



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 09:41 PM UTC

PDB ID : 9EKD / pdb_00009ekd
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 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

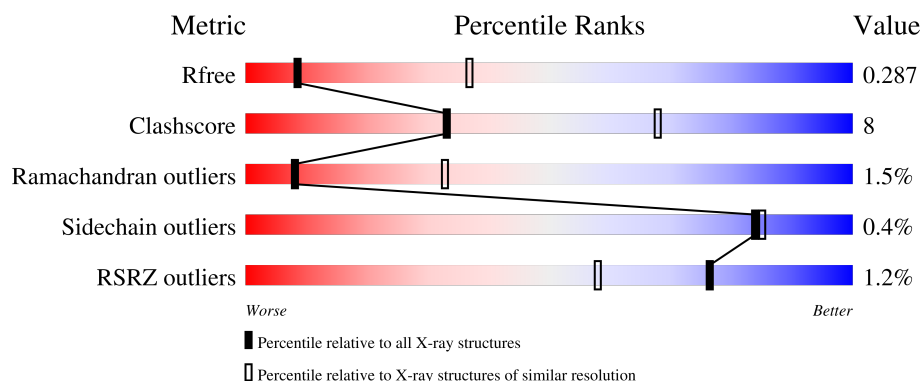
1 Overall quality at a glance

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}	180053	1303 (3.30-3.26)
Clashscore	190562	1354 (3.30-3.26)
Ramachandran outliers	187476	1334 (3.30-3.26)
Sidechain outliers	187428	1333 (3.30-3.26)
RSRZ outliers	180081	1303 (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 ≥ 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	 75% 11% 14%
1	B	104	 69% 15% 14%
2	C	409	 2% 74% 20% 5%
2	D	409	 2% 71% 23% 6%

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:

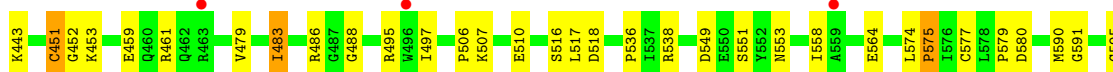
Chain	Residue	Modelled	Actual	Comment	Reference
C	654	ALA	SER	engineered mutation	UNP P00736
C	706	GLY	-	expression tag	UNP P00736
C	707	SER	-	expression tag	UNP P00736
C	708	GLY	-	expression tag	UNP P00736
C	709	HIS	-	expression tag	UNP P00736
C	710	HIS	-	expression tag	UNP P00736
C	711	HIS	-	expression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



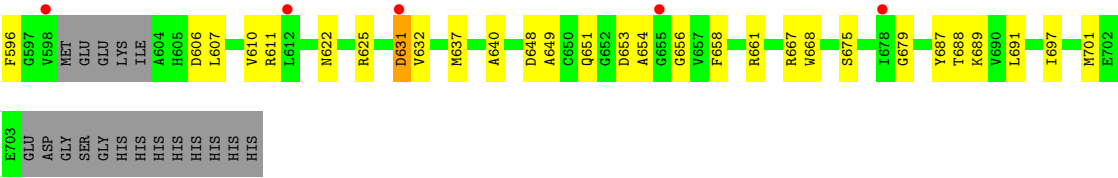
- | | | | | | | | | | | | | | | |
|------|------|------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| SER | E24 | D25 | H31 | L36 | D40 | R45 | V46 | D47 | E50 | Y51 | E58 | E61 | I62 | T63 | V64 | V68 | I79 | Y99 | I107 | Y111 | P112 | GLU | ASN | MET | GLY | SER | GLY |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

- | | | | | | | | | |
|------|-----|-----|-----|-----|------|------|------|------|------|
| K308 | D316 | T319 | I320 | I321 | Q322 | I323 | I324 | Q327 | I333 | F334 | I335 | A336 | T337 | C338 | E346 | Q349 | T355 | A356 | I357 | H365 | I373 | K374 | D375 | D386 | Y389 | M393 | T397 | Y398 | Y405 | Y410 | R416 | ALA | GLY | SER | ARG | E421 | K436 | M437 | K440 | C441 |
|------|-----|-----|-----|-----|------|------|------|------|------|



