



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 10:34 PM UTC

PDB ID : 5YCO / pdb_00005yco
Title : Complex structure of PCNA with UHRF2
Authors : Wu, M.; Chen, W.; Hang, T.; Wang, C.; Zhang, X.; Zang, J.
Deposited on : 2017-09-07
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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

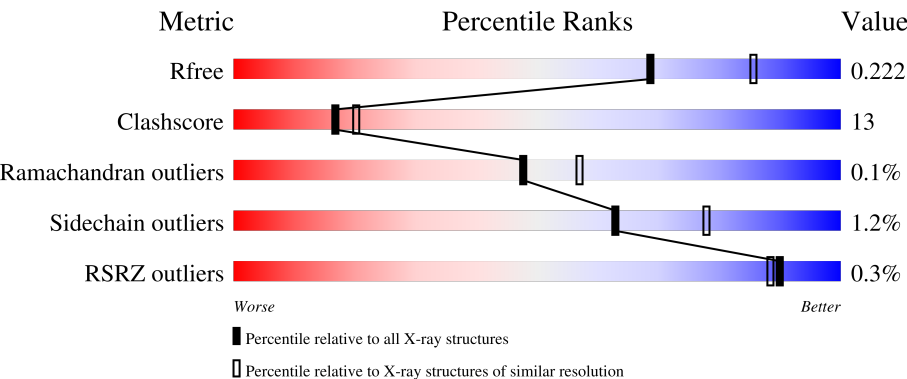
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance i

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}	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	72%19%• 7%
1	B	269	% 77%14%• 7%
1	C	269	72%18%• 8%
1	D	269	74%18%• 7%
2	E	17	24%18%6%53%

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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	-
4	SO4	C	302	-	-	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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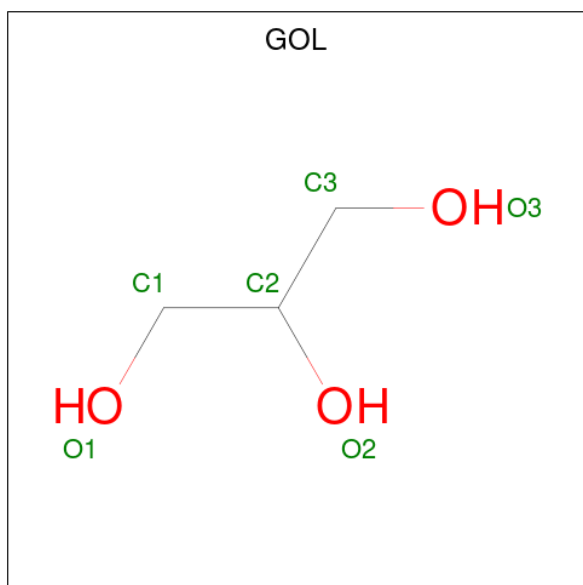
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Chain	Residue	Modelled	Actual	Comment	Reference
C	267	HIS	-	expression tag	UNP P12004
C	268	HIS	-	expression tag	UNP P12004
C	269	HIS	-	expression tag	UNP P12004
D	262	LEU	-	expression tag	UNP P12004
D	263	GLU	-	expression tag	UNP P12004
D	264	HIS	-	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 (CCD ID: GOL) (formula: $C_3H_8O_3$).



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 (CCD ID: SO4) (formula: O₄S).



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.

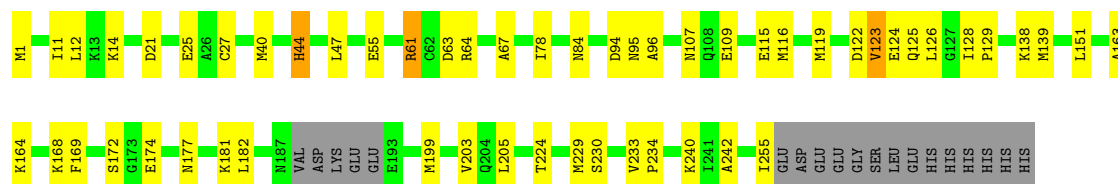
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	82	Total 82	O 82	0	0
5	B	82	Total 82	O 82	0	0
5	C	75	Total 75	O 75	0	0
5	D	84	Total 84	O 84	0	0
5	E	1	Total 1	O 1	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

