



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 16, 2018 – 10:46 pm GMT

PDB ID : 3ZC2
Title : STRUCTURE OF AN ACTIVITY SUPPRESSING FAB FRAGMENT TO
CYTOCHROME P450 AROMATASE
Authors : Sawicki, M.W.; Ng, P.C.; Burkhart, B.; Pletnev, V.; Higashiyama, T.; Osawa,
Y.; Ghosh, D.
Deposited on : 1999-04-21
Resolution : 3.00 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
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk30686

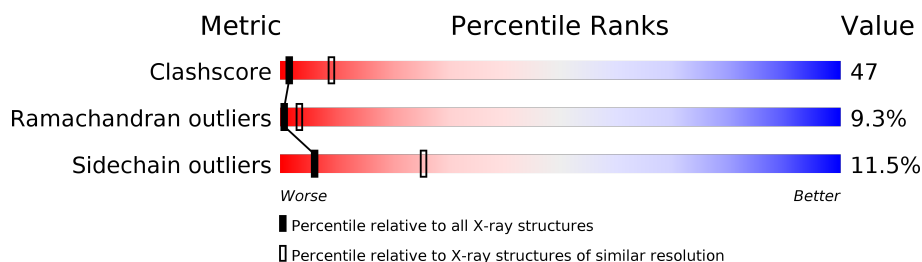
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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))
Clashscore	122078	2167 (3.00-3.00)
Ramachandran outliers	120005	2101 (3.00-3.00)
Sidechain outliers	119972	2104 (3.00-3.00)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	217	
2	B	218	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3326 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 IGG1 ANTIBODY 32C2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	217	Total	C	N	O	S	0	0	0
			1673	1040	288	338	7			

- Molecule 2 is a protein called IGG1 ANTIBODY 32C2.

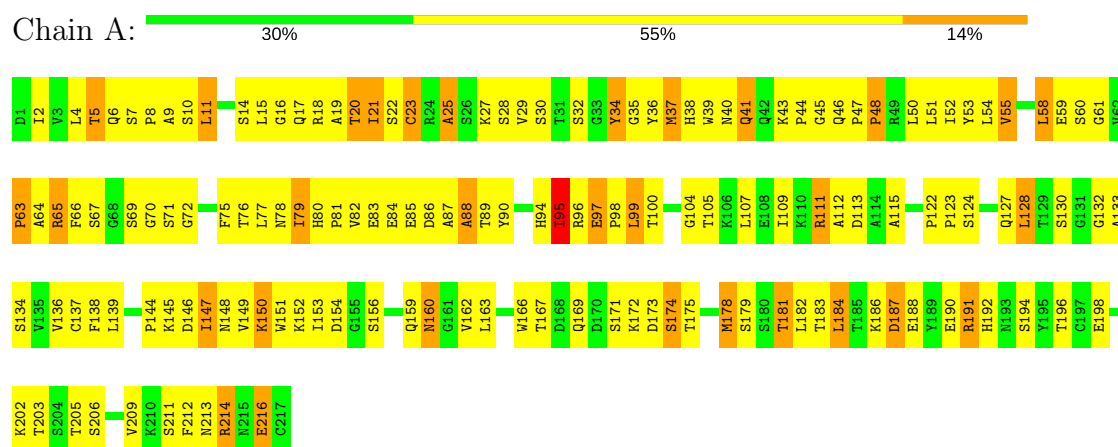
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	218	Total	C	N	O	S	0	0	0
			1653	1048	266	333	6			

3 Residue-property plots

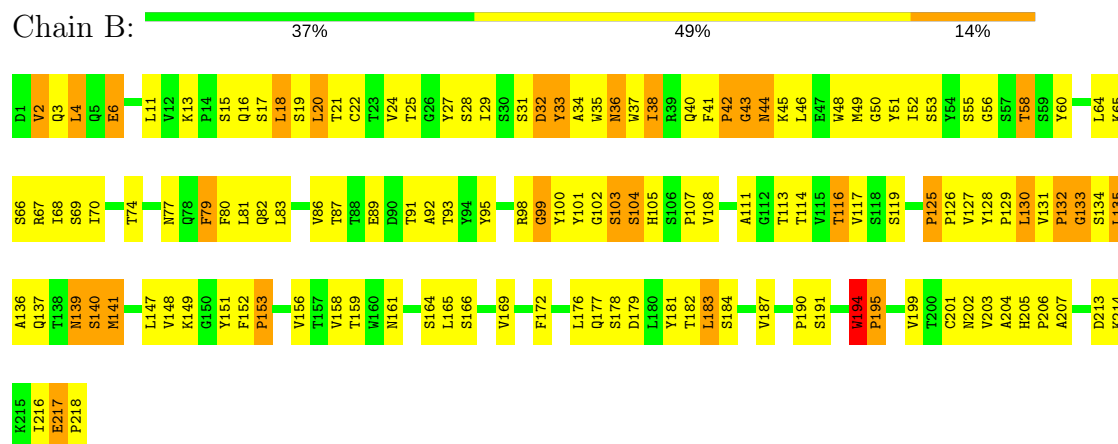
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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.

