



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 4, 2025 – 12:09 PM EST

PDB ID : 9EKD  
Title : Structure of a C1r Zymogen Fragment Bound to SALO  
Authors : Duan, H.; Geisbrecht, B.V.  
Deposited on : 2024-12-02  
Resolution : 3.28 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

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<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>.

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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	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

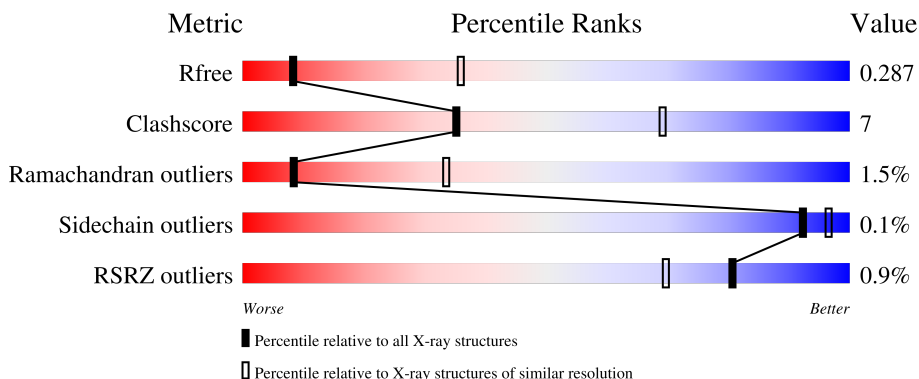
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.28 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))
$R_{free}$	164625	1214 (3.30-3.26)
Clashscore	180529	1265 (3.30-3.26)
Ramachandran outliers	177936	1264 (3.30-3.26)
Sidechain outliers	177891	1263 (3.30-3.26)
RSRZ outliers	164620	1215 (3.30-3.26)

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  $\geq 3$ , 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	104	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 11%, green 75%, grey 14%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>75%</span> <span>11%</span> <span>14%</span> </div> </div>
1	B	104	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 15%, green 69%, grey 14%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>69%</span> <span>15%</span> <span>14%</span> </div> </div>
2	C	409	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 19%, green 75%, grey 5%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>75%</span> <span>19%</span> <span>5%</span> </div> </div>
2	D	409	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 22%, green 72%, grey 6%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>72%</span> <span>22%</span> <span>6%</span> </div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7644 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 Salivary anti-complement protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	89	Total	C	N	O	S	0	0	0
			725	450	110	157	8			
1	B	89	Total	C	N	O	S	0	0	0
			725	450	110	157	8			

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	116	GLY	-	expression tag	UNP Q5WPZ4
A	117	SER	-	expression tag	UNP Q5WPZ4
A	118	GLY	-	expression tag	UNP Q5WPZ4
A	119	HIS	-	expression tag	UNP Q5WPZ4
A	120	HIS	-	expression tag	UNP Q5WPZ4
A	121	HIS	-	expression tag	UNP Q5WPZ4
A	122	HIS	-	expression tag	UNP Q5WPZ4
A	123	HIS	-	expression tag	UNP Q5WPZ4
A	124	HIS	-	expression tag	UNP Q5WPZ4
A	125	HIS	-	expression tag	UNP Q5WPZ4
A	126	HIS	-	expression tag	UNP Q5WPZ4
B	116	GLY	-	expression tag	UNP Q5WPZ4
B	117	SER	-	expression tag	UNP Q5WPZ4
B	118	GLY	-	expression tag	UNP Q5WPZ4
B	119	HIS	-	expression tag	UNP Q5WPZ4
B	120	HIS	-	expression tag	UNP Q5WPZ4
B	121	HIS	-	expression tag	UNP Q5WPZ4
B	122	HIS	-	expression tag	UNP Q5WPZ4
B	123	HIS	-	expression tag	UNP Q5WPZ4
B	124	HIS	-	expression tag	UNP Q5WPZ4
B	125	HIS	-	expression tag	UNP Q5WPZ4
B	126	HIS	-	expression tag	UNP Q5WPZ4

- Molecule 2 is a protein called Complement C1r subcomponent.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	389	Total 3111	C 1964	N 552	O 571	S 24	0	0	0
2	D	386	Total 3083	C 1948	N 546	O 566	S 23	0	0	0

