



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:23 PM GMT

PDB ID : 1FDP
Title : PROENZYME OF HUMAN COMPLEMENT FACTOR D, RECOMBINANT PROFACTOR D
Authors : Jing, H.; Macon, K.J.; Moore, D.; Delucas, L.J.; Volanakis, J.E.; Narayana, S.V.L.
Deposited on : 1998-12-03
Resolution : 2.10 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
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

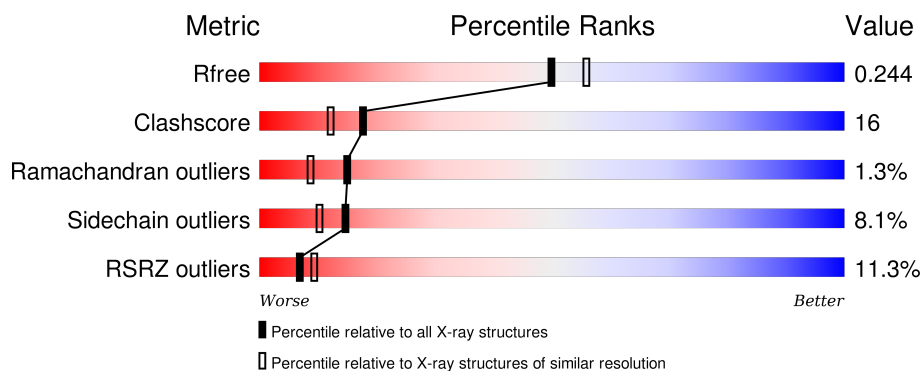
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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}	91344	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	235	<div> <div>15%</div> <div>68%</div> <div>23%</div> <div>• 6%</div> </div>
1	B	235	<div> <div>8%</div> <div>63%</div> <div>20%</div> <div>• 14%</div> </div>
1	C	235	<div> <div>9%</div> <div>57%</div> <div>23%</div> <div>• • 15%</div> </div>
1	D	235	<div> <div>7%</div> <div>58%</div> <div>23%</div> <div>• 15%</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6764 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 PROENZYME OF COMPLEMENT FACTOR D.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	221	Total	C	N	O	S	0	0	0
			1654	1025	309	310	10			
1	B	201	Total	C	N	O	S	0	0	0
			1497	936	272	281	8			
1	C	199	Total	C	N	O	S	0	0	0
			1490	933	270	279	8			
1	D	200	Total	C	N	O	S	0	0	0
			1492	934	270	280	8			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	11	PRO	ARG	CONFLICT	UNP P00746
B	11	PRO	ARG	CONFLICT	UNP P00746
C	11	PRO	ARG	CONFLICT	UNP P00746
D	11	PRO	ARG	CONFLICT	UNP P00746

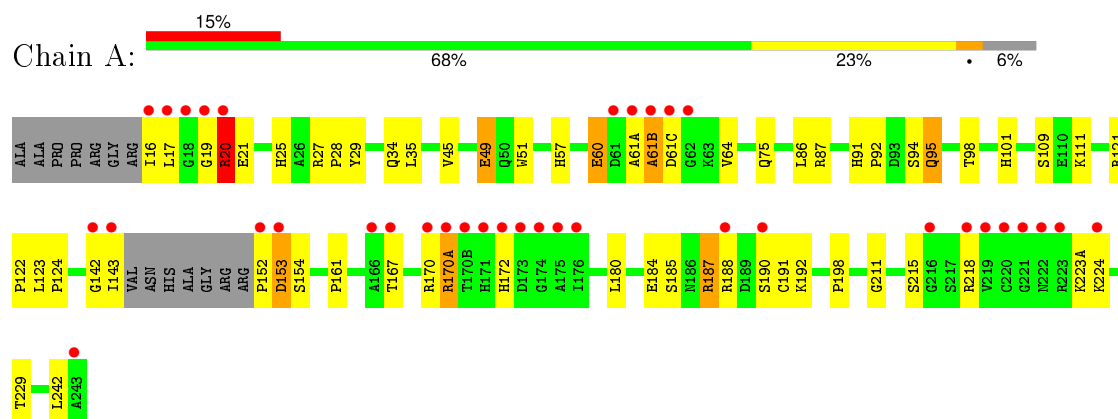
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	177	Total	O	0	0
			177	177		
2	B	156	Total	O	0	0
			156	156		
2	C	142	Total	O	0	0
			142	142		
2	D	156	Total	O	0	0
			156	156		