- K308
 C309
 D316
 T319
 I320
 I321
 Q322
 Q327
 F334
 I335
 A336
 T337
 E346
 Q349
 T356
 A356
 I357
 C358
 I373
 D386
 F387
 R388
 Y398
 Q403
 Q404
 T415
 ARG
 ALA
 GLY
 SER
 ARG
 E421
 S422
 E423
 Q424
 M437
 K440
 C441
 E442
 K443
 C451
 G452
 K453





4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	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	1996 reflections (8.33%)	wwPDB-VP
Wilson B-factor (Å ²)	128.1	Xtriage
Anisotropy	0.157	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 113.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.31$	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 ²)	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.*

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: 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	0.07	0/718	0.20	0/968
1	B	0.08	0/718	0.20	0/968
2	C	0.09	0/3191	0.25	0/4321
2	D	0.08	0/3163	0.25	0/4285
All	All	0.08	0/7790	0.24	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	46	0
2	D	3083	0	2965	55	0
All	All	7644	0	7298	116	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 8.

All (116) 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
2:D:437:ASN:H	2:D:441:GLY:HA2	1.57	0.70
2:C:610:VAL:HG11	2:C:651:GLN:HB3	1.75	0.68
2:D:595:GLY:HA3	2:D:653:ASP:HB2	1.77	0.66
2:D:322:GLN:HB2	2:D:335:ILE:HG13	1.77	0.66
2:C:308:LYS:HE3	2:C:327:GLN:HB2	1.79	0.65
2:C:553:ASN:HA	2:C:632:VAL:HG11	1.79	0.65
2:D:637:MET:O	2:D:689:LYS:NZ	2.33	0.61
2:D:335:ILE:HG22	2:D:355:THR:HB	1.82	0.60
1:B:51:TYS:HE1	2:D:463:ARG:HA	1.84	0.60
2:D:320:ILE:HG13	2:D:337:THR:HG23	1.84	0.60
2:C:322:GLN:HB2	2:C:335:ILE:HG13	1.83	0.59
1:B:36:LEU:HD22	2:D:590:MET:HE1	1.86	0.58
2:D:537:ILE:HD12	2:D:561:LEU:HB3	1.85	0.58
2:C:452:GLY:N	2:C:577:CYS:SG	2.77	0.57
2:D:451:CYS:SG	2:D:452:GLY:N	2.77	0.56
2:C:579:PRO:HB2	2:C:691:LEU:HD13	1.88	0.55
2:D:560:LEU:HD11	2:D:697:ILE:HG23	1.87	0.55
2:D:648:ASP:OD1	2:D:649:ALA:N	2.40	0.55
1:B:47:ASP:HB3	1:B:50:GLU:HG2	1.89	0.54
2:D:580:ASP:N	2:D:580:ASP:OD1	2.40	0.54
2:C:536:PRO:HG2	2:C:564:GLU:HB3	1.90	0.53
2:D:440:LYS:HZ1	2:D:443:LYS:H	1.55	0.53
2:C:451:CYS:HA	2:C:575:PRO:HG2	1.90	0.53
2:D:486:ARG:NH2	2:D:596:PHE:O	2.39	0.53
2:D:476:PRO:HB2	2:D:574:LEU:H	1.73	0.53
2:C:346:GLU:O	2:C:349:GLN:NE2	2.42	0.52
2:D:453:LYS:HE2	2:D:667:ARG:HG2	1.91	0.52
2:D:536:PRO:HG2	2:D:564:GLU:HB3	1.91	0.52
1:A:76:VAL:HG13	1:A:107:ILE:HD11	1.90	0.52
2:D:456:ASN:O	2:D:474:ASN:ND2	2.43	0.52
2:D:459:GLU:HG3	2:D:461:ARG:H	1.75	0.52
1:B:107:ILE:HG12	1:B:111:TYR:HE2	1.75	0.51
2:D:423:GLU:HG3	2:D:424:GLN:HG3	1.92	0.51
2:C:495:ARG:HH21	2:C:538:ARG:HH11	1.58	0.51
2:D:346:GLU:O	2:D:349:GLN:NE2	2.43	0.51
1:A:25:ASP:N	1:A:25:ASP:OD1	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:648:ASP:OD1	2:C:649:ALA:N	2.44	0.50
2:D:334:PHE:CE1	2:D:356:ALA:HB3	2.47	0.50
2:C:410:TYR:HD1	2:C:574:LEU:HD21	1.75	0.50
1:A:107:ILE:HG12	1:A:111:TYR:HE1	1.77	0.50
2:C:479:VAL:HG11	2:C:497:ILE:HD12	1.94	0.49
2:C:459:GLU:HG3	2:C:461:ARG:H	1.77	0.49
2:D:502:HIS:ND1	2:D:557:ASP:OD2	2.44	0.49
1:B:58:GLU:HA	1:B:61:GLU:HG2	1.95	0.49
