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2018 – 10:56 PM EST

PDB ID : 5XNP  
Title : Crystal structures of human SALM5 in complex with human PTPdelta  
Authors : Liu, H.; Lin, Z.; Xu, F.  
Deposited on : 2017-05-24  
Resolution : 3.73 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-20030736  
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-20030736

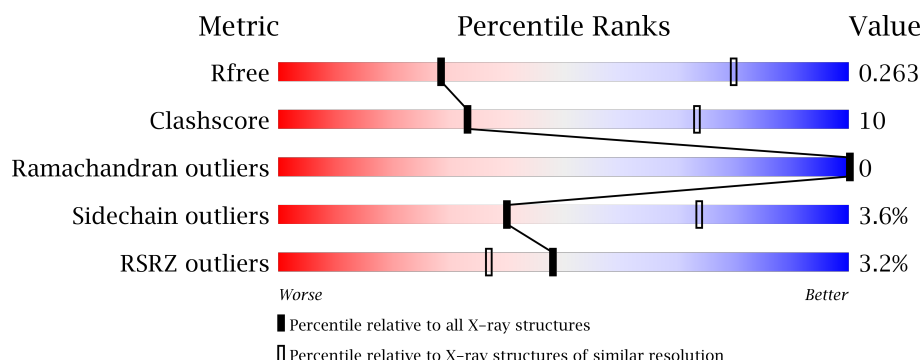
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.73 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	1264 (3.94-3.50)
Clashscore	112137	1408 (3.94-3.50)
Ramachandran outliers	110173	1353 (3.94-3.50)
Sidechain outliers	110143	1350 (3.94-3.50)
RSRZ outliers	101464	1293 (3.94-3.50)

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	361	<div> <div>2%</div> <div>72%</div> <div>26%</div> <div>.</div> </div>
1	B	361	<div> <div>3%</div> <div>70%</div> <div>28%</div> <div>.</div> </div>
2	D	291	<div> <div>4%</div> <div>79%</div> <div>20%</div> <div>.</div> </div>
2	E	291	<div> <div>3%</div> <div>81%</div> <div>18%</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
4	NA	A	404	-	-	-	X
4	NA	B	404	-	-	-	X
7	SO4	A	415	-	-	X	-

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 10418 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 Leucine-rich repeat and fibronectin type-III domain-containing protein 5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	361	Total	C	N	O	S	0	0	0
			2839	1793	500	530	16			
1	B	361	Total	C	N	O	S	0	0	0
			2839	1793	500	530	16			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	14	PRO	-	expression tag	UNP Q96NI6
A	15	GLY	-	expression tag	UNP Q96NI6
A	16	ASP	-	expression tag	UNP Q96NI6
A	17	PRO	-	expression tag	UNP Q96NI6
B	14	PRO	-	expression tag	UNP Q96NI6
B	15	GLY	-	expression tag	UNP Q96NI6
B	16	ASP	-	expression tag	UNP Q96NI6
B	17	PRO	-	expression tag	UNP Q96NI6

- Molecule 2 is a protein called Receptor-type tyrosine-protein phosphatase delta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	291	Total	C	N	O	S	0	0	0
			2244	1394	400	437	13			
2	E	291	Total	C	N	O	S	0	0	0
			2244	1394	400	437	13			

There are 18 discrepancies between the modelled and reference sequences:

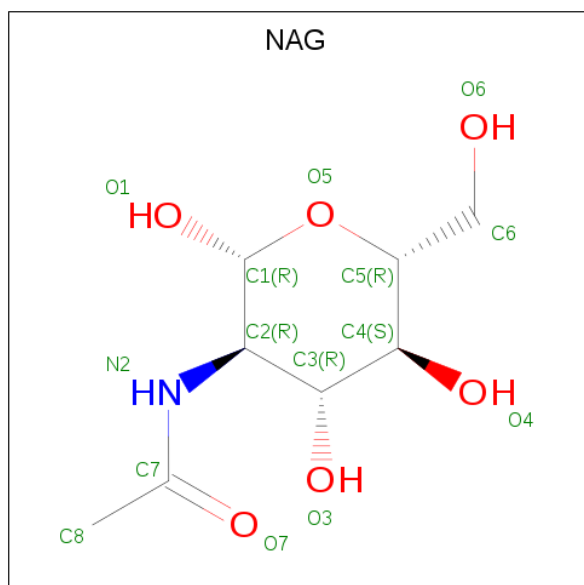
Chain	Residue	Modelled	Actual	Comment	Reference
D	?	-	GLU	deletion	UNP P23468
D	?	-	SER	deletion	UNP P23468
D	?	-	ILE	deletion	UNP P23468

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Chain	Residue	Modelled	Actual	Comment	Reference
D	?	-	GLY	deletion	UNP P23468
D	?	-	GLY	deletion	UNP P23468
D	?	-	THR	deletion	UNP P23468
D	?	-	PRO	deletion	UNP P23468
D	?	-	ILE	deletion	UNP P23468
D	?	-	ARG	deletion	UNP P23468
E	?	-	GLU	deletion	UNP P23468
E	?	-	SER	deletion	UNP P23468
E	?	-	ILE	deletion	UNP P23468
E	?	-	GLY	deletion	UNP P23468
E	?	-	GLY	deletion	UNP P23468
E	?	-	THR	deletion	UNP P23468
E	?	-	PRO	deletion	UNP P23468
E	?	-	ILE	deletion	UNP P23468
E	?	-	ARG	deletion	UNP P23468