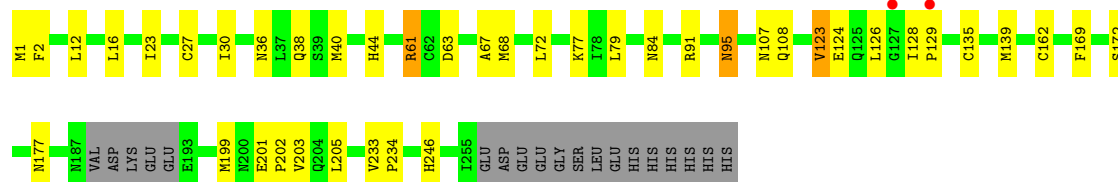
• Molecule 1: Proliferating cell nuclear antigen

Chain A: 



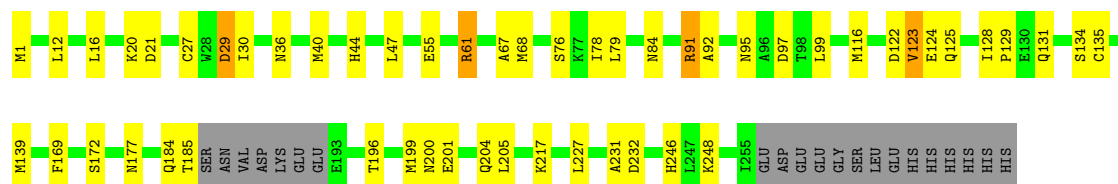
• Molecule 1: Proliferating cell nuclear antigen

Chain B: 



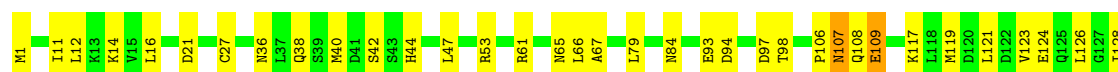
• Molecule 1: Proliferating cell nuclear antigen

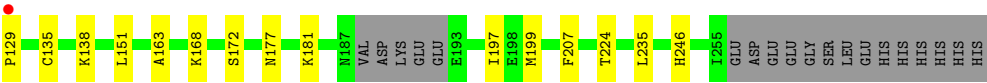
Chain C: 



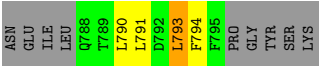
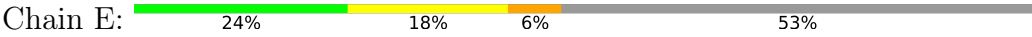
• Molecule 1: Proliferating cell nuclear antigen

Chain D: 

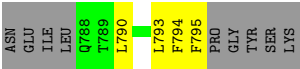
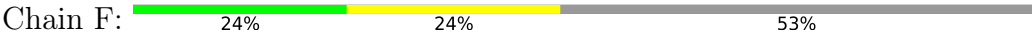




● Molecule 2: E3 ubiquitin-protein ligase UHRF2



● 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, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	2.39 (at 2.20Å)	Xtriage
Refinement program	PHENIX 1.11.1_2575	Depositor
R, R_{free}	0.204 , 0.220 0.204 , 0.222	Depositor DCC
R_{free} test set	4857 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	41.0	Xtriage
Anisotropy	0.015	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 31.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	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 ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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	0.56	3/1946 (0.2%)	0.74	3/2628 (0.1%)
1	B	0.59	3/1942 (0.2%)	0.74	6/2623 (0.2%)
1	C	0.62	2/1954 (0.1%)	0.96	16/2637 (0.6%)
1	D	0.43	0/1966	0.71	7/2653 (0.3%)
2	E	0.49	0/71	1.03	0/95
2	F	0.44	0/71	0.98	0/95
All	All	0.55	8/7950 (0.1%)	0.80	32/10731 (0.3%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	91[A]	ARG	CA-C	7.28	1.62	1.52
1	C	91[B]	ARG	CA-C	7.28	1.62	1.52
1	A	44	HIS	CG-ND1	-6.14	1.31	1.38
1	B	44	HIS	CG-ND1	-6.06	1.31	1.38
1	B	44	HIS	CD2-NE2	-5.62	1.31	1.37
1	A	44	HIS	CD2-NE2	-5.57	1.31	1.37
1	A	61	ARG	C-O	-5.14	1.17	1.23
1	B	61	ARG	N-CA	-5.12	1.40	1.46

