



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 11:56 PM GMT

PDB ID : 1Z6A  
Title : Sulfolobus solfataricus SWI2/SNF2 ATPase core domain  
Authors : Duerr, H.; Koerner, C.; Mueller, M.; Hickmann, V.; Hopfner, K.P.  
Deposited on : 2005-03-22  
Resolution : 3.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

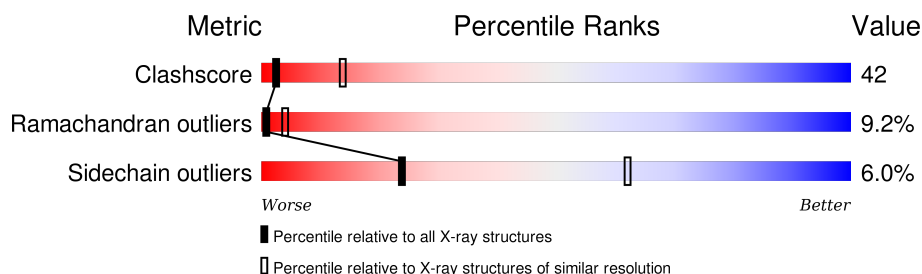
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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))
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	500	<div> <div style="width: 35%; background-color: green;"></div> <div style="width: 52%; background-color: yellow;"></div> <div style="width: 9%; background-color: orange;"></div> <div style="width: 4%; background-color: grey;"></div> </div> <div> <div style="width: 35%;"></div> <div style="width: 52%;"></div> <div style="width: 9%;"></div> <div style="width: 4%;"></div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3874 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 Helicase of the snf2/rad54 family.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	480	Total	C	N	O	S	62	0	0
			3831	2467	644	707	13			

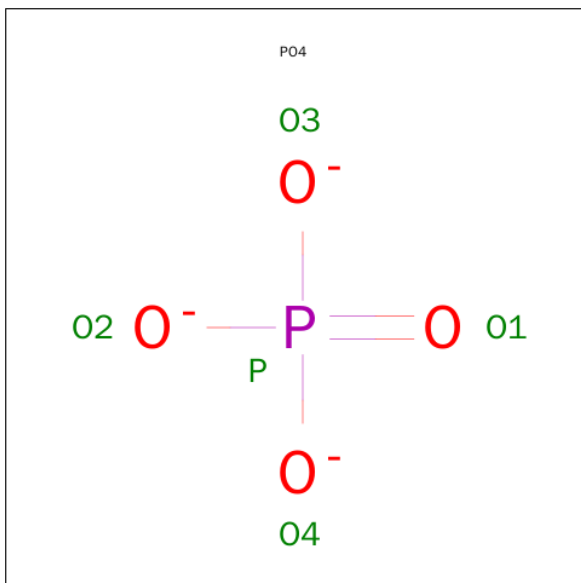
There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-12	MET	-	EXPRESSION TAG	UNP Q97XQ5
A	-11	GLY	-	EXPRESSION TAG	UNP Q97XQ5
A	-10	SER	-	EXPRESSION TAG	UNP Q97XQ5
A	-9	SER	-	EXPRESSION TAG	UNP Q97XQ5
A	-8	HIS	-	EXPRESSION TAG	UNP Q97XQ5
A	-7	HIS	-	EXPRESSION TAG	UNP Q97XQ5
A	-6	HIS	-	EXPRESSION TAG	UNP Q97XQ5
A	-5	HIS	-	EXPRESSION TAG	UNP Q97XQ5
A	-4	HIS	-	EXPRESSION TAG	UNP Q97XQ5
A	-3	HIS	-	EXPRESSION TAG	UNP Q97XQ5
A	-2	SER	-	EXPRESSION TAG	UNP Q97XQ5
A	-1	SER	-	EXPRESSION TAG	UNP Q97XQ5
A	0	GLY	-	EXPRESSION TAG	UNP Q97XQ5
A	1	LEU	-	EXPRESSION TAG	UNP Q97XQ5
A	2	VAL	-	EXPRESSION TAG	UNP Q97XQ5
A	3	PRO	-	EXPRESSION TAG	UNP Q97XQ5
A	4	ARG	-	EXPRESSION TAG	UNP Q97XQ5
A	5	GLY	-	EXPRESSION TAG	UNP Q97XQ5
A	6	SER	-	EXPRESSION TAG	UNP Q97XQ5
A	7	HIS	-	EXPRESSION TAG	UNP Q97XQ5
A	8	MET	-	EXPRESSION TAG	UNP Q97XQ5
A	9	ALA	-	EXPRESSION TAG	UNP Q97XQ5
A	11	SER	-	EXPRESSION TAG	UNP Q97XQ5
A	12	LYS	-	EXPRESSION TAG	UNP Q97XQ5

- Molecule 2 is MERCURY (II) ION (three-letter code: HG) (formula: Hg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	3	Total Hg 3 3	0	0

