



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 11:49 PM UTC

PDB ID : 2VR3 / pdb_00002vr3
Title : Structural and Biochemical Characterization of Fibrinogen binding to ClfA from *Staphylococcus aureus*
Authors : Ganesh, V.K.; Rivera, J.J.; Smeds, E.; Bowden, M.G.; Wann, E.R.; Gurudappa, S.; Fitzgerald, J.R.; Hook, M.
Deposited on : 2008-03-25
Resolution : 1.95 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
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

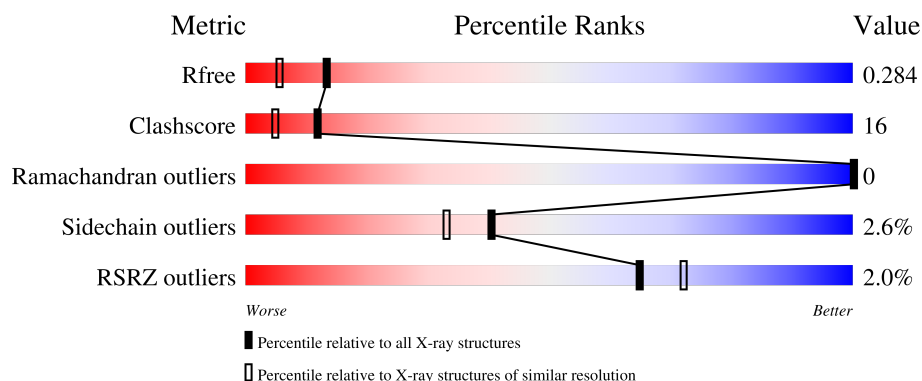
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.95 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	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

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	329	 2% 69% 22% • 6%
1	B	329	 2% 68% 25% • 5%
2	C	13	 8% 77% 15% 8%
2	D	13	 77% 23%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5226 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 CLUMPING FACTOR A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	308	Total	C	N	O	S	0	0	0
			2269	1432	369	463	5			
1	B	311	Total	C	N	O	S	0	0	1
			2289	1443	371	470	5			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	327	CYS	ASP	engineered mutation	UNP Q2G015
A	541	CYS	LYS	engineered mutation	UNP Q2G015
B	327	CYS	ASP	engineered mutation	UNP Q2G015
B	541	CYS	LYS	engineered mutation	UNP Q2G015

- Molecule 2 is a protein called FIBRINOGEN GAMMA-CHAIN.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	12	Total	C	N	O	0	0	0
			70	42	14	14			
2	D	13	Total	C	N	O	0	0	0
			71	42	14	15			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	410	ALA	ASP	engineered mutation	UNP P02679
D	410	ALA	ASP	engineered mutation	UNP P02679

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	249	Total	O	0	0
			249	249		

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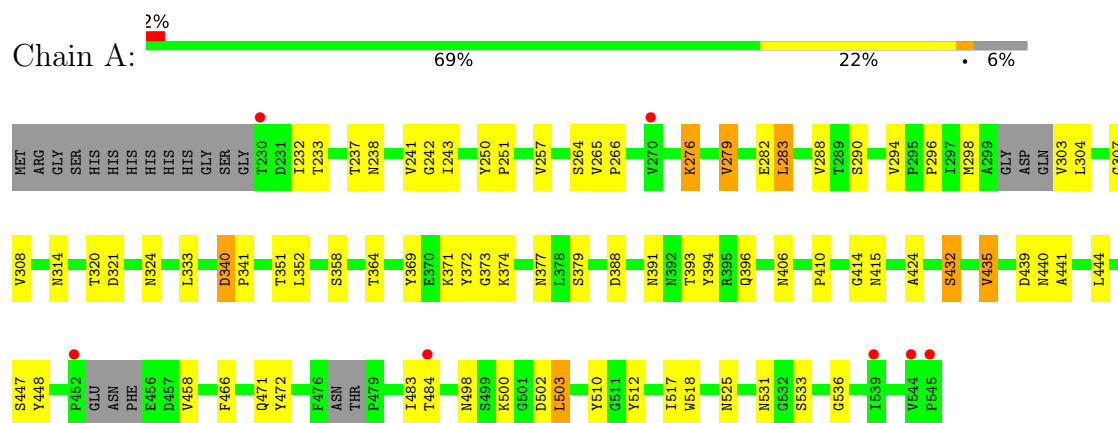
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	262	Total 262	O 262	0	0
3	C	10	Total 10	O 10	0	0
3	D	6	Total 6	O 6	0	0