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	124	GLU	O-C-N	-12.22	109.68	122.64
1	C	124	GLU	O-C-N	-11.62	109.42	122.55
1	C	91[A]	ARG	CA-C-O	11.45	133.37	119.98
1	C	91[B]	ARG	CA-C-O	11.45	133.37	119.98
1	A	124	GLU	O-C-N	-11.16	109.94	122.55
1	C	122	ASP	CA-C-N	-10.70	108.94	122.43
1	C	122	ASP	C-N-CA	-10.70	108.94	122.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	123	VAL	CA-C-N	9.36	135.61	122.41
1	A	123	VAL	C-N-CA	9.36	135.61	122.41
1	C	123	VAL	CA-C-N	9.17	135.34	122.41
1	C	123	VAL	C-N-CA	9.17	135.34	122.41
1	C	123	VAL	O-C-N	8.32	133.09	122.77
1	B	123	VAL	CA-C-N	7.73	134.87	123.12
1	B	123	VAL	C-N-CA	7.73	134.87	123.12
1	D	123	VAL	CB-CA-C	7.10	119.32	111.80
1	D	106	PRO	CA-C-N	7.07	130.61	120.79
1	D	106	PRO	C-N-CA	7.07	130.61	120.79
1	B	124	GLU	CA-C-N	-6.70	110.54	122.74
1	B	124	GLU	C-N-CA	-6.70	110.54	122.74
1	D	107	ASN	O-C-N	6.40	128.93	122.08
1	C	124	GLU	CA-C-N	-6.39	111.62	122.67
1	C	124	GLU	C-N-CA	-6.39	111.62	122.67
1	C	91[A]	ARG	N-CA-C	5.80	123.15	110.80
1	C	91[B]	ARG	N-CA-C	5.80	123.15	110.80
1	B	123	VAL	N-CA-C	-5.55	99.49	107.37
1	D	124	GLU	CA-C-N	-5.35	115.17	122.93
1	D	124	GLU	C-N-CA	-5.35	115.17	122.93
1	D	123	VAL	N-CA-C	-5.34	99.79	107.37
1	C	123	VAL	N-CA-C	-5.33	99.41	107.73
1	C	92	ALA	N-CA-CB	5.21	119.82	110.80
1	C	29	ASP	CA-C-N	-5.17	116.44	123.10
1	C	29	ASP	C-N-CA	-5.17	116.44	123.10

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	57	0
1	B	1917	0	1929	47	0
1	C	1923	0	1948	55	0
1	D	1935	0	1960	37	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	2	0
5	C	75	0	0	3	0
5	D	84	0	0	3	0
5	E	1	0	0	0	0
All	All	8224	0	7940	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 13.

