



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 12:00 PM UTC

PDB ID : 5X5W / pdb_00005x5w
Title : Crystal structure of pseudorabies virus glycoprotein D
Authors : Li, A.; Lu, G.; Qi, J.; Wu, L.; Tian, K.; Luo, T.; Shi, Y.; Yan, J.; Gao, G.F.
Deposited on : 2017-02-17
Resolution : 2.70 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

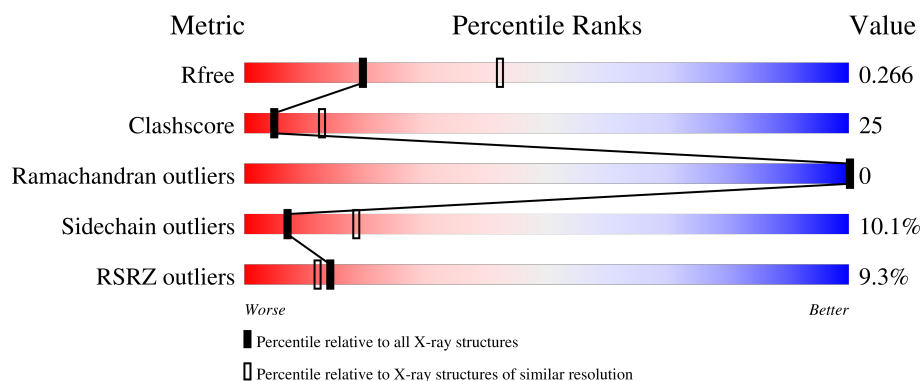
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	402	2% 42% 14% . 42%
1	C	402	4% 39% 16% .. 42%
2	B	107	20% 56% 31% 12% .
2	D	107	15% 55% 36% 7% .

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5542 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 GD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	233	Total	C	N	O	S	0	0	0
			1896	1219	330	336	11			
1	C	233	Total	C	N	O	S	0	0	0
			1902	1222	333	336	11			

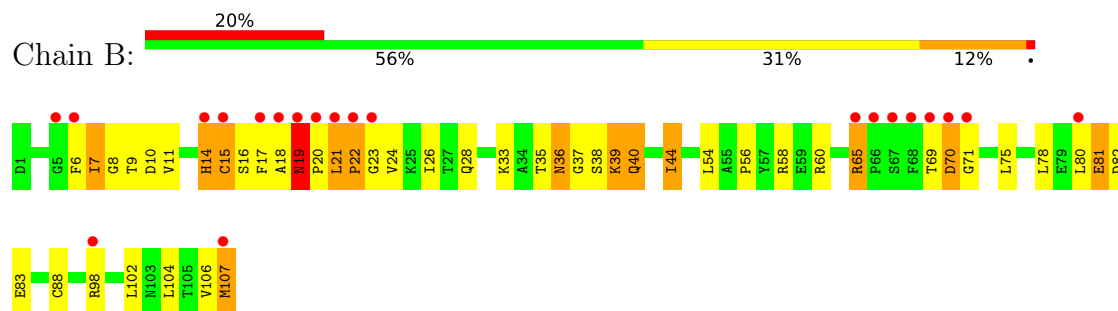
- Molecule 2 is a protein called Nectin-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	107	Total	C	N	O	S	0	0	0
			830	529	141	155	5			
2	D	107	Total	C	N	O	S	0	0	0
			829	528	138	158	5			

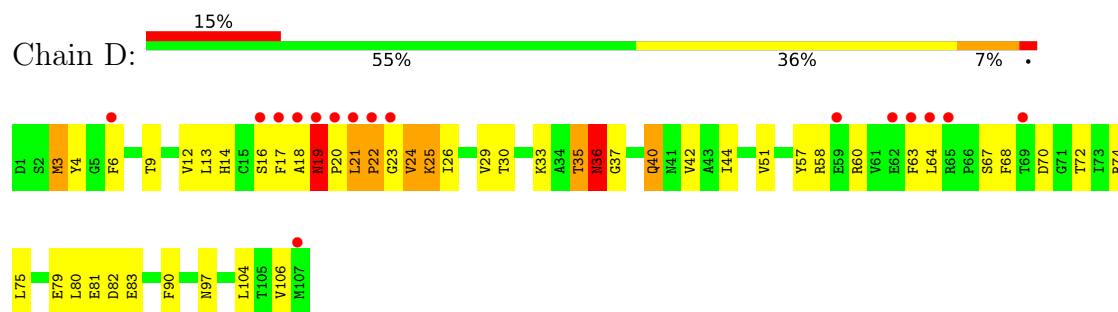
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	33	Total	O	0	0
			33	33		
3	B	9	Total	O	0	0
			9	9		
3	C	31	Total	O	0	0
			31	31		
3	D	12	Total	O	0	0
			12	12		

