



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 27, 2017 – 02:09 PM EST

PDB ID : 5YCO  
Title : Complex structure of PCNA with UHRF2  
Authors : Wu, M.; Chen, W.; Hang, T.; Wang, C.; Zhang, X.; Zang, J.  
Deposited on : unknown  
Resolution : 2.20 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-20030345  
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-20030345

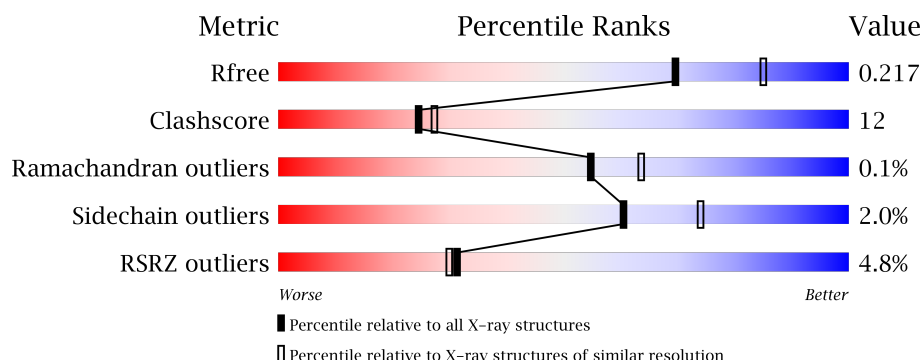
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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	4002 (2.20-2.20)
Clashscore	112137	4730 (2.20-2.20)
Ramachandran outliers	110173	4656 (2.20-2.20)
Sidechain outliers	110143	4657 (2.20-2.20)
RSRZ outliers	101464	4033 (2.20-2.20)

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	269	<div> <div>6%</div> <div>72% 19% 7%</div> </div>
1	B	269	<div> <div>4%</div> <div>77% 15% 7%</div> </div>
1	C	269	<div> <div>3%</div> <div>72% 19% 8%</div> </div>
1	D	269	<div> <div>4%</div> <div>75% 17% 7%</div> </div>
2	E	17	<div> <div>6%</div> <div>24% 18% 6% 53%</div> </div>

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Mol	Chain	Length	Quality of chain
2	F	17	

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
3	GOL	A	301	-	-	X	X
3	GOL	B	301	-	-	-	X
3	GOL	C	301	-	-	-	X
4	SO4	B	303	-	-	-	X
4	SO4	C	302	-	-	X	-
4	SO4	C	303	-	-	-	X
4	SO4	D	302	-	-	X	-

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8224 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 Proliferating cell nuclear antigen.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	250	Total	C	N	O	S	0	0	0
			1921	1208	316	381	16			
1	B	250	Total	C	N	O	S	0	0	0
			1917	1206	316	379	16			
1	C	248	Total	C	N	O	S	0	2	0
			1923	1211	319	377	16			
1	D	250	Total	C	N	O	S	0	2	0
			1935	1218	320	381	16			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	262	LEU	-	expression tag	UNP P12004
A	263	GLU	-	expression tag	UNP P12004
A	264	HIS	-	expression tag	UNP P12004
A	265	HIS	-	expression tag	UNP P12004
A	266	HIS	-	expression tag	UNP P12004
A	267	HIS	-	expression tag	UNP P12004
A	268	HIS	-	expression tag	UNP P12004
A	269	HIS	-	expression tag	UNP P12004
B	262	LEU	-	expression tag	UNP P12004
B	263	GLU	-	expression tag	UNP P12004
B	264	HIS	-	expression tag	UNP P12004
B	265	HIS	-	expression tag	UNP P12004
B	266	HIS	-	expression tag	UNP P12004
B	267	HIS	-	expression tag	UNP P12004
B	268	HIS	-	expression tag	UNP P12004
B	269	HIS	-	expression tag	UNP P12004
C	262	LEU	-	expression tag	UNP P12004
C	263	GLU	-	expression tag	UNP P12004
C	264	HIS	-	expression tag	UNP P12004
C	265	HIS	-	expression tag	UNP P12004
C	266	HIS	-	expression tag	UNP P12004

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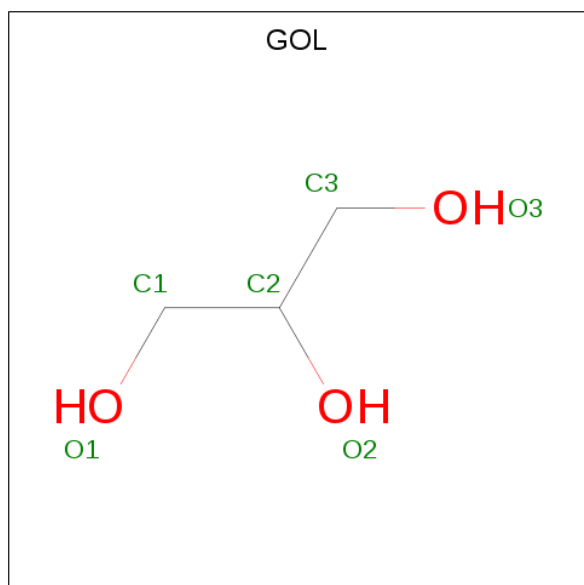
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Chain	Residue	Modelled	Actual	Comment	Reference
C	267	HIS	-	expression tag	UNP P12004
C	268	HIS	-	expression tag	UNP P12004
C	269	HIS	-	expression tag	UNP P12004
D	262	LEU	-	expression tag	UNP P12004
D	263	GLU	-	expression tag	UNP P12004
D	264	HIS	-	expression tag	UNP P12004
D	265	HIS	-	expression tag	UNP P12004
D	266	HIS	-	expression tag	UNP P12004
D	267	HIS	-	expression tag	UNP P12004
D	268	HIS	-	expression tag	UNP P12004
D	269	HIS	-	expression tag	UNP P12004

