



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 4, 2021 – 04:07 PM EDT

PDB ID : 6XAY
Title : Structure of a fragment of human fibronectin containing the 10th, 11th and 12th type III domains
Authors : Mou, T.C.; Nepomuceno, P.A.; Sprang, S.R.; Briknarova, K.
Deposited on : 2020-06-05
Resolution : 2.48 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.23.2
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.23.2

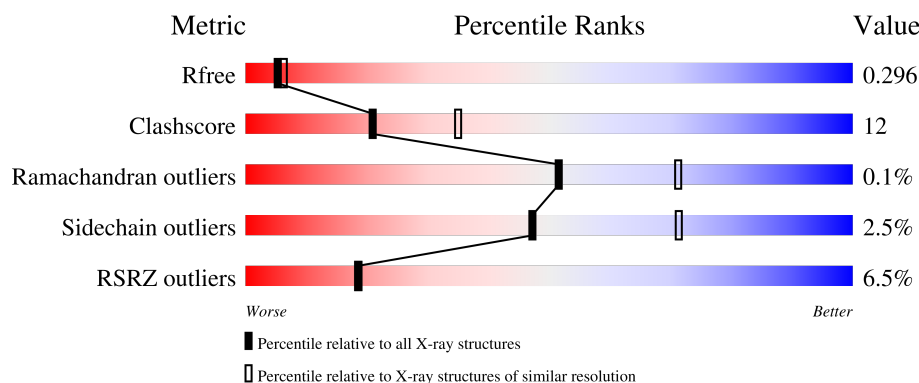
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.48 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}	130704	5857 (2.50-2.46)
Clashscore	141614	6594 (2.50-2.46)
Ramachandran outliers	138981	6469 (2.50-2.46)
Sidechain outliers	138945	6471 (2.50-2.46)
RSRZ outliers	127900	5738 (2.50-2.46)

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	280	
1	B	280	
1	C	280	
1	D	280	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8315 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 Fibronectin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	272	Total	C	N	O	S	0	0	0
			2042	1286	336	416	4			
1	B	269	Total	C	N	O	S	0	0	0
			2022	1274	332	412	4			
1	C	271	Total	C	N	O	S	0	0	0
			2036	1283	335	414	4			
1	D	272	Total	C	N	O	S	0	0	0
			2042	1286	336	416	4			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1443	GLY	-	expression tag	UNP P02751
A	1444	SER	-	expression tag	UNP P02751
A	1445	HIS	-	expression tag	UNP P02751
A	1446	MET	-	expression tag	UNP P02751
A	1643	GLY	VAL	engineered mutation	UNP P02751
B	1443	GLY	-	expression tag	UNP P02751
B	1444	SER	-	expression tag	UNP P02751
B	1445	HIS	-	expression tag	UNP P02751
B	1446	MET	-	expression tag	UNP P02751
B	1643	GLY	VAL	engineered mutation	UNP P02751
C	1443	GLY	-	expression tag	UNP P02751
C	1444	SER	-	expression tag	UNP P02751
C	1445	HIS	-	expression tag	UNP P02751
C	1446	MET	-	expression tag	UNP P02751
C	1643	GLY	VAL	engineered mutation	UNP P02751
D	1443	GLY	-	expression tag	UNP P02751
D	1444	SER	-	expression tag	UNP P02751
D	1445	HIS	-	expression tag	UNP P02751
D	1446	MET	-	expression tag	UNP P02751
D	1643	GLY	VAL	engineered mutation	UNP P02751

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

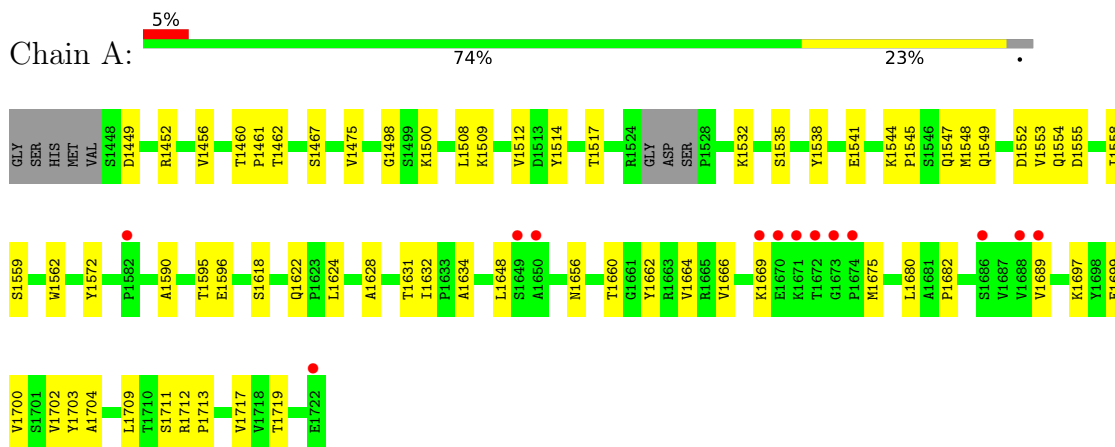
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	44	Total	O	0	0
			44	44		
3	B	20	Total	O	0	0
			20	20		
3	C	27	Total	O	0	0
			27	27		
3	D	46	Total	O	0	0
			46	46		