● Molecule 2: Nectin-1



● Molecule 2: Nectin-1



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	79.94Å 98.11Å 128.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.17 – 2.70 38.17 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.2 (38.17-2.70) 99.8 (38.17-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.77 (at 2.69Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.238 , 0.266 0.240 , 0.266	Depositor DCC
R_{free} test set	1431 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	37.1	Xtriage
Anisotropy	1.187	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 37.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.53$, $\langle L^2 \rangle = 0.37$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	5542	wwPDB-VP
Average B, all atoms (Å ²)	46.0	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 46.40 % 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 1.1519e-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](#)

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	0.89	2/1964 (0.1%)	0.96	6/2690 (0.2%)
1	C	1.10	12/1970 (0.6%)	1.11	23/2697 (0.9%)
2	B	1.24	3/848 (0.4%)	1.11	9/1152 (0.8%)
2	D	0.92	1/847 (0.1%)	1.12	11/1152 (1.0%)
All	All	1.03	18/5629 (0.3%)	1.06	49/7691 (0.6%)

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	74	ASP	C-N	8.54	1.40	1.33
1	C	28	PHE	C-N	7.69	1.40	1.33
1	C	241	ASN	N-CA	-5.92	1.38	1.46
1	C	46	VAL	C-N	5.85	1.40	1.33
1	C	133	MET	C-O	-5.83	1.17	1.24
1	A	165	ARG	C-O	-5.79	1.17	1.24
1	C	52	GLY	C-N	5.77	1.40	1.33
1	C	29	PRO	C-N	5.74	1.40	1.33
1	C	187	GLN	CA-C	-5.46	1.46	1.52
1	A	30	PRO	C-N	5.27	1.40	1.33
1	C	30	PRO	N-CD	5.17	1.54	1.47
2	B	39	LYS	CA-C	-5.15	1.46	1.52
2	D	20	PRO	N-CD	5.11	1.54	1.47
1	C	205	CYS	C-O	-5.11	1.18	1.24
2	B	20	PRO	N-CD	5.09	1.54	1.47
1	C	142	MET	C-O	-5.08	1.17	1.24
1	C	48	SER	C-N	5.06	1.40	1.34
2	B	14	HIS	CA-C	-5.04	1.46	1.52

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	185	GLU	N-CA-C	-9.60	98.15	110.53
2	B	70	ASP	CB-CA-C	9.11	128.55	110.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	241	ASN	N-CA-C	-8.89	102.97	112.93
2	D	24	VAL	N-CA-C	8.13	120.49	108.45
1	C	28	PHE	CA-C-N	-8.12	113.73	119.66
1	C	28	PHE	C-N-CA	-8.12	113.73	119.66
1	C	238	TYR	CB-CA-C	-8.06	95.20	110.67
1	C	29	PRO	O-C-N	7.74	124.87	121.31
2	B	21	LEU	CB-CA-C	-7.67	95.96	109.61
2	D	21	LEU	CB-CA-C	-7.66	95.98	109.61
1	C	85	VAL	N-CA-C	-7.20	103.65	110.42
2	D	24	VAL	CB-CA-C	-7.04	98.54	110.71
1	C	238	TYR	N-CA-C	6.77	119.67	111.82
1	C	46	VAL	CA-C-N	-6.73	113.37	120.03
1	C	46	VAL	C-N-CA	-6.73	113.37	120.03
1	C	29	PRO	CA-C-N	-6.72	113.46	120.38
1	C	29	PRO	C-N-CA	-6.72	113.46	120.38
2	D	23	GLY	CA-C-N	6.67	132.31	122.71
2	D	23	GLY	C-N-CA	6.67	132.31	122.71
1	C	52	GLY	CA-C-N	-6.62	113.45	120.66
1	C	52	GLY	C-N-CA	-6.62	113.45	120.66
1	C	185	GLU	N-CA-C	-6.60	98.48	109.24
1	C	74	ASP	CA-C-N	-6.56	113.46	120.94
1	C	74	ASP	C-N-CA	-6.56	113.46	120.94
1	C	48	SER	CA-C-N	-6.24	113.26	119.56
1	C	48	SER	C-N-CA	-6.24	113.26	119.56
1	A	30	PRO	CA-C-N	-6.14	113.34	119.92
1	A	30	PRO	C-N-CA	-6.14	113.34	119.92
2	B	16	SER	N-CA-C	6.06	120.53	111.81
1	C	187	GLN	N-CA-C	-6.05	99.04	108.90
2	B	21	LEU	N-CA-C	6.01	118.73	110.01
2	B	69	THR	N-CA-C	-6.01	105.80	113.01
2	D	21	LEU	N-CA-C	5.99	118.70	110.01
1	A	228	PRO	CA-C-N	-5.88	113.62	119.56
1	A	228	PRO	C-N-CA	-5.88	113.62	119.56
2	D	36	ASN	N-CA-C	5.86	118.27	107.73
2	D	19	ASN	CA-C-N	-5.62	112.81	119.84
2	D	19	ASN	C-N-CA	-5.62	112.81	119.84
2	B	19	ASN	CA-C-N	-5.62	112.82	119.84
2	B	19	ASN	C-N-CA	-5.62	112.82	119.84
1	A	201	LYS	CB-CA-C	-5.54	110.21	116.63
2	B	40	GLN	N-CA-C	-5.39	101.10	109.24
1	C	228	PRO	CA-C-N	-5.35	114.16	119.56
1	C	228	PRO	C-N-CA	-5.35	114.16	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	53	PRO	CA-N-CD	-5.29	104.60	112.00
2	B	22	PRO	CA-N-CD	-5.22	104.69	112.00
2	D	22	PRO	CA-N-CD	-5.21	104.70	112.00
2	D	22	PRO	O-C-N	-5.21	117.88	122.93
1	C	201	LYS	CB-CA-C	-5.11	110.66	116.54