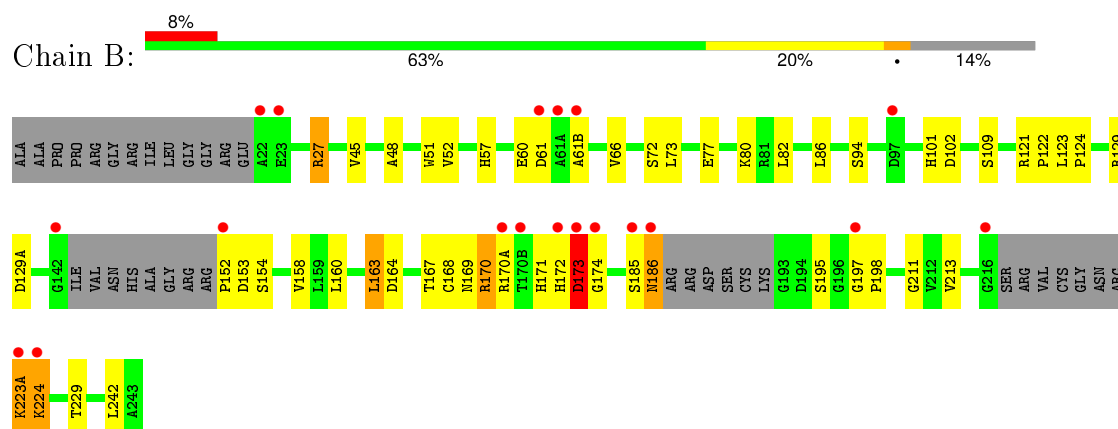
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

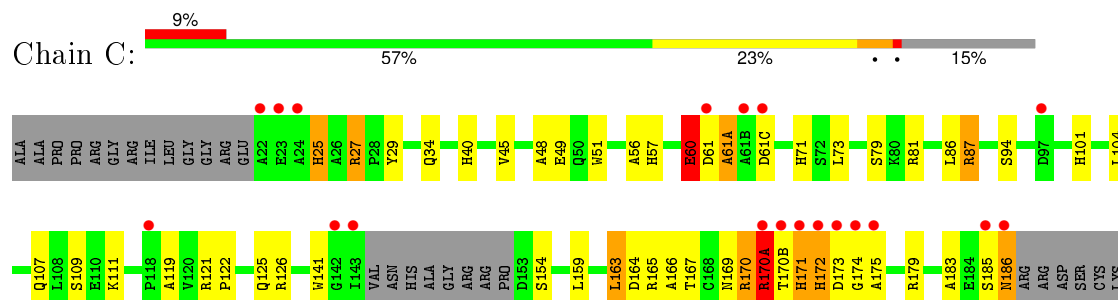
• Molecule 1: PROENZYME OF COMPLEMENT FACTOR D