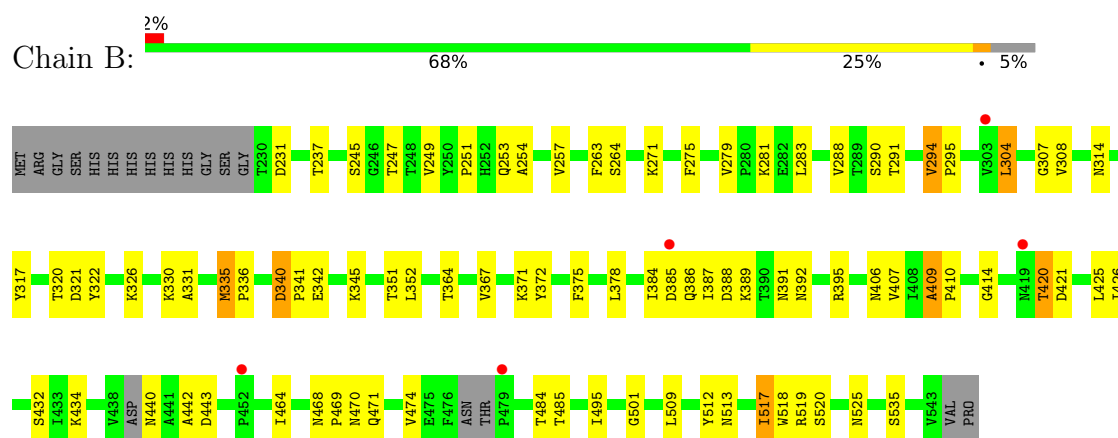
3 Residue-property plots

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

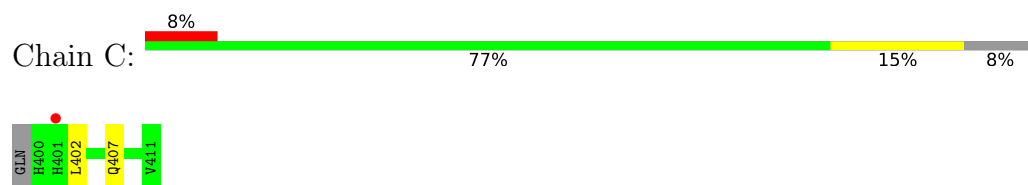
• Molecule 1: CLUMPING FACTOR A



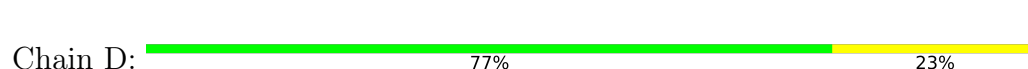
• Molecule 1: CLUMPING FACTOR A



• Molecule 2: FIBRINOGEN GAMMA-CHAIN



• Molecule 2: FIBRINOGEN GAMMA-CHAIN



Q399	
Q407	
A408	
G409	
A410	
V411	

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	35.43Å 61.84Å 81.78Å 85.44° 81.84° 82.45°	Depositor
Resolution (Å)	15.00 – 1.95 15.00 – 1.95	Depositor EDS
% Data completeness (in resolution range)	93.2 (15.00-1.95) 92.9 (15.00-1.95)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.11 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.211 , 0.279 0.213 , 0.284	Depositor DCC
R_{free} test set	941 reflections (1.92%)	wwPDB-VP
Wilson B-factor (Å ²)	21.0	Xtriage
Anisotropy	0.196	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.44 , 87.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	5226	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 16.96% 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](#)