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	654	ALA	SER	engineered mutation	UNP P00736
C	706	GLY	-	expression tag	UNP P00736
C	707	SER	-	expression tag	UNP P00736
C	708	GLY	-	expression tag	UNP P00736
C	709	HIS	-	expression tag	UNP P00736
C	710	HIS	-	expression tag	UNP P00736
C	711	HIS	-	expression tag	UNP P00736
C	712	HIS	-	expression tag	UNP P00736
C	713	HIS	-	expression tag	UNP P00736
C	714	HIS	-	expression tag	UNP P00736
C	715	HIS	-	expression tag	UNP P00736
C	716	HIS	-	expression tag	UNP P00736
D	654	ALA	SER	engineered mutation	UNP P00736
D	706	GLY	-	expression tag	UNP P00736
D	707	SER	-	expression tag	UNP P00736
D	708	GLY	-	expression tag	UNP P00736
D	709	HIS	-	expression tag	UNP P00736
D	710	HIS	-	expression tag	UNP P00736
D	711	HIS	-	expression tag	UNP P00736
D	712	HIS	-	expression tag	UNP P00736
D	713	HIS	-	expression tag	UNP P00736
D	714	HIS	-	expression tag	UNP P00736
D	715	HIS	-	expression tag	UNP P00736
D	716	HIS	-	expression tag	UNP P00736



- Molecule 1: Salivary anti-complement protein



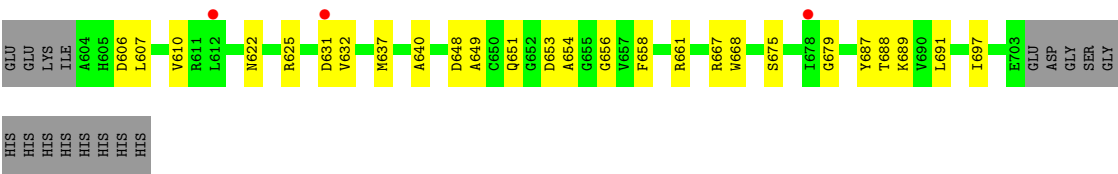
- |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |     |      |      |      |     |     |     |     |     |     |     |     |     |     |     |     |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| SER | E24 | D25 | H31 | L36 | D40 | R45 | V46 | D47 | E50 | Y51 | E58 | E61 | I62 | T63 | V64 | V68 | I79 | Y99 | I107 | Y111 | P112 | GLU | ASN | MET | GLY | SER | GLY | HIS | HIS | HIS | HIS | HIS | HIS |
|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|