- Molecule 3 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	D	1	Total	C	N	O	0	0
			14	8	1	5		
3	E	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

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

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	6	Total	Ca	0	0
			6	6		
5	A	6	Total	Ca	0	0
			6	6		

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	3	Total	Cl	0	0
			3	3		
6	A	3	Total	Cl	0	0
			3	3		
6	D	3	Total	Cl	0	0
			3	3		
6	E	3	Total	Cl	0	0
			3	3		

- Molecule 7 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

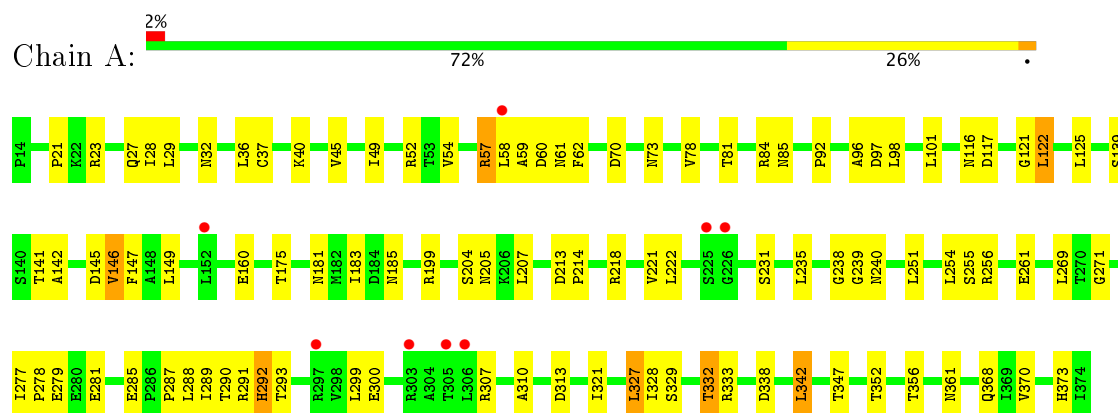
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	32	Total	O	0	0
			32	32		
8	B	35	Total	O	0	0
			35	35		
8	D	14	Total	O	0	0
			14	14		
8	E	13	Total	O	0	0
			13	13		

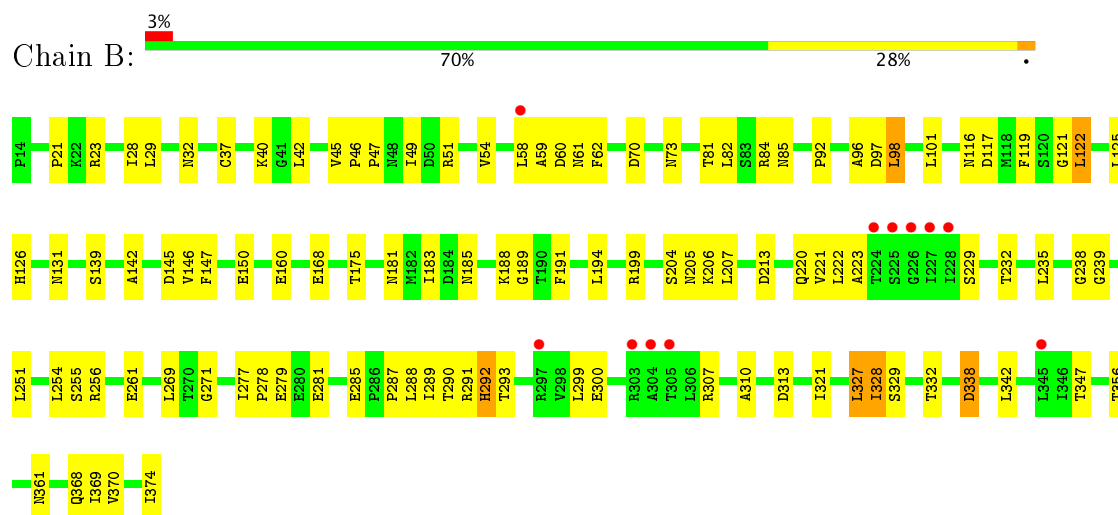
### 3 Residue-property plots

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

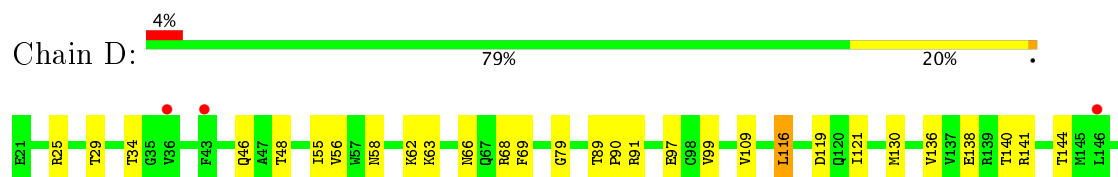
- Molecule 1: Leucine-rich repeat and fibronectin type-III domain-containing protein 5