- Molecule 2 is a protein called E3 ubiquitin-protein ligase UHRF2.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	8	Total	C	N	O	0	0	0
			70	49	9	12			
2	F	8	Total	C	N	O	0	0	0
			70	49	9	12			

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



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

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

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



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

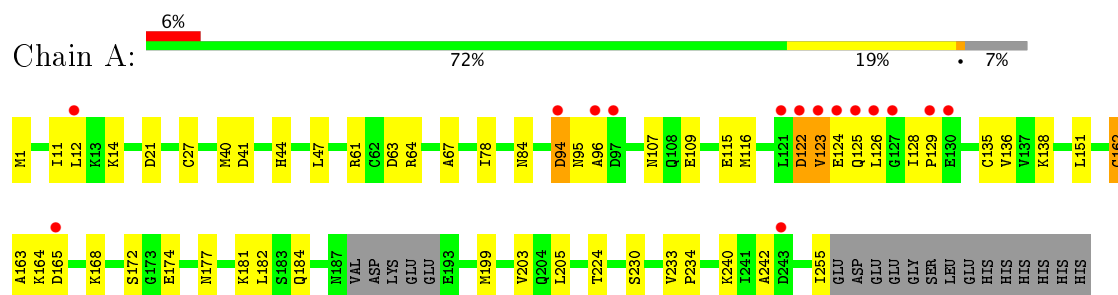
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	82	Total 82	O 82	0	0
5	B	82	Total 82	O 82	0	0
5	C	75	Total 75	O 75	0	0
5	D	84	Total 84	O 84	0	0
5	E	1	Total 1	O 1	0	0

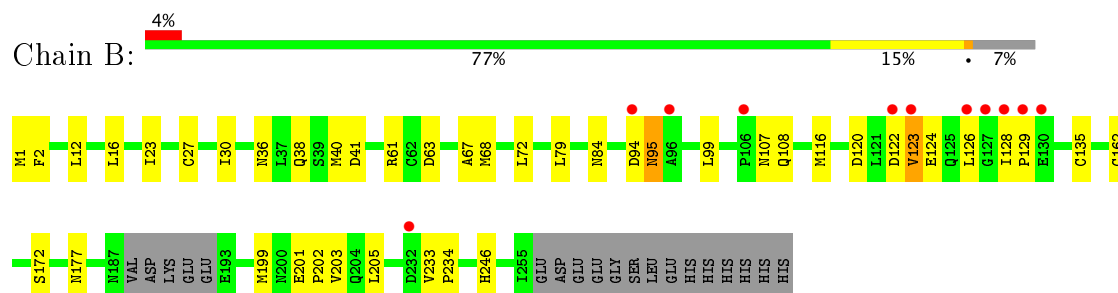
### 3 Residue-property plots [i](#)

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.

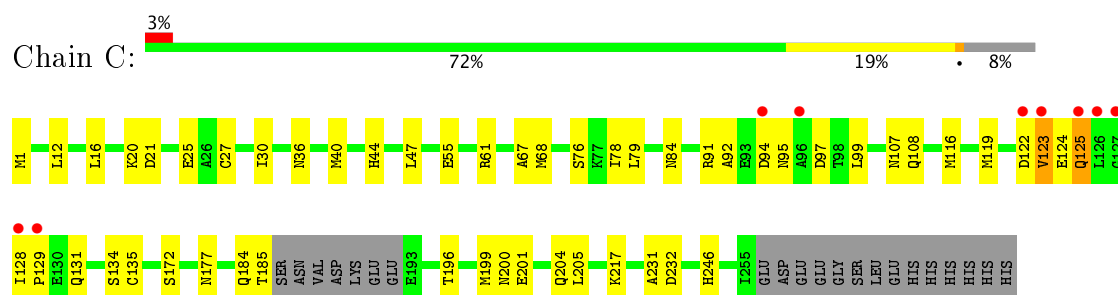
- Molecule 1: Proliferating cell nuclear antigen