Note EDS was not executed.

• Molecule 1: IGG1 ANTIBODY 32C2



• Molecule 2: IGG1 ANTIBODY 32C2



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	154.89Å 73.51Å 36.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	99.00 – 3.00	Depositor
% Data completeness (in resolution range)	88.3 (99.00-3.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
Refinement program	CNS 0.4	Depositor
R, R_{free}	0.213 , 0.317	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3326	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

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	0.41	0/1711	0.67	0/2325
2	B	0.42	0/1701	0.71	0/2334
All	All	0.42	0/3412	0.69	0/4659

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	1673	0	1610	166	0
2	B	1653	0	1603	156	0
All	All	3326	0	3213	310	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 47.

All (310) 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:A:58:LEU:HD13	1:A:63:PRO:HB2	1.28	1.11
1:A:30:SER:HB3	1:A:72:GLY:H	1.20	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:163:LEU:HD11	2:B:177:GLN:HG3	1.43	0.98
1:A:80:HIS:HB2	1:A:81:PRO:HD3	1.45	0.96
1:A:136:VAL:HG22	1:A:181:THR:HG23	1.46	0.96
2:B:4:LEU:HB3	2:B:24:VAL:HG22	1.48	0.96
2:B:125:PRO:HB3	2:B:151:TYR:HB3	1.51	0.92
2:B:91:THR:HG23	2:B:116:THR:HA	1.50	0.92
1:A:30:SER:CB	1:A:72:GLY:H	1.85	0.90
2:B:158:VAL:HG22	2:B:203:VAL:HG22	1.55	0.88
2:B:33:TYR:HA	2:B:101:TYR:H	1.39	0.86
1:A:18:ARG:NH1	1:A:18:ARG:HB2	1.93	0.84
1:A:36:TYR:HB3	1:A:55:VAL:HG23	1.60	0.83
1:A:19:ALA:HB3	1:A:79:ILE:HG23	1.61	0.82
2:B:4:LEU:N	2:B:4:LEU:HD23	1.95	0.82
1:A:58:LEU:HD13	1:A:63:PRO:CB	2.09	0.81
2:B:31:SER:O	2:B:32:ASP:HB2	1.80	0.81
2:B:194:TRP:HB3	2:B:195:PRO:HD3	1.61	0.81
1:A:38:HIS:CE1	1:A:50:LEU:HD13	2.18	0.79
1:A:58:LEU:HB3	1:A:63:PRO:HB3	1.64	0.79
2:B:127:VAL:HG23	2:B:214:LYS:HD2	1.65	0.79
2:B:149:LYS:HG3	2:B:182:THR:OG1	1.85	0.77
2:B:166:SER:O	2:B:169:VAL:HG12	1.83	0.77
1:A:163:LEU:HD11	2:B:177:GLN:CG	2.15	0.77