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



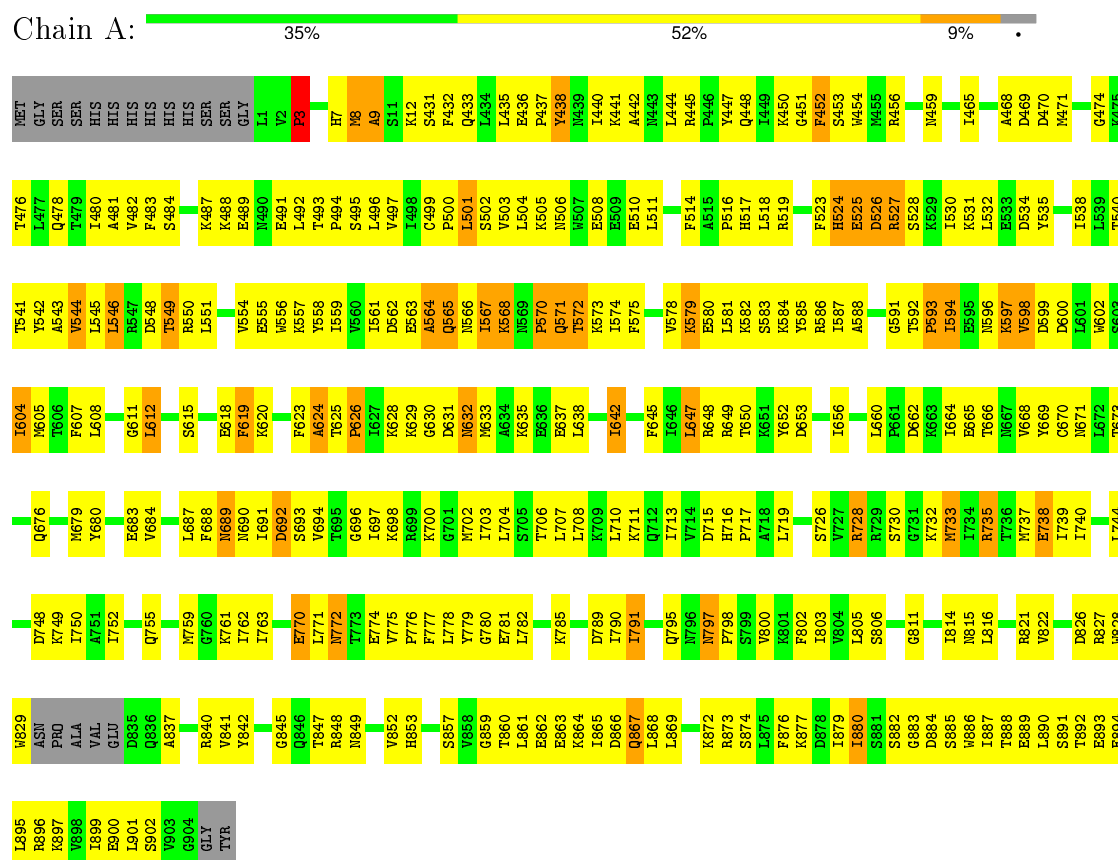
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O P 5 4 1	0	0
3	A	1	Total O P 5 4 1	0	0
3	A	1	Total O P 5 4 1	0	0
3	A	1	Total O P 5 4 1	0	0
3	A	1	Total O P 5 4 1	0	0
3	A	1	Total O P 5 4 1	0	0
3	A	1	Total O P 5 4 1	0	0
3	A	1	Total O P 5 4 1	0	0

### 3 Residue-property plots

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

Note EDS was not executed.

- Molecule 1: Helicase of the snf2/rad54 family



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	83.89Å 83.89Å 227.54Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.00	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-3.00)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	CNS	Depositor
R, $R_{free}$	0.240 , 0.297	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3874	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	91.0	wwPDB-VP

## 5 Model quality [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, HG

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	0.41	0/3898	0.67	1/5252 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	3	PRO	N-CA-CB	5.79	110.25	103.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3831	0	3926	321	1
2	A	3	0	0	0	0
3	A	40	0	0	2	0
All	All	3874	0	3926	321	1

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 42.