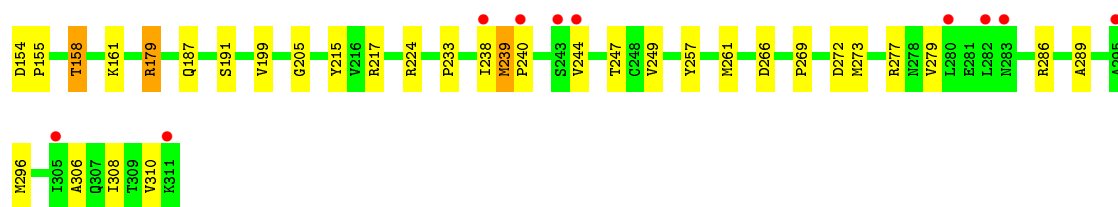
- Molecule 1: Leucine-rich repeat and fibronectin type-III domain-containing protein 5



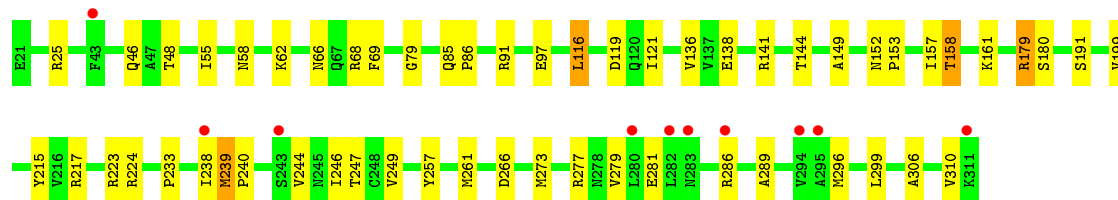
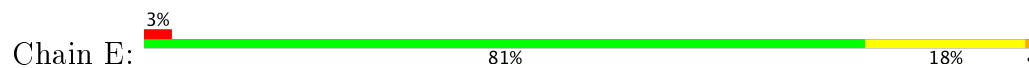
- Molecule 2: Receptor-type tyrosine-protein phosphatase delta







- Molecule 2: Receptor-type tyrosine-protein phosphatase delta



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 2 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	249.38Å 249.38Å 249.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.91 – 3.73 48.91 – 3.73	Depositor EDS
% Data completeness (in resolution range)	99.1 (48.91-3.73) 99.1 (48.91-3.73)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.32 (at 3.77Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, $R_{free}$	0.232 , 0.264 0.229 , 0.263	Depositor DCC
$R_{free}$ test set	1316 reflections (4.92%)	DCC
Wilson B-factor (Å <sup>2</sup> )	122.4	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 89.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.440 for -l,-k,-h	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	10418	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	133.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.57% 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: SO4, NA, CA, 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	0.27	1/2900 (0.0%)	0.48	0/3947
1	B	0.28	0/2900	0.52	0/3947
2	D	0.25	0/2287	0.46	0/3109
2	E	0.25	0/2287	0.46	0/3109
All	All	0.27	1/10374 (0.0%)	0.48	0/14112