1:A:28:SER:HA	1:A:72:GLY:O	1.84	0.77
1:A:136:VAL:HG22	1:A:181:THR:CG2	2.15	0.77
1:A:30:SER:HB3	1:A:72:GLY:N	1.97	0.76
2:B:20:LEU:HD23	2:B:20:LEU:H	1.49	0.76
2:B:158:VAL:HA	2:B:202:ASN:O	1.86	0.76
1:A:67:SER:HB2	1:A:78:ASN:ND2	2.01	0.75
1:A:150:LYS:HZ2	1:A:198:GLU:C	1.91	0.74
1:A:133:ALA:O	1:A:184:LEU:HD12	1.88	0.73
1:A:58:LEU:HD21	1:A:66:PHE:O	1.86	0.73
2:B:126:PRO:HD2	2:B:149:LYS:O	1.89	0.72
1:A:41:GLN:HG2	1:A:51:LEU:HD11	1.71	0.72
2:B:48:TRP:CZ2	2:B:50:GLY:HA2	2.25	0.72
2:B:44:ASN:HD22	2:B:45:LYS:NZ	1.87	0.72
2:B:32:ASP:HB3	2:B:33:TYR:HD1	1.54	0.72
2:B:16:GLN:HG2	2:B:17:SER:H	1.55	0.72
2:B:133:GLY:O	2:B:135:LEU:HD23	1.90	0.71
2:B:137:GLN:C	2:B:139:ASN:H	1.94	0.71
2:B:40:GLN:HG3	2:B:46:LEU:HD12	1.73	0.71
2:B:18:LEU:HD11	2:B:20:LEU:HD22	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:198:GLU:HG2	1:A:209:VAL:HG22	1.75	0.68
2:B:68:ILE:HD11	2:B:81:LEU:HD11	1.74	0.68
2:B:35:TRP:O	2:B:52:ILE:HG22	1.93	0.68
1:A:20:THR:OG1	1:A:78:ASN:HB3	1.94	0.67
1:A:95:ILE:HG21	2:B:103:SER:O	1.94	0.67
1:A:45:GLY:O	1:A:46:GLN:HG3	1.95	0.67
1:A:124:SER:OG	1:A:127:GLN:HB2	1.95	0.67
2:B:67:ARG:NH2	2:B:83:LEU:HD11	2.09	0.67
1:A:186:LYS:HE2	1:A:190:GLU:CD	2.15	0.67
1:A:55:VAL:HG11	1:A:71:SER:OG	1.94	0.67
2:B:40:GLN:OE1	2:B:46:LEU:HD11	1.96	0.66
1:A:163:LEU:HD21	2:B:177:GLN:HG2	1.77	0.66
1:A:52:ILE:HG22	1:A:53:TYR:N	2.11	0.66
2:B:15:SER:N	2:B:86:VAL:O	2.18	0.66
2:B:22:CYS:SG	2:B:79:PHE:CE1	2.89	0.66
1:A:10:SER:O	1:A:11:LEU:HB2	1.96	0.65
2:B:183:LEU:C	2:B:183:LEU:HD23	2.16	0.65
2:B:129:PRO:HD3	2:B:214:LYS:HD3	1.78	0.65
1:A:145:LYS:O	1:A:147:ILE:HG22	1.95	0.65
1:A:8:PRO:HD2	1:A:21:ILE:CG2	2.26	0.65
2:B:32:ASP:HB3	2:B:33:TYR:CD1	2.32	0.65
2:B:22:CYS:HB2	2:B:37:TRP:CH2	2.32	0.64
1:A:54:LEU:O	1:A:55:VAL:HB	1.96	0.64
2:B:176:LEU:N	2:B:176:LEU:HD23	2.12	0.64
1:A:186:LYS:HE2	1:A:190:GLU:OE1	1.98	0.63
1:A:16:GLY:HA2	1:A:81:PRO:HA	1.80	0.63
2:B:6:GLU:CD	2:B:6:GLU:H	2.02	0.63
1:A:18:ARG:HB2	1:A:18:ARG:HH11	1.62	0.63