All (321) 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:571:GLN:HG2	1:A:572:THR:H	1.11	1.07
1:A:568:LYS:O	1:A:570:PRO:HD3	1.53	1.07
1:A:650:THR:HG22	1:A:652:TYR:H	1.19	1.02
1:A:546:LEU:HD21	1:A:573:LYS:HE3	1.44	0.97
1:A:791:ILE:HD11	1:A:814:ILE:HG23	1.47	0.96
1:A:860:THR:HG22	1:A:862:GLU:H	1.29	0.95
1:A:650:THR:HG22	1:A:652:TYR:N	1.86	0.90
1:A:531:LYS:HG2	1:A:534:ASP:HB2	1.52	0.90
1:A:542:TYR:HB3	1:A:574:ILE:HD13	1.55	0.87
1:A:592:THR:O	1:A:594:ILE:HG13	1.73	0.87
1:A:571:GLN:HG2	1:A:572:THR:N	1.91	0.84
1:A:625:THR:OG1	1:A:626:PRO:HD3	1.77	0.83
1:A:759:MET:HE3	1:A:762:ILE:HB	1.61	0.81
1:A:519:ARG:HD2	1:A:535:TYR:HE2	1.43	0.81
1:A:748:ASP:OD2	1:A:821:ARG:NH1	2.13	0.81
1:A:883:GLY:HA2	1:A:886:TRP:HE1	1.45	0.81
1:A:650:THR:CG2	1:A:652:TYR:H	1.94	0.81
1:A:814:ILE:HD12	1:A:842:TYR:CE2	2.16	0.80
1:A:837:ALA:O	1:A:841:VAL:HG23	1.81	0.80
1:A:867:GLN:HG2	1:A:868:LEU:N	1.95	0.80
1:A:491:GLU:C	1:A:557:LYS:HD3	2.02	0.79
1:A:555:GLU:HG2	1:A:582:LYS:HE2	1.64	0.79
1:A:600:ASP:O	1:A:604:ILE:HG13	1.82	0.78
1:A:715:ASP:HA	1:A:732:LYS:HD2	1.64	0.78
1:A:454:TRP:CZ3	1:A:647:LEU:HB2	2.18	0.78
1:A:527:ARG:CZ	1:A:530:ILE:HG12	2.14	0.78
1:A:797:ASN:HD22	1:A:798:PRO:HD2	1.48	0.77
1:A:478:GLN:O	1:A:482:VAL:HG23	1.86	0.76
1:A:740:ILE:HD12	1:A:802:PHE:HE2	1.51	0.75
1:A:638:LEU:HG	1:A:642:ILE:HD11	1.67	0.75
1:A:592:THR:HG22	1:A:648:ARG:CZ	2.18	0.74
1:A:700:LYS:HE2	1:A:888:THR:OG1	1.87	0.74
1:A:504:LEU:HD21	1:A:508:GLU:OE1	1.88	0.74
1:A:495:SER:OG	1:A:558:TYR:HB2	1.87	0.74
1:A:638:LEU:O	1:A:642:ILE:HG13	1.86	0.74
1:A:593:PRO:HA	1:A:597:LYS:NZ	2.03	0.73
1:A:873:ARG:HG3	1:A:876:PHE:HD2	1.52	0.73
1:A:519:ARG:HD2	1:A:535:TYR:CE2	2.23	0.72
1:A:873:ARG:HA	1:A:876:PHE:HB3	1.71	0.72
1:A:863:GLU:O	1:A:866:ASP:HB3	1.91	0.71
1:A:631:ASP:OD1	1:A:633:MET:HB2	1.91	0.71
1:A:668:VAL:HG11	1:A:739:ILE:HD12	1.73	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:9:ALA:HA	1:A:432:PHE:CE1	2.27	0.70
1:A:873:ARG:HG2	1:A:877:LYS:HB2	1.73	0.70
1:A:869:LEU:HD21	1:A:886:TRP:CH2	2.27	0.70
1:A:563:GLU:O	1:A:564:ALA:O	2.10	0.69
1:A:597:LYS:NZ	1:A:597:LYS:HB3	2.07	0.69
1:A:504:LEU:O	1:A:508:GLU:HG3	1.93	0.69
1:A:676:GLN:OE1	1:A:730:SER:HA	1.92	0.69
1:A:527:ARG:HD2	1:A:530:ILE:CD1	2.23	0.69
1:A:465:ILE:HG22	1:A:645:PHE:HA	1.75	0.69
1:A:653:ASP:O	1:A:656:ILE:HG22	1.92	0.68
1:A:476:THR:O	1:A:480:ILE:HD13	1.94	0.68
1:A:726:SER:HB2	1:A:728:ARG:HE	1.58	0.68
1:A:749:LYS:HE2	1:A:800:VAL:O	1.94	0.67
1:A:499:CYS:HB2	1:A:503:VAL:CG2	2.23	0.67
1:A:527:ARG:HD2	1:A:530:ILE:HD11	1.76	0.67
1:A:740:ILE:HD11	1:A:752:ILE:HD11	1.77	0.67
1:A:440:ILE:HD11	1:A:481:ALA:HA	1.74	0.66
1:A:688:PHE:HE1	1:A:896:ARG:HB2	1.59	0.66
1:A:883:GLY:O	1:A:887:ILE:HG13	1.96	0.65
1:A:444:LEU:H	1:A:444:LEU:HD12	1.60	0.65
1:A:556:TRP:O	1:A:583:SER:HA	1.95	0.65