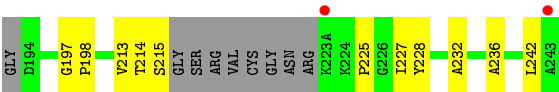


• Molecule 1: PROENZYME OF COMPLEMENT FACTOR D

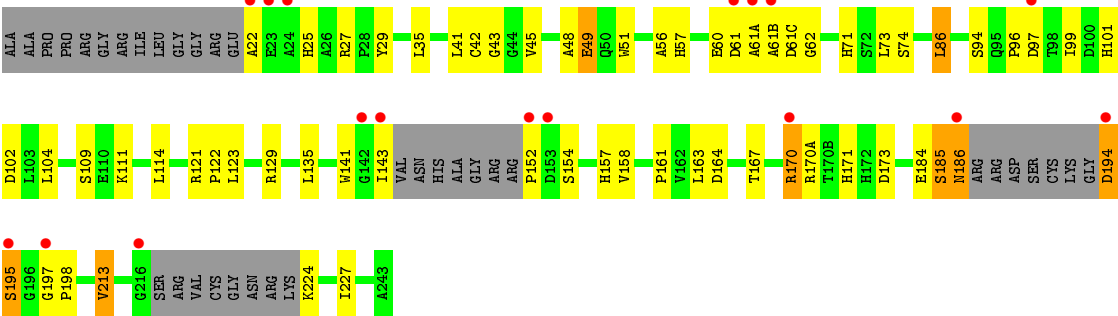


• Molecule 1: PROENZYME OF COMPLEMENT FACTOR D





● Molecule 1: PROENZYME OF COMPLEMENT FACTOR D



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	65.05Å 70.32Å 86.30Å 90.00° 101.98° 90.00°	Depositor
Resolution (Å)	30.00 – 2.10 28.99 – 2.10	Depositor EDS
% Data completeness (in resolution range)	98.5 (30.00-2.10) 98.3 (28.99-2.10)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.22 (at 2.10Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.204 , 0.251 0.200 , 0.244	Depositor DCC
R_{free} test set	4399 reflections (10.06%)	DCC
Wilson B-factor (Å ²)	20.4	Xtriage
Anisotropy	0.486	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 61.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 43713 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6764	wwPDB-VP
Average B, all atoms (Å ²)	24.0	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 32.83 % 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 8.8262e-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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	0.53	0/1685	0.72	2/2289 (0.1%)
1	B	0.50	0/1528	0.68	0/2083
1	C	0.46	0/1520	0.75	1/2073 (0.0%)
1	D	0.53	0/1523	0.74	2/2078 (0.1%)
All	All	0.51	0/6256	0.72	5/8523 (0.1%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	121	ARG	NE-CZ-NH2	7.47	124.04	120.30
1	A	170(A)	ARG	NE-CZ-NH2	7.33	123.97	120.30
1	C	170(A)	ARG	NE-CZ-NH2	7.28	123.94	120.30
1	A	20	ARG	NE-CZ-NH2	6.68	123.64	120.30
1	D	170(A)	ARG	NE-CZ-NH2	6.27	123.43	120.30

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	1654	0	1634	47	0
1	B	1497	0	1474	44	0
1	C	1490	0	1471	52	0
1	D	1492	0	1469	52	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	177	0	0	3	1
2	B	156	0	0	3	0
2	C	142	0	0	7	0
2	D	156	0	0	8	1
All	All	6764	0	6048	194	1