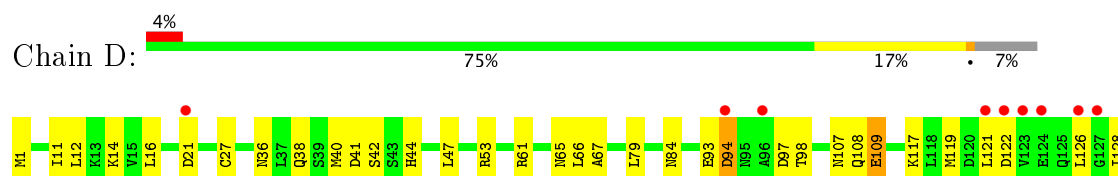
- Molecule 1: Proliferating cell nuclear antigen



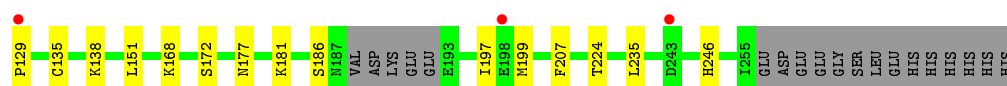
- Molecule 1: Proliferating cell nuclear antigen



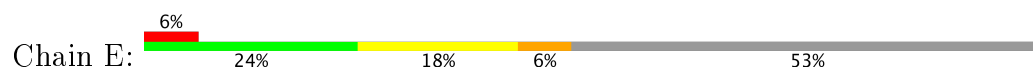
- Molecule 1: Proliferating cell nuclear antigen



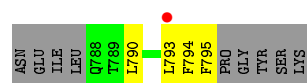




- Molecule 2: E3 ubiquitin-protein ligase UHRF2



- Molecule 2: E3 ubiquitin-protein ligase UHRF2



## 4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	202.51Å 202.51Å 123.94Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	41.31 – 2.20 41.31 – 2.20	Depositor EDS
% Data completeness (in resolution range)	98.1 (41.31-2.20) 98.0 (41.31-2.20)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.39 (at 2.20Å)	Xtriage
Refinement program	PHENIX 1.11.1_2575	Depositor
R, $R_{free}$	0.204 , 0.220 0.201 , 0.217	Depositor DCC
$R_{free}$ test set	4855 reflections (5.14%)	DCC
Wilson B-factor (Å <sup>2</sup> )	41.0	Xtriage
Anisotropy	0.015	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 32.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.019 for -2/3*h-1/3*k-4/3*l,-1/3*h-2/3*k+4/3*l,-1/3*h+1/3*k+1/3*l 0.019 for -h,1/3*h-1/3*k-4/3*l,-1/3*h-2/3*k+1/3*l 0.018 for -1/3*h+1/3*k+4/3*l,-k,2/3*h+1/3*k+1/3*l 0.460 for -h,2/3*h+1/3*k+4/3*l,1/3*h+2/3*k-1/3*l 0.457 for -1/3*h-2/3*k+4/3*l,-2/3*h-1/3*k-4/3*l,1/3*h-1/3*k-1/3*l 0.457 for 1/3*h+2/3*k-4/3*l,-k,-2/3*h-1/3*k-1/3*l 0.020 for h,-h-k,-l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	8224	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.86% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, 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	0.50	0/1946	0.71	5/2628 (0.2%)
1	B	0.50	0/1942	0.71	5/2623 (0.2%)
1	C	0.53	0/1954	0.80	9/2637 (0.3%)
1	D	0.44	0/1966	0.67	2/2653 (0.1%)
2	E	0.54	0/71	0.85	0/95
2	F	0.44	0/71	0.82	0/95
All	All	0.49	0/7950	0.73	21/10731 (0.2%)

There are no bond length outliers.

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	124	GLU	O-C-N	-8.30	109.42	122.70
1	B	124	GLU	O-C-N	-8.14	109.68	122.70
1	A	124	GLU	O-C-N	-7.98	109.94	122.70
1	C	92	ALA	N-CA-CB	6.94	119.82	110.10
1	C	123	VAL	O-C-N	6.49	133.09	122.70
1	C	91[A]	ARG	CA-C-O	6.32	133.37	120.10
1	C	91[B]	ARG	CA-C-O	6.32	133.37	120.10
1	C	123	VAL	CA-C-N	-5.93	104.15	117.20
1	A	123	VAL	C-N-CA	5.57	135.61	121.70
1	C	123	VAL	C-N-CA	5.46	135.34	121.70
1	B	123	VAL	C-N-CA	5.27	134.87	121.70
1	B	122	ASP	CB-CG-OD2	5.22	123.00	118.30
1	D	94	ASP	CB-CG-OD2	5.20	122.98	118.30
1	D	122	ASP	CB-CG-OD2	5.20	122.98	118.30
1	B	94	ASP	CB-CG-OD2	5.19	122.97	118.30
1	C	122	ASP	CB-CG-OD2	5.17	122.96	118.30
1	A	94	ASP	CB-CG-OD2	5.17	122.95	118.30
1	A	122	ASP	CB-CG-OD1	5.16	122.94	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	122	ASP	C-N-CA	-5.10	108.94	121.70
1	A	162	CYS	CA-CB-SG	-5.06	104.89	114.00
1	B	124	GLU	CA-C-N	5.01	128.21	117.20