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	0.93	2/2313 (0.1%)	1.15	9/3173 (0.3%)
1	B	0.93	1/2333 (0.0%)	1.15	9/3197 (0.3%)
2	C	1.15	0/69	1.21	1/89 (1.1%)
2	D	1.06	0/70	0.99	0/91
All	All	0.94	3/4785 (0.1%)	1.15	19/6550 (0.3%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	250	TYR	CA-C	-6.02	1.46	1.52
1	A	279	VAL	CA-CB	5.93	1.58	1.54
1	B	367	VAL	CA-CB	5.04	1.59	1.53

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	340	ASP	CA-C-N	12.27	132.00	119.24
1	A	340	ASP	C-N-CA	12.27	132.00	119.24
1	B	420	THR	N-CA-C	-8.43	97.98	110.46
1	B	409	ALA	CA-C-N	7.45	129.39	120.23
1	B	409	ALA	C-N-CA	7.45	129.39	120.23
1	A	466	PHE	CA-C-N	6.61	126.32	119.64
1	A	466	PHE	C-N-CA	6.61	126.32	119.64
1	B	340	ASP	CA-C-N	6.46	126.38	119.28
1	B	340	ASP	C-N-CA	6.46	126.38	119.28
1	B	335	MET	CA-C-N	5.91	125.84	119.76
1	B	335	MET	C-N-CA	5.91	125.84	119.76
1	B	294	VAL	CA-C-N	5.86	126.41	120.38
1	B	294	VAL	C-N-CA	5.86	126.41	120.38
2	C	402	LEU	N-CA-C	5.68	117.90	108.13
1	A	424	ALA	N-CA-C	5.59	118.12	110.24
1	A	243	ILE	N-CA-C	5.33	115.54	107.75
1	A	276	LYS	N-CA-C	5.19	116.87	108.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	498	ASN	N-CA-C	-5.04	107.18	113.38
1	A	444	LEU	N-CA-C	5.03	118.15	110.20

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2269	0	2111	62	0
1	B	2289	0	2125	84	0
2	C	70	0	67	2	0
2	D	71	0	59	3	0
3	A	249	0	0	14	0
3	B	262	0	0	20	0
3	C	10	0	0	0	0
3	D	6	0	0	0	0
All	All	5226	0	4362	143	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 16.