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 (194) 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:194:ASP:OD1	1:D:197:GLY:HA3	1.50	1.09
1:B:197:GLY:O	1:B:213:VAL:HG23	1.64	0.95
1:B:169:ASN:OD1	1:B:174:GLY:HA2	1.67	0.92
1:B:170(A):ARG:HD3	1:B:173:ASP:HA	1.56	0.87
1:D:157:HIS:HD2	2:D:362:HOH:O	1.57	0.86
1:C:179:ARG:HD2	2:C:369:HOH:O	1.76	0.85
1:C:197:GLY:O	1:C:213:VAL:HG23	1.80	0.81
1:D:194:ASP:HB3	2:D:256:HOH:O	1.81	0.81
1:B:45:VAL:HG21	1:B:198:PRO:HB3	1.62	0.81
1:B:61(B):ALA:HB2	2:B:388:HOH:O	1.81	0.80
1:D:213:VAL:HB	2:D:378:HOH:O	1.81	0.79
1:D:167:THR:HA	1:D:170:ARG:HD3	1.64	0.78
1:C:45:VAL:HG21	1:C:198:PRO:HB3	1.65	0.78
1:D:161:PRO:HG2	1:D:184:GLU:HG2	1.66	0.78
1:D:45:VAL:HG21	1:D:198:PRO:HB3	1.68	0.75
1:C:71:HIS:CD2	1:C:154:SER:HB2	2.22	0.74
1:C:45:VAL:HG22	1:C:198:PRO:HG3	1.69	0.74
1:C:61:ASP:O	1:C:61(A):ALA:HB2	1.86	0.74
1:A:16:ILE:C	1:A:16:ILE:CB	2.56	0.73
1:D:194:ASP:CG	1:D:197:GLY:HA3	2.09	0.73
1:A:91:HIS:CG	1:A:92:PRO:HD2	2.23	0.73
1:C:171:HIS:O	1:C:172:HIS:HB3	1.89	0.72
1:A:16:ILE:N	1:A:16:ILE:CB	2.52	0.72
1:B:123:LEU:HD12	1:B:124:PRO:HD2	1.70	0.72
1:C:185:SER:C	1:C:186:ASN:HD22	1.93	0.71
1:D:57:HIS:ND1	1:D:102:ASP:OD2	2.24	0.70
1:B:86:LEU:HG	1:B:109:SER:HA	1.73	0.70
1:D:185:SER:HB2	1:D:224:LYS:O	1.92	0.69
1:C:167:THR:CG2	1:C:170(A):ARG:HE	2.05	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:57:HIS:O	1:A:60:GLU:HB2	1.92	0.69
1:D:161:PRO:HG2	1:D:184:GLU:CG	2.23	0.67
1:D:71:HIS:NE2	1:D:154:SER:HB2	2.08	0.67
1:A:61(A):ALA:C	1:A:61(C):ASP:H	1.97	0.67
1:A:91:HIS:ND1	1:A:92:PRO:HD2	2.11	0.66
1:D:49:GLU:HB3	1:D:111:LYS:HG2	1.78	0.65
1:C:49:GLU:HB3	1:C:111:LYS:HG2	1.79	0.65
1:B:185:SER:O	1:B:186:ASN:HB2	1.96	0.65
1:B:170(A):ARG:HA	1:B:173:ASP:HA	1.79	0.64
1:A:45:VAL:CG2	1:A:198:PRO:HG3	2.27	0.64
1:A:121:ARG:HG3	1:A:121:ARG:HH11	1.63	0.64
1:C:25:HIS:HD2	2:C:254:HOH:O	1.80	0.64
1:A:188:ARG:HG3	1:A:192:LYS:HB2	1.80	0.63
1:A:16:ILE:C	1:A:16:ILE:N	2.51	0.63
1:C:61:ASP:O	1:C:61(A):ALA:CB	2.47	0.63
1:D:71:HIS:CD2	1:D:154:SER:HB2	2.34	0.62
1:B:45:VAL:CG2	1:B:198:PRO:HG3	2.30	0.62
1:C:34:GLN:HG2	1:C:40:HIS:HA	1.82	0.62
1:A:45:VAL:HG22	1:A:198:PRO:HG3	1.82	0.62
1:A:86:LEU:HG	1:A:109:SER:HA	1.80	0.61
1:D:35:LEU:HB2	1:D:41:LEU:HD22	1.82	0.61
1:D:197:GLY:O	2:D:378:HOH:O	2.16	0.61
1:C:57:HIS:O	1:C:60:GLU:HB2	2.00	0.61
1:B:45:VAL:CG2	1:B:198:PRO:HB3	2.31	0.60
1:B:169:ASN:OD1	1:B:174:GLY:CA	2.46	0.60
1:C:167:THR:HA	1:C:170:ARG:HD3	1.83	0.60
1:C:167:THR:HG22	1:C:170(A):ARG:HE	1.66	0.60
1:C:236:ALA:HB3	2:C:271:HOH:O	2.02	0.59
1:C:185:SER:HB2	1:C:225:PRO:HA	1.85	0.59
1:C:94:SER:HB3	1:C:101:HIS:O	2.02	0.59
1:A:152:PRO:O	1:A:153:ASP:HB2	2.03	0.58
1:B:185:SER:HB2	1:B:224:LYS:O	2.04	0.57
1:A:16:ILE:HG12	1:A:16:ILE:C	2.24	0.57
1:A:187:ARG:NH1	1:A:223(A):LYS:HE2	2.19	0.57
1:A:16:ILE:CG1	1:A:16:ILE:C	2.73	0.57