2:D:483:ILE:HG12	2:D:517:LEU:HA	1.93	0.49
2:D:489:GLY:N	2:D:656:GLY:HA2	2.28	0.48
2:D:594:SER:HB2	2:D:607:LEU:HD11	1.95	0.48
2:C:483:ILE:HG12	2:C:517:LEU:HA	1.96	0.48
2:C:334:PHE:CE1	2:C:356:ALA:HB3	2.49	0.47
2:C:604:ALA:O	2:C:605:HIS:ND1	2.47	0.47
2:D:488:GLY:N	2:D:654:ALA:HB1	2.29	0.47
2:D:579:PRO:HB2	2:D:691:LEU:HD13	1.95	0.47
2:C:386:ASP:HB3	2:C:405:TYR:CZ	2.49	0.47
2:C:389:TYR:HB2	2:C:393:MET:HG2	1.97	0.47
2:C:453:LYS:HE2	2:C:667:ARG:HG2	1.97	0.47
2:D:476:PRO:HB2	2:D:574:LEU:N	2.30	0.47
2:C:640:ALA:HB3	2:C:687:TYR:HE2	1.80	0.47
2:C:580:ASP:OD1	2:C:580:ASP:N	2.47	0.46
2:D:500:ALA:HB3	2:D:503:THR:HG23	1.98	0.46
1:B:25:ASP:N	1:B:25:ASP:OD1	2.48	0.46
1:B:40:ASP:OD1	1:B:45:ARG:NH2	2.48	0.46
1:A:36:LEU:HD22	2:C:590:MET:HE1	1.98	0.46
2:C:558:ILE:HD11	2:C:697:ILE:HD11	1.98	0.46
2:D:622:ASN:HA	2:D:625:ARG:NE	2.31	0.46
2:D:610:VAL:HG11	2:D:651:GLN:HB3	1.97	0.45
2:D:622:ASN:HA	2:D:625:ARG:HE	1.81	0.45
2:C:436:LYS:HZ3	2:C:441:GLY:HA3	1.82	0.45
2:C:316:ASP:OD1	2:C:319:THR:OG1	2.34	0.45
2:C:637:MET:O	2:C:689:LYS:NZ	2.49	0.44
2:C:321:ILE:HB	2:C:324:LEU:HG	1.99	0.44
2:D:451:CYS:HA	2:D:575:PRO:HG2	2.00	0.44
2:C:506:PRO:HB2	2:C:510:GLU:H	1.82	0.44
1:B:63:THR:HB	1:B:68:VAL:HB	2.00	0.44
2:D:316:ASP:OD1	2:D:319:THR:OG1	2.29	0.44
2:D:622:ASN:O	2:D:625:ARG:HG2	2.18	0.44
1:A:58:GLU:HA	1:A:61:GLU:HG2	2.00	0.44
2:C:507:LYS:HE3	2:C:551:SER:HA	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:309:CYS:SG	2:D:358:CYS:HB2	2.58	0.44
2:D:386:ASP:HB3	2:D:405:TYR:CZ	2.53	0.44
2:D:479:VAL:HG11	2:D:497:ILE:HD12	1.99	0.43
1:A:41:CYS:SG	1:A:48:PRO:HG3	2.59	0.43
2:C:373:ILE:HD11	2:C:398:TYR:HB3	2.01	0.43
2:D:640:ALA:HB3	2:D:687:TYR:HE1	1.83	0.43
2:C:335:ILE:HG22	2:C:355:THR:HB	2.01	0.43
1:B:79:ILE:HG21	1:B:107:ILE:HB	2.01	0.43
2:D:558:ILE:HD11	2:D:697:ILE:HD11	2.01	0.43
2:C:591:GLY:HA3	2:C:658:PHE:CE2	2.53	0.42
2:D:501:ALA:N	2:D:557:ASP:OD1	2.52	0.42
2:D:675:SER:HB2	2:D:688:THR:HG23	2.01	0.42
1:B:61:GLU:HA	1:B:64:VAL:HG22	2.01	0.42
2:C:440:LYS:HZ1	2:C:443:LYS:H	1.66	0.42
2:C:590:MET:HE3	2:C:611:ARG:HG2	2.01	0.42
2:C:375:ASP:HA	2:C:397:THR:HA	2.01	0.42
2:D:519:VAL:HG11	2:D:537:ILE:HD11	2.02	0.42
2:D:487:GLY:C	2:D:654:ALA:HB1	2.44	0.42
2:C:488:GLY:N	2:C:654:ALA:HB1	2.35	0.41
2:D:373:ILE:HD11	2:D:398:TYR:HB3	2.01	0.41
2:D:591:GLY:HA3	2:D:658:PHE:CE2	2.56	0.41
2:D:661:ARG:HB3	2:D:668:TRP:CE2	2.56	0.41
2:C:337:THR:OG1	2:C:338:CYS:N	2.54	0.41
2:D:349:GLN:H	2:D:349:GLN:CD	2.28	0.41
2:D:388:ARG:HH21	2:D:403:GLN:HG2	1.86	0.41
2:C:356:ALA:HA	2:C:365:HIS:CE1	2.56	0.41
2:C:486:ARG:NH2	2:C:597:GLY:O	2.41	0.41
2:D:496:TRP:CD1	2:D:701:MET:HE3	2.55	0.41
2:C:333:TYR:HB3	2:C:357:VAL:HG12	2.03	0.41
2:C:549:ASP:N	2:C:549:ASP:OD1	2.54	0.41
1:A:32:ASP:O	1:A:36:LEU:HG	2.20	0.40
2:C:483:ILE:HG23	2:C:517:LEU:HA	2.02	0.40
1:B:31:HIS:HB2	1:B:99:TYR:CZ	2.56	0.40
2:D:590:MET:HE3	2:D:611:ARG:HG2	2.02	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	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	26
2	D	380/409 (93%)	336 (88%)	38 (10%)	6 (2%)	7	31
All	All	935/1026 (91%)	833 (89%)	88 (9%)	14 (2%)	8	33