All (143) 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:B:386:GLN:HG2	3:B:2157:HOH:O	1.54	1.05
1:B:384:ILE:H	2:D:407:GLN:HE22	1.11	0.97
1:A:279:VAL:H	1:A:314:ASN:HD22	1.11	0.96
1:A:290:SER:O	3:A:2050:HOH:O	1.83	0.95
1:B:281:LYS:NZ	3:B:2045:HOH:O	2.01	0.94
1:B:432:SER:OG	3:B:2195:HOH:O	1.82	0.90
1:A:279:VAL:H	1:A:314:ASN:ND2	1.71	0.87
1:A:406:ASN:OD1	1:A:484:THR:HG22	1.73	0.86
1:B:281:LYS:NZ	3:B:2044:HOH:O	2.08	0.85
1:B:281:LYS:HE3	3:B:2044:HOH:O	1.78	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:531:ASN:H	1:B:247:THR:HG23	1.43	0.83
1:A:531:ASN:H	1:B:247:THR:CG2	1.91	0.83
1:A:276:LYS:O	3:A:2036:HOH:O	1.98	0.81
1:B:281:LYS:CE	3:B:2044:HOH:O	2.28	0.80
1:A:303:VAL:N	3:A:2061:HOH:O	2.15	0.80
1:A:283:LEU:HD11	1:A:352:LEU:HD22	1.64	0.80
1:B:279:VAL:H	1:B:314:ASN:HD22	1.29	0.79
1:A:372:TYR:OH	3:A:2128:HOH:O	2.00	0.78
1:B:231:ASP:OD2	3:B:2002:HOH:O	2.04	0.74
1:B:271:LYS:HG3	1:B:321:ASP:N	2.02	0.74
1:B:322:TYR:O	1:B:326:LYS:HG2	1.88	0.74
1:B:388:ASP:N	3:B:2157:HOH:O	2.21	0.73
1:B:468:ASN:HB3	1:B:469:PRO:HD2	1.71	0.72
1:A:320:THR:HG22	1:A:321:ASP:N	2.04	0.71
1:B:519:ARG:HG3	3:B:2247:HOH:O	1.91	0.70
1:B:304:LEU:HD13	1:B:322:TYR:CD2	2.28	0.69
1:A:410:PRO:HG3	1:A:483:ILE:HG12	1.73	0.69
1:B:519:ARG:NH1	3:B:2247:HOH:O	2.25	0.68
1:A:447:SER:O	1:A:448:TYR:HB2	1.94	0.67
1:B:387:ILE:CA	3:B:2157:HOH:O	2.45	0.65
1:A:320:THR:HG22	1:A:321:ASP:H	1.61	0.65
1:B:387:ILE:C	3:B:2157:HOH:O	2.38	0.65
1:B:464:ILE:HG12	1:B:474:VAL:HG22	1.78	0.65
1:B:421:ASP:O	1:B:501:GLY:HA3	1.97	0.65
1:A:432:SER:OG	3:A:2180:HOH:O	2.14	0.65
1:B:468:ASN:HB3	1:B:469:PRO:CD	2.26	0.64
1:A:351:THR:OG1	1:A:364:THR:OG1	2.08	0.64
1:A:415:ASN:OD1	1:A:471:GLN:HG3	1.97	0.64
1:B:389:LYS:NZ	3:B:2159:HOH:O	2.30	0.64
1:B:426:ILE:H	1:B:470:ASN:HD22	1.45	0.64
1:B:271:LYS:HG3	1:B:321:ASP:CA	2.27	0.64
1:B:249:VAL:O	1:B:251:PRO:HD3	1.98	0.63
1:A:304:LEU:HD13	1:A:536:GLY:HA3	1.81	0.63
1:B:294:VAL:HB	1:B:295:PRO:HD2	1.81	0.62
1:A:525:ASN:ND2	3:A:2239:HOH:O	2.16	0.61
1:A:303:VAL:CA	3:A:2061:HOH:O	2.47	0.60
1:B:341:PRO:HD2	3:B:2099:HOH:O	2.00	0.60
1:A:303:VAL:HA	3:A:2061:HOH:O	2.01	0.60
1:A:396:GLN:HE21	1:A:525:ASN:ND2	2.02	0.58
1:A:251:PRO:HG2	1:A:369:TYR:CE1	2.39	0.58
1:B:294:VAL:HB	1:B:295:PRO:CD	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:414:GLY:HA3	1:A:472:TYR:CE1	2.39	0.58
1:A:374:LYS:NZ	3:A:2133:HOH:O	2.38	0.56
1:B:512:TYR:HD1	1:B:517:ILE:C	2.13	0.56
1:A:320:THR:CG2	1:A:321:ASP:N	2.68	0.56
1:A:320:THR:CG2	1:A:321:ASP:H	2.18	0.55
1:B:409:ALA:N	1:B:410:PRO:CD	2.69	0.55
1:B:420:THR:O	3:B:2184:HOH:O	2.18	0.55
1:A:283:LEU:N	1:A:283:LEU:CD1	2.70	0.55
1:A:351:THR:HA	1:A:364:THR:HA	1.90	0.54
1:B:512:TYR:CD1	1:B:517:ILE:C	2.88	0.52
1:A:282:GLU:C	1:A:283:LEU:HD12	2.36	0.51
1:B:406:ASN:CG	1:B:484:THR:HG22	2.36	0.51
1:A:377:ASN:ND2	1:A:406:ASN:O	2.40	0.51
1:B:342:GLU:O	1:B:342:GLU:HG2	2.10	0.51
1:B:519:ARG:HB3	2:D:399:GLN:O	2.11	0.50
1:A:237:THR:OG1	1:A:264:SER:HB2	2.12	0.50
1:B:351:THR:HA	1:B:364:THR:HA	1.94	0.50
1:B:385:ASP:HB2	1:B:395:ARG:HB3	1.94	0.49
1:B:513:ASN:OD1	1:B:517:ILE:HG23	2.12	0.49
1:B:384:ILE:HD11	1:B:525:ASN:HB3	1.94	0.49
1:A:265:VAL:HG13	1:A:266:PRO:HD2	1.94	0.49
1:A:321:ASP:O	1:A:324:ASN:HB2	2.12	0.49
1:A:396:GLN:NE2	1:A:525:ASN:ND2	2.60	0.49
1:B:406:ASN:ND2	3:B:2171:HOH:O	2.39	0.48
1:A:502:ASP:HB2	3:A:2148:HOH:O	2.13	0.48
1:B:283:LEU:HG	1:B:352:LEU:HD22	1.96	0.48