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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	1921	0	1933	54	0
1	B	1917	0	1929	44	0
1	C	1923	0	1948	54	0
1	D	1935	0	1960	36	0
2	E	70	0	69	5	0
2	F	70	0	69	7	0
3	A	6	0	8	4	0
3	B	6	0	8	0	0
3	C	6	0	8	0	0
3	D	6	0	8	3	0
4	A	10	0	0	1	0
4	B	10	0	0	2	0
4	C	10	0	0	3	0
4	D	10	0	0	3	0
5	A	82	0	0	2	0
5	B	82	0	0	1	0
5	C	75	0	0	2	0
5	D	84	0	0	3	0
5	E	1	0	0	0	0
All	All	8224	0	7940	193	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 12.

All (193) 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:C:246:HIS:ND1	4:C:302:SO4:O2	1.58	1.33
1:B:199:MET:HE2	1:B:201:GLU:C	1.61	1.19
1:D:119:MET:HE2	1:D:121:LEU:HD21	1.34	1.07
1:C:123:VAL:CG2	1:C:125:GLN:HE21	1.70	1.04
1:C:30:ILE:HD11	1:C:68:MET:CE	1.88	1.04
1:A:1:MET:N	1:A:64:ARG:HH12	1.57	1.02
1:B:199:MET:CE	1:B:201:GLU:CA	2.36	1.02
1:B:199:MET:HE2	1:B:201:GLU:CA	1.92	1.00
1:C:128:ILE:HD12	1:C:129:PRO:HD2	1.43	1.00
1:B:199:MET:CE	1:B:201:GLU:C	2.32	0.98
1:C:30:ILE:HD11	1:C:68:MET:HE2	1.50	0.94
1:B:199:MET:HE1	1:B:201:GLU:HA	1.54	0.89
1:D:119:MET:CE	1:D:121:LEU:HD21	2.03	0.87
1:C:200:ASN:C	1:C:201:GLU:OE1	2.13	0.87
1:C:1:MET:HG2	1:C:61:ARG:HH12	1.38	0.87
1:C:134:SER:HB3	1:C:201:GLU:HG2	1.59	0.85
1:C:30:ILE:HD11	1:C:68:MET:HE1	1.58	0.84
1:D:65:ASN:O	1:D:66:LEU:HD23	1.78	0.82
1:A:125:GLN:C	1:A:126:LEU:HD12	2.00	0.82
1:B:128:ILE:HD12	1:B:129:PRO:HD2	1.61	0.82
1:B:199:MET:HE1	1:B:201:GLU:CA	2.07	0.81
1:A:233:VAL:HG23	1:A:234:PRO:HD2	1.63	0.79
1:A:1:MET:H2	1:A:64:ARG:HH12	1.27	0.79
1:C:1:MET:HB3	1:C:61:ARG:NH1	1.97	0.79
1:A:182:LEU:HD22	1:D:109:GLU:OE1	1.83	0.77
1:B:199:MET:HE2	1:B:201:GLU:N	1.99	0.77
1:A:135:CYS:HG	1:A:162:CYS:HG	1.31	0.77
1:C:123:VAL:HG21	1:C:125:GLN:HE21	1.50	0.77
1:C:123:VAL:CG2	1:C:125:GLN:NE2	2.49	0.76
1:D:14:LYS:HD2	3:D:301:GOL:H11	1.68	0.75
1:B:199:MET:CE	1:B:201:GLU:N	2.50	0.75
1:C:200:ASN:CB	1:C:201:GLU:OE1	2.35	0.74
1:B:40:MET:HE3	2:E:793:LEU:HB2	1.70	0.73
1:A:64:ARG:NH2	1:A:94:ASP:OD1	2.22	0.73
2:E:793:LEU:HD12	2:E:793:LEU:H	1.52	0.73
1:A:123:VAL:CG1	1:A:125:GLN:HE21	2.02	0.72
1:B:95:ASN:ND2	1:B:95:ASN:H	1.88	0.72
1:B:199:MET:CE	1:B:202:PRO:N	2.53	0.71
2:F:790:LEU:H	2:F:793:LEU:HD22	1.57	0.69
1:D:65:ASN:C	1:D:66:LEU:HD23	2.13	0.69
1:B:95:ASN:H	1:B:95:ASN:HD22	1.40	0.69