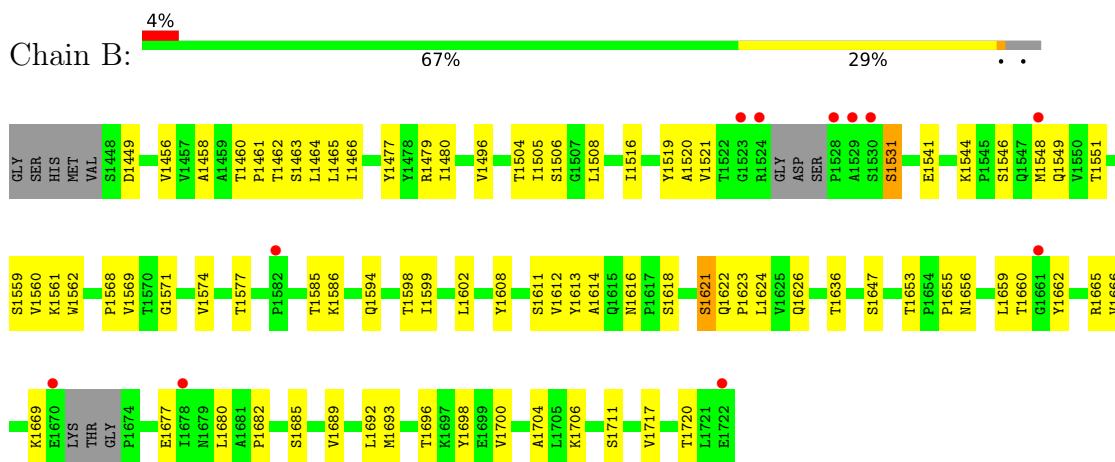
3 Residue-property plots

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.

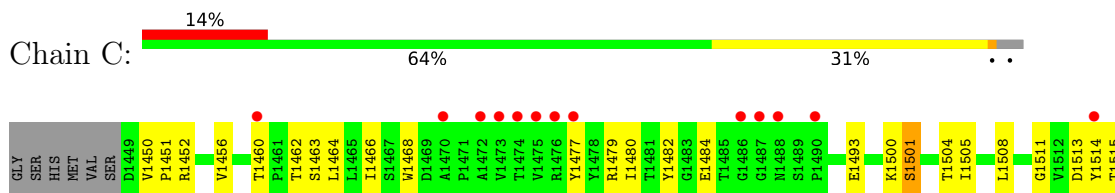
• Molecule 1: Fibronectin



• Molecule 1: Fibronectin

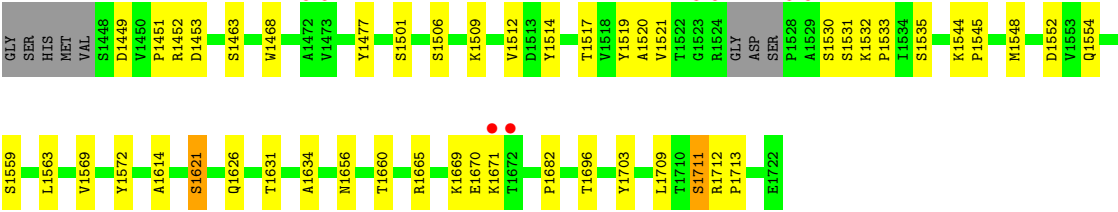
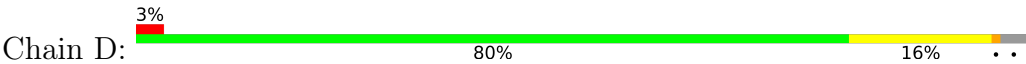