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	1896	0	1799	71	0
1	C	1902	0	1810	91	0
2	B	830	0	816	60	0
2	D	829	0	812	50	0
3	A	33	0	0	28	0
3	B	9	0	0	11	0
3	C	31	0	0	40	0
3	D	12	0	0	12	0
All	All	5542	0	5237	269	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 25.

All (269) 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:B:6:PHE:CE1	2:B:107:MET:HE3	1.83	1.12
1:C:163:GLN:CA	3:C:503:HOH:O	1.99	1.11
2:B:9:THR:HG22	2:B:10:ASP:N	1.53	1.10
2:D:74:ARG:NH1	3:D:201:HOH:O	1.81	1.09
2:B:9:THR:HG22	2:B:10:ASP:H	1.08	1.08
2:B:7:ILE:HD12	2:B:7:ILE:H	1.19	1.07
1:A:184:PRO:CA	3:A:502:HOH:O	2.04	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:164:TYR:N	3:C:503:HOH:O	1.87	1.06
1:C:121:GLN:HE22	1:C:125:ARG:NE	1.52	1.06
1:C:179:PHE:HZ	3:C:514:HOH:O	1.38	1.06
1:A:184:PRO:CB	3:A:502:HOH:O	2.03	1.05
1:C:33:TYR:CD1	3:C:505:HOH:O	2.10	1.04
1:C:163:GLN:HA	3:C:503:HOH:O	1.57	1.04
2:D:64:LEU:HD12	2:D:72:THR:CG2	1.88	1.04
1:C:60:ARG:NE	3:C:504:HOH:O	1.91	1.03
1:C:121:GLN:NE2	1:C:125:ARG:HG2	1.74	1.03
1:A:184:PRO:C	3:A:502:HOH:O	2.02	1.02
1:A:185:GLU:N	3:A:502:HOH:O	1.91	1.02
1:C:33:TYR:N	3:C:505:HOH:O	1.93	1.01
1:C:33:TYR:CB	3:C:505:HOH:O	2.08	1.01
1:A:158:ARG:HH12	1:A:186:GLY:C	1.69	1.01
1:A:209:ASP:CB	3:A:505:HOH:O	2.07	1.01
2:B:14:HIS:CG	3:B:202:HOH:O	2.14	1.00
2:B:9:THR:CG2	2:B:10:ASP:H	1.74	1.00
2:B:28:GLN:CG	3:B:201:HOH:O	2.07	0.99
2:B:28:GLN:HG2	3:B:201:HOH:O	1.63	0.99
1:A:87:HIS:HB2	1:A:89:ARG:NH1	1.77	0.99
1:C:185:GLU:HA	3:C:513:HOH:O	1.63	0.98
1:C:146:GLU:OE2	3:C:501:HOH:O	1.82	0.98
2:D:70:ASP:HA	3:D:203:HOH:O	1.62	0.98
1:A:209:ASP:CA	3:A:505:HOH:O	2.11	0.98
2:B:6:PHE:CE1	2:B:107:MET:CE	2.47	0.97
1:A:209:ASP:N	3:A:505:HOH:O	1.97	0.96
2:D:21:LEU:HB3	2:D:22:PRO:HD2	1.47	0.96
2:B:21:LEU:HB3	2:B:22:PRO:HD2	1.47	0.95
1:C:121:GLN:HE22	1:C:125:ARG:CD	1.81	0.93
1:C:121:GLN:NE2	1:C:125:ARG:CD	2.32	0.92
1:A:158:ARG:NH1	1:A:186:GLY:C	2.27	0.92
2:B:14:HIS:CB	3:B:202:HOH:O	2.17	0.91
2:D:64:LEU:HD12	2:D:72:THR:HG22	1.53	0.90
1:C:236:TYR:CZ	1:C:240:LYS:NZ	2.41	0.89
2:B:21:LEU:HB3	2:B:22:PRO:CD	2.03	0.89
2:B:28:GLN:NE2	3:B:201:HOH:O	2.03	0.88
2:D:21:LEU:HB3	2:D:22:PRO:CD	2.03	0.88
2:B:21:LEU:O	2:B:24:VAL:HG22	1.72	0.87
1:C:121:GLN:NE2	1:C:125:ARG:CG	2.37	0.87
1:A:209:ASP:HB2	3:A:505:HOH:O	1.72	0.86
1:C:133:MET:CE	1:C:218:MET:HG2	2.06	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:133:MET:HE2	1:C:218:MET:HG2	1.55	0.85