1:A:561:ILE:HD11	1:A:578:VAL:HG11	1.78	0.64
1:A:728:ARG:CD	1:A:728:ARG:H	2.10	0.64
1:A:571:GLN:CG	1:A:572:THR:H	1.98	0.64
1:A:859:GLY:O	1:A:901:LEU:HD12	1.98	0.64
1:A:703:ILE:CG2	1:A:888:THR:HG22	2.28	0.63
1:A:441:LYS:HD2	1:A:441:LYS:N	2.12	0.63
1:A:688:PHE:O	1:A:691:ILE:HG22	1.97	0.63
1:A:593:PRO:HA	1:A:597:LYS:HZ2	1.63	0.62
1:A:733:MET:O	1:A:737:MET:HG2	1.99	0.62
1:A:527:ARG:HD3	1:A:550:ARG:CB	2.30	0.62
1:A:704:LEU:O	1:A:708:LEU:HG	2.00	0.61
1:A:791:ILE:CD1	1:A:814:ILE:HA	2.30	0.61
1:A:860:THR:CG2	1:A:861:LEU:HD23	2.31	0.61
1:A:735:ARG:HA	1:A:738:GLU:HG3	1.81	0.61
1:A:459:ASN:HB3	1:A:585:TYR:HD2	1.63	0.61
1:A:471:MET:O	1:A:821:ARG:NH2	2.34	0.60
1:A:865:ILE:O	1:A:869:LEU:HG	2.02	0.60
1:A:555:GLU:HG2	1:A:582:LYS:CE	2.31	0.60
1:A:484:SER:O	1:A:487:LYS:HB3	2.02	0.60
1:A:523:PHE:HB3	1:A:540:THR:OG1	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:580:GLU:HG3	1:A:580:GLU:O	2.01	0.60
1:A:673:THR:H	1:A:676:GLN:NE2	2.00	0.59
1:A:527:ARG:HH21	1:A:550:ARG:CB	2.15	0.59
1:A:602:TRP:HB2	1:A:619:PHE:CD2	2.38	0.59
1:A:480:ILE:O	1:A:483:PHE:HB2	2.03	0.59
1:A:444:LEU:H	1:A:444:LEU:CD1	2.16	0.59
1:A:711:LYS:NZ	1:A:755:GLN:HE22	2.01	0.59
1:A:465:ILE:HG22	1:A:645:PHE:CA	2.33	0.58
1:A:891:SER:O	1:A:893:GLU:N	2.36	0.58
1:A:541:THR:HG22	1:A:542:TYR:N	2.17	0.58
1:A:715:ASP:OD2	1:A:732:LYS:HE3	2.03	0.58
1:A:887:ILE:O	1:A:890:LEU:HG	2.02	0.58
1:A:688:PHE:HE2	1:A:899:ILE:HD11	1.67	0.58
1:A:444:LEU:N	1:A:444:LEU:HD12	2.17	0.58
1:A:8:MET:O	1:A:9:ALA:HB2	2.03	0.58
1:A:857:SER:O	1:A:860:THR:HB	2.04	0.58
1:A:620:LYS:HA	1:A:624:ALA:HB3	1.85	0.58
1:A:715:ASP:HB3	1:A:759:MET:SD	2.44	0.57
1:A:797:ASN:HD22	1:A:798:PRO:CD	2.17	0.57
1:A:660:LEU:HD22	1:A:664:ILE:HD11	1.87	0.57
1:A:592:THR:O	1:A:594:ILE:N	2.29	0.57
1:A:688:PHE:C	1:A:690:ASN:H	2.07	0.57
1:A:775:VAL:HG12	1:A:775:VAL:O	2.04	0.57
1:A:563:GLU:OE2	1:A:570:PRO:HB2	2.04	0.57
1:A:687:LEU:O	1:A:691:ILE:HB	2.04	0.57
1:A:827:ARG:HH22	1:A:866:ASP:HB2	1.68	0.57
1:A:899:ILE:HG13	1:A:900:GLU:N	2.19	0.57
1:A:849:ASN:HB2	3:A:961:PO4:O2	2.04	0.57
1:A:689:ASN:N	1:A:689:ASN:HD22	2.02	0.56
1:A:548:ASP:CG	1:A:549:THR:H	2.09	0.56
1:A:890:LEU:HB2	1:A:895:LEU:HD13	1.88	0.56
1:A:543:ALA:C	1:A:545:LEU:H	2.09	0.56
1:A:578:VAL:C	1:A:580:GLU:H	2.09	0.55
1:A:564:ALA:HB1	1:A:565:GLN:NE2	2.21	0.55
1:A:795:GLN:HE21	1:A:815:ASN:ND2	2.05	0.55
1:A:586:ARG:NH2	1:A:608:LEU:O	2.40	0.55
1:A:540:THR:HG23	1:A:544:VAL:HB	1.89	0.55
1:A:605:MET:HG3	1:A:642:ILE:HG21	1.89	0.55
1:A:680:TYR:O	1:A:684:VAL:HG23	2.06	0.55
1:A:445:ARG:HD3	1:A:447:TYR:HE2	1.71	0.55
1:A:527:ARG:NH2	1:A:530:ILE:HG12	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:814:ILE:HG22	1:A:816:LEU:HG	1.89	0.54
1:A:829:TRP:CB	1:A:883:GLY:HA3	2.38	0.54
1:A:770:GLU:O	1:A:771:LEU:HD23	2.07	0.54