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	240	ASN	C-N	5.59	1.44	1.34

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	2839	0	2847	68	0
1	B	2839	0	2847	69	0
2	D	2244	0	2228	38	0
2	E	2244	0	2228	36	0
3	A	42	0	39	0	0
3	B	42	0	39	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	14	0	13	0	0
3	E	14	0	13	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	6	0	0	0	0
5	B	6	0	0	0	0
6	A	3	0	0	0	0
6	B	3	0	0	0	0
6	D	3	0	0	0	0
6	E	3	0	0	0	0
7	A	10	0	0	4	0
7	B	10	0	0	0	0
8	A	32	0	0	1	0
8	B	35	0	0	0	0
8	D	14	0	0	3	0
8	E	13	0	0	2	0
All	All	10418	0	10254	201	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 (201) 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:292:HIS:CE1	1:A:368:GLN:HE22	1.75	1.05
1:B:292:HIS:CE1	1:B:368:GLN:HE22	1.78	1.01
2:E:25:ARG:HG2	2:E:48:THR:HG22	1.56	0.88
2:D:25:ARG:HG2	2:D:48:THR:HG22	1.56	0.87
1:A:292:HIS:CE1	1:A:368:GLN:NE2	2.45	0.85
1:B:292:HIS:CG	1:B:368:GLN:HE22	1.95	0.83
1:B:292:HIS:CE1	1:B:368:GLN:NE2	2.48	0.82
1:A:96:ALA:HA	1:A:121:GLY:HA3	1.62	0.81
2:E:233:PRO:HB2	2:E:306:ALA:HB2	1.64	0.80
1:A:292:HIS:CG	1:A:368:GLN:HE22	1.99	0.80
1:A:59:ALA:HB2	1:A:81:THR:HG22	1.63	0.79
1:A:204:SER:H	1:A:239:GLY:HA3	1.50	0.77
2:D:257:TYR:HB3	2:D:273:MET:HG2	1.65	0.77
2:D:25:ARG:HG2	2:D:48:THR:CG2	2.14	0.77
1:A:290:THR:HG22	1:A:291:ARG:HG3	1.67	0.76
1:B:96:ALA:HA	1:B:121:GLY:HA3	1.68	0.76
1:A:292:HIS:CD2	1:A:368:GLN:HE22	2.04	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:292:HIS:CD2	1:B:368:GLN:HE22	2.04	0.75
2:D:233:PRO:HB2	2:D:306:ALA:HB2	1.68	0.74
1:B:59:ALA:HB2	1:B:81:THR:HG22	1.69	0.74
1:A:28:ILE:HD12	1:A:29:LEU:HD23	1.70	0.74
2:E:25:ARG:HG2	2:E:48:THR:CG2	2.17	0.74
1:B:290:THR:HG22	1:B:291:ARG:HG3	1.70	0.73
2:E:257:TYR:HB3	2:E:273:MET:HG2	1.69	0.73
2:E:158:THR:HG23	2:E:199:VAL:HB	1.71	0.72
1:B:101:LEU:HD23	1:B:122:LEU:HD11	1.72	0.71
1:B:191:PHE:HA	1:B:194:LEU:HD23	1.72	0.71
1:A:101:LEU:HD23	1:A:122:LEU:HD11	1.71	0.71
1:B:204:SER:H	1:B:239:GLY:HA3	1.56	0.70
2:D:158:THR:HG23	2:D:199:VAL:HB	1.72	0.69
2:D:289:ALA:O	8:D:501:HOH:O	2.10	0.68
1:B:238:GLY:HA2	1:B:261:GLU:HB3	1.77	0.67
2:E:224:ARG:HB2	2:E:299:LEU:HD21	1.76	0.67
2:D:240:PRO:HG3	2:D:310:VAL:HB	1.76	0.67
2:E:240:PRO:HG3	2:E:310:VAL:HB	1.75	0.67
1:A:292:HIS:CD2	7:A:415:SO4:O4	2.48	0.66
2:E:138:GLU:HB2	2:E:141:ARG:HD2	1.77	0.66
2:D:138:GLU:HB2	2:D:141:ARG:HD2	1.78	0.66
1:B:287:PRO:HG3	1:B:361:ASN:HB2	1.78	0.65
1:A:73:ASN:N	1:A:97:ASP:OD2	2.21	0.65
1:B:292:HIS:ND1	1:B:368:GLN:NE2	2.45	0.64
1:A:287:PRO:HG3	1:A:361:ASN:HB2	1.79	0.64
2:E:247:THR:HA	2:E:279:VAL:HG12	1.80	0.63
2:D:66:ASN:HB3	2:D:69:PHE:HD2	1.64	0.63
2:E:62:LYS:HD2	8:E:506:HOH:O	1.99	0.63
1:A:292:HIS:ND1	1:A:368:GLN:NE2	2.45	0.63
2:E:244:VAL:O	2:E:281:GLU:HA	2.00	0.61
1:B:73:ASN:N	1:B:97:ASP:OD2	2.22	0.61
2:E:238:ILE:HD13	2:E:244:VAL:HB	1.81	0.61
1:A:122:LEU:HG	1:A:125:LEU:HD22	1.83	0.61
2:D:238:ILE:HD13	2:D:244:VAL:HB	1.83	0.61
2:E:66:ASN:HB3	2:E:69:PHE:HD2	1.65	0.60
1:B:292:HIS:CG	1:B:368:GLN:NE2	2.68	0.60
2:E:136:VAL:HG22	2:E:215:TYR:HB2	1.84	0.59
1:B:222:LEU:HB3	1:B:255:SER:HB3	1.85	0.59
1:B:98:LEU:H	1:B:98:LEU:HD22	1.68	0.59
2:D:136:VAL:HG22	2:D:215:TYR:HB2	1.84	0.59
1:A:238:GLY:HA2	1:A:261:GLU:HB3	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:289:ILE:HD13	1:B:310:ALA:HB2	1.85	0.59