1:D:94:SER:HB3	1:D:101:HIS:O	2.05	0.57
1:B:51:TRP:CG	1:B:242:LEU:HD22	2.40	0.57
1:B:73:LEU:HD12	1:B:152:PRO:HB2	1.86	0.57
1:B:123:LEU:HD12	1:B:124:PRO:CD	2.34	0.57
1:C:86:LEU:HG	1:C:109:SER:HA	1.86	0.57
1:C:45:VAL:CG2	1:C:198:PRO:HB3	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:VAL:HG21	1:A:198:PRO:HB3	1.88	0.56
1:A:95:GLN:HG3	1:A:98:THR:HG22	1.88	0.56
1:C:170(A):ARG:O	1:C:171:HIS:ND1	2.38	0.55
1:A:123:LEU:HD12	1:A:124:PRO:HD2	1.88	0.55
1:B:223(A):LYS:HD2	1:B:223(A):LYS:O	2.06	0.55
1:C:186:ASN:HD22	1:C:186:ASN:N	2.04	0.55
1:C:170(B):THR:OG1	1:C:174:GLY:HA2	2.07	0.55
1:A:61(A):ALA:O	1:A:61(C):ASP:N	2.39	0.55
1:A:19:GLY:O	1:A:21:GLU:N	2.40	0.55
1:C:27:ARG:HG2	1:C:29:TYR:OH	2.07	0.55
1:D:45:VAL:CG2	1:D:198:PRO:HG3	2.38	0.54
1:C:25:HIS:CD2	2:C:254:HOH:O	2.57	0.54
1:D:35:LEU:HD11	1:D:62:GLY:HA3	1.88	0.54
1:D:48:ALA:HB3	1:D:51:TRP:HB2	1.89	0.53
1:D:45:VAL:CG2	1:D:198:PRO:HB3	2.36	0.53
1:B:73:LEU:HB2	1:B:152:PRO:O	2.08	0.53
1:B:169:ASN:CG	1:B:174:GLY:HA2	2.29	0.53
1:A:161:PRO:HD2	1:A:184:GLU:HB2	1.91	0.52
1:A:61(A):ALA:C	1:A:61(C):ASP:N	2.63	0.52
1:C:73:LEU:HG	1:C:141:TRP:CD1	2.44	0.52
1:A:49:GLU:HB3	1:A:111:LYS:HG2	1.90	0.52
1:A:142:GLY:O	1:A:152:PRO:HB3	2.09	0.52
1:B:185:SER:OG	1:B:186:ASN:N	2.43	0.52
1:D:74:SER:CB	1:D:152:PRO:HB2	2.40	0.52
1:A:60:GLU:OE1	1:A:60:GLU:HA	2.10	0.52
1:B:185:SER:CB	1:B:224:LYS:O	2.58	0.52
1:B:48:ALA:HB3	1:B:51:TRP:HB2	1.92	0.52
1:B:45:VAL:HG22	1:B:198:PRO:HG3	1.90	0.52
1:A:94:SER:HB3	1:A:101:HIS:O	2.10	0.52
1:D:194:ASP:CG	1:D:197:GLY:CA	2.77	0.51
1:A:35:LEU:HD21	1:A:61(B):ALA:HB3	1.92	0.51
1:C:185:SER:C	1:C:186:ASN:ND2	2.62	0.51
1:D:60:GLU:OE2	1:D:96:PRO:HA	2.11	0.51
1:C:170:ARG:O	1:C:170:ARG:HG2	2.09	0.51
1:A:16:ILE:HG12	1:A:17:LEU:N	2.26	0.50
1:D:74:SER:HB3	1:D:152:PRO:HB2	1.91	0.50
1:C:170:ARG:O	1:C:171:HIS:HB3	2.11	0.50
1:A:16:ILE:CG2	1:A:16:ILE:N	2.74	0.50
1:C:48:ALA:HB3	1:C:51:TRP:HB2	1.94	0.50
1:D:114:LEU:HD22	1:D:122:PRO:HD3	1.94	0.50
1:D:114:LEU:CD2	1:D:122:PRO:HD3	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:167:THR:HG23	1:C:170:ARG:CZ	2.42	0.50
1:A:21:GLU:HG3	2:A:359:HOH:O	2.11	0.50
1:D:61(A):ALA:O	1:D:61(B):ALA:C	2.50	0.49
1:C:56:ALA:HA	1:C:104:LEU:HB2	1.94	0.49
1:B:27:ARG:HG3	2:B:311:HOH:O	2.13	0.49
1:A:188:ARG:HD2	1:A:192:LYS:HD2	1.94	0.49
1:A:25:HIS:O	1:A:28:PRO:HD3	2.13	0.48
1:A:17:LEU:O	1:A:17:LEU:HD23	2.13	0.48
1:C:175:ALA:N	2:C:307:HOH:O	2.44	0.48
1:B:77:GLU:HB2	1:B:80:LYS:HG3	1.95	0.48
1:A:143:ILE:HG12	1:A:188:ARG:NH2	2.29	0.48
1:D:71:HIS:HE2	1:D:154:SER:HB2	1.77	0.48
1:D:25:HIS:HD2	2:D:250:HOH:O	1.96	0.48
1:B:163:LEU:HD22	1:B:168:CYS:HB2	1.96	0.47
1:B:173:ASP:N	1:B:173:ASP:OD1	2.48	0.47
1:D:143:ILE:CG2	1:D:194:ASP:N	2.77	0.47
1:D:74:SER:OG	1:D:152:PRO:HB2	2.14	0.47
1:D:143:ILE:HG22	1:D:194:ASP:N	2.30	0.47
1:B:45:VAL:HG21	1:B:198:PRO:CB	2.39	0.47