1:C:40:MET:HE2	1:C:44:HIS:CG	2.28	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:64:ARG:CZ	1:A:94:ASP:OD1	2.42	0.67
1:C:40:MET:HG3	1:C:47:LEU:HD12	1.74	0.67
1:B:1:MET:HG2	1:B:61:ARG:HH12	1.60	0.67
1:A:11:ILE:HG12	3:A:301:GOL:H12	1.75	0.67
1:A:1:MET:HG2	1:A:61:ARG:HH22	1.60	0.66
1:A:84:ASN:OD1	5:A:401:HOH:O	2.14	0.66
1:C:123:VAL:HG22	1:C:125:GLN:HE21	1.55	0.66
1:C:1:MET:CG	1:C:61:ARG:HH12	2.08	0.66
1:A:233:VAL:CG2	1:A:234:PRO:HD2	2.25	0.66
1:B:123:VAL:HG23	1:B:123:VAL:O	1.95	0.65
1:C:95:ASN:OD1	1:C:97:ASP:OD1	2.14	0.65
2:F:793:LEU:H	2:F:793:LEU:HD12	1.61	0.65
1:A:40:MET:HE2	1:A:44:HIS:CG	2.32	0.65
1:D:84:ASN:ND2	4:D:303:SO4:O3	2.30	0.65
1:C:204:GLN:C	1:C:205:LEU:HD23	2.18	0.65
1:C:1:MET:HG2	1:C:61:ARG:NH1	2.11	0.64
1:B:123:VAL:CG2	1:B:123:VAL:O	2.45	0.64
1:C:204:GLN:O	1:C:205:LEU:HD23	1.99	0.63
1:B:199:MET:HE3	1:B:202:PRO:N	2.13	0.63
1:C:200:ASN:HB2	1:C:201:GLU:OE1	1.97	0.63
1:B:199:MET:HE3	1:B:202:PRO:CD	2.30	0.62
1:C:30:ILE:CD1	1:C:68:MET:CE	2.74	0.61
1:B:135:CYS:SG	1:B:203:VAL:HG23	2.41	0.61
1:B:199:MET:CE	1:B:201:GLU:HA	2.13	0.61
1:D:119:MET:O	5:D:402:HOH:O	2.16	0.61
1:A:27:CYS:SG	1:A:123:VAL:HG22	2.41	0.60
1:A:174:GLU:O	1:D:117:LYS:NZ	2.31	0.60
1:D:53:ARG:NH1	4:D:302:SO4:O2	2.32	0.60
2:F:794:PHE:O	2:F:795:PHE:CD1	2.55	0.60
1:A:233:VAL:HG23	1:A:234:PRO:CD	2.30	0.60
1:D:128:ILE:HD12	1:D:129:PRO:HD2	1.85	0.59
1:C:84:ASN:ND2	4:C:303:SO4:O1	2.36	0.58
1:D:36:ASN:OD1	5:D:401:HOH:O	2.16	0.58
1:C:1:MET:CG	1:C:61:ARG:NH1	2.67	0.57
2:F:790:LEU:HB2	2:F:793:LEU:HD13	1.85	0.57
1:C:246:HIS:CE1	4:C:302:SO4:O2	2.50	0.57
1:A:11:ILE:HG13	3:A:301:GOL:H31	1.87	0.57
2:F:790:LEU:HB2	2:F:793:LEU:CD1	2.35	0.57
1:A:1:MET:N	1:A:64:ARG:NH1	2.41	0.57
1:A:230:SER:HB2	1:A:233:VAL:HG11	1.87	0.57
1:A:233:VAL:CG2	1:A:234:PRO:CD	2.82	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:203:VAL:HG12	1:A:205:LEU:HG	1.86	0.56
1:C:1:MET:CB	1:C:61:ARG:NH1	2.68	0.56
1:A:64:ARG:NH1	1:A:94:ASP:OD1	2.39	0.56
1:A:126:LEU:HD12	1:A:126:LEU:N	2.20	0.55
1:A:21:ASP:HB2	5:A:410:HOH:O	2.05	0.55
1:D:246:HIS:ND1	4:D:302:SO4:O3	2.34	0.55
1:D:21:ASP:HB2	5:D:405:HOH:O	2.05	0.55
1:B:172:SER:HB3	1:B:177:ASN:HB3	1.88	0.55
1:C:123:VAL:HG21	1:C:125:GLN:NE2	2.19	0.55
1:C:1:MET:HB3	1:C:61:ARG:HH11	1.69	0.55
1:C:25:GLU:OE1	1:C:119:MET:HE1	2.06	0.55