1:A:96:ARG:HG2	1:A:96:ARG:HH11	1.64	0.63
1:A:4:LEU:HD11	1:A:94:HIS:HB3	1.81	0.63
1:A:94:HIS:ND1	1:A:95:ILE:N	2.48	0.62
2:B:141:MET:HE2	2:B:190:PRO:HA	1.81	0.62
2:B:38:ILE:HG23	2:B:48:TRP:HA	1.82	0.62
1:A:214:ARG:HH11	1:A:214:ARG:CB	2.11	0.62
2:B:204:ALA:O	2:B:206:PRO:HD3	2.00	0.62
2:B:131:VAL:HG11	2:B:217:GLU:O	2.00	0.62
2:B:202:ASN:ND2	2:B:213:ASP:OD2	2.33	0.61
1:A:94:HIS:C	1:A:95:ILE:HD13	2.20	0.61
1:A:41:GLN:O	1:A:48:PRO:HA	2.00	0.61
1:A:134:SER:HB3	1:A:183:THR:HG23	1.82	0.61
2:B:103:SER:O	2:B:104:SER:HB2	1.99	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:194:TRP:HH2	2:B:216:ILE:O	1.84	0.61
1:A:127:GLN:HG3	2:B:128:TYR:CE2	2.35	0.60
1:A:159:GLN:OE1	1:A:159:GLN:HA	2.01	0.60
1:A:83:GLU:HB3	1:A:86:ASP:CG	2.22	0.60
1:A:152:LYS:HA	1:A:156:SER:O	2.01	0.60
2:B:147:LEU:HD12	2:B:148:VAL:N	2.16	0.59
2:B:4:LEU:H	2:B:4:LEU:HD23	1.63	0.59
1:A:160:ASN:HD22	1:A:160:ASN:H	1.50	0.59
2:B:79:PHE:HD1	2:B:79:PHE:H	1.51	0.59
1:A:95:ILE:HG21	2:B:104:SER:HB2	1.83	0.59
1:A:35:GLY:HA3	1:A:96:ARG:HH12	1.67	0.59
2:B:20:LEU:N	2:B:20:LEU:HD23	2.16	0.59
2:B:44:ASN:C	2:B:45:LYS:HD2	2.23	0.59
1:A:87:ALA:HA	1:A:107:LEU:HD12	1.85	0.59
1:A:97:GLU:HA	1:A:99:LEU:HD23	1.85	0.59
1:A:169:GLN:OE1	1:A:174:SER:HB3	2.03	0.58
2:B:83:LEU:HD12	2:B:86:VAL:HG22	1.85	0.58
2:B:201:CYS:O	2:B:213:ASP:HA	2.03	0.58
1:A:160:ASN:HD22	1:A:160:ASN:N	2.01	0.58
1:A:95:ILE:HG22	1:A:99:LEU:HD13	1.86	0.58
2:B:194:TRP:CB	2:B:195:PRO:HD3	2.32	0.58
2:B:194:TRP:HB3	2:B:195:PRO:CD	2.34	0.58
2:B:44:ASN:HD22	2:B:45:LYS:HZ2	1.52	0.57
2:B:4:LEU:CB	2:B:24:VAL:HG22	2.31	0.57
1:A:167:THR:HG23	2:B:172:PHE:CD2	2.40	0.57
2:B:45:LYS:O	2:B:46:LEU:HD12	2.05	0.57
1:A:173:ASP:O	1:A:175:THR:N	2.38	0.57
1:A:99:LEU:HD23	1:A:99:LEU:N	2.20	0.57
1:A:65:ARG:NH2	1:A:83:GLU:OE1	2.37	0.56
1:A:144:PRO:HG3	1:A:202:LYS:HD3	1.86	0.56
2:B:98:ARG:O	2:B:98:ARG:HG2	2.05	0.56
1:A:98:PRO:O	1:A:100:THR:HG23	2.05	0.55
2:B:93:THR:HG23	2:B:114:THR:HG22	1.87	0.55
2:B:29:ILE:HD13	2:B:29:ILE:N	2.22	0.55