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:C:246:HIS:ND1	4:C:302:SO4:O2	1.58	1.33
1:B:199:MET:HE2	1:B:201:GLU:CA	1.63	1.27
1:B:199:MET:HE2	1:B:201:GLU:N	1.57	1.20
1:C:30:ILE:CD1	1:C:68:MET:HE2	1.80	1.10
1:D:119:MET:HE2	1:D:121:LEU:HD21	1.31	1.05
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:B:199:MET:CE	1:B:201:GLU:C	2.32	1.03
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:C	1.84	1.01
1:C:30:ILE:HD11	1:C:68:MET:HE2	1.01	1.01
1:C:128:ILE:HD12	1:C:129:PRO:HD2	1.43	1.00
1:C:200:ASN:C	1:C:201:GLU:OE1	2.13	0.92
1:D:119:MET:CE	1:D:121:LEU:HD21	2.03	0.87
1:A:125:GLN:C	1:A:126:LEU:HD12	2.00	0.87
1:C:1:MET:HG2	1:C:61:ARG:HH12	1.38	0.87
1:B:199:MET:HE3	1:B:202:PRO:N	1.91	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:134:SER:HB3	1:C:201:GLU:HG2	1.59	0.85
1:B:30:ILE:HD11	1:B:68:MET:HE2	1.60	0.83
1:D:65:ASN:O	1:D:66:LEU:HD23	1.78	0.82
1:B:128:ILE:HD12	1:B:129:PRO:HD2	1.61	0.82
1:A:1:MET:H2	1:A:64:ARG:HH12	1.28	0.80
1:A:233:VAL:HG23	1:A:234:PRO:HD2	1.63	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:C:123:VAL:HG21	1:C:125:GLN:HE21	1.50	0.77
1:B:199:MET:CE	1:B:201:GLU:HA	2.13	0.76
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:C:200:ASN:CB	1:C:201:GLU:OE1	2.35	0.74
1:D:65:ASN:C	1:D:66:LEU:HD23	2.13	0.73
1:A:64:ARG:NH2	1:A:94:ASP:OD1	2.22	0.73
1:B:199:MET:HE3	1:B:201:GLU:C	2.08	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
2:F:790:LEU:H	2:F:793:LEU:HD22	1.57	0.69
1:C:204:GLN:C	1:C:205:LEU:HD23	2.18	0.69
1:B:95:ASN:H	1:B:95:ASN:HD22	1.40	0.69
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:B:199:MET:CE	1:B:202:PRO:N	2.53	0.66
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:B:40:MET:HE3	2:E:793:LEU:HB2	1.76	0.66
1:C:1:MET:CG	1:C:61:ARG:HH12	2.08	0.66
1:C:123:VAL:HG22	1:C:125:GLN:HE21	1.55	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:D:84:ASN:ND2	4:D:303:SO4:O3	2.30	0.65
1:C:1:MET:HG2	1:C:61:ARG:NH1	2.11	0.64
1:B:123:VAL:O	1:B:123:VAL:CG2	2.45	0.64
1:C:204:GLN:O	1:C:205:LEU:HD23	1.99	0.63
1:C:200:ASN:HB2	1:C:201:GLU:OE1	1.97	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:135:CYS:SG	1:B:203:VAL:HG23	2.41	0.61
1:C:40:MET:HE2	1:C:44:HIS:CG	2.35	0.61
1:B:199:MET:CE	1:B:201:GLU:N	2.50	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:B:1:MET:HE1	1:B:91:ARG:HD3	1.84	0.59
1:D:128:ILE:HD12	1:D:129:PRO:HD2	1.85	0.59
1:A:163:ALA:C	1:A:199:MET:SD	2.86	0.59
1:C:84:ASN:ND2	4:C:303:SO4:O1	2.36	0.58
1:B:199:MET:HE1	1:B:201:GLU:HA	1.85	0.58
1:D:36:ASN:OD1	5:D:401:HOH:O	2.16	0.58
1:A:40:MET:HE2	1:A:44:HIS:CG	2.39	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
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:21:ASP:HB2	5:A:410:HOH:O	2.05	0.55
1:A:126:LEU:HD12	1:A:126:LEU:N	2.20	0.55
1:D:246:HIS:ND1	4:D:302:SO4:O3	2.34	0.55
1:C:248:LYS:NZ	5:C:404:HOH:O	2.38	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:1:MET:HB3	1:C:61:ARG:HH11	1.69	0.55
1:C:123:VAL:HG21	1:C:125:GLN:NE2	2.19	0.55