1:A:163:ALA:C	1:A:199:MET:SD	2.86	0.54
1:B:84:ASN:ND2	4:B:303:SO4:O3	2.40	0.54
1:B:246:HIS:ND1	4:B:302:SO4:O3	2.23	0.53
1:B:107:ASN:O	1:B:108:GLN:HB2	2.09	0.53
1:C:128:ILE:HD12	1:C:129:PRO:CD	2.28	0.53
1:D:40:MET:HG3	1:D:47:LEU:HD12	1.90	0.53
1:B:61:ARG:HD3	1:B:63:ASP:OD1	2.09	0.53
1:B:1:MET:HG2	1:B:61:ARG:NH1	2.24	0.52
1:A:40:MET:CE	1:A:44:HIS:CG	2.92	0.52
1:D:38:GLN:NE2	1:D:126:LEU:HB2	2.24	0.52
2:F:793:LEU:CD1	2:F:793:LEU:H	2.23	0.51
1:A:164:LYS:N	1:A:199:MET:SD	2.83	0.51
1:C:30:ILE:CD1	1:C:68:MET:HE2	2.32	0.51
1:D:172:SER:HB3	1:D:177:ASN:HB3	1.93	0.51
1:D:38:GLN:HE21	1:D:126:LEU:HB2	1.76	0.51
1:A:40:MET:HG3	1:A:47:LEU:HD12	1.93	0.51
1:C:231:ALA:O	1:C:232:ASP:HB2	2.11	0.51
1:C:99:LEU:HD23	1:C:116:MET:HE2	1.92	0.51
1:A:115:GLU:OE1	1:C:177:ASN:ND2	2.43	0.50
1:C:27:CYS:SG	1:C:67:ALA:HB1	2.52	0.50
1:A:230:SER:HB2	1:A:233:VAL:CG1	2.41	0.50
1:B:126:LEU:HD23	2:E:794:PHE:O	2.12	0.50
1:A:128:ILE:HD12	1:A:129:PRO:HD2	1.94	0.50
1:C:30:ILE:CD1	1:C:68:MET:HE1	2.33	0.50
1:C:135:CYS:SG	1:C:199:MET:HG3	2.51	0.49
1:C:21:ASP:HB2	5:C:410:HOH:O	2.12	0.49
1:A:107:ASN:OD1	1:A:109:GLU:HG2	2.12	0.49
1:A:1:MET:H3	1:A:64:ARG:HH12	1.54	0.49
1:B:135:CYS:SG	1:B:162:CYS:HB3	2.53	0.49
1:C:36:ASN:ND2	5:C:401:HOH:O	2.15	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:42:SER:O	1:D:44:HIS:HD2	1.95	0.49
1:C:123:VAL:HG13	1:C:123:VAL:O	2.11	0.49
1:D:93:GLU:H	1:D:93:GLU:CD	2.17	0.49
1:D:11:ILE:HG12	3:D:301:GOL:H32	1.94	0.48
1:D:27:CYS:SG	1:D:67:ALA:HB1	2.53	0.48
1:A:95:ASN:CG	1:A:96:ALA:N	2.68	0.47
1:B:38:GLN:OE1	1:B:126:LEU:HB2	2.15	0.47
1:B:128:ILE:HD12	1:B:129:PRO:CD	2.41	0.47
1:A:123:VAL:CG1	1:A:125:GLN:NE2	2.76	0.47
1:D:97:ASP:HB3	1:D:98:THR:HG23	1.97	0.46
1:D:168:LYS:HD3	1:D:181:LYS:HE2	1.97	0.46
1:B:203:VAL:HG12	1:B:205:LEU:HG	1.97	0.46
1:B:199:MET:CE	1:B:202:PRO:CD	2.92	0.46
1:C:200:ASN:O	1:C:201:GLU:OE1	2.33	0.46
1:A:233:VAL:HG22	1:A:234:PRO:N	2.31	0.46
1:C:78:ILE:CD1	1:C:116:MET:HB3	2.45	0.46
1:A:138:LYS:HE3	1:A:224:THR:HG21	1.98	0.45
1:A:14:LYS:HD2	3:A:301:GOL:H32	1.97	0.45
1:C:129:PRO:O	1:C:131:GLN:HG2	2.17	0.45
1:A:168:LYS:HD3	1:A:181:LYS:HE2	1.97	0.45
1:B:30:ILE:HD11	1:B:68:MET:CE	2.47	0.45
1:C:201:GLU:N	1:C:201:GLU:OE1	2.50	0.45
1:A:11:ILE:CG1	3:A:301:GOL:H31	2.46	0.45
2:E:791:LEU:HA	2:E:794:PHE:HD2	1.82	0.45