1:A:740:ILE:HD12	1:A:802:PHE:CE2	2.38	0.54
1:A:625:THR:O	1:A:629:LYS:HB2	2.08	0.54
1:A:483:PHE:O	1:A:492:LEU:HD22	2.07	0.54
1:A:847:THR:O	1:A:848:ARG:HG3	2.07	0.54
1:A:822:VAL:HB	1:A:852:VAL:HG22	1.89	0.54
1:A:859:GLY:HA2	1:A:864:LYS:HZ2	1.71	0.54
1:A:860:THR:HG22	1:A:861:LEU:HD23	1.89	0.54
1:A:688:PHE:CE2	1:A:899:ILE:HD11	2.43	0.54
1:A:615:SER:OG	1:A:618:GLU:HB2	2.07	0.54
1:A:564:ALA:C	1:A:566:ASN:H	2.10	0.54
1:A:531:LYS:HG2	1:A:534:ASP:CB	2.34	0.54
1:A:791:ILE:HD13	1:A:815:ASN:H	1.73	0.53
1:A:578:VAL:O	1:A:580:GLU:N	2.38	0.53
1:A:827:ARG:NH2	1:A:866:ASP:HB2	2.23	0.53
1:A:883:GLY:HA2	1:A:886:TRP:NE1	2.18	0.53
1:A:587:ILE:HG22	1:A:588:ALA:N	2.23	0.53
1:A:516:PRO:C	1:A:518:LEU:H	2.11	0.53
1:A:499:CYS:HB2	1:A:503:VAL:HG23	1.90	0.53
1:A:821:ARG:NE	1:A:853:HIS:NE2	2.54	0.53
1:A:687:LEU:CD1	1:A:702:MET:HG2	2.39	0.53
1:A:440:ILE:CD1	1:A:481:ALA:HA	2.39	0.52
1:A:496:LEU:HD12	1:A:497:VAL:H	1.74	0.52
1:A:730:SER:HB3	1:A:733:MET:HB2	1.91	0.52
1:A:551:LEU:HG	1:A:556:TRP:HZ2	1.74	0.52
1:A:527:ARG:O	1:A:528:SER:HB2	2.09	0.52
1:A:717:PRO:C	1:A:719:LEU:N	2.61	0.52
1:A:506:ASN:O	1:A:510:GLU:HG3	2.10	0.52
1:A:771:LEU:O	1:A:772:ASN:C	2.48	0.52
1:A:541:THR:HG22	1:A:543:ALA:H	1.75	0.52
1:A:543:ALA:O	1:A:545:LEU:N	2.43	0.51
1:A:890:LEU:HD12	1:A:895:LEU:HD12	1.93	0.51
1:A:895:LEU:O	1:A:899:ILE:HG12	2.10	0.51
1:A:579:LYS:HG2	1:A:579:LYS:O	2.11	0.51
1:A:598:VAL:HG12	1:A:599:ASP:N	2.24	0.51
1:A:680:TYR:CD1	1:A:901:LEU:HB2	2.46	0.51
1:A:540:THR:CG2	1:A:541:THR:N	2.74	0.50
1:A:623:PHE:CD2	1:A:638:LEU:HB2	2.46	0.50
1:A:602:TRP:HB2	1:A:619:PHE:CE2	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:523:PHE:O	1:A:544:VAL:HG11	2.11	0.50
1:A:648:ARG:HH21	1:A:648:ARG:HG3	1.76	0.50
1:A:578:VAL:O	1:A:581:LEU:HG	2.11	0.50
1:A:441:LYS:O	1:A:442:ALA:HB2	2.11	0.50
1:A:650:THR:O	1:A:656:ILE:HG21	2.12	0.49
1:A:827:ARG:HH12	1:A:866:ASP:CG	2.16	0.49
1:A:541:THR:CG2	1:A:542:TYR:N	2.75	0.49
1:A:620:LYS:HA	1:A:624:ALA:CB	2.41	0.49
1:A:791:ILE:HD13	1:A:814:ILE:HA	1.94	0.49
1:A:543:ALA:C	1:A:545:LEU:N	2.66	0.49
1:A:468:ALA:HB3	1:A:648:ARG:HB2	1.94	0.49
1:A:527:ARG:NE	1:A:530:ILE:HG12	2.28	0.49
1:A:666:THR:OG1	1:A:853:HIS:ND1	2.45	0.49
1:A:504:LEU:C	1:A:504:LEU:HD23	2.32	0.49
1:A:597:LYS:O	1:A:600:ASP:N	2.45	0.49
1:A:740:ILE:HG23	1:A:802:PHE:CE2	2.48	0.49
1:A:571:GLN:HA	1:A:575:PHE:CD1	2.47	0.49
1:A:795:GLN:HE21	1:A:815:ASN:HD21	1.61	0.49
1:A:668:VAL:HG11	1:A:739:ILE:CD1	2.40	0.49
1:A:459:ASN:HB3	1:A:585:TYR:CD2	2.46	0.49
1:A:505:LYS:HE2	1:A:863:GLU:OE1	2.12	0.48
1:A:776:PRO:HB2	1:A:790:ILE:HG23	1.95	0.48
1:A:435:LEU:HB2	1:A:452:PHE:CE2	2.48	0.48
1:A:474:GLY:O	1:A:478:GLN:HG3	2.13	0.48
1:A:605:MET:HA	1:A:605:MET:HE3	1.95	0.48
1:A:438:TYR:HB3	1:A:484:SER:OG	2.13	0.48
1:A:532:LEU:HD22	1:A:538:ILE:HD13	1.95	0.48