All (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
2	C	451	CYS
2	C	631	ASP
2	C	679	GLY
2	D	631	ASP
2	C	516	SER
2	C	518	ASP
2	C	575	PRO
2	C	440	LYS
2	D	679	GLY

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	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%)	86	86
2	D	330/349 (95%)	328 (99%)	2 (1%)	78	82
All	All	827/888 (93%)	824 (100%)	3 (0%)	84	85

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	320	ILE
2	D	593	VAL
2	D	631	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
2	C	322	GLN
2	C	378	GLN
2	C	403	GLN
2	C	512	GLN
2	C	618	GLN
2	D	384	ASN
2	D	403	GLN
2	D	407	HIS
2	D	618	GLN
2	D	692	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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
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 [i](#)

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 ⓘ

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, 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	88/104 (84%)	-0.36	0 100 100	103, 154, 188, 229	0
1	B	88/104 (84%)	-0.22	0 100 100	132, 197, 254, 347	0
2	C	389/409 (95%)	-0.19	4 (1%) 79 63	92, 143, 210, 280	0
2	D	386/409 (94%)	-0.03	7 (1%) 67 49	81, 130, 202, 286	0
All	All	951/1026 (92%)	-0.15	11 (1%) 76 58	81, 142, 220, 347	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	598	VAL	3.3
2	D	631	ASP	3.1
2	C	496	TRP	2.8
2	D	594	SER	2.5
2	D	612	LEU	2.5
2	C	701	MET	2.4
2	C	559	ALA	2.4
2	D	404	TYR	2.3
2	D	678	ILE	2.2
2	D	655	GLY	2.1
2	C	463	ARG	2.0

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

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
1	TYS	B	51	16/17	0.82	0.17	178,205,226,245	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
1	TYS	A	51	16/17	0.93	0.14	120,130,163,166	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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.