• Molecule 1: Fibronectin





● Molecule 1: Fibronectin



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	125.08Å 440.37Å 60.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.40 – 2.48 38.13 – 2.48	Depositor EDS
% Data completeness (in resolution range)	92.1 (37.40-2.48) 92.2 (38.13-2.48)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.84 (at 2.48Å)	Xtriage
Refinement program	PHENIX 1.16	Depositor
R, R_{free}	0.246 , 0.296 0.246 , 0.296	Depositor DCC
R_{free} test set	1998 reflections (3.61%)	wwPDB-VP
Wilson B-factor (Å ²)	41.8	Xtriage
Anisotropy	0.624	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 54.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	8315	wwPDB-VP
Average B, all atoms (Å ²)	72.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 39.23 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.2757e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

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	0.29	0/2087	0.50	0/2866
1	B	0.30	0/2066	0.50	0/2836
1	C	0.31	0/2081	0.55	0/2858
1	D	0.31	0/2087	0.51	0/2866
All	All	0.30	0/8321	0.52	0/11426

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	2042	0	2057	45	0
1	B	2022	0	2034	61	0
1	C	2036	0	2052	72	0
1	D	2042	0	2057	36	0
2	A	12	0	16	2	0
2	B	18	0	24	2	0
2	D	6	0	8	1	0
3	A	44	0	0	1	0
3	B	20	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	27	0	0	1	0
3	D	46	0	0	0	0
All	All	8315	0	8248	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 12.