1:C:163:GLN:C	3:C:503:HOH:O	2.08	0.85
2:D:16:SER:O	3:D:202:HOH:O	1.93	0.85
1:A:155:ALA:O	3:A:503:HOH:O	1.94	0.85
1:C:60:ARG:CD	3:C:504:HOH:O	2.21	0.84
1:C:74:ASP:OD1	1:C:76:GLN:N	2.10	0.84
1:C:32:ALA:HB3	3:C:505:HOH:O	1.78	0.83
1:C:162:GLY:O	3:C:503:HOH:O	1.96	0.82
1:A:185:GLU:O	3:A:502:HOH:O	1.96	0.82
1:A:87:HIS:HB2	1:A:89:ARG:HH11	1.44	0.82
2:B:14:HIS:ND1	3:B:202:HOH:O	2.11	0.81
1:C:100:ARG:NH2	1:C:142:MET:HE1	1.94	0.81
1:A:95:HIS:ND1	3:A:510:HOH:O	2.13	0.81
1:C:186:GLY:HA2	3:C:513:HOH:O	1.81	0.80
2:B:33:LYS:HG2	2:B:35:THR:HG23	1.62	0.80
1:C:236:TYR:OH	1:C:240:LYS:NZ	2.17	0.78
1:A:252:ALA:O	3:A:506:HOH:O	2.02	0.78
1:A:141:TYR:OH	3:A:501:HOH:O	2.02	0.77
1:C:60:ARG:HD2	3:C:504:HOH:O	1.80	0.77
1:C:127:ARG:NH2	3:C:502:HOH:O	1.85	0.77
2:D:70:ASP:OD1	3:D:203:HOH:O	2.01	0.77
2:D:35:THR:O	2:D:37:GLY:HA2	1.83	0.77
1:A:158:ARG:NH2	1:A:158:ARG:HG3	1.99	0.77
1:A:181:VAL:O	3:A:507:HOH:O	2.02	0.77
1:C:33:TYR:HB3	3:C:505:HOH:O	1.78	0.77
2:B:102:LEU:C	2:B:102:LEU:HD12	2.11	0.76
1:A:158:ARG:HG3	1:A:158:ARG:HH21	1.50	0.75
1:C:166:ARG:NH2	3:C:514:HOH:O	2.18	0.75
1:C:166:ARG:CZ	3:C:514:HOH:O	2.35	0.75
1:C:121:GLN:NE2	1:C:125:ARG:NE	2.33	0.75
1:A:148:GLU:O	3:A:509:HOH:O	2.05	0.74
1:A:210:SER:N	3:A:505:HOH:O	2.07	0.74
2:D:16:SER:HB3	3:D:203:HOH:O	1.88	0.73
2:D:4:TYR:O	3:D:204:HOH:O	2.07	0.72
2:B:14:HIS:HB2	3:B:202:HOH:O	1.83	0.72
1:C:59:THR:O	3:C:508:HOH:O	2.08	0.71
1:C:186:GLY:N	3:C:507:HOH:O	2.20	0.70
2:D:64:LEU:CD1	2:D:72:THR:HG22	2.19	0.70
1:C:121:GLN:HE21	1:C:125:ARG:HG2	1.53	0.70
1:C:127:ARG:NH1	3:C:502:HOH:O	2.24	0.70
1:C:158:ARG:NE	3:C:513:HOH:O	2.23	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:46:VAL:HG23	1:C:215:VAL:O	1.91	0.70
2:D:83:GLU:HG3	2:D:106:VAL:H	1.57	0.69
1:C:179:PHE:CZ	3:C:514:HOH:O	2.21	0.69
2:D:64:LEU:HD12	2:D:72:THR:HG21	1.73	0.69
1:A:225:TYR:HB3	1:A:229:PRO:HG2	1.74	0.68
2:B:102:LEU:HD12	2:B:102:LEU:O	1.91	0.68
1:A:149:LEU:O	1:A:166:ARG:NH1	2.21	0.68
1:C:182:ALA:O	3:C:510:HOH:O	2.12	0.68
1:C:202:PHE:O	3:C:509:HOH:O	2.11	0.68
1:A:210:SER:CB	3:A:517:HOH:O	2.42	0.67
2:D:35:THR:HB	3:D:207:HOH:O	1.95	0.66
2:B:65:ARG:O	2:B:65:ARG:HG2	1.92	0.66
2:D:40:GLN:NE2	3:D:206:HOH:O	2.28	0.66
1:C:149:LEU:O	1:C:166:ARG:NH1	2.29	0.66
1:C:211:PHE:O	3:C:511:HOH:O	2.14	0.65
2:D:18:ALA:N	3:D:202:HOH:O	2.31	0.64