2:B:135:LEU:HD12	2:B:137:GLN:HB2	1.88	0.55
2:B:4:LEU:HD21	2:B:108:VAL:HG12	1.89	0.55
1:A:52:ILE:HG22	1:A:53:TYR:H	1.72	0.55
1:A:41:GLN:HG2	1:A:51:LEU:HD21	1.89	0.54
1:A:65:ARG:O	1:A:79:ILE:HA	2.07	0.54
2:B:34:ALA:N	2:B:101:TYR:HB2	2.22	0.54
2:B:52:ILE:HD13	2:B:58:THR:HG22	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:178:MET:HG2	1:A:179:SER:N	2.23	0.54
2:B:91:THR:CG2	2:B:116:THR:HA	2.31	0.54
1:A:113:ASP:OD2	1:A:202:LYS:HE2	2.07	0.54
2:B:22:CYS:SG	2:B:79:PHE:HE1	2.31	0.54
2:B:4:LEU:HD21	2:B:108:VAL:CG1	2.38	0.54
1:A:196:THR:HA	1:A:211:SER:CB	2.38	0.53
1:A:59:GLU:HG3	1:A:60:SER:N	2.23	0.53
2:B:41:PHE:HB2	2:B:45:LYS:HB2	1.90	0.53
2:B:86:VAL:HG12	2:B:117:VAL:HG11	1.90	0.53
1:A:109:ILE:HD11	1:A:174:SER:OG	2.09	0.53
1:A:137:CYS:HB2	1:A:151:TRP:CH2	2.43	0.53
1:A:150:LYS:HE3	1:A:150:LYS:N	2.24	0.53
1:A:39:TRP:O	1:A:51:LEU:HB2	2.09	0.53
2:B:40:GLN:HG3	2:B:46:LEU:CD1	2.39	0.53
1:A:196:THR:HA	1:A:211:SER:HB2	1.90	0.53
1:A:53:TYR:HE2	1:A:59:GLU:OE1	1.92	0.53
2:B:95:TYR:HE1	2:B:111:ALA:O	1.92	0.53
2:B:27:TYR:CD1	2:B:28:SER:N	2.77	0.53
2:B:27:TYR:CE1	2:B:31:SER:HB3	2.44	0.53
2:B:194:TRP:O	2:B:195:PRO:C	2.47	0.52
1:A:38:HIS:ND1	1:A:52:ILE:O	2.41	0.52
1:A:95:ILE:HA	1:A:99:LEU:HD22	1.91	0.52
2:B:194:TRP:CH2	2:B:216:ILE:O	2.61	0.52
1:A:80:HIS:CB	1:A:81:PRO:HD3	2.28	0.52
1:A:4:LEU:CD2	1:A:25:ALA:HB2	2.40	0.52
2:B:43:GLY:O	2:B:45:LYS:N	2.43	0.52
1:A:190:GLU:HA	1:A:214:ARG:HH21	1.75	0.52
1:A:59:GLU:HG3	1:A:60:SER:H	1.75	0.52
1:A:96:ARG:NH1	1:A:96:ARG:HG2	2.21	0.52
2:B:65:LYS:O	2:B:66:SER:HB2	2.10	0.52
1:A:166:TRP:CD1	1:A:178:MET:HB2	2.45	0.52
1:A:50:LEU:HD11	2:B:107:PRO:HD2	1.91	0.52
1:A:7:SER:O	1:A:21:ILE:HG22	2.10	0.51
2:B:33:TYR:CD2	2:B:100:TYR:HD1	2.28	0.51
1:A:69:SER:OG	1:A:70:GLY:N	2.44	0.51
2:B:139:ASN:O	2:B:140:SER:CB	2.58	0.51
2:B:60:TYR:HE1	2:B:70:ILE:HG13	1.76	0.51
2:B:151:TYR:CZ	2:B:156:VAL:HG21	2.45	0.51
2:B:65:LYS:O	2:B:66:SER:CB	2.59	0.51
1:A:83:GLU:HB3	1:A:86:ASP:OD1	2.11	0.51