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:D:1548:MET:CE	1:D:1626:GLN:HB3	1.90	1.01
1:C:1542:ILE:HD12	1:C:1542:ILE:H	1.25	0.98
1:C:1515:THR:HA	1:C:1537:ASN:HB2	1.48	0.93
1:D:1548:MET:HE3	1:D:1626:GLN:HB3	1.50	0.93
1:C:1574:VAL:HG12	1:C:1612:VAL:HG12	1.56	0.88
1:B:1460:THR:HG22	1:B:1462:THR:H	1.42	0.84
1:A:1669:LYS:HD2	1:A:1717:VAL:HG21	1.64	0.79
1:C:1549:GLN:HE21	1:C:1561:LYS:HD3	1.48	0.79
1:A:1452:ARG:HH21	1:D:1665:ARG:HH12	1.33	0.77
1:D:1548:MET:HE2	1:D:1626:GLN:HB3	1.66	0.77
1:A:1669:LYS:HE3	1:A:1699:GLU:OE1	1.84	0.76
1:C:1542:ILE:H	1:C:1542:ILE:CD1	1.98	0.76
1:B:1462:THR:HG21	1:C:1547:GLN:HB3	1.67	0.76
1:B:1505:ILE:HG22	1:B:1508:LEU:HD11	1.68	0.76
1:A:1460:THR:HG22	1:A:1462:THR:H	1.50	0.74
1:D:1552:ASP:HB3	1:D:1559:SER:HB2	1.69	0.74
1:C:1480:ILE:N	1:C:1493:GLU:OE1	2.21	0.72
1:C:1561:LYS:HG3	1:C:1596:GLU:HB3	1.72	0.71
1:C:1542:ILE:HD12	1:C:1542:ILE:N	2.03	0.70
1:C:1456:VAL:HG21	1:C:1464:LEU:HD12	1.72	0.69
1:C:1542:ILE:HD13	1:C:1619:GLY:O	1.92	0.69
1:C:1511:GLY:O	1:C:1539:ARG:NH1	2.27	0.68
1:C:1569:VAL:HG12	1:C:1571:GLY:H	1.60	0.67
1:D:1452:ARG:HD2	1:D:1453:ASP:H	1.60	0.67
1:C:1464:LEU:HD23	1:C:1508:LEU:HD22	1.77	0.66
1:C:1493:GLU:OE2	1:C:1493:GLU:HA	1.96	0.66
1:C:1549:GLN:HG3	1:C:1561:LYS:HB3	1.78	0.65
1:B:1504:THR:HG21	1:C:1551:THR:HA	1.77	0.65
1:C:1482:TYR:HB3	1:C:1516:ILE:HD13	1.79	0.64
1:C:1517:THR:HG22	1:C:1535:SER:HB2	1.80	0.64
1:B:1548:MET:HG3	1:B:1562:TRP:HB3	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1801:GOL:H2	1:D:1544:LYS:HE3	1.81	0.63
1:B:1669:LYS:HE2	1:B:1717:VAL:HG21	1.81	0.62
1:C:1572:TYR:HB2	1:C:1590:ALA:HB3	1.81	0.62
1:B:1689:VAL:HG13	1:B:1692:LEU:HD11	1.82	0.62
1:B:1594:GLN:NE2	2:B:1801:GOL:O3	2.32	0.62
1:C:1613:TYR:CZ	1:C:1623:PRO:HB3	2.35	0.61
1:C:1574:VAL:HG23	1:C:1588:LYS:HB3	1.81	0.61
1:C:1532:LYS:HG2	1:C:1533:PRO:HD2	1.82	0.61
1:B:1463:SER:OG	1:C:1549:GLN:HB3	2.01	0.61
1:B:1548:MET:HB2	1:B:1624:LEU:HD21	1.82	0.61
1:A:1595:THR:HG23	1:A:1596:GLU:HG3	1.82	0.60
1:D:1449:ASP:N	1:D:1449:ASP:OD1	2.34	0.60
1:D:1631:THR:HA	1:D:1709:LEU:HD22	1.83	0.60
1:A:1452:ARG:NH2	3:A:1902:HOH:O	2.29	0.60
1:C:1631:THR:HA	1:C:1709:LEU:HD22	1.84	0.60
1:B:1465:LEU:HD13	1:B:1504:THR:HG23	1.83	0.59
1:C:1632:ILE:HG13	1:C:1711:SER:HB3	1.84	0.59
1:B:1636:THR:HG23	1:B:1653:THR:HB	1.84	0.59
1:C:1542:ILE:CD1	1:C:1619:GLY:O	2.50	0.59
1:B:1706:LYS:NZ	3:B:1901:HOH:O	2.36	0.58
1:B:1461:PRO:HD3	1:B:1541:GLU:HB3	1.85	0.58
1:A:1662:TYR:HB2	1:A:1680:LEU:HB2	1.86	0.58
1:C:1568:PRO:O	1:C:1616:ASN:ND2	2.37	0.58
1:B:1456:VAL:HA	1:B:1466:ILE:HA	1.87	0.57
1:A:1664:VAL:HG22	1:A:1702:VAL:HG22	1.87	0.57
1:A:1666:VAL:HG21	1:A:1689:VAL:HG11	1.87	0.56
1:B:1693:MET:O	1:B:1720:THR:HG21	2.05	0.56
1:A:1509:LYS:HB2	1:A:1512:VAL:HG21	1.87	0.56
1:B:1614:ALA:H	1:B:1621:SER:HB3	1.69	0.56
1:B:1551:THR:HG22	1:C:1504:THR:HG21	1.87	0.56
1:D:1517:THR:HG22	1:D:1535:SER:HB2	1.87	0.56
1:B:1569:VAL:HG12	1:B:1571:GLY:H	1.70	0.56
1:D:1671:LYS:HD2	1:D:1696:THR:HG23	1.87	0.56
1:A:1666:VAL:HG12	1:A:1700:VAL:HG22	1.87	0.56
1:B:1602:LEU:HD12	1:B:1608:TYR:CZ	2.40	0.55
1:A:1631:THR:HA	1:A:1709:LEU:HD23	1.88	0.55
1:C:1482:TYR:HA	1:C:1515:THR:O	2.07	0.55
1:A:1697:LYS:HD3	1:A:1719:THR:HG22	1.90	0.54