1:C:165:ARG:HD2	2:C:322:HOH:O	2.14	0.47
1:D:74:SER:HG	1:D:152:PRO:HB2	1.80	0.47
1:D:22:ALA:HB3	2:D:376:HOH:O	2.14	0.46
1:B:211:GLY:HA2	1:B:229:THR:O	2.16	0.46
1:B:72:SER:O	1:B:80:LYS:HE2	2.16	0.46
1:D:29:TYR:CD2	1:D:123:LEU:HD13	2.51	0.46
1:D:158:VAL:HG21	1:D:186:ASN:ND2	2.31	0.46
1:A:45:VAL:CG2	1:A:198:PRO:HB3	2.45	0.46
1:C:164:ASP:OD1	1:C:166:ALA:HB3	2.16	0.46
1:A:27:ARG:HD2	2:A:328:HOH:O	2.17	0.45
1:B:27:ARG:CG	1:B:27:ARG:HH11	2.29	0.45
1:A:91:HIS:CE1	1:A:92:PRO:HD2	2.52	0.45
1:A:51:TRP:CG	1:A:242:LEU:HD22	2.52	0.45
1:B:52:VAL:HG21	1:B:66:VAL:HG11	1.99	0.45
1:D:43:GLY:HA3	1:D:194:ASP:OD2	2.16	0.44
1:D:73:LEU:HG	1:D:141:TRP:CD1	2.51	0.44
1:A:27:ARG:HG2	1:A:29:TYR:OH	2.17	0.44
1:C:159:LEU:HA	1:C:159:LEU:HD23	1.89	0.44
1:D:42:CYS:SG	1:D:195:SER:HB3	2.58	0.44
1:A:75:GLN:NE2	2:A:293:HOH:O	2.50	0.44
1:C:51:TRP:CG	1:C:242:LEU:HD22	2.52	0.44
1:C:169:ASN:OD1	1:C:174:GLY:HA3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:87:ARG:HD2	1:C:107:GLN:OE1	2.18	0.43
1:B:167:THR:O	1:B:170:ARG:HB2	2.18	0.43
1:D:194:ASP:CB	2:D:256:HOH:O	2.52	0.43
1:D:157:HIS:ND1	2:D:357:HOH:O	2.22	0.43
1:B:172:HIS:O	1:B:173:ASP:C	2.57	0.43
1:C:171:HIS:O	1:C:171:HIS:CD2	2.72	0.43
1:A:170(A):ARG:NH2	1:A:184:GLU:OE2	2.50	0.43
1:D:86:LEU:HD13	1:D:109:SER:HA	2.01	0.42
1:D:194:ASP:HB2	1:D:195:SER:H	1.60	0.42
1:D:74:SER:HB3	1:D:152:PRO:CB	2.50	0.42
1:C:121:ARG:HA	1:C:122:PRO:HD3	1.88	0.42
1:B:129:ARG:HG2	1:B:129(A):ASP:O	2.19	0.42
1:D:99:ILE:HD11	1:D:227:ILE:HG21	2.02	0.42
1:B:45:VAL:CG2	1:B:198:PRO:CG	2.97	0.42
1:D:161:PRO:HG2	1:D:184:GLU:HG3	2.01	0.42
1:A:180:LEU:HD23	1:A:229:THR:HA	2.02	0.42
1:A:211:GLY:HA2	1:A:229:THR:O	2.20	0.42
1:B:51:TRP:CD1	1:B:242:LEU:HD22	2.54	0.42
1:D:45:VAL:HG21	1:D:198:PRO:CB	2.45	0.42
1:C:173:ASP:O	1:C:175:ALA:N	2.48	0.42
1:A:34:GLN:O	1:A:64:VAL:HA	2.20	0.41
1:B:167:THR:O	1:B:171:HIS:ND1	2.53	0.41
1:B:168:CYS:SG	1:B:172:HIS:HD2	2.42	0.41
1:A:152:PRO:O	1:A:153:ASP:CB	2.68	0.41
1:B:121:ARG:HA	1:B:122:PRO:HD3	1.94	0.41
1:C:45:VAL:HG22	1:C:198:PRO:CG	2.47	0.41
1:C:213:VAL:HG22	1:C:228:TYR:CE2	2.56	0.41
1:D:171:HIS:O	1:D:224:LYS:HD3	2.21	0.41
1:C:49:GLU:OE1	1:C:111:LYS:HD3	2.20	0.41
1:C:163:LEU:HD12	1:C:183:ALA:C	2.41	0.41
1:C:79:SER:CB	1:C:119:ALA:HB3	2.50	0.41
1:B:57:HIS:ND1	1:B:102:ASP:OD2	2.48	0.41
1:B:154:SER:HB2	2:B:391:HOH:O	2.21	0.41
1:C:121:ARG:HB3	2:C:347:HOH:O	2.21	0.40
1:C:214:THR:HG22	1:C:227:ILE:O	2.21	0.40
1:C:125:GLN:O	1:C:232:ALA:HA	2.21	0.40
1:D:135:LEU:HD23	1:D:135:LEU:HA	1.96	0.40
1:D:56:ALA:HA	1:D:104:LEU:HB2	2.04	0.40
1:B:158:VAL:HG23	1:B:160:LEU:HG	2.03	0.40
1:A:121:ARG:HA	1:A:122:PRO:HD3	1.94	0.40
1:B:94:SER:HB3	1:B:101:HIS:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:81:ARG:HE	1:D:129:ARG:NH2	2.20	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:372:HOH:O	2:D:385:HOH:O[1_545]	2.03	0.17