1:A:87:HIS:CB	1:A:89:ARG:NH1	2.58	0.63
1:A:79:ARG:NE	3:A:515:HOH:O	2.32	0.63
1:A:163:GLN:OE1	1:A:178:ASP:OD2	2.17	0.63
2:D:21:LEU:O	2:D:24:VAL:HB	1.98	0.62
2:D:29:VAL:CG2	2:D:68:PHE:HD2	2.13	0.62
2:B:7:ILE:H	2:B:7:ILE:CD1	1.98	0.62
1:C:51:VAL:HG12	1:C:176:LEU:HD11	1.83	0.61
2:D:64:LEU:CG	2:D:72:THR:HG22	2.30	0.61
2:B:60:ARG:NH2	2:B:82:ASP:OD2	2.31	0.61
1:A:131:THR:O	1:A:133:MET:HE2	2.00	0.61
1:C:33:TYR:HD1	3:C:505:HOH:O	1.62	0.61
1:C:236:TYR:CE2	1:C:240:LYS:NZ	2.68	0.61
2:D:36:ASN:N	3:D:207:HOH:O	2.34	0.61
2:B:7:ILE:HD12	2:B:7:ILE:N	2.04	0.60
1:C:51:VAL:HG22	1:C:51:VAL:O	2.01	0.60
1:C:137:PRO:O	3:C:512:HOH:O	2.16	0.60
1:C:225:TYR:HB3	1:C:229:PRO:HG2	1.85	0.59
2:B:28:GLN:CB	3:B:201:HOH:O	2.43	0.59
2:D:12:VAL:HG13	2:D:72:THR:HG23	1.84	0.58
2:D:17:PHE:CD1	2:D:18:ALA:N	2.71	0.58
2:B:17:PHE:CD1	2:B:18:ALA:N	2.71	0.58
1:C:236:TYR:CE2	1:C:240:LYS:HE2	2.38	0.58
1:A:87:HIS:HB2	1:A:89:ARG:HH12	1.64	0.58
1:C:184:PRO:O	3:C:513:HOH:O	2.16	0.58
1:A:138:SER:OG	3:A:501:HOH:O	1.90	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:28:GLN:HB3	3:B:201:HOH:O	2.02	0.57
1:C:162:GLY:C	3:C:503:HOH:O	2.45	0.57
2:D:16:SER:OG	3:D:205:HOH:O	2.18	0.57
2:D:21:LEU:CB	2:D:22:PRO:CD	2.70	0.57
2:D:33:LYS:NZ	2:D:81:GLU:O	2.38	0.57
1:A:193:ARG:NH2	3:A:504:HOH:O	1.95	0.57
2:B:6:PHE:HE1	2:B:107:MET:HE3	1.58	0.57
1:C:121:GLN:NE2	1:C:125:ARG:HD3	2.16	0.57
1:C:206:TRP:HA	3:C:520:HOH:O	2.04	0.57
1:C:33:TYR:CG	3:C:505:HOH:O	2.28	0.57
1:C:49:PRO:HD3	1:C:99:TYR:CE1	2.40	0.56
2:B:6:PHE:CE1	2:B:107:MET:HE1	2.40	0.56
1:A:193:ARG:HD3	1:A:237:TRP:CZ2	2.40	0.56
1:C:133:MET:HE3	1:C:223:PRO:HG3	1.88	0.56
2:B:6:PHE:O	2:B:9:THR:HB	2.07	0.55
2:B:6:PHE:CD1	2:B:107:MET:HE3	2.37	0.55
1:A:138:SER:HA	3:A:501:HOH:O	2.06	0.55
1:A:235:ASN:O	1:A:239:ARG:HG2	2.05	0.55
2:D:29:VAL:CG2	2:D:68:PHE:CD2	2.90	0.55
1:A:218:MET:HE2	2:B:44:ILE:CD1	2.38	0.54
1:A:70:ALA:HB1	1:A:72:ILE:HD12	1.89	0.54
2:D:17:PHE:CD1	2:D:17:PHE:C	2.85	0.54
2:B:33:LYS:NZ	2:B:81:GLU:O	2.41	0.54
1:C:33:TYR:HE2	1:C:126:CYS:O	1.91	0.54
2:B:6:PHE:CZ	2:B:107:MET:HE1	2.43	0.54
2:B:17:PHE:CD1	2:B:17:PHE:C	2.85	0.54
2:D:17:PHE:HD1	2:D:18:ALA:N	2.06	0.54
1:A:207:SER:OG	3:A:505:HOH:O	2.17	0.54
2:B:17:PHE:HD1	2:B:18:ALA:N	2.06	0.54
1:C:98:TRP:HB2	1:C:110:TYR:HB3	1.90	0.54
2:D:60:ARG:NH2	2:D:82:ASP:OD2	2.38	0.53
1:A:208:ASP:HB3	1:C:243:ARG:HD2	1.90	0.53
1:A:210:SER:HA	3:A:517:HOH:O	2.09	0.53