2:B:13:LYS:HE2	2:B:16:GLN:OE1	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:47:PRO:HB3	2:B:95:TYR:CE1	2.46	0.51
1:A:128:LEU:HD12	1:A:133:ALA:HB2	1.93	0.50
1:A:6:GLN:HB2	1:A:23:CYS:SG	2.51	0.50
2:B:139:ASN:O	2:B:140:SER:HB3	2.11	0.50
2:B:36:ASN:HB3	2:B:51:TYR:HB3	1.94	0.50
2:B:41:PHE:HD2	2:B:45:LYS:HB3	1.76	0.50
2:B:95:TYR:CE1	2:B:111:ALA:O	2.64	0.50
1:A:84:GLU:H	1:A:84:GLU:CD	2.14	0.50
2:B:87:THR:O	2:B:117:VAL:HG11	2.11	0.50
1:A:52:ILE:CG2	1:A:53:TYR:N	2.75	0.50
1:A:81:PRO:O	1:A:83:GLU:N	2.45	0.50
2:B:141:MET:HA	2:B:191:SER:H	1.77	0.50
1:A:20:THR:HA	1:A:77:LEU:O	2.12	0.49
1:A:8:PRO:HD2	1:A:21:ILE:HG23	1.94	0.49
2:B:161:ASN:O	2:B:164:SER:HB3	2.12	0.49
1:A:83:GLU:OE1	1:A:86:ASP:OD1	2.29	0.49
2:B:137:GLN:C	2:B:139:ASN:N	2.64	0.49
2:B:187:VAL:HG13	2:B:187:VAL:O	2.12	0.49
1:A:128:LEU:O	1:A:186:LYS:HD3	2.12	0.49
1:A:83:GLU:HB3	1:A:86:ASP:OD2	2.13	0.49
2:B:176:LEU:HD22	2:B:181:TYR:CE1	2.47	0.49
2:B:194:TRP:CB	2:B:195:PRO:CD	2.90	0.49
2:B:51:TYR:HD1	2:B:52:ILE:N	2.10	0.49
1:A:196:THR:HG23	1:A:211:SER:HB3	1.95	0.49
1:A:75:PHE:CD1	1:A:75:PHE:N	2.80	0.49
2:B:129:PRO:O	2:B:130:LEU:HD12	2.13	0.49
1:A:115:ALA:HB2	1:A:203:THR:HG21	1.95	0.48
1:A:28:SER:O	1:A:96:ARG:HD2	2.13	0.48
1:A:149:VAL:C	1:A:150:LYS:HE3	2.33	0.48
2:B:21:THR:HG1	2:B:80:PHE:HE1	1.59	0.48
2:B:178:SER:OG	2:B:179:ASP:N	2.46	0.48
2:B:135:LEU:HD12	2:B:137:GLN:CB	2.44	0.48
1:A:194:SER:HA	1:A:213:ASN:HA	1.94	0.48
1:A:214:ARG:HH11	1:A:214:ARG:HB2	1.78	0.48
2:B:194:TRP:CZ3	2:B:199:VAL:HG23	2.47	0.48
1:A:58:LEU:CB	1:A:63:PRO:HB3	2.41	0.48
2:B:4:LEU:HD11	2:B:108:VAL:O	2.14	0.48
1:A:22:SER:HB3	1:A:76:THR:HG22	1.96	0.47
1:A:83:GLU:HG2	1:A:84:GLU:N	2.29	0.47
1:A:8:PRO:HD2	1:A:21:ILE:HG22	1.97	0.47
2:B:98:ARG:O	2:B:99:GLY:C	2.53	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34:TYR:CD1	2:B:103:SER:OG	2.67	0.47
1:A:43:LYS:O	1:A:45:GLY:N	2.48	0.47
1:A:94:HIS:ND1	1:A:94:HIS:C	2.67	0.47
2:B:13:LYS:N	2:B:13:LYS:HD3	2.29	0.47
1:A:216:GLU:HG2	1:A:216:GLU:O	2.15	0.47