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	217/235 (92%)	201 (93%)	12 (6%)	4 (2%)	11	5
1	B	193/235 (82%)	186 (96%)	5 (3%)	2 (1%)	19	13
1	C	191/235 (81%)	179 (94%)	8 (4%)	4 (2%)	9	3
1	D	192/235 (82%)	184 (96%)	8 (4%)	0	100	100
All	All	793/940 (84%)	750 (95%)	33 (4%)	10 (1%)	15	9

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	20	ARG
1	A	61(B)	ALA
1	C	60	GLU
1	C	61(A)	ALA
1	C	171	HIS
1	A	153	ASP
1	B	173	ASP
1	C	172	HIS
1	A	60	GLU

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Mol	Chain	Res	Type
1	B	153	ASP

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	176/186 (95%)	161 (92%)	15 (8%)	13	9
1	B	160/186 (86%)	148 (92%)	12 (8%)	17	13
1	C	160/186 (86%)	149 (93%)	11 (7%)	19	15
1	D	160/186 (86%)	145 (91%)	15 (9%)	11	7
All	All	656/744 (88%)	603 (92%)	53 (8%)	15	10

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	ARG
1	A	49	GLU
1	A	87	ARG
1	A	95	GLN
1	A	154	SER
1	A	167	THR
1	A	170	ARG
1	A	172	HIS
1	A	185	SER
1	A	187	ARG
1	A	190	SER
1	A	191	CYS
1	A	215	SER
1	A	218	ARG
1	A	224	LYS
1	B	27	ARG
1	B	60	GLU
1	B	61	ASP
1	B	82	LEU
1	B	163	LEU

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Mol	Chain	Res	Type
1	B	164	ASP
1	B	170	ARG
1	B	173	ASP
1	B	186	ASN
1	B	195	SER
1	B	223(A)	LYS
1	B	224	LYS
1	C	25	HIS
1	C	27	ARG
1	C	60	GLU
1	C	61(C)	ASP
1	C	87	ARG
1	C	126	ARG
1	C	163	LEU
1	C	170	ARG
1	C	170(A)	ARG
1	C	186	ASN
1	C	215	SER
1	D	27	ARG
1	D	49	GLU
1	D	61	ASP
1	D	61(C)	ASP
1	D	86	LEU
1	D	97	ASP
1	D	163	LEU
1	D	164	ASP
1	D	170	ARG
1	D	173	ASP
1	D	185	SER
1	D	186	ASN
1	D	194	ASP
1	D	195	SER
1	D	213	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	75	GLN
1	B	186	ASN
1	C	25	HIS
1	C	57	HIS
1	C	172	HIS