1:A:673:THR:H	1:A:676:GLN:HE21	1.62	0.48
1:A:605:MET:SD	1:A:642:ILE:HG21	2.53	0.48
1:A:580:GLU:CG	1:A:580:GLU:O	2.62	0.48
1:A:883:GLY:CA	1:A:886:TRP:HE1	2.21	0.48
1:A:487:LYS:C	1:A:489:GLU:H	2.16	0.48
1:A:777:PHE:O	1:A:790:ILE:HD13	2.14	0.47
1:A:593:PRO:HA	1:A:597:LYS:HZ1	1.77	0.47
1:A:814:ILE:HB	1:A:842:TYR:CD2	2.49	0.47
1:A:597:LYS:NZ	1:A:597:LYS:CB	2.77	0.47
1:A:638:LEU:CG	1:A:642:ILE:HD11	2.40	0.47
1:A:559:ILE:HD12	1:A:583:SER:HB3	1.95	0.47
1:A:542:TYR:O	1:A:545:LEU:HB3	2.14	0.47
1:A:523:PHE:HB3	1:A:540:THR:HG1	1.77	0.47
1:A:605:MET:HA	1:A:605:MET:CE	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:551:LEU:HG	1:A:556:TRP:CZ2	2.49	0.47
1:A:565:GLN:H	1:A:565:GLN:CD	2.18	0.47
1:A:597:LYS:HZ3	1:A:597:LYS:HB3	1.78	0.47
1:A:680:TYR:CE2	1:A:710:LEU:HG	2.50	0.47
1:A:631:ASP:C	1:A:633:MET:H	2.18	0.47
1:A:628:LYS:C	1:A:630:GLY:H	2.18	0.47
1:A:882:SER:O	1:A:886:TRP:CD1	2.67	0.47
1:A:797:ASN:ND2	1:A:798:PRO:HD2	2.25	0.47
1:A:433:GLN:O	1:A:435:LEU:N	2.48	0.47
1:A:698:LYS:O	1:A:698:LYS:HG3	2.14	0.47
1:A:562:ASP:OD2	3:A:958:PO4:O4	2.32	0.47
1:A:689:ASN:ND2	1:A:689:ASN:N	2.62	0.47
1:A:514:PHE:C	1:A:516:PRO:HD3	2.35	0.47
1:A:697:ILE:HG13	1:A:697:ILE:O	2.15	0.47
1:A:653:ASP:HB2	1:A:656:ILE:HG22	1.96	0.46
1:A:827:ARG:NH2	1:A:862:GLU:O	2.49	0.46
1:A:491:GLU:O	1:A:557:LYS:HD3	2.14	0.46
1:A:584:LYS:HG2	1:A:585:TYR:CE1	2.50	0.46
1:A:594:ILE:HG22	1:A:596:ASN:OD1	2.16	0.46
1:A:755:GLN:N	1:A:826:ASP:OD1	2.46	0.46
1:A:717:PRO:C	1:A:719:LEU:H	2.19	0.46
1:A:759:MET:O	1:A:763:ILE:HG13	2.16	0.46
1:A:795:GLN:NE2	1:A:815:ASN:ND2	2.64	0.46
1:A:544:VAL:HG12	1:A:544:VAL:O	2.14	0.45
1:A:496:LEU:HD12	1:A:497:VAL:N	2.31	0.45
1:A:840:ARG:NH2	1:A:840:ARG:HG3	2.31	0.45
1:A:771:LEU:O	1:A:772:ASN:O	2.34	0.45
1:A:791:ILE:HD11	1:A:814:ILE:CG2	2.33	0.45
1:A:864:LYS:NZ	1:A:902:SER:HB2	2.32	0.45
1:A:728:ARG:CD	1:A:728:ARG:N	2.78	0.45
1:A:620:LYS:HG2	1:A:625:THR:HG23	1.97	0.45
1:A:431:SER:O	1:A:432:PHE:HB2	2.16	0.45
1:A:666:THR:HG1	1:A:853:HIS:CE1	2.35	0.45
1:A:504:LEU:HD23	1:A:504:LEU:O	2.16	0.45
1:A:688:PHE:CE1	1:A:896:ARG:HB2	2.45	0.44
1:A:493:THR:HA	1:A:494:PRO:HA	1.77	0.44
1:A:814:ILE:O	1:A:842:TYR:HA	2.17	0.44
1:A:696:GLY:C	1:A:698:LYS:H	2.21	0.44
1:A:779:TYR:HA	1:A:806:SER:O	2.18	0.44
1:A:894:GLU:O	1:A:897:LYS:HB2	2.17	0.44
1:A:662:ASP:OD1	1:A:845:GLY:O	2.35	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:540:THR:HG23	1:A:541:THR:N	2.33	0.44
1:A:744:LEU:HD11	1:A:802:PHE:CZ	2.53	0.44
1:A:761:LYS:HG3	1:A:777:PHE:HE2	1.82	0.44
1:A:632:ASN:HD22	1:A:635:LYS:HD3	1.83	0.44
1:A:648:ARG:O	1:A:648:ARG:HG2	2.17	0.44
1:A:566:ASN:O	1:A:567:ILE:C	2.56	0.44
1:A:530:ILE:HG23	1:A:532:LEU:HG	1.98	0.43
1:A:465:ILE:CA	1:A:608:LEU:HD13	2.48	0.43
1:A:450:LYS:O	1:A:451:GLY:C	2.54	0.43
1:A:688:PHE:C	1:A:690:ASN:N	2.72	0.43