2:E:249:VAL:HG22	2:E:277:ARG:HG3	1.85	0.59
1:B:21:PRO:HG3	1:B:49:ILE:HG12	1.84	0.58
1:A:289:ILE:HD13	1:A:310:ALA:HB2	1.85	0.58
1:B:221:VAL:HG13	1:B:229:SER:HB2	1.85	0.58
1:A:292:HIS:CG	1:A:368:GLN:NE2	2.71	0.58
1:B:338:ASP:N	1:B:338:ASP:OD1	2.37	0.57
1:A:21:PRO:HG3	1:A:49:ILE:HG12	1.87	0.57
1:B:60:ASP:OD2	1:B:84:ARG:NH1	2.38	0.57
1:B:321:ILE:HB	1:B:356:THR:HB	1.86	0.56
1:A:321:ILE:HB	1:A:356:THR:HB	1.85	0.56
1:B:285:GLU:N	1:B:313:ASP:O	2.38	0.56
1:B:285:GLU:O	1:B:361:ASN:ND2	2.39	0.56
1:A:36:LEU:HD22	1:A:57:ARG:HD2	1.87	0.56
2:E:246:ILE:O	2:E:279:VAL:HA	2.05	0.55
1:A:139:SER:HB2	1:A:142:ALA:HB2	1.89	0.55
1:A:292:HIS:HD2	7:A:415:SO4:O4	1.87	0.55
1:A:59:ALA:HB2	1:A:81:THR:CG2	2.34	0.55
2:E:161:LYS:NZ	2:E:191:SER:O	2.40	0.55
1:A:269:LEU:HD22	1:A:277:ILE:HD13	1.87	0.55
2:D:249:VAL:HG22	2:D:277:ARG:HG3	1.88	0.55
1:A:285:GLU:O	1:A:361:ASN:ND2	2.41	0.54
1:A:278:PRO:HG2	1:A:281:GLU:HG3	1.90	0.54
1:B:59:ALA:HB2	1:B:81:THR:CG2	2.36	0.54
2:D:308:ILE:N	8:D:501:HOH:O	2.28	0.54
1:A:221:VAL:HG23	1:A:231:SER:HB2	1.89	0.54
1:A:235:LEU:O	1:A:256:ARG:NH2	2.41	0.54
1:A:279:GLU:O	2:D:217:ARG:NH2	2.41	0.53
1:A:300:GLU:HG3	1:A:347:THR:O	2.09	0.53
2:D:68:ARG:HH21	2:D:91:ARG:HH21	1.56	0.53
1:B:82:LEU:O	1:B:85:ASN:ND2	2.42	0.52
1:B:300:GLU:HG3	1:B:347:THR:O	2.09	0.52
1:B:279:GLU:O	2:E:217:ARG:NH2	2.42	0.52
1:B:269:LEU:HD22	1:B:277:ILE:HD13	1.92	0.52
1:B:278:PRO:HG2	1:B:281:GLU:HG3	1.91	0.52
1:B:122:LEU:HG	1:B:125:LEU:HD22	1.92	0.52
1:B:235:LEU:O	1:B:256:ARG:NH2	2.43	0.52
1:B:139:SER:HB2	1:B:142:ALA:HB2	1.92	0.51
1:A:288:LEU:HD11	2:D:296:MET:HB3	1.91	0.51
2:E:261:MET:HG2	2:E:266:ASP:HA	1.93	0.51
2:D:55:ILE:HG13	2:D:79:GLY:HA2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:251:LEU:HD12	1:B:254:LEU:HD12	1.93	0.50
1:A:60:ASP:OD2	1:A:84:ARG:NH1	2.45	0.50
2:D:179:ARG:H	2:D:179:ARG:HD2	1.76	0.50
1:A:116:ASN:HA	1:A:142:ALA:HA	1.94	0.49
1:B:32:ASN:HB3	1:B:54:VAL:HB	1.93	0.49
1:B:327:LEU:HD23	1:B:328:ILE:H	1.78	0.49
1:A:327:LEU:HD11	2:D:130:MET:CE	2.42	0.49
2:E:46:GLN:HA	2:E:79:GLY:HA3	1.95	0.49
1:A:27:GLN:HB3	1:A:29:LEU:HG	1.93	0.49
2:D:46:GLN:HA	2:D:79:GLY:HA3	1.93	0.49
1:B:92:PRO:HB3	1:B:117:ASP:HB2	1.94	0.49
1:B:37:CYS:HB2	1:B:58:LEU:HD23	1.94	0.49
2:E:55:ILE:HG13	2:E:79:GLY:HA2	1.95	0.49
1:A:181:ASN:O	1:A:205:ASN:HA	2.13	0.48
2:D:247:THR:HA	2:D:279:VAL:HG12	1.94	0.48
1:A:32:ASN:HB3	1:A:54:VAL:HB	1.95	0.48
1:A:45:VAL:HG11	1:A:70:ASP:HB3	1.96	0.48
2:D:161:LYS:NZ	2:D:191:SER:O	2.46	0.48
2:D:116:LEU:HD12	2:D:121:ILE:HD13	1.94	0.48
1:A:175:THR:HG22	1:A:199:ARG:HB3	1.95	0.48
2:E:289:ALA:O	8:E:501:HOH:O	2.20	0.47
2:E:116:LEU:HD12	2:E:121:ILE:HD13	1.96	0.47
2:E:68:ARG:HH21	2:E:91:ARG:HH21	1.63	0.47
1:B:168:GLU:HA	1:B:194:LEU:HD21	1.96	0.47
2:E:58:ASN:HB2	2:E:97:GLU:HB3	1.97	0.47
1:A:62:PHE:CE2	1:B:239:GLY:HA2	2.50	0.46
1:B:126:HIS:ND1	1:B:150:GLU:OE2	2.48	0.46
1:A:239:GLY:HA2	1:B:62:PHE:CE2	2.51	0.46
1:B:175:THR:HG22	1:B:199:ARG:HB3	1.96	0.46
1:A:251:LEU:HD12	1:A:254:LEU:HD12	1.98	0.46
2:E:179:ARG:HH21	2:E:179:ARG:HB3	1.80	0.46
1:A:78:VAL:O	1:A:101:LEU:HD12	2.16	0.46
1:A:92:PRO:HB3	1:A:117:ASP:HB2	1.97	0.46
1:B:181:ASN:O	1:B:205:ASN:HA	2.16	0.46
2:D:56:VAL:HG13	2:D:63:LYS:HD3	1.98	0.45
1:A:222:LEU:HB3	1:A:255:SER:HB3	1.97	0.45
2:D:239:MET:H	2:D:239:MET:HG2	1.61	0.45
1:A:37:CYS:HB2	1:A:58:LEU:HD23	1.99	0.45