- K308 K320 K321 K322 K323 K324 K327 K333 K334 K335 K336 K337 K338 K346 K349 K356 K358 K359 K365 K373 K374 K375 K386 K389 K393 K397 K398 K399 K405 K410 K416 K418 K419 K420 K421 K422 K423 K424 K425 K426 K427 K428 K429 K430 K431 K432 K433 K434 K435 K436 K437 K438 K439 K440 K441 K442 K443 K444 K445 K446 K447 K448 K449 K450 K451 K452 K453 K454 K455 K456 K457 K458 K459 K460 K461 K462 K463 K464 K465 K466 K467 K468 K469 K470 K471 K472 K473 K474 K475 K476 K477 K478 K479 K480 K481 K482 K483 K484 K485 K486 K487 K488 K489 K490 K491 K492 K493 K494 K495 K496 K497 K498 K499 K500 K501 K502 K503 K504 K505 K506 K507 K508 K509 K510 K511 K512 K513 K514 K515 K516 K517 K518 K519 K520 K521 K522 K523 K524 K525 K526 K527 K528 K529 K530 K531 K532 K533 K534 K535 K536 K537 K538 K539 K540 K541 K542 K543 K544 K545 K546 K547 K548 K549 K550 K551 K552 K553 K554 K555 K556 K557 K558 K559 K560 K561 K562 K563 K564 K565 K566 K567 K568 K569 K570 K571 K572 K573 K574 K575 K576 K577 K578 K579 K580 K581 K582 K583 K584 K585 K586 K587 K588 K589 K590 K591 K592 K593 K594 K595 K596 K597 K598 K599 K600 K601 K602 K603 K604 K605 K606 K607 K608 K609 K610 K611 K612 K613 K614 K615 K616 K617 K618 K619 K620 K621 K622 K623 K624 K625 K626 K627 K628 K629 K630 K631 K632 K633 K634 K635 K636 K637 K638 K639 K640 K641 K642 K643 K644 K645 K646 K647 K648 K649 K650 K651 K652 K653 K654 K655 K656 K657 K658 K659 K660 K661 K662 K663 K664 K665 K666 K667 K668 K669 K670 K671 K672 K673 K674 K675 K676 K677 K678 K679 K680 K681 K682 K683 K684 K685 K686 K687 K688 K689 K690 K691 K692 K693 K694 K695 K696 K697 K698 K699 K700 K701 K702 K703 K704 K705 K706 K707 K708 K709 K710 K711 K712 K713 K714 K715 K716 K717 K718 K719 K720 K721 K722 K723 K724 K725 K726 K727 K728 K729 K730 K731 K732 K733 K734 K735 K736 K737 K738 K739 K740 K741 K742 K743 K744 K745 K746 K747 K748 K749 K750 K751 K752 K753 K754 K755 K756 K757 K758 K759 K760 K761 K762 K763 K764 K765 K766 K767 K768 K769 K770 K771 K772 K773 K774 K775 K776 K777 K778 K779 K780 K781 K782 K783 K784 K785 K786 K787 K788 K789 K790 K791 K792 K793 K794 K795 K796 K797 K798 K799 K800 K801 K802 K803 K804 K805 K806 K807 K808 K809 K810 K811 K812 K813 K814 K815 K816 K817 K818 K819 K820 K821 K822 K823 K824 K825 K826 K827 K828 K829 K830 K831 K832 K833 K834 K835 K836 K837 K838 K839 K840 K841 K842 K843 K844 K845 K846 K847 K848 K849 K850 K851 K852 K853 K854 K855 K856 K857 K858 K859 K860 K861 K862 K863 K864 K865 K866 K867 K868 K869 K870 K871 K872 K873 K874 K875 K876 K877 K878 K879 K880 K881 K882 K883 K884 K885 K886 K887 K888 K889 K890 K891 K892 K893 K894 K895 K896 K897 K898 K899 K900 K901 K902 K903 K904 K905 K906 K907 K908 K909 K910 K911 K912 K913 K914 K915 K916 K917 K918 K919 K920 K921 K922 K923 K924 K925 K926 K927 K928 K929 K930 K931 K932 K933 K934 K935 K936 K937 K938 K939 K940 K941 K942 K943 K944 K945 K946 K947 K948 K949 K950 K951 K952 K953 K954 K955 K956 K957 K958 K959 K960 K961 K962 K963 K964 K965 K966 K967 K968 K969 K970 K971 K972 K973 K974 K975 K976 K977 K978 K979 K980 K981 K982 K983 K984 K985 K986 K987 K988 K989 K990 K991 K992 K993 K994 K995 K996 K997 K998 K999



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|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|------|------|------|------|------|------|------|
| K308 | C309 | I320 | I321 | Q322 | Q327 | F334 | I335 | A336 | I337 | E346 | Q349 | T355 | A356 | V357 | C358 | I373 | D386 | F387 | R388 | Y398 | Q403 | Y404 | Y405 | T415 | ARG | ALA | GLY | GLY | SER | ARG | E421 | S422 | E423 | Q424 | Q424 | N437 | K440 | G441 | E442 | Q451 | G452 | K453 | N456 | E459 |
|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|------|-----|-----|-----|-----|-----|-----|------|------|------|------|------|------|------|------|------|------|------|------|------|------|





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## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	117.83Å 117.83Å 190.58Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.29 – 3.28 49.29 – 3.28	Depositor EDS
% Data completeness (in resolution range)	98.0 (49.29-3.28) 98.0 (49.29-3.28)	Depositor EDS
$R_{merge}$	0.23	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.63 (at 3.25Å)	Xtriage
Refinement program	PHENIX 1.21rc1_5127	Depositor
R, $R_{free}$	0.242 , 0.286 0.242 , 0.287	Depositor DCC
$R_{free}$ test set	21962 reflections (8.50%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	128.1	Xtriage
Anisotropy	0.157	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 113.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.029 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	7644	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	149.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.07% 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: TYS

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	0.23	0/718	0.39	0/968
1	B	0.24	0/718	0.38	0/968
2	C	0.24	0/3191	0.47	0/4321
2	D	0.24	0/3163	0.47	0/4285
All	All	0.24	0/7790	0.45	0/10542

There are no bond length outliers.