1:C:1553:VAL:HG12	1:C:1631:THR:HG23	1.89	0.54
1:C:1574:VAL:HG21	1:C:1597:MET:HG2	1.88	0.54
1:D:1548:MET:HE2	1:D:1626:GLN:CB	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1517:THR:HG1	1:A:1535:SER:HG	1.54	0.54
1:C:1660:THR:C	1:C:1682:PRO:HG3	2.28	0.54
1:A:1669:LYS:CE	1:A:1699:GLU:OE1	2.55	0.53
1:D:1477:TYR:CZ	1:D:1521:VAL:HG21	2.43	0.53
1:A:1656:ASN:HA	1:B:1685:SER:HB3	1.90	0.53
1:D:1703:TYR:CE2	1:D:1713:PRO:HB3	2.43	0.53
1:C:1482:TYR:CB	1:C:1516:ILE:HD13	2.38	0.53
1:C:1460:THR:HG22	1:C:1462:THR:H	1.74	0.52
1:C:1663:ARG:NH1	3:C:1804:HOH:O	2.41	0.52
1:A:1553:VAL:HG12	1:A:1631:THR:HG23	1.91	0.52
1:B:1626:GLN:NE2	3:B:1902:HOH:O	2.43	0.52
1:A:1562:TRP:O	1:A:1595:THR:OG1	2.28	0.52
1:D:1660:THR:C	1:D:1682:PRO:HG3	2.30	0.51
1:B:1460:THR:HB	1:B:1463:SER:HB2	1.91	0.51
1:B:1460:THR:HG21	1:C:1548:MET:O	2.10	0.51
1:B:1660:THR:HG23	1:B:1706:LYS:HA	1.91	0.51
1:C:1548:MET:HB2	1:C:1624:LEU:HD21	1.92	0.51
1:C:1576:THR:HG22	1:C:1610:VAL:HG13	1.92	0.51
1:D:1449:ASP:OD1	1:D:1532:LYS:NZ	2.36	0.51
1:B:1621:SER:OG	1:B:1622:GLN:O	2.28	0.51
1:B:1696:THR:HB	1:B:1698:TYR:CE2	2.45	0.51
1:A:1552:ASP:HB3	1:A:1559:SER:HB2	1.93	0.51
1:A:1632:ILE:HG13	1:A:1711:SER:HB2	1.92	0.50
1:A:1452:ARG:NH2	1:D:1665:ARG:HH12	2.05	0.50
1:C:1573:ARG:NH1	1:C:1620:GLU:OE2	2.45	0.50
1:A:1456:VAL:HG11	1:A:1538:TYR:CG	2.47	0.50
1:A:1660:THR:C	1:A:1682:PRO:HG3	2.32	0.50
1:C:1542:ILE:HD13	1:C:1619:GLY:C	2.32	0.50
1:D:1519:TYR:CE2	1:D:1533:PRO:HB3	2.45	0.50
1:B:1574:VAL:HG22	1:B:1612:VAL:HG13	1.94	0.49
1:A:1545:PRO:HG3	1:A:1572:TYR:HE2	1.77	0.49
1:C:1451:PRO:HG3	1:C:1520:ALA:HB2	1.94	0.49
1:A:1460:THR:HG21	1:D:1548:MET:O	2.12	0.49
1:C:1664:VAL:HG12	1:C:1702:VAL:HG22	1.95	0.49
1:C:1515:THR:HA	1:C:1537:ASN:CB	2.33	0.49
1:B:1480:ILE:HD11	1:B:1496:VAL:HG22	1.95	0.49
1:C:1501:SER:O	1:C:1501:SER:OG	2.30	0.48
1:A:1544:LYS:HE3	2:D:1801:GOL:H31	1.95	0.48
1:B:1666:VAL:HG12	1:B:1700:VAL:HG23	1.95	0.48
1:C:1484:GLU:HA	1:C:1513:ASP:O	2.12	0.48
1:B:1599:ILE:HG22	1:B:1602:LEU:HD21	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1451:PRO:HG3	1:D:1520:ALA:HB2	1.95	0.48
1:A:1549:GLN:HG2	1:D:1463:SER:HB3	1.95	0.48
1:B:1662:TYR:HB2	1:B:1680:LEU:HB2	1.94	0.48
1:A:1512:VAL:HG23	1:A:1514:TYR:CE2	2.49	0.48
1:B:1574:VAL:HG13	1:B:1612:VAL:HG22	1.96	0.48
1:A:1634:ALA:HA	1:A:1711:SER:OG	2.14	0.48
1:B:1704:ALA:HB3	1:B:1711:SER:HB3	1.94	0.47
1:D:1569:VAL:HG11	1:D:1614:ALA:HB1	1.96	0.47
1:C:1460:THR:O	1:C:1540:THR:HG23	2.14	0.47
1:B:1568:PRO:O	1:B:1616:ASN:ND2	2.48	0.47
1:A:1549:GLN:OE1	1:D:1506:SER:HB2	2.15	0.47
1:B:1660:THR:C	1:B:1682:PRO:HG3	2.34	0.47
1:C:1544:LYS:HG3	1:C:1622:GLN:O	2.15	0.47
1:C:1663:ARG:HB2	1:C:1705:LEU:HD11	1.95	0.47
1:B:1611:SER:HB3	1:B:1623:PRO:HB2	1.97	0.47
1:B:1665:ARG:HG3	1:B:1677:GLU:HG3	1.97	0.47
1:D:1614:ALA:HB3	1:D:1621:SER:HB3	1.97	0.46
1:B:1611:SER:HA	1:B:1624:LEU:O	2.16	0.46
1:B:1669:LYS:HB2	1:B:1669:LYS:HE3	1.66	0.46
1:B:1655:PRO:HG2	1:B:1659:LEU:HD11	1.97	0.46
1:D:1711:SER:OG	1:D:1712:ARG:O	2.34	0.46
1:B:1520:ALA:H	1:B:1531:SER:HB3	1.80	0.46
1:D:1512:VAL:HG23	1:D:1514:TYR:CE2	2.51	0.46
1:D:1669:LYS:HB3	1:D:1670:GLU:OE1	2.15	0.45
1:A:1572:TYR:HB2	1:A:1590:ALA:HB3	1.99	0.45