1:B:51:ARG:HB3	1:B:73:ASN:O	2.15	0.45
2:D:58:ASN:HB2	2:D:97:GLU:HB3	1.97	0.45
1:A:285:GLU:N	1:A:313:ASP:O	2.43	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:256:ARG:NH1	8:A:501:HOH:O	2.31	0.45
1:A:327:LEU:HD11	2:D:130:MET:HE2	1.99	0.45
2:E:179:ARG:NH2	2:E:179:ARG:HB3	2.31	0.45
1:A:292:HIS:NE2	7:A:415:SO4:S	2.89	0.45
1:A:328:ILE:HG22	1:A:329:SER:H	1.82	0.45
1:A:23:ARG:NH1	1:B:271:GLY:O	2.50	0.45
2:D:240:PRO:HB3	2:D:286:ARG:HA	1.99	0.45
1:B:220:GLN:HA	1:B:256:ARG:HG2	1.98	0.45
2:D:89:THR:HA	2:D:90:PRO:HA	1.83	0.45
1:B:223:ALA:HB2	1:B:229:SER:OG	2.17	0.44
2:E:240:PRO:HB3	2:E:286:ARG:HA	1.99	0.44
2:D:261:MET:HG2	2:D:266:ASP:HA	1.98	0.44
1:B:291:ARG:C	1:B:292:HIS:ND1	2.71	0.44
1:A:160:GLU:O	1:A:183:ILE:HA	2.18	0.44
1:A:214:PRO:O	1:A:218:ARG:HG3	2.18	0.43
1:B:23:ARG:HE	1:B:42:LEU:HD23	1.83	0.43
2:E:149:ALA:HB3	2:E:157:ILE:HD11	2.00	0.43
1:B:28:ILE:HD12	1:B:29:LEU:HD23	2.00	0.43
2:E:152:ASN:HA	2:E:153:PRO:HA	1.92	0.43
1:A:328:ILE:HD12	1:A:342:LEU:HD11	1.99	0.43
1:A:61:ASN:O	1:A:85:ASN:HA	2.18	0.43
2:D:34:THR:HB	2:D:205:GLY:HA2	2.01	0.43
1:A:293:THR:HG23	1:A:307:ARG:HB2	2.00	0.43
1:B:46:PRO:HA	1:B:47:PRO:HD3	1.91	0.43
1:B:61:ASN:O	1:B:85:ASN:HA	2.18	0.43
1:B:288:LEU:HD11	2:E:296:MET:HB3	2.01	0.43
2:E:179:ARG:HG2	2:E:180:SER:H	1.83	0.43
1:A:291:ARG:C	1:A:292:HIS:ND1	2.73	0.42
1:A:292:HIS:CD2	7:A:415:SO4:S	3.12	0.42
1:A:116:ASN:HB2	1:A:141:THR:OG1	2.19	0.42
1:A:332:THR:HG23	1:A:333:ARG:HG3	2.02	0.42
1:A:352:THR:HG23	1:A:373:HIS:HA	2.01	0.42
1:B:160:GLU:O	1:B:183:ILE:HA	2.19	0.42
2:D:62:LYS:HD2	8:D:510:HOH:O	2.19	0.42
1:B:206:LYS:HD3	1:B:206:LYS:HA	1.80	0.42
1:B:45:VAL:HG11	1:B:70:ASP:HB3	2.02	0.42
1:B:368:GLN:HG2	1:B:369:ILE:H	1.84	0.42
2:E:239:MET:HG2	2:E:239:MET:H	1.62	0.42
1:A:146:VAL:HB	1:A:149:LEU:HD21	2.02	0.42
1:B:40:LYS:HA	1:B:40:LYS:HD3	1.74	0.42
1:B:293:THR:HG23	1:B:307:ARG:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:328:ILE:HG22	1:B:329:SER:H	1.85	0.41
2:D:140:THR:HA	2:D:187:GLN:HA	2.02	0.41
1:A:185:ASN:HA	1:A:207:LEU:HD22	2.02	0.41
1:A:40:LYS:HA	1:A:40:LYS:HD3	1.76	0.41
1:B:119:PHE:HA	1:B:122:LEU:HD23	2.02	0.41
1:B:185:ASN:HA	1:B:207:LEU:HD22	2.01	0.41
2:D:269:PRO:HG2	2:D:272:ASP:OD1	2.20	0.41
2:D:119:ASP:OD1	2:D:119:ASP:N	2.48	0.41
2:E:66:ASN:HA	2:E:66:ASN:HD22	1.75	0.41
2:D:56:VAL:HB	2:D:99:VAL:HB	2.02	0.41
1:B:292:HIS:CD2	1:B:368:GLN:NE2	2.83	0.41
2:D:154:ASP:HA	2:D:155:PRO:HD3	1.95	0.41
2:E:119:ASP:N	2:E:119:ASP:OD1	2.46	0.40
1:B:188:LYS:HG3	1:B:189:GLY:N	2.36	0.40
1:B:347:THR:HB	1:B:374:ILE:HD13	2.03	0.40
1:A:271:GLY:O	1:B:23:ARG:NH1	2.54	0.40
1:A:338:ASP:OD1	1:A:338:ASP:N	2.54	0.40
1:B:116:ASN:HA	1:B:142:ALA:HA	2.04	0.40
2:D:29:THR:HB	2:D:109:VAL:HG11	2.03	0.40
2:E:85:GLN:HA	2:E:86:PRO:HA	1.86	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	359/361 (99%)	349 (97%)	10 (3%)	0	100	100
1	B	359/361 (99%)	352 (98%)	7 (2%)	0	100	100
2	D	289/291 (99%)	283 (98%)	6 (2%)	0	100	100
2	E	289/291 (99%)	283 (98%)	6 (2%)	0	100	100
All	All	1296/1304 (99%)	1267 (98%)	29 (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	325/325 (100%)	311 (96%)	14 (4%)	33	70
1	B	325/325 (100%)	309 (95%)	16 (5%)	29	66
2	D	252/252 (100%)	246 (98%)	6 (2%)	54	82
2	E	252/252 (100%)	246 (98%)	6 (2%)	54	82
All	All	1154/1154 (100%)	1112 (96%)	42 (4%)	40	74