2:B:17:PHE:HB3	3:B:205:HOH:O	2.08	0.53
1:C:133:MET:HE2	1:C:218:MET:CG	2.35	0.53
2:B:7:ILE:C	2:B:9:THR:H	2.16	0.53
1:C:164:TYR:HD1	3:C:503:HOH:O	1.91	0.52
2:B:7:ILE:HD11	2:B:107:MET:C	2.35	0.52
2:B:18:ALA:HB1	2:B:19:ASN:HD22	1.76	0.51
2:D:18:ALA:HB1	2:D:19:ASN:HD22	1.76	0.51
2:B:83:GLU:HG3	2:B:106:VAL:HG23	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:15:CYS:HB2	2:B:71:GLY:HA3	1.92	0.50
2:B:9:THR:CG2	2:B:10:ASP:N	2.27	0.50
2:B:24:VAL:HG23	2:B:24:VAL:O	2.10	0.50
1:C:138:SER:OG	3:C:506:HOH:O	1.93	0.50
1:A:158:ARG:HH11	1:A:185:GLU:C	2.21	0.49
1:C:147:ASP:O	1:C:149:LEU:HD22	2.12	0.49
1:C:147:ASP:CG	3:C:515:HOH:O	2.55	0.49
1:A:184:PRO:HB3	3:A:502:HOH:O	1.92	0.49
1:A:65:PRO:HG3	1:A:187:GLN:HB2	1.95	0.49
1:C:51:VAL:HG21	1:C:174:ASN:HD22	1.78	0.49
1:C:100:ARG:HB2	1:C:107:HIS:HB2	1.93	0.49
1:A:98:TRP:CZ2	1:A:166:ARG:HD3	2.48	0.49
1:C:195:ASP:OD1	1:C:195:ASP:N	2.43	0.49
1:C:236:TYR:CE2	1:C:240:LYS:CE	2.96	0.49
1:A:33:TYR:HE2	1:A:126:CYS:O	1.96	0.49
1:A:92:TYR:CE2	1:A:117:CYS:HB2	2.48	0.48
1:A:138:SER:CA	3:A:501:HOH:O	2.61	0.48
1:A:138:SER:CB	3:A:501:HOH:O	2.53	0.48
1:C:29:PRO:HD2	1:C:229:PRO:HB3	1.93	0.48
2:D:67:SER:OG	2:D:68:PHE:N	2.44	0.48
2:B:33:LYS:HG2	2:B:35:THR:CG2	2.37	0.48
2:D:29:VAL:HG23	2:D:68:PHE:CE2	2.49	0.48
2:B:22:PRO:HA	2:B:23:GLY:HA2	1.60	0.48
2:D:6:PHE:O	2:D:9:THR:OG1	2.29	0.48
2:D:35:THR:C	2:D:37:GLY:HA2	2.39	0.48
2:B:18:ALA:C	2:B:19:ASN:ND2	2.73	0.47
2:D:17:PHE:C	2:D:17:PHE:HD1	2.22	0.47
1:A:117:CYS:HA	1:A:126:CYS:HA	1.95	0.47
2:B:17:PHE:C	2:B:17:PHE:HD1	2.22	0.47
1:A:219:ARG:HG2	1:A:220:PHE:CE2	2.49	0.47
1:C:51:VAL:HG21	1:C:174:ASN:ND2	2.30	0.47
2:D:30:THR:HG23	2:D:44:ILE:HG12	1.95	0.47
2:D:18:ALA:C	2:D:19:ASN:ND2	2.73	0.47
1:A:158:ARG:NH1	1:A:186:GLY:N	2.62	0.47
2:B:56:PRO:O	3:B:204:HOH:O	2.20	0.47
1:C:49:PRO:HB2	1:C:165:ARG:HD2	1.96	0.47
2:D:3:MET:HE3	2:D:3:MET:HB3	1.85	0.47
1:C:239:ARG:O	1:C:239:ARG:HG3	2.14	0.47
1:A:89:ARG:HH11	1:A:89:ARG:CG	2.28	0.46
2:B:6:PHE:CD1	2:B:107:MET:CE	2.96	0.46
2:B:83:GLU:HG3	2:B:106:VAL:H	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:133:MET:HE3	1:C:218:MET:HG2	1.95	0.46
2:B:33:LYS:HE2	2:B:35:THR:HG22	1.98	0.46
2:B:65:ARG:HE	2:B:70:ASP:CB	2.29	0.46
2:D:29:VAL:HG23	2:D:68:PHE:CD2	2.50	0.46
1:C:51:VAL:CG1	1:C:176:LEU:HD11	2.45	0.46
1:C:121:GLN:CD	1:C:125:ARG:HD3	2.41	0.45
2:B:102:LEU:C	2:B:102:LEU:CD1	2.85	0.45