1:C:1452:ARG:HA	1:C:1534:ILE:HD13	1.98	0.45
1:B:1464:LEU:HD12	1:B:1516:ILE:HD11	1.98	0.45
1:A:1703:TYR:CE2	1:A:1713:PRO:HB3	2.52	0.45
1:B:1461:PRO:CD	1:B:1541:GLU:HB3	2.46	0.45
1:C:1466:ILE:HD13	1:C:1480:ILE:HG21	1.98	0.45
1:B:1549:GLN:O	1:B:1560:VAL:HA	2.16	0.45
1:B:1548:MET:HA	1:B:1561:LYS:O	2.17	0.45
1:D:1634:ALA:HA	1:D:1711:SER:OG	2.17	0.45
2:A:1801:GOL:H2	1:D:1544:LYS:CE	2.47	0.44
1:C:1482:TYR:OH	1:C:1505:ILE:HD11	2.18	0.44
1:C:1479:ARG:O	1:C:1518:VAL:HA	2.15	0.44
1:D:1545:PRO:HG3	1:D:1572:TYR:HE2	1.82	0.44
1:C:1642:GLN:HB3	1:C:1649:SER:HB2	1.99	0.44
1:D:1554:GLN:C	1:D:1631:THR:HG22	2.38	0.44
1:A:1618:SER:O	1:A:1618:SER:OG	2.30	0.44
1:B:1463:SER:O	1:B:1464:LEU:HD23	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1505:ILE:HG13	1:C:1508:LEU:HD11	2.00	0.43
1:C:1450:VAL:HG22	1:C:1451:PRO:O	2.19	0.43
1:C:1576:THR:HA	1:C:1609:VAL:O	2.18	0.43
1:A:1532:LYS:HB3	1:A:1532:LYS:HE3	1.80	0.43
1:C:1466:ILE:HD12	1:C:1468:TRP:HZ3	1.83	0.43
1:C:1613:TYR:CE1	1:C:1623:PRO:HB3	2.52	0.43
1:A:1656:ASN:HA	1:B:1685:SER:CB	2.48	0.43
1:B:1477:TYR:CZ	1:B:1521:VAL:HG21	2.54	0.43
1:C:1599:ILE:O	1:C:1602:LEU:HD13	2.19	0.43
1:D:1532:LYS:HD2	1:D:1532:LYS:H	1.83	0.43
1:A:1500:LYS:HD3	1:A:1500:LYS:HA	1.81	0.43
1:C:1576:THR:HG21	1:C:1599:ILE:HD13	2.00	0.43
1:B:1544:LYS:HG2	2:B:1803:GOL:H12	2.01	0.43
1:C:1668:PRO:HB2	1:C:1671:LYS:O	2.18	0.43
1:B:1618:SER:O	1:B:1618:SER:OG	2.34	0.42
1:A:1666:VAL:HA	1:A:1699:GLU:O	2.19	0.42
1:B:1458:ALA:CB	1:C:1550:VAL:HG11	2.50	0.42
1:B:1577:THR:HG23	1:B:1585:THR:HG22	2.02	0.42
1:C:1477:TYR:CE1	1:C:1521:VAL:HG21	2.55	0.42
1:D:1468:TRP:O	1:D:1501:SER:OG	2.37	0.42
1:B:1548:MET:HB2	1:B:1624:LEU:CD2	2.49	0.42
1:B:1613:TYR:CZ	1:B:1623:PRO:HB3	2.54	0.42
1:C:1666:VAL:HG13	1:C:1700:VAL:HG22	2.01	0.42
1:B:1614:ALA:N	1:B:1621:SER:HB3	2.34	0.42
1:B:1559:SER:OG	1:B:1598:THR:HG22	2.19	0.42
1:C:1552:ASP:HB3	1:C:1559:SER:OG	2.20	0.42
1:D:1509:LYS:HB2	1:D:1512:VAL:HG21	2.01	0.42
1:D:1563:LEU:HD23	1:D:1563:LEU:HA	1.88	0.42
1:A:1548:MET:HE2	1:A:1624:LEU:HG	2.02	0.41
1:A:1558:ILE:HD13	1:A:1628:ALA:HB3	2.02	0.41
1:C:1542:ILE:HG12	1:C:1616:ASN:HB3	2.01	0.41
1:D:1521:VAL:HA	1:D:1530:SER:HA	2.02	0.41
1:A:1475:VAL:O	1:A:1498:GLY:HA3	2.21	0.41
1:A:1704:ALA:HB3	1:A:1711:SER:HB2	2.03	0.41
1:B:1465:LEU:HD13	1:B:1504:THR:CG2	2.50	0.41
1:A:1508:LEU:HD22	1:A:1514:TYR:CE1	2.55	0.41
1:C:1704:ALA:O	1:C:1705:LEU:HD23	2.21	0.41
1:C:1508:LEU:HD23	1:C:1514:TYR:CZ	2.56	0.41
1:C:1660:THR:O	1:C:1682:PRO:HG3	2.21	0.41
1:A:1541:GLU:OE1	1:A:1622:GLN:NE2	2.47	0.41
1:A:1461:PRO:HD3	1:A:1541:GLU:OE2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1648:LEU:HD23	1:A:1648:LEU:HA	1.86	0.41
1:B:1621:SER:OG	1:B:1622:GLN:N	2.54	0.41
1:C:1456:VAL:HA	1:C:1466:ILE:HA	2.03	0.41
1:B:1586:LYS:HE2	1:B:1586:LYS:HB2	1.91	0.40
1:C:1644:THR:OG1	1:C:1647:SER:HB2	2.21	0.40
1:B:1479:ARG:HB2	1:B:1519:TYR:HD2	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	268/280 (96%)	257 (96%)	10 (4%)	1 (0%)	34	52
1	B	263/280 (94%)	252 (96%)	11 (4%)	0	100	100
1	C	267/280 (95%)	250 (94%)	17 (6%)	0	100	100
1	D	268/280 (96%)	257 (96%)	11 (4%)	0	100	100
All	All	1066/1120 (95%)	1016 (95%)	49 (5%)	1 (0%)	51	71