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	52	ARG
1	A	57	ARG
1	A	98	LEU
1	A	122	LEU
1	A	145	ASP
1	A	146	VAL
1	A	147	PHE
1	A	213	ASP
1	A	292	HIS
1	A	299	LEU
1	A	327	LEU
1	A	332	THR
1	A	342	LEU
1	A	370	VAL
1	B	98	LEU
1	B	122	LEU
1	B	131	ASN
1	B	145	ASP
1	B	146	VAL
1	B	147	PHE
1	B	213	ASP
1	B	232	THR

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Mol	Chain	Res	Type
1	B	292	HIS
1	B	299	LEU
1	B	327	LEU
1	B	328	ILE
1	B	332	THR
1	B	338	ASP
1	B	342	LEU
1	B	370	VAL
2	D	116	LEU
2	D	144	THR
2	D	158	THR
2	D	179	ARG
2	D	224	ARG
2	D	239	MET
2	E	116	LEU
2	E	144	THR
2	E	158	THR
2	E	179	ARG
2	E	223	ARG
2	E	239	MET

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	368	GLN
1	B	368	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 38 ligands modelled in this entry, 26 are monoatomic - leaving 12 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$
3	NAG	A	401	1	14,14,15	0.20	0	15,19,21	0.45	0
3	NAG	A	402	1	14,14,15	0.35	0	15,19,21	0.54	0
3	NAG	A	403	1	14,14,15	0.28	0	15,19,21	0.50	0
7	SO4	A	414	-	4,4,4	0.15	0	6,6,6	0.07	0
7	SO4	A	415	-	4,4,4	0.82	0	6,6,6	1.31	1 (16%)
3	NAG	B	401	1	14,14,15	0.17	0	15,19,21	0.47	0
3	NAG	B	402	1	14,14,15	0.31	0	15,19,21	0.47	0
3	NAG	B	403	1	14,14,15	0.22	0	15,19,21	0.52	0
7	SO4	B	414	-	4,4,4	0.13	0	6,6,6	0.08	0
7	SO4	B	415	-	4,4,4	0.82	0	6,6,6	1.31	1 (16%)
3	NAG	D	401	2	14,14,15	0.26	0	15,19,21	0.50	0
3	NAG	E	401	2	14,14,15	0.26	0	15,19,21	0.45	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
3	NAG	A	401	1	-	0/6/23/26	0/1/1/1
3	NAG	A	402	1	-	0/6/23/26	0/1/1/1
3	NAG	A	403	1	-	0/6/23/26	0/1/1/1
7	SO4	A	414	-	-	0/0/0/0	0/0/0/0
7	SO4	A	415	-	-	0/0/0/0	0/0/0/0
3	NAG	B	401	1	-	0/6/23/26	0/1/1/1
3	NAG	B	402	1	-	0/6/23/26	0/1/1/1
3	NAG	B	403	1	-	0/6/23/26	0/1/1/1
7	SO4	B	414	-	-	0/0/0/0	0/0/0/0
7	SO4	B	415	-	-	0/0/0/0	0/0/0/0
3	NAG	D	401	2	-	0/6/23/26	0/1/1/1
3	NAG	E	401	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
7	B	415	SO4	O4-S-O1	2.92	125.38	109.26
7	A	415	SO4	O4-S-O2	2.92	125.38	109.26

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	415	SO4	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 ⓘ