1:A:900:GLU:HG2	1:A:901:LEU:O	2.18	0.43
1:A:586:ARG:HG2	1:A:607:PHE:CZ	2.53	0.43
1:A:857:SER:OG	1:A:862:GLU:OE2	2.28	0.43
1:A:504:LEU:CD2	1:A:508:GLU:OE1	2.63	0.43
1:A:488:LYS:HG3	1:A:488:LYS:O	2.17	0.43
1:A:592:THR:C	1:A:594:ILE:H	2.19	0.43
1:A:594:ILE:HG13	1:A:594:ILE:H	1.64	0.43
1:A:623:PHE:C	1:A:626:PRO:HD2	2.39	0.43
1:A:611:GLY:O	1:A:612:LEU:C	2.57	0.43
1:A:884:ASP:HA	1:A:887:ILE:HD12	2.01	0.43
1:A:450:LYS:O	1:A:453:SER:N	2.51	0.43
1:A:778:LEU:HD23	1:A:805:LEU:HD23	2.00	0.43
1:A:814:ILE:HB	1:A:842:TYR:HD2	1.83	0.43
1:A:827:ARG:HA	1:A:827:ARG:HD2	1.70	0.43
1:A:829:TRP:HB2	1:A:883:GLY:HA3	1.99	0.43
1:A:716:HIS:O	1:A:719:LEU:HB2	2.19	0.43
1:A:578:VAL:C	1:A:580:GLU:N	2.73	0.43
1:A:888:THR:OG1	1:A:889:GLU:OE2	2.32	0.43
1:A:698:LYS:O	1:A:698:LYS:CG	2.66	0.43
1:A:527:ARG:NH2	1:A:550:ARG:CB	2.81	0.42
1:A:706:THR:O	1:A:707:LEU:C	2.57	0.42
1:A:448:GLN:O	1:A:452:PHE:HB3	2.20	0.42
1:A:563:GLU:C	1:A:564:ALA:O	2.58	0.42
1:A:691:ILE:HG23	1:A:692:ASP:N	2.33	0.42
1:A:436:GLU:O	1:A:437:PRO:C	2.57	0.42
1:A:860:THR:HG22	1:A:861:LEU:N	2.34	0.42
1:A:679:MET:HE2	1:A:713:ILE:HG12	2.02	0.42
1:A:500:PRO:O	1:A:501:LEU:C	2.58	0.42
1:A:525:GLU:HB2	1:A:526:ASP:H	1.60	0.42
1:A:637:GLU:HA	1:A:637:GLU:OE1	2.18	0.42
1:A:441:LYS:N	1:A:441:LYS:CD	2.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:564:ALA:C	1:A:566:ASN:N	2.73	0.42
1:A:872:LYS:HG2	1:A:874:SER:OG	2.20	0.42
1:A:571:GLN:CG	1:A:572:THR:N	2.67	0.42
1:A:605:MET:SD	1:A:642:ILE:CG2	3.08	0.42
1:A:740:ILE:HA	1:A:740:ILE:HD13	1.82	0.42
1:A:785:LYS:O	1:A:789:ASP:CG	2.58	0.42
1:A:499:CYS:HA	1:A:500:PRO:HD3	1.93	0.41
1:A:869:LEU:HD21	1:A:886:TRP:CZ2	2.54	0.41
1:A:493:THR:O	1:A:557:LYS:HD2	2.20	0.41
1:A:503:VAL:HA	1:A:506:ASN:OD1	2.20	0.41
1:A:840:ARG:HG3	1:A:840:ARG:HH21	1.84	0.41
1:A:593:PRO:O	1:A:594:ILE:C	2.58	0.41
1:A:873:ARG:HG3	1:A:876:PHE:CD2	2.43	0.41
1:A:602:TRP:CD1	1:A:619:PHE:HB2	2.55	0.41
1:A:774:GLU:HG2	1:A:776:PRO:HD3	2.02	0.41
1:A:469:ASP:O	1:A:470:ASP:C	2.58	0.41
1:A:505:LYS:HG2	1:A:669:TYR:CE2	2.55	0.41
1:A:3:PRO:O	1:A:648:ARG:NE	2.54	0.41
1:A:624:ALA:O	1:A:625:THR:C	2.58	0.41
1:A:555:GLU:HG2	1:A:582:LYS:NZ	2.36	0.41
1:A:571:GLN:HA	1:A:575:PHE:CE1	2.56	0.41
1:A:759:MET:HE2	1:A:763:ILE:HG13	2.03	0.41
1:A:597:LYS:O	1:A:598:VAL:C	2.58	0.40
1:A:880:ILE:HG21	1:A:886:TRP:CG	2.56	0.40
1:A:750:ILE:HD12	1:A:750:ILE:N	2.36	0.40
1:A:8:MET:O	1:A:9:ALA:CB	2.68	0.40
1:A:886:TRP:C	1:A:888:THR:N	2.75	0.40
1:A:559:ILE:O	1:A:559:ILE:HG22	2.21	0.40
1:A:774:GLU:HG2	1:A:775:VAL:N	2.36	0.40
1:A:564:ALA:O	1:A:566:ASN:N	2.54	0.40
1:A:597:LYS:HZ2	1:A:597:LYS:HB3	1.82	0.40
1:A:869:LEU:O	1:A:873:ARG:HB2	2.22	0.40
1:A:551:LEU:O	1:A:554:VAL:N	2.53	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:872:LYS:NZ	1:A:872:LYS:NZ[8_665]	2.15	0.05