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1547	GLN

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	238/244 (98%)	232 (98%)	6 (2%)	47	71
1	B	236/244 (97%)	229 (97%)	7 (3%)	41	65
1	C	237/244 (97%)	230 (97%)	7 (3%)	41	65
1	D	238/244 (98%)	234 (98%)	4 (2%)	60	81
All	All	949/976 (97%)	925 (98%)	24 (2%)	47	71

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1449	ASP
1	A	1467	SER
1	A	1554	GLN
1	A	1555	ASP
1	A	1675	MET
1	A	1712	ARG
1	B	1449	ASP
1	B	1506	SER
1	B	1531	SER
1	B	1546	SER
1	B	1621	SER
1	B	1647	SER
1	B	1656	ASN
1	C	1463	SER
1	C	1500	LYS
1	C	1501	SER
1	C	1537	ASN
1	C	1539	ARG
1	C	1588	LYS
1	C	1676	LYS
1	D	1531	SER
1	D	1621	SER
1	D	1656	ASN
1	D	1711	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1549	GLN
1	B	1594	GLN

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Mol	Chain	Res	Type
1	B	1656	ASN
1	C	1715	GLN
1	D	1656	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

6 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	$\# Z > 2$
2	GOL	A	1801	-	5,5,5	0.97	0	5,5,5	1.08	0
2	GOL	D	1801	-	5,5,5	0.84	0	5,5,5	1.03	0
2	GOL	B	1803	-	5,5,5	0.94	0	5,5,5	1.05	0
2	GOL	A	1802	-	5,5,5	1.03	1 (20%)	5,5,5	1.03	0
2	GOL	B	1801	-	5,5,5	0.88	0	5,5,5	1.04	0
2	GOL	B	1802	-	5,5,5	0.96	0	5,5,5	0.95	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
2	GOL	A	1801	-	-	2/4/4/4	-
2	GOL	D	1801	-	-	0/4/4/4	-
2	GOL	B	1803	-	-	3/4/4/4	-
2	GOL	A	1802	-	-	0/4/4/4	-
2	GOL	B	1801	-	-	0/4/4/4	-
2	GOL	B	1802	-	-	0/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1802	GOL	O2-C2	-2.02	1.37	1.43