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Mol	Chain	Res	Type
1	C	186	ASN
1	D	25	HIS

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 carbohydrates 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	221/235 (94%)	0.71	36 (16%) 2 3	7, 19, 54, 64	0
1	B	201/235 (85%)	0.40	19 (9%) 10 14	9, 21, 48, 56	0
1	C	199/235 (84%)	0.60	21 (10%) 8 11	9, 21, 52, 64	0
1	D	200/235 (85%)	0.39	17 (8%) 13 18	7, 19, 45, 54	0
All	All	821/940 (87%)	0.53	93 (11%) 7 9	7, 20, 50, 64	0

All (93) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	172	HIS	12.0
1	C	173	ASP	9.1
1	A	171	HIS	8.4
1	A	172	HIS	8.3
1	C	22	ALA	7.7
1	A	61	ASP	7.5
1	A	143	ILE	7.5
1	A	17	LEU	6.9
1	B	170(A)	ARG	6.8
1	A	175	ALA	6.8
1	C	171	HIS	6.5
1	D	152	PRO	6.4
1	B	22	ALA	6.3
1	A	16	ILE	6.3
1	D	61(A)	ALA	5.9
1	A	170(B)	THR	5.9
1	B	61(A)	ALA	5.8
1	A	222	ASN	5.6
1	B	61(B)	ALA	5.4
1	D	22	ALA	5.2
1	C	170(B)	THR	5.1

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Mol	Chain	Res	Type	RSRZ
1	C	174	GLY	5.1
1	B	170(B)	THR	5.0
1	C	61	ASP	4.9
1	A	188	ARG	4.8
1	A	20	ARG	4.6
1	C	24	ALA	4.6
1	C	143	ILE	4.6
1	D	23	GLU	4.4
1	A	174	GLY	4.2
1	C	175	ALA	4.2
1	A	61(B)	ALA	4.2
1	D	61(B)	ALA	4.2
1	B	142	GLY	4.2
1	D	24	ALA	4.0
1	B	61	ASP	4.0
1	C	61(C)	ASP	3.9
1	C	97	ASP	3.9
1	D	194	ASP	3.9
1	B	186	ASN	3.8
1	A	224	LYS	3.8
1	C	61(B)	ALA	3.8
1	A	223	ARG	3.7
1	C	186	ASN	3.7
1	A	18	GLY	3.7
1	B	173	ASP	3.7
1	B	223(A)	LYS	3.7
1	A	170	ARG	3.7
1	C	142	GLY	3.6
1	B	172	HIS	3.6
1	D	142	GLY	3.6
1	D	97	ASP	3.6
1	B	224	LYS	3.5
1	A	220	CYS	3.5
1	A	19	GLY	3.4
1	A	61(A)	ALA	3.2
1	D	186	ASN	3.2
1	C	23	GLU	3.1
1	A	173	ASP	3.0
1	B	216	GLY	3.0
1	A	166	ALA	3.0
1	C	243	ALA	3.0
1	B	23	GLU	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	216	GLY	2.9
1	A	142	GLY	2.9
1	D	153	ASP	2.8
1	A	218	ARG	2.7
1	C	223(A)	LYS	2.7
1	D	197	GLY	2.7
1	C	170(A)	ARG	2.6
1	D	61	ASP	2.6
1	A	243	ALA	2.5
1	D	195	SER	2.5
1	B	97	ASP	2.5
1	B	174	GLY	2.5
1	A	170(A)	ARG	2.4
1	D	170	ARG	2.4
1	A	219	VAL	2.4
1	A	61(C)	ASP	2.4
1	D	143	ILE	2.4
1	B	152	PRO	2.3
1	A	190	SER	2.3
1	A	167	THR	2.2
1	C	185	SER	2.2
1	A	153	ASP	2.2
1	B	197	GLY	2.2
1	A	62	GLY	2.1
1	C	118	PRO	2.1
1	A	216	GLY	2.1
1	A	221	GLY	2.1
1	A	176	ILE	2.0
1	A	152	PRO	2.0
1	B	185	SER	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.