1:C:98:TRP:CZ2	1:C:166:ARG:HD3	2.52	0.44
1:C:133:MET:CE	1:C:223:PRO:HG3	2.48	0.44
1:A:132:PRO:HD3	1:A:226:GLN:NE2	2.32	0.44
2:B:35:THR:O	2:B:36:ASN:HB2	2.17	0.44
1:A:193:ARG:HD3	1:A:237:TRP:CE2	2.52	0.44
1:A:89:ARG:NH1	1:A:89:ARG:HG3	2.31	0.44
1:A:239:ARG:C	1:A:241:ASN:N	2.75	0.44
2:B:107:MET:HE3	2:B:107:MET:HB2	1.68	0.44
1:C:73:SER:HB3	3:C:514:HOH:O	2.17	0.44
1:C:100:ARG:HH21	1:C:142:MET:HE1	1.81	0.44
2:D:3:MET:HE1	2:D:13:LEU:HD23	1.99	0.44
1:C:147:ASP:OD1	3:C:515:HOH:O	2.21	0.44
1:A:69:VAL:HB	1:A:153:MET:HB3	2.00	0.44
2:B:7:ILE:HG22	2:B:8:GLY:N	2.33	0.43
1:A:66:CYS:SG	1:A:190:PRO:HD2	2.58	0.43
2:B:26:ILE:HD12	2:B:26:ILE:N	2.33	0.43
1:C:77:VAL:O	1:C:77:VAL:HG22	2.17	0.43
1:C:187:GLN:N	3:C:507:HOH:O	1.99	0.43
1:A:92:TYR:CZ	1:A:117:CYS:HB2	2.54	0.43
1:A:87:HIS:CB	1:A:89:ARG:HH11	2.23	0.43
1:C:47:PRO:O	1:C:99:TYR:OH	2.34	0.43
1:A:195:ASP:OD1	1:A:195:ASP:N	2.37	0.42
1:C:165:ARG:HD3	1:C:176:LEU:HD22	2.00	0.42
2:D:90:PHE:O	2:D:97:ASN:HA	2.19	0.42
2:B:35:THR:C	2:B:37:GLY:H	2.27	0.42
1:A:79:ARG:HD3	3:A:515:HOH:O	2.19	0.42
2:D:12:VAL:CG1	2:D:72:THR:HG23	2.48	0.42
2:D:24:VAL:CG1	2:D:25:LYS:N	2.77	0.42
1:C:236:TYR:O	1:C:240:LYS:HD3	2.20	0.42
1:A:158:ARG:HH12	1:A:187:GLN:N	2.13	0.42
2:D:12:VAL:HG12	2:D:14:HIS:CD2	2.53	0.42
2:D:42:VAL:HG22	2:D:57:TYR:CE2	2.54	0.42
1:A:39:TRP:C	1:A:40:GLN:HG2	2.44	0.42
1:C:219:ARG:HG2	1:C:220:PHE:CE2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:158:ARG:HH21	1:A:158:ARG:CG	2.22	0.42
1:A:193:ARG:CD	1:A:237:TRP:CZ2	3.02	0.42
2:D:17:PHE:CE2	2:D:26:ILE:HG12	2.54	0.42
1:C:84:ALA:HB2	1:C:89:ARG:HH21	1.85	0.42
2:D:63:PHE:C	2:D:64:LEU:HD23	2.45	0.41
1:A:71:LEU:H	1:A:71:LEU:HD12	1.86	0.41
1:A:89:ARG:NH1	1:A:89:ARG:CG	2.80	0.41
1:A:239:ARG:C	1:A:241:ASN:H	2.28	0.41
2:D:35:THR:HB	2:D:36:ASN:H	1.48	0.41
2:D:17:PHE:C	3:D:202:HOH:O	2.63	0.41
1:A:104:GLY:HA2	1:C:239:ARG:O	2.21	0.41
2:B:21:LEU:CB	2:B:22:PRO:CD	2.70	0.40
1:C:132:PRO:HD3	1:C:226:GLN:NE2	2.36	0.40
2:B:7:ILE:C	2:B:9:THR:N	2.78	0.40
1:C:100:ARG:NH2	1:C:142:MET:CE	2.75	0.40
1:A:79:ARG:CD	3:A:515:HOH:O	2.69	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	231/402 (58%)	218 (94%)	13 (6%)	0	100	100
1	C	231/402 (58%)	212 (92%)	19 (8%)	0	100	100
2	B	105/107 (98%)	91 (87%)	14 (13%)	0	100	100
2	D	105/107 (98%)	94 (90%)	11 (10%)	0	100	100
All	All	672/1018 (66%)	615 (92%)	57 (8%)	0	100	100