1:A:37:MET:HG3	1:A:38:HIS:H	1.80	0.47
1:A:107:LEU:O	1:A:107:LEU:HD13	2.15	0.47
1:A:94:HIS:O	1:A:95:ILE:HG23	2.14	0.47
1:A:136:VAL:HG12	1:A:137:CYS:N	2.29	0.47
1:A:14:SER:O	1:A:15:LEU:C	2.54	0.46
1:A:34:TYR:HB3	2:B:103:SER:OG	2.15	0.46
2:B:20:LEU:N	2:B:20:LEU:CD2	2.78	0.46
1:A:21:ILE:O	1:A:76:THR:HA	2.15	0.46
2:B:152:PHE:HA	2:B:153:PRO:HA	1.67	0.46
1:A:52:ILE:CG2	1:A:53:TYR:H	2.28	0.46
2:B:67:ARG:NH2	2:B:83:LEU:CD1	2.77	0.46
1:A:205:THR:OG1	1:A:206:SER:N	2.47	0.46
1:A:162:VAL:O	1:A:163:LEU:HD23	2.16	0.46
1:A:41:GLN:CG	1:A:51:LEU:HD11	2.44	0.45
2:B:141:MET:HG3	2:B:190:PRO:HA	1.98	0.45
2:B:44:ASN:HD22	2:B:45:LYS:HZ3	1.61	0.45
2:B:113:THR:O	2:B:113:THR:HG23	2.15	0.45
2:B:205:HIS:CE1	2:B:207:ALA:HB3	2.51	0.45
2:B:19:SER:HA	2:B:81:LEU:O	2.16	0.45
1:A:67:SER:O	1:A:78:ASN:OD1	2.35	0.45
1:A:111:ARG:HG2	1:A:174:SER:O	2.16	0.45
1:A:18:ARG:HB2	1:A:18:ARG:CZ	2.45	0.45
2:B:35:TRP:HB2	2:B:52:ILE:HG23	1.97	0.45
1:A:186:LYS:O	1:A:190:GLU:HG3	2.16	0.45
1:A:30:SER:HA	1:A:36:TYR:HA	1.99	0.45
1:A:85:GLU:HG3	1:A:171:SER:OG	2.16	0.45
1:A:127:GLN:O	1:A:128:LEU:C	2.55	0.45
1:A:139:LEU:HD12	1:A:139:LEU:N	2.32	0.45
2:B:4:LEU:CD2	2:B:4:LEU:N	2.67	0.45
1:A:80:HIS:HB2	1:A:81:PRO:CD	2.33	0.44
2:B:152:PHE:CE2	2:B:153:PRO:HB3	2.52	0.44
1:A:196:THR:CA	1:A:211:SER:HB2	2.48	0.44
2:B:183:LEU:HD23	2:B:184:SER:N	2.32	0.44
2:B:89:GLU:H	2:B:89:GLU:CD	2.21	0.44
2:B:40:GLN:O	2:B:92:ALA:HB1	2.17	0.44
1:A:2:ILE:HD11	1:A:25:ALA:HB1	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:TYR:O	1:A:104:GLY:HA2	2.18	0.44
2:B:164:SER:O	2:B:165:LEU:HB2	2.17	0.44
1:A:123:PRO:HB2	1:A:128:LEU:HD13	1.99	0.44
1:A:127:GLN:NE2	1:A:134:SER:OG	2.50	0.44
1:A:194:SER:HB3	1:A:213:ASN:OD1	2.17	0.44
1:A:54:LEU:O	1:A:55:VAL:CB	2.66	0.44
2:B:51:TYR:CD1	2:B:51:TYR:C	2.91	0.44
1:A:87:ALA:O	1:A:88:ALA:HB2	2.18	0.43
1:A:9:ALA:O	1:A:105:THR:HA	2.18	0.43
2:B:34:ALA:HB2	2:B:101:TYR:HB2	1.98	0.43
2:B:159:THR:OG1	2:B:202:ASN:HB2	2.18	0.43
1:A:188:GLU:O	1:A:191:ARG:HB3	2.17	0.43