1:A:78:ILE:CD1	1:A:116:MET:HB3	2.48	0.44
1:C:200:ASN:HB3	1:C:201:GLU:OE1	2.16	0.44
1:D:135:CYS:SG	1:D:199:MET:HG2	2.58	0.44
1:B:135:CYS:HB3	1:B:162:CYS:SG	2.57	0.44
1:D:11:ILE:CG1	3:D:301:GOL:H12	2.48	0.44
1:A:240:LYS:NZ	1:A:242:ALA:HA	2.33	0.44
1:A:123:VAL:HG13	1:A:125:GLN:NE2	2.33	0.44
1:A:172:SER:HB3	1:A:177:ASN:HB3	2.00	0.43
1:D:197:ILE:HG22	1:D:199:MET:HB2	2.00	0.43
1:A:95:ASN:CG	1:A:96:ALA:H	2.22	0.43
1:D:16:LEU:HG	1:D:79:LEU:HD12	2.00	0.43
1:B:36:ASN:OD1	5:B:401:HOH:O	2.21	0.43
2:E:790:LEU:HD23	2:E:790:LEU:HA	1.73	0.43
1:A:84:ASN:ND2	4:A:303:SO4:O4	2.50	0.43
1:D:207:PHE:CZ	1:D:235:LEU:HB2	2.54	0.43
1:B:2:PHE:CD2	1:B:30:ILE:HD13	2.54	0.42
1:A:27:CYS:SG	1:A:123:VAL:CG2	3.07	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:172:SER:HB3	1:C:177:ASN:HB3	2.00	0.42
1:D:38:GLN:HE22	1:D:126:LEU:C	2.21	0.42
1:D:1:MET:HG2	1:D:61:ARG:HH22	1.85	0.42
2:F:790:LEU:N	2:F:793:LEU:HD22	2.31	0.42
1:A:27:CYS:SG	1:A:67:ALA:HB1	2.59	0.42
1:C:55:GLU:H	1:C:55:GLU:CD	2.23	0.42
1:A:61:ARG:NH1	1:A:63:ASP:OD1	2.52	0.41
1:C:107:ASN:O	1:C:108:GLN:HB2	2.20	0.41
1:B:23:ILE:HG13	1:B:72:LEU:HD12	2.02	0.41
1:A:135:CYS:SG	1:A:136:VAL:N	2.93	0.41
1:B:27:CYS:SG	1:B:67:ALA:HB1	2.61	0.41
1:B:99:LEU:HD23	1:B:116:MET:HE2	2.03	0.41
1:A:182:LEU:HB3	1:D:109:GLU:OE1	2.20	0.41
1:B:199:MET:CE	1:B:202:PRO:HD3	2.50	0.41
1:B:199:MET:HE2	1:B:201:GLU:O	2.13	0.41
1:D:138:LYS:HE3	1:D:224:THR:HG21	2.01	0.41
1:D:151:LEU:HA	1:D:151:LEU:HD23	1.75	0.41
1:A:151:LEU:HA	1:A:151:LEU:HD23	1.87	0.41
1:B:16:LEU:HG	1:B:79:LEU:HD12	2.03	0.41
1:C:184:GLN:HG3	1:C:196:THR:HA	2.03	0.41
1:D:107:ASN:O	1:D:108:GLN:HB2	2.19	0.41
1:C:16:LEU:HG	1:C:79:LEU:HD12	2.03	0.41
1:C:1:MET:CB	1:C:61:ARG:HH12	2.31	0.40
1:D:1:MET:N	1:D:94:ASP:OD1	2.50	0.40
1:B:233:VAL:HG22	1:B:234:PRO:HD2	2.04	0.40
1:B:95:ASN:ND2	1:B:95:ASN:N	2.60	0.40
1:A:109:GLU:OE1	1:C:185:THR:HG22	2.21	0.40
1:C:20:LYS:HD3	1:C:76:SER:OG	2.22	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	246/269 (91%)	241 (98%)	4 (2%)	1 (0%)	38	41
1	B	246/269 (91%)	244 (99%)	2 (1%)	0	100	100
1	C	246/269 (91%)	239 (97%)	7 (3%)	0	100	100
1	D	248/269 (92%)	244 (98%)	4 (2%)	0	100	100
2	E	6/17 (35%)	6 (100%)	0	0	100	100
2	F	6/17 (35%)	4 (67%)	2 (33%)	0	100	100
All	All	998/1110 (90%)	978 (98%)	19 (2%)	1 (0%)	55	63