There are no Ramachandran outliers to report.

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	200/328 (61%)	187 (94%)	13 (6%)	15	37
1	C	201/328 (61%)	187 (93%)	14 (7%)	14	34
2	B	90/92 (98%)	70 (78%)	20 (22%)	1	3
2	D	91/92 (99%)	79 (87%)	12 (13%)	4	10
All	All	582/840 (69%)	523 (90%)	59 (10%)	7	18

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	89	ARG
1	A	93	ARG
1	A	117	CYS
1	A	125	ARG
1	A	149	LEU
1	A	158	ARG
1	A	183	LEU
1	A	185	GLU
1	A	209	ASP
1	A	212	LYS
1	A	219	ARG
1	A	222	THR
1	A	233	VAL
2	B	7	ILE
2	B	11	VAL
2	B	15	CYS
2	B	19	ASN
2	B	36	ASN
2	B	38	SER
2	B	39	LYS
2	B	40	GLN
2	B	44	ILE
2	B	54	LEU
2	B	58	ARG

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Mol	Chain	Res	Type
2	B	65	ARG
2	B	75	LEU
2	B	78	LEU
2	B	80	LEU
2	B	81	GLU
2	B	88	CYS
2	B	98	ARG
2	B	104	LEU
2	B	107	MET
1	C	30	PRO
1	C	44	THR
1	C	45	THR
1	C	46	VAL
1	C	77	VAL
1	C	81	LEU
1	C	133	MET
1	C	146	GLU
1	C	149	LEU
1	C	187	GLN
1	C	188	GLU
1	C	193	ARG
1	C	219	ARG
1	C	240	LYS
2	D	3	MET
2	D	19	ASN
2	D	25	LYS
2	D	35	THR
2	D	36	ASN
2	D	40	GLN
2	D	51	VAL
2	D	58	ARG
2	D	75	LEU
2	D	79	GLU
2	D	80	LEU
2	D	104	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	58	HIS
1	A	87	HIS
1	A	95	HIS

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Mol	Chain	Res	Type
1	A	160	ASN
1	A	163	GLN
1	A	196	GLN
2	B	19	ASN
2	B	36	ASN
2	B	97	ASN
1	C	121	GLN
1	C	160	ASN
1	C	174	ASN
1	C	197	HIS
2	D	19	ASN
2	D	32	GLN
2	D	41	ASN
2	D	97	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 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	233/402 (57%)	0.32	10 (4%) 40 36	19, 38, 79, 112	0
1	C	233/402 (57%)	0.42	16 (6%) 23 20	18, 40, 86, 112	0
2	B	107/107 (100%)	0.95	21 (19%) 3 2	27, 46, 119, 133	0
2	D	107/107 (100%)	0.91	16 (14%) 5 4	26, 45, 87, 151	0
All	All	680/1018 (66%)	0.55	63 (9%) 14 12	18, 42, 88, 151	0

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	71	GLY	7.7
2	D	17	PHE	5.2
2	D	20	PRO	4.9
2	B	67	SER	4.6
2	D	23	GLY	4.5
2	B	69	THR	4.5
2	B	20	PRO	4.4
1	C	125	ARG	4.4
2	D	19	ASN	4.3
2	D	22	PRO	4.2
2	B	70	ASP	4.2
2	B	65	ARG	4.1
1	A	63	GLU	3.9
2	D	21	LEU	3.9
2	D	16	SER	3.8
1	A	195	ASP	3.8
1	C	258	ASP	3.6
1	C	195	ASP	3.6
2	D	64	LEU	3.4
2	D	65	ARG	3.3
2	B	21	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	187	GLN	3.2
1	C	32	ALA	3.2
2	D	6	PHE	3.2
1	C	212	LYS	3.2
1	C	34	PRO	2.9
2	B	66	PRO	2.9
2	B	18	ALA	2.9
1	C	63	GLU	2.9
2	B	17	PHE	2.8
2	B	107	MET	2.8
1	A	27	THR	2.8
2	B	15	CYS	2.8
1	A	258	ASP	2.8
2	B	22	PRO	2.7
2	B	5	GLY	2.7
2	D	69	THR	2.7
1	C	198	ARG	2.7
2	B	19	ASN	2.7
2	D	18	ALA	2.7
1	C	127	ARG	2.7
1	C	240	LYS	2.6
1	A	32	ALA	2.6
2	B	68	PHE	2.6
1	A	198	ARG	2.5
2	B	14	HIS	2.5
1	A	26	PRO	2.5
1	C	247	ARG	2.4
2	D	62	GLU	2.4
2	B	6	PHE	2.4
1	C	185	GLU	2.4
1	C	239	ARG	2.3
1	C	26	PRO	2.3
1	C	83	GLU	2.2
2	D	59	GLU	2.2
1	C	86	ALA	2.2
1	A	88	ARG	2.2
2	B	98	ARG	2.1
2	D	107	MET	2.1
2	D	63	PHE	2.1
1	A	83	GLU	2.1
2	B	80	LEU	2.0
2	B	23	GLY	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 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.