2:B:136:ALA:HA	2:B:139:ASN:OD1	2.18	0.43
2:B:27:TYR:HE1	2:B:31:SER:HB3	1.83	0.43
2:B:131:VAL:HA	2:B:132:PRO:HD3	1.80	0.43
1:A:67:SER:HB2	1:A:78:ASN:HD21	1.78	0.43
2:B:53:SER:C	2:B:55:SER:N	2.72	0.43
1:A:39:TRP:N	1:A:39:TRP:CD1	2.87	0.43
1:A:4:LEU:O	1:A:5:THR:C	2.56	0.43
2:B:29:ILE:HG12	2:B:77:ASN:HA	2.00	0.43
2:B:53:SER:O	2:B:56:GLY:N	2.43	0.43
1:A:30:SER:HB2	1:A:75:PHE:CE2	2.54	0.42
1:A:4:LEU:HD23	1:A:25:ALA:HB2	2.00	0.42
2:B:68:ILE:HA	2:B:82:GLN:O	2.19	0.42
2:B:135:LEU:HB2	2:B:136:ALA:H	1.60	0.42
1:A:138:PHE:C	1:A:139:LEU:HD12	2.40	0.42
1:A:18:ARG:CB	1:A:18:ARG:HH11	2.29	0.42
1:A:212:PHE:C	1:A:212:PHE:CD1	2.92	0.42
2:B:176:LEU:N	2:B:176:LEU:CD2	2.81	0.42
2:B:3:GLN:HB2	2:B:25:THR:OG1	2.19	0.42
2:B:51:TYR:CD1	2:B:52:ILE:N	2.87	0.42
2:B:11:LEU:HD13	2:B:11:LEU:C	2.39	0.42
2:B:28:SER:O	2:B:31:SER:HB3	2.18	0.42
2:B:52:ILE:O	2:B:52:ILE:HG23	2.20	0.42
2:B:2:VAL:HG12	2:B:4:LEU:HD22	2.01	0.42
1:A:154:ASP:HB2	1:A:192:HIS:HD2	1.84	0.42
2:B:166:SER:O	2:B:169:VAL:CG1	2.62	0.42
1:A:130:SER:C	1:A:132:GLY:H	2.24	0.41
1:A:41:GLN:HB3	1:A:51:LEU:HD11	2.01	0.41
2:B:33:TYR:CD2	2:B:100:TYR:HA	2.55	0.41
2:B:16:GLN:HG2	2:B:17:SER:N	2.30	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:93:THR:HA	2:B:114:THR:HA	2.01	0.41
1:A:63:PRO:O	1:A:64:ALA:HB3	2.21	0.41
1:A:111:ARG:HD3	1:A:112:ALA:O	2.20	0.41
1:A:87:ALA:HA	1:A:107:LEU:CD1	2.49	0.41
2:B:49:MET:HE1	2:B:81:LEU:HD21	2.03	0.41
1:A:147:ILE:O	1:A:147:ILE:HG23	2.20	0.41
1:A:34:TYR:CG	2:B:103:SER:OG	2.74	0.41
1:A:45:GLY:C	1:A:46:GLN:HG3	2.42	0.41
2:B:126:PRO:HG2	2:B:126:PRO:O	2.20	0.41
2:B:172:PHE:O	2:B:183:LEU:HG	2.21	0.41
2:B:18:LEU:HD12	2:B:19:SER:N	2.36	0.41
1:A:122:PRO:HA	1:A:123:PRO:HD3	1.96	0.40
1:A:187:ASP:O	1:A:188:GLU:C	2.58	0.40
1:A:153:ILE:HG22	1:A:192:HIS:CD2	2.56	0.40
1:A:203:THR:HG22	1:A:203:THR:O	2.20	0.40
1:A:20:THR:O	1:A:20:THR:HG22	2.20	0.40
1:A:83:GLU:N	1:A:86:ASP:OD2	2.54	0.40
2:B:101:TYR:CG	2:B:102:GLY:N	2.88	0.40
2:B:217:GLU:O	2:B:218:