### 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	361/361 (100%)	0.23	8 (2%) 62 50	77, 118, 196, 250	0
1	B	361/361 (100%)	0.26	11 (3%) 51 38	78, 119, 201, 263	0
2	D	291/291 (100%)	0.29	13 (4%) 34 25	100, 132, 209, 228	0
2	E	291/291 (100%)	0.23	10 (3%) 46 35	98, 132, 212, 235	0
All	All	1304/1304 (100%)	0.25	42 (3%) 48 37	77, 127, 203, 263	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	282	LEU	6.0
2	E	282	LEU	5.1
1	B	225	SER	4.6
1	B	226	GLY	4.2
2	D	311	LYS	4.0
2	E	311	LYS	3.9
2	D	243	SER	3.5
2	D	280	LEU	3.5
2	D	240	PRO	3.3
2	D	283	ASN	3.2
1	B	227	ILE	3.2
1	A	297	ARG	3.2
1	B	303	ARG	3.1
1	B	297	ARG	3.1
2	E	238	ILE	3.1
1	B	224	THR	3.0
2	D	244	VAL	2.9
2	E	243	SER	2.9
1	A	305	THR	2.8
1	B	228	ILE	2.8
2	D	295	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	306	LEU	2.7
1	A	226	GLY	2.6
2	D	36	VAL	2.6
2	E	286	ARG	2.5
2	E	43	PHE	2.5
2	E	280	LEU	2.4
2	E	283	ASN	2.3
1	A	58	LEU	2.3
1	B	305	THR	2.3
2	D	305	ILE	2.3
1	A	225	SER	2.2
2	D	238	ILE	2.2
2	E	295	ALA	2.2
2	D	43	PHE	2.2
1	B	304	ALA	2.2
2	E	294	VAL	2.2
2	D	146	LEU	2.1
1	B	345	LEU	2.1
1	A	152	LEU	2.0
1	B	58	LEU	2.0
1	A	303	ARG	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
4	NA	B	404	1/1	0.96	1.49	40.61	107,107,107,107	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	NA	A	404	1/1	0.94	0.99	21.62	107,107,107,107	0
6	CL	B	413	1/1	0.67	0.26	0.38	111,111,111,111	0
6	CL	A	413	1/1	0.67	0.24	-0.16	112,112,112,112	0
5	CA	B	408	1/1	0.82	0.22	-0.47	144,144,144,144	0
3	NAG	D	401	14/15	0.79	0.23	-0.52	188,208,216,218	0
7	SO4	A	415	5/5	0.77	0.19	-0.86	179,188,196,207	0
7	SO4	B	415	5/5	0.81	0.17	-1.06	185,188,191,210	0
5	CA	B	405	1/1	0.88	0.17	-1.82	98,98,98,98	0
5	CA	A	405	1/1	0.94	0.11	-3.07	95,95,95,95	0
3	NAG	A	403	14/15	0.88	0.24	-	177,183,187,188	0
7	SO4	B	414	5/5	0.79	0.23	-	128,139,158,160	0
5	CA	A	406	1/1	0.66	0.12	-	162,162,162,162	0
3	NAG	A	401	14/15	0.75	0.41	-	179,201,209,217	0
5	CA	A	407	1/1	0.42	0.20	-	162,162,162,162	0
5	CA	A	410	1/1	0.91	0.12	-	148,148,148,148	0
5	CA	A	408	1/1	0.87	0.10	-	146,146,146,146	0
6	CL	B	412	1/1	0.69	0.26	-	174,174,174,174	0
5	CA	B	410	1/1	0.50	0.20	-	152,152,152,152	0
3	NAG	B	403	14/15	0.82	0.28	-	184,192,201,210	0
3	NAG	E	401	14/15	0.69	0.32	-	192,209,216,222	0
6	CL	E	403	1/1	0.85	0.17	-	146,146,146,146	0
7	SO4	A	414	5/5	0.74	0.25	-	125,131,150,152	0
5	CA	A	409	1/1	0.80	0.26	-	114,114,114,114	0
5	CA	B	406	1/1	0.79	0.17	-	147,147,147,147	0
3	NAG	B	402	14/15	0.77	0.31	-	172,189,195,202	0
6	CL	E	402	1/1	0.86	0.19	-	157,157,157,157	0
6	CL	D	404	1/1	0.85	0.18	-	141,141,141,141	0
6	CL	E	404	1/1	0.45	0.19	-	158,158,158,158	0
6	CL	A	412	1/1	0.81	0.24	-	128,128,128,128	0
3	NAG	A	402	14/15	0.78	0.21	-	171,200,209,210	0
6	CL	D	402	1/1	0.77	0.22	-	152,152,152,152	0
5	CA	B	409	1/1	0.83	0.27	-	111,111,111,111	0
3	NAG	B	401	14/15	0.71	0.50	-	176,198,207,216	0
5	CA	B	407	1/1	0.62	0.16	-	154,154,154,154	0
6	CL	A	411	1/1	0.94	0.47	-	98,98,98,98	0
6	CL	D	403	1/1	0.91	0.10	-	152,152,152,152	0
6	CL	B	411	1/1	0.89	0.33	-	97,97,97,97	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.