## 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	476/500 (95%)	350 (74%)	82 (17%)	44 (9%)	<b>1</b> <b>4</b>

All (44) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3	PRO
1	A	8	MET
1	A	9	ALA
1	A	525	GLU
1	A	526	ASP
1	A	564	ALA
1	A	567	ILE
1	A	572	THR
1	A	879	ILE
1	A	885	SER
1	A	892	THR
1	A	527	ARG
1	A	544	VAL
1	A	546	LEU
1	A	570	PRO
1	A	571	GLN
1	A	579	LYS
1	A	772	ASN
1	A	780	GLY
1	A	880	ILE
1	A	438	TYR
1	A	517	HIS
1	A	565	GLN
1	A	568	LYS
1	A	593	PRO
1	A	612	LEU
1	A	624	ALA
1	A	689	ASN

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Mol	Chain	Res	Type
1	A	770	GLU
1	A	12	LYS
1	A	524	HIS
1	A	549	THR
1	A	683	GLU
1	A	693	SER
1	A	694	VAL
1	A	782	LEU
1	A	811	GLY
1	A	7	HIS
1	A	591	GLY
1	A	598	VAL
1	A	619	PHE
1	A	781	GLU
1	A	594	ILE
1	A	626	PRO

### 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	419/446 (94%)	394 (94%)	25 (6%)	24 62

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	452	PHE
1	A	456	ARG
1	A	501	LEU
1	A	502	SER
1	A	511	LEU
1	A	524	HIS
1	A	597	LYS
1	A	604	ILE
1	A	632	ASN
1	A	642	ILE

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Mol	Chain	Res	Type
1	A	647	LEU
1	A	649	ARG
1	A	665	GLU
1	A	670	CYS
1	A	671	ASN
1	A	692	ASP
1	A	728	ARG
1	A	733	MET
1	A	735	ARG
1	A	738	GLU
1	A	791	ILE
1	A	797	ASN
1	A	803	ILE
1	A	828	TRP
1	A	867	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	459	ASN
1	A	478	GLN
1	A	565	GLN
1	A	571	GLN
1	A	632	ASN
1	A	676	GLN
1	A	689	ASN
1	A	712	GLN
1	A	755	GLN
1	A	797	ASN
1	A	815	ASN
1	A	836	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 11 ligands modelled in this entry, 3 are monoatomic - leaving 8 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	PO4	A	954	-	4,4,4	1.12	0	6,6,6	0.27	0
3	PO4	A	955	-	4,4,4	1.13	0	6,6,6	0.27	0
3	PO4	A	956	-	4,4,4	1.13	0	6,6,6	0.27	0
3	PO4	A	957	-	4,4,4	1.06	0	6,6,6	0.27	0
3	PO4	A	958	-	4,4,4	1.16	0	6,6,6	0.27	0
3	PO4	A	959	-	4,4,4	1.11	0	6,6,6	0.27	0
3	PO4	A	960	-	4,4,4	1.14	0	6,6,6	0.27	0
3	PO4	A	961	-	4,4,4	1.12	0	6,6,6	0.27	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	PO4	A	954	-	-	0/0/0/0	0/0/0/0
3	PO4	A	955	-	-	0/0/0/0	0/0/0/0
3	PO4	A	956	-	-	0/0/0/0	0/0/0/0
3	PO4	A	957	-	-	0/0/0/0	0/0/0/0
3	PO4	A	958	-	-	0/0/0/0	0/0/0/0
3	PO4	A	959	-	-	0/0/0/0	0/0/0/0
3	PO4	A	960	-	-	0/0/0/0	0/0/0/0
3	PO4	A	961	-	-	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.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	958	PO4	1	0
3	A	961	PO4	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 [i](#)

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

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers [i](#)

EDS was not executed - this section will therefore be empty.