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	725	0	671	7	0
1	B	725	0	671	11	0
2	C	3111	0	2991	43	0
2	D	3083	0	2965	51	0
All	All	7644	0	7298	109	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 7.

The worst 5 of 109 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)
2:D:308:LYS:HE3	2:D:327:GLN:HB2	1.68	0.75
2:C:437:ASN:H	2:C:441:GLY:HA2	1.53	0.74
2:D:553:ASN:HA	2:D:632:VAL:HG11	1.70	0.73
2:C:595:GLY:HA3	2:C:653:ASP:HB2	1.72	0.72
2:C:320:ILE:HG13	2:C:337:THR:HG23	1.71	0.70

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	86/104 (83%)	83 (96%)	3 (4%)	0	100	100
1	B	86/104 (83%)	84 (98%)	2 (2%)	0	100	100
2	C	383/409 (94%)	330 (86%)	45 (12%)	8 (2%)	5	27
2	D	380/409 (93%)	336 (88%)	38 (10%)	6 (2%)	8	32
All	All	935/1026 (91%)	833 (89%)	88 (9%)	14 (2%)	8	33

5 of 14 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	483	ILE
2	D	451	CYS
2	D	509	HIS
2	D	483	ILE
2	D	606	ASP

### 5.3.2 Protein sidechains [i](#)

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	82/95 (86%)	82 (100%)	0	100	100
1	B	82/95 (86%)	82 (100%)	0	100	100
2	C	333/349 (95%)	332 (100%)	1 (0%)	91	94
2	D	330/349 (95%)	330 (100%)	0	100	100
All	All	827/888 (93%)	826 (100%)	1 (0%)	92	96

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	410	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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
1	TYS	B	51	1	15,16,17	1.60	2 (13%)	15,22,24	0.86	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	TYS	A	51	1	15,16,17	1.61	2 (13%)	15,22,24	0.87	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
1	TYS	B	51	1	-	2/10/11/13	0/1/1/1
1	TYS	A	51	1	-	3/10/11/13	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	51	TYS	OH-S	5.07	1.68	1.58
1	B	51	TYS	OH-S	5.04	1.68	1.58
1	A	51	TYS	OH-CZ	-3.23	1.37	1.42
1	B	51	TYS	OH-CZ	-3.19	1.37	1.42

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	51	TYS	CZ-OH-S-O1
1	A	51	TYS	CZ-OH-S-O2
1	A	51	TYS	CZ-OH-S-O3
1	B	51	TYS	CZ-OH-S-O3
1	B	51	TYS	CZ-OH-S-O2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	51	TYS	1	0

## 5.5 Carbohydrates

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 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, 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	88/104 (84%)	-0.51	0 100 100	103, 154, 188, 229	0
1	B	88/104 (84%)	-0.37	0 100 100	132, 197, 254, 347	0
2	C	389/409 (95%)	-0.34	3 (0%) 82 72	92, 143, 210, 280	0
2	D	386/409 (94%)	-0.18	6 (1%) 70 56	81, 130, 202, 286	0
All	All	951/1026 (92%)	-0.30	9 (0%) 81 70	81, 142, 220, 347	0

The worst 5 of 9 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	598	VAL	3.2
2	D	631	ASP	3.0
2	C	496	TRP	2.6
2	D	594	SER	2.3
2	D	612	LEU	2.3

### 6.2 Non-standard residues in protein, DNA, RNA chains [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, 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	B-factors(Å <sup>2</sup> )	Q<0.9
1	TYS	B	51	16/17	0.82	0.17	178,205,226,245	0
1	TYS	A	51	16/17	0.93	0.14	120,130,163,166	0

### 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.