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1803	GOL	C1-C2-C3-O3
2	B	1803	GOL	O2-C2-C3-O3
2	A	1801	GOL	O1-C1-C2-C3
2	A	1801	GOL	O1-C1-C2-O2
2	B	1803	GOL	O1-C1-C2-C3

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1801	GOL	2	0
2	D	1801	GOL	1	0
2	B	1803	GOL	1	0
2	B	1801	GOL	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	272/280 (97%)	0.15	13 (4%) 30 32	38, 55, 102, 145	0
1	B	269/280 (96%)	0.40	11 (4%) 37 39	48, 81, 113, 156	0
1	C	271/280 (96%)	0.75	38 (14%) 2 2	28, 91, 139, 185	0
1	D	272/280 (97%)	0.00	8 (2%) 51 54	29, 53, 102, 146	0
All	All	1084/1120 (96%)	0.33	70 (6%) 18 18	28, 67, 122, 185	0

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1674	PRO	6.5
1	C	1476	ARG	5.9
1	C	1593	ASP	5.5
1	C	1522	THR	5.5
1	B	1523	GLY	5.4
1	D	1523	GLY	5.2
1	A	1673	GLY	4.8
1	C	1568	PRO	4.5
1	C	1523	GLY	4.5
1	D	1524	ARG	4.4
1	C	1521	VAL	4.2
1	C	1514	TYR	4.2
1	B	1722	GLU	4.0
1	C	1470	ALA	3.9
1	C	1519	TYR	3.9
1	C	1487	GLY	3.8
1	B	1530	SER	3.7
1	D	1672	THR	3.7
1	C	1564	PRO	3.6
1	C	1590	ALA	3.6
1	B	1529	ALA	3.6

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Mol	Chain	Res	Type	RSRZ
1	C	1589	THR	3.6
1	D	1472	ALA	3.6
1	C	1524	ARG	3.5
1	C	1673	GLY	3.5
1	C	1530	SER	3.4
1	A	1582	PRO	3.3
1	C	1516	ILE	3.3
1	C	1722	GLU	3.3
1	B	1528	PRO	3.2
1	A	1669	LYS	3.2
1	C	1671	LYS	3.1
1	C	1477	TYR	3.1
1	B	1524	ARG	3.0
1	A	1670	GLU	3.0
1	A	1672	THR	3.0
1	C	1560	VAL	2.9
1	A	1722	GLU	2.9
1	B	1582	PRO	2.9
1	C	1475	VAL	2.9
1	C	1529	ALA	2.9
1	C	1571	GLY	2.8
1	B	1661	GLY	2.8
1	C	1473	VAL	2.8
1	A	1671	LYS	2.7
1	C	1474	THR	2.7
1	B	1678	ILE	2.7
1	C	1486	GLY	2.6
1	A	1649	SER	2.6
1	C	1472	ALA	2.6
1	C	1597	MET	2.5
1	A	1689	VAL	2.5
1	A	1650	ALA	2.4
1	A	1686	SER	2.4
1	D	1528	PRO	2.4
1	D	1671	LYS	2.4
1	C	1686	SER	2.4
1	D	1473	VAL	2.4
1	C	1619	GLY	2.4
1	C	1599	ILE	2.3
1	C	1674	PRO	2.3
1	C	1460	THR	2.3
1	D	1529	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	1670	GLU	2.2
1	B	1670	GLU	2.2
1	B	1548	MET	2.2
1	C	1488	ASN	2.1
1	A	1688	VAL	2.0
1	C	1490	PRO	2.0
1	C	1520	ALA	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 monosaccharides 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(\AA^2)	Q<0.9
2	GOL	B	1803	6/6	0.78	0.30	83,102,126,131	0
2	GOL	B	1802	6/6	0.83	0.32	85,95,124,142	0
2	GOL	A	1801	6/6	0.94	0.31	44,60,76,84	0
2	GOL	B	1801	6/6	0.95	0.19	65,69,84,91	6
2	GOL	A	1802	6/6	0.96	0.22	43,50,62,69	6
2	GOL	D	1801	6/6	0.98	0.29	43,43,69,84	0

6.5 Other polymers [i](#)

There are no such residues in this entry.