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	122	ASP

### 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	218/236 (92%)	213 (98%)	5 (2%)	56	69
1	B	217/236 (92%)	213 (98%)	4 (2%)	64	77
1	C	218/236 (92%)	214 (98%)	4 (2%)	64	77
1	D	220/236 (93%)	216 (98%)	4 (2%)	64	77
2	E	8/16 (50%)	7 (88%)	1 (12%)	5	4
2	F	8/16 (50%)	8 (100%)	0	100	100
All	All	889/976 (91%)	871 (98%)	18 (2%)	60	74

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	LEU
1	A	41	ASP
1	A	165	ASP
1	A	184	GLN

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Mol	Chain	Res	Type
1	A	255	ILE
1	B	12	LEU
1	B	41	ASP
1	B	95	ASN
1	B	120	ASP
1	C	12	LEU
1	C	94	ASP
1	C	125	GLN
1	C	217	LYS
1	D	12	LEU
1	D	41	ASP
1	D	109	GLU
1	D	186	SER
2	E	793	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	125	GLN
1	C	125	GLN
1	C	204	GLN
1	D	24	ASN
1	D	38	GLN
1	D	44	HIS

### 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

12 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	$\# Z  > 2$
3	GOL	A	301	-	5,5,5	0.38	0	5,5,5	0.69	0
4	SO4	A	302	1	4,4,4	0.32	0	6,6,6	0.31	0
4	SO4	A	303	-	4,4,4	0.23	0	6,6,6	0.13	0
3	GOL	B	301	-	5,5,5	0.34	0	5,5,5	0.42	0
4	SO4	B	302	1	4,4,4	0.23	0	6,6,6	0.41	0
4	SO4	B	303	-	4,4,4	0.18	0	6,6,6	0.20	0
3	GOL	C	301	-	5,5,5	0.34	0	5,5,5	0.30	0
4	SO4	C	302	1	4,4,4	0.39	0	6,6,6	0.39	0
4	SO4	C	303	-	4,4,4	0.19	0	6,6,6	0.42	0
3	GOL	D	301	-	5,5,5	0.47	0	5,5,5	0.66	0
4	SO4	D	302	-	4,4,4	0.22	0	6,6,6	0.11	0
4	SO4	D	303	-	4,4,4	0.26	0	6,6,6	0.24	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	GOL	A	301	-	-	0/4/4/4	0/0/0/0
4	SO4	A	302	1	-	0/0/0/0	0/0/0/0
4	SO4	A	303	-	-	0/0/0/0	0/0/0/0
3	GOL	B	301	-	-	0/4/4/4	0/0/0/0
4	SO4	B	302	1	-	0/0/0/0	0/0/0/0
4	SO4	B	303	-	-	0/0/0/0	0/0/0/0
3	GOL	C	301	-	-	0/4/4/4	0/0/0/0
4	SO4	C	302	1	-	0/0/0/0	0/0/0/0
4	SO4	C	303	-	-	0/0/0/0	0/0/0/0
3	GOL	D	301	-	-	0/4/4/4	0/0/0/0
4	SO4	D	302	-	-	0/0/0/0	0/0/0/0
4	SO4	D	303	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	301	GOL	4	0
4	A	303	SO4	1	0
4	B	302	SO4	1	0
4	B	303	SO4	1	0
4	C	302	SO4	2	0
4	C	303	SO4	1	0
3	D	301	GOL	3	0
4	D	302	SO4	2	0
4	D	303	SO4	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å <sup>2</sup> )	Q<0.9
1	A	250/269 (92%)	0.43	15 (6%)	23 22	28, 44, 79, 101	6 (2%)
1	B	250/269 (92%)	0.49	11 (4%)	35 33	28, 44, 80, 99	5 (2%)
1	C	248/269 (92%)	0.45	9 (3%)	43 41	28, 45, 79, 97	10 (4%)
1	D	250/269 (92%)	0.49	12 (4%)	31 30	29, 44, 78, 99	16 (6%)
2	E	8/17 (47%)	1.04	1 (12%)	4 4	59, 68, 72, 82	0
2	F	8/17 (47%)	0.98	1 (12%)	4 4	62, 66, 76, 81	0
All	All	1014/1110 (91%)	0.48	49 (4%)	31 30	28, 45, 81, 101	37 (3%)

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	127	GLY	6.5
1	D	126	LEU	6.4
1	B	129	PRO	6.1
1	D	129	PRO	5.4
1	A	94	ASP	5.2
1	A	129	PRO	4.9
1	C	94	ASP	4.6
1	B	94	ASP	4.4
1	D	94	ASP	4.4
1	C	129	PRO	4.4
1	B	126	LEU	4.3
1	C	127	GLY	4.2
1	B	96	ALA	4.0
1	A	123	VAL	3.8
1	A	96	ALA	3.6
1	C	96	ALA	3.6
1	A	126	LEU	3.6
1	D	96	ALA	3.5
1	D	123	VAL	3.4

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Mol	Chain	Res	Type	RSRZ
1	C	125	GLN	3.1
1	C	128	ILE	3.1
1	C	126	LEU	3.0
1	A	130	GLU	3.0
1	D	124	GLU	3.0
1	B	122	ASP	2.8
1	A	127	GLY	2.8
1	B	128	ILE	2.7
2	E	794	PHE	2.5
2	F	793	LEU	2.5
1	A	122	ASP	2.5
1	B	130	GLU	2.5
1	C	122	ASP	2.5
1	B	106	PRO	2.4
1	B	123	VAL	2.4
1	A	243	ASP	2.3
1	D	21	ASP	2.3
1	D	243	ASP	2.2
1	A	125	GLN	2.2
1	A	12	LEU	2.2
1	D	121	LEU	2.2
1	A	124	GLU	2.2
1	B	232	ASP	2.1
1	D	122	ASP	2.1
1	A	97	ASP	2.1
1	D	198	GLU	2.1
1	A	121	LEU	2.1
1	D	127	GLY	2.1
1	A	165	ASP	2.0
1	C	123	VAL	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands [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	SO4	B	303	5/5	0.85	0.28	8.17	54,57,74,76	0
3	GOL	B	301	6/6	0.91	0.27	5.95	45,47,55,58	0
3	GOL	A	301	6/6	0.92	0.20	4.31	47,49,53,58	0
3	GOL	C	301	6/6	0.87	0.23	2.29	45,49,54,56	0
4	SO4	C	303	5/5	0.94	0.18	2.14	53,57,75,77	0
4	SO4	B	302	5/5	0.89	0.16	0.61	64,65,74,76	0
3	GOL	D	301	6/6	0.84	0.15	-0.11	46,48,50,58	0
4	SO4	D	302	5/5	0.94	0.10	-1.53	61,62,75,76	0
4	SO4	C	302	5/5	0.93	0.08	-2.80	58,66,75,76	0
4	SO4	A	302	5/5	0.95	0.11	-	64,65,71,76	0
4	SO4	D	303	5/5	0.88	0.17	-	57,61,76,80	0
4	SO4	A	303	5/5	0.90	0.22	-	56,66,78,78	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.