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:D:93:GLU:H	1:D:93:GLU:CD	2.17	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:163:ALA:HA	1:D:199:MET:HE3	1.89	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:95:ASN:CG	1:A:96:ALA:N	2.68	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:H	2:F:793:LEU:CD1	2.23	0.51
1:A:164:LYS:N	1:A:199:MET:SD	2.83	0.51
1:C:99:LEU:HD23	1:C:116:MET:HE2	1.91	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: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:A:1:MET:H3	1:A:64:ARG:HH12	1.53	0.49
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: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
1:D:42:SER:O	1:D:44:HIS:HD2	1.95	0.49
1:C:123:VAL:O	1:C:123:VAL:HG13	2.11	0.49
1:D:11:ILE:HG12	3:D:301:GOL:H32	1.94	0.48
1:A:95:ASN:CG	1:A:96:ALA:H	2.22	0.48
1:D:27:CYS:SG	1:D:67:ALA:HB1	2.53	0.48
1:B:199:MET:CE	1:B:202:PRO:CD	2.92	0.47
1:B:199:MET:HE1	1:B:202:PRO:HD3	1.95	0.47
1:C:199:MET:HE3	1:C:201:GLU:HA	1.97	0.47
1:D:38:GLN:HE22	1:D:126:LEU:C	2.21	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:C:55:GLU:H	1:C:55:GLU:CD	2.23	0.46
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:C:200:ASN:O	1:C:201:GLU:OE1	2.33	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:78:ILE:CD1	1:C:116:MET:HB3	2.45	0.46
1:A:14:LYS:HD2	3:A:301:GOL:H32	1.97	0.45
1:A:138:LYS:HE3	1:A:224:THR:HG21	1.98	0.45
1:B:139:MET:HE1	1:B:169:PHE:HZ	1.80	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: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:55:GLU:H	1:A:55:GLU:CD	2.25	0.45
1:A:78:ILE:CD1	1:A:116:MET:HB3	2.48	0.44
1:A:233:VAL:HG22	1:A:234:PRO:N	2.31	0.44
1:C:139:MET:HE1	1:C:169:PHE:HZ	1.82	0.44
1:B:199:MET:HE2	1:B:201:GLU:H	1.65	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:A:25:GLU:CD	1:A:119:MET:HE1	2.43	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: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
1:D:1:MET:N	1:D:94:ASP:OD1	2.50	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:B:199:MET:HE3	1:B:202:PRO:CD	2.47	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
1:C:172:SER:HB3	1:C:177:ASN:HB3	2.00	0.42
1:C:139:MET:HE3	1:C:227:LEU:HD11	2.01	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:40:MET:HE2	1:C:44:HIS:HA	2.01	0.42
1:A:61:ARG:NH1	1:A:63:ASP:OD1	2.52	0.41
1:B:23:ILE:HG13	1:B:72:LEU:HD12	2.02	0.41
1:A:139:MET:HE1	1:A:169:PHE:HZ	1.85	0.41
1:B:27:CYS:SG	1:B:67:ALA:HB1	2.61	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:138:LYS:HE3	1:D:224:THR:HG21	2.01	0.41
1:A:229:MET:HE3	1:A:229:MET:HB2	1.91	0.41
1:B:77:LYS:NZ	5:B:402:HOH:O	2.40	0.41
1:D:151:LEU:HD23	1:D:151:LEU:HA	1.75	0.41
1:A:151:LEU:HD23	1:A:151:LEU:HA	1.87	0.41
1:A:240:LYS:HZ3	1:A:242:ALA:HA	1.84	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:C:201:GLU:OE1	1:C:201:GLU:N	2.50	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:29:ASP:CG	1:C:125:GLN:HE22	2.28	0.41
1:C:1:MET:CB	1:C:61:ARG:HH12	2.31	0.40
1:B:95:ASN:ND2	1:B:95:ASN:N	2.60	0.40
1:B:233:VAL:HG22	1:B:234:PRO:HD2	2.04	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