1:B:307:GLY:C	1:B:308:VAL:HG23	2.38	0.48
1:B:409:ALA:N	1:B:410:PRO:HD3	2.28	0.48
1:B:443:ASP:N	1:B:443:ASP:OD1	2.47	0.48
1:B:307:GLY:O	1:B:308:VAL:HG23	2.14	0.47
1:B:371:LYS:CG	1:B:372:TYR:H	2.28	0.47
1:B:434:LYS:CD	3:B:2206:HOH:O	2.63	0.47
1:B:513:ASN:OD1	1:B:517:ILE:CG2	2.63	0.47
1:A:512:TYR:HA	1:A:517:ILE:O	2.14	0.47
1:A:510:TYR:HB3	1:A:518:TRP:CZ2	2.50	0.47
1:A:500:LYS:HA	3:A:2225:HOH:O	2.13	0.46
1:A:283:LEU:CD1	1:A:352:LEU:HD22	2.41	0.46
1:B:263:PHE:CZ	1:B:331:ALA:HB3	2.50	0.46
1:A:288:VAL:CG1	2:C:407:GLN:HB3	2.45	0.46
1:B:279:VAL:H	1:B:314:ASN:ND2	2.04	0.46
1:B:414:GLY:O	1:B:471:GLN:HA	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:263:PHE:CE2	1:B:331:ALA:HB3	2.52	0.45
1:B:340:ASP:HA	1:B:341:PRO:HD3	1.82	0.45
1:A:396:GLN:NE2	1:A:525:ASN:HD22	2.15	0.45
1:A:435:VAL:HG22	1:A:458:VAL:HG23	1.97	0.45
1:A:371:LYS:HA	3:A:2130:HOH:O	2.17	0.45
1:B:290:SER:O	1:B:291:THR:CG2	2.64	0.45
1:A:439:ASP:N	3:A:2184:HOH:O	2.50	0.44
1:B:388:ASP:OD1	1:B:388:ASP:C	2.60	0.44
1:B:371:LYS:CG	1:B:372:TYR:N	2.81	0.44
1:B:425:LEU:O	3:B:2186:HOH:O	2.21	0.44
1:A:232:ILE:O	1:A:233:THR:C	2.60	0.44
1:B:275:PHE:CE1	1:B:317:TYR:HB2	2.53	0.44
1:A:394:TYR:CG	1:A:503:LEU:HD21	2.53	0.44
1:B:237:THR:OG1	1:B:264:SER:HB2	2.18	0.43
1:A:288:VAL:HG11	2:C:407:GLN:HB2	2.00	0.43
1:A:388:ASP:OD1	1:A:388:ASP:C	2.61	0.43
1:B:245:SER:HB3	1:B:257:VAL:HG13	2.00	0.43
1:B:253:GLN:O	1:B:254:ALA:HB3	2.19	0.43
1:B:307:GLY:O	1:B:308:VAL:CG2	2.67	0.43
1:B:375:PHE:CE2	1:B:519:ARG:HD3	2.54	0.43
1:B:342:GLU:O	1:B:342:GLU:CG	2.66	0.43
1:A:388:ASP:OD2	1:A:391:ASN:ND2	2.52	0.43
1:A:283:LEU:N	1:A:283:LEU:HD12	2.33	0.42
1:A:298:MET:SD	1:A:303:VAL:HG22	2.59	0.42
1:B:271:LYS:HG3	1:B:320:THR:C	2.43	0.42
1:B:294:VAL:CB	1:B:295:PRO:CD	2.96	0.42
1:B:378:LEU:CD2	1:B:407:VAL:HG13	2.49	0.42
1:B:288:VAL:HG12	2:D:409:GLY:HA3	2.01	0.42
1:A:296:PRO:HG2	1:A:298:MET:HE2	2.00	0.42
1:A:340:ASP:HA	1:A:341:PRO:HD2	1.54	0.42
1:B:391:ASN:O	1:B:392:ASN:HB2	2.20	0.42
1:B:426:ILE:H	1:B:470:ASN:ND2	2.13	0.42
1:B:335:MET:HA	1:B:336:PRO:HD3	1.83	0.42
1:A:531:ASN:H	1:B:247:THR:HG21	1.75	0.42
1:A:296:PRO:HD3	3:A:2056:HOH:O	2.20	0.41
1:B:512:TYR:HA	1:B:517:ILE:O	2.19	0.41
1:A:373:GLY:O	1:A:379:SER:HA	2.20	0.41
1:B:342:GLU:O	1:B:345:LYS:HE2	2.21	0.41
1:B:517:ILE:HG13	1:B:518:TRP:N	2.35	0.41
1:A:294:VAL:CG2	1:A:307:GLY:HA3	2.50	0.41
1:B:432:SER:CB	3:B:2195:HOH:O	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:237:THR:O	1:A:238:ASN:HB2	2.21	0.41
1:A:241:VAL:HG12	1:A:242:GLY:N	2.35	0.41
1:B:519:ARG:CG	3:B:2247:HOH:O	2.62	0.41
1:A:440:ASN:O	1:A:441:ALA:C	2.64	0.40
1:B:271:LYS:HG3	1:B:321:ASP:HA	2.03	0.40
1:A:333:LEU:HD12	1:A:533:SER:O	2.21	0.40
1:B:512:TYR:CE1	1:B:518:TRP:HB2	2.57	0.40
1:B:440:ASN:C	1:B:442:ALA:N	2.78	0.40
1:B:330:LYS:C	1:B:330:LYS:CD	2.94	0.40
1:B:509:LEU:O	1:B:520:SER:HA	2.21	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	300/329 (91%)	289 (96%)	11 (4%)	0	100	100
1	B	305/329 (93%)	291 (95%)	14 (5%)	0	100	100
2	C	10/13 (77%)	10 (100%)	0	0	100	100
2	D	11/13 (85%)	11 (100%)	0	0	100	100
All	All	626/684 (92%)	601 (96%)	25 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	242/288 (84%)	234 (97%)	8 (3%)	33	24
1	B	242/288 (84%)	237 (98%)	5 (2%)	47	41
2	C	4/7 (57%)	4 (100%)	0	100	100
2	D	3/7 (43%)	3 (100%)	0	100	100
All	All	491/590 (83%)	478 (97%)	13 (3%)	40	33