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	246/269 (91%)	241 (98%)	4 (2%)	1 (0%)	30	34
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	F	6/17 (35%)	4 (67%)	2 (33%)	0	100	100
All	All	998/1110 (90%)	978 (98%)	19 (2%)	1 (0%)	48	57

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%)	216 (99%)	2 (1%)	70	84
1	B	217/236 (92%)	215 (99%)	2 (1%)	70	84
1	C	218/236 (92%)	213 (98%)	5 (2%)	44	59
1	D	220/236 (93%)	218 (99%)	2 (1%)	70	84
2	E	8/16 (50%)	7 (88%)	1 (12%)	4	4
2	F	8/16 (50%)	8 (100%)	0	100	100
All	All	889/976 (91%)	877 (99%)	12 (1%)	63	76

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	LEU
1	A	255	ILE
1	B	12	LEU
1	B	95	ASN
1	C	12	LEU
1	C	61	ARG
1	C	91[A]	ARG
1	C	91[B]	ARG
1	C	217	LYS
1	D	12	LEU

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Mol	Chain	Res	Type
1	D	109	GLU
2	E	793	LEU

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

Mol	Chain	Res	Type
1	A	125	GLN
1	B	36	ASN
1	B	38	GLN
1	B	204	GLN
1	C	8	GLN
1	C	125	GLN
1	C	204	GLN
1	D	24	ASN
1	D	36	ASN
1	D	38	GLN
1	D	44	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	$\# Z > 2$
4	SO4	B	302	-	4,4,4	0.27	0	6,6,6	0.43	0
4	SO4	B	303	-	4,4,4	0.24	0	6,6,6	0.21	0
4	SO4	C	303	-	4,4,4	0.27	0	6,6,6	0.43	0
3	GOL	A	301	-	5,5,5	0.43	0	5,5,5	0.75	0
4	SO4	C	302	-	4,4,4	0.41	0	6,6,6	0.39	0
4	SO4	D	303	-	4,4,4	0.33	0	6,6,6	0.19	0
4	SO4	A	302	-	4,4,4	0.37	0	6,6,6	0.28	0
4	SO4	D	302	-	4,4,4	0.29	0	6,6,6	0.14	0
3	GOL	C	301	-	5,5,5	0.38	0	5,5,5	0.34	0
3	GOL	B	301	-	5,5,5	0.40	0	5,5,5	0.47	0
4	SO4	A	303	-	4,4,4	0.29	0	6,6,6	0.18	0
3	GOL	D	301	-	5,5,5	0.52	0	5,5,5	0.71	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	D	301	-	-	2/4/4/4	-
3	GOL	B	301	-	-	2/4/4/4	-
3	GOL	C	301	-	-	1/4/4/4	-
3	GOL	A	301	-	-	4/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	301	GOL	O1-C1-C2-C3
3	A	301	GOL	C1-C2-C3-O3
3	D	301	GOL	O1-C1-C2-C3
3	A	301	GOL	O1-C1-C2-O2
3	A	301	GOL	O2-C2-C3-O3
3	D	301	GOL	O1-C1-C2-O2
3	B	301	GOL	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
3	B	301	GOL	O1-C1-C2-C3
3	C	301	GOL	O1-C1-C2-O2

There are no ring outliers.

9 monomers are involved in 16 short contacts:

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

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th 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 ²)	Q<0.9
1	A	250/269 (92%)	-0.74	0 100 100	28, 44, 77, 94	6 (2%)
1	B	250/269 (92%)	-0.72	2 (0%) 82 80	28, 44, 77, 96	5 (2%)
1	C	248/269 (92%)	-0.72	0 100 100	22, 44, 76, 95	11 (4%)
1	D	250/269 (92%)	-0.74	1 (0%) 88 87	21, 43, 77, 96	18 (7%)
2	E	8/17 (47%)	0.36	0 100 100	59, 68, 72, 82	0
2	F	8/17 (47%)	0.16	0 100 100	62, 66, 76, 81	0
All	All	1014/1110 (91%)	-0.71	3 (0%) 90 88	21, 44, 77, 96	40 (3%)

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	129	PRO	2.5
1	B	129	PRO	2.1
1	B	127	GLY	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 oligosaccharides 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. The B-factors column lists the minimum,

median, 95th 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	B-factors(Å ²)	Q<0.9
4	SO4	B	302	5/5	0.96	0.06	64,65,74,76	0
3	GOL	C	301	6/6	0.98	0.08	45,49,54,56	0
3	GOL	D	301	6/6	0.98	0.09	46,48,50,58	0
4	SO4	A	303	5/5	0.98	0.06	56,66,78,78	0
3	GOL	B	301	6/6	0.98	0.06	45,47,55,58	0
4	SO4	B	303	5/5	0.98	0.12	54,57,74,76	0
4	SO4	D	302	5/5	0.98	0.05	61,62,75,76	0
4	SO4	D	303	5/5	0.98	0.07	57,61,76,80	0
4	SO4	C	302	5/5	0.99	0.04	58,66,75,76	0
4	SO4	C	303	5/5	0.99	0.05	53,57,75,77	0
4	SO4	A	302	5/5	0.99	0.04	64,65,71,76	0
3	GOL	A	301	6/6	0.99	0.07	47,49,53,58	0

6.5 Other polymers [i](#)

There are no such residues in this entry.