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	257	VAL
1	A	283	LEU
1	A	308	VAL
1	A	358	SER
1	A	393	THR
1	A	432	SER
1	A	435	VAL
1	A	503	LEU
1	B	304	LEU
1	B	485	THR
1	B	495	ILE
1	B	517	ILE
1	B	535	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	238	ASN
1	A	314	ASN
1	A	362	ASN
1	A	396	GLN
1	A	419	ASN
1	A	463	ASN
1	A	468	ASN
1	A	492	ASN
1	A	525	ASN
1	B	260	ASN
1	B	314	ASN
1	B	406	ASN

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Mol	Chain	Res	Type
1	B	468	ASN
1	B	470	ASN
1	B	515	ASN
2	D	407	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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, 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	308/329 (93%)	0.39	7 (2%) 61 68	17, 30, 41, 53	0
1	B	311/329 (94%)	0.33	5 (1%) 70 77	17, 30, 43, 48	0
2	C	12/13 (92%)	0.40	1 (8%) 17 20	18, 25, 44, 49	0
2	D	13/13 (100%)	0.40	0 100 100	18, 23, 44, 49	0
All	All	644/684 (94%)	0.36	13 (2%) 65 72	17, 30, 43, 53	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	539	ILE	2.9
1	A	230	THR	2.7
1	B	303	VAL	2.6
1	A	452	PRO	2.6
2	C	401	HIS	2.5
1	A	484	THR	2.4
1	B	479	PRO	2.4
1	B	452	PRO	2.4
1	B	419	ASN	2.2
1	A	544	VAL	2.1
1	A	545	PRO	2.1
1	B	385	ASP	2.1
1	A	270	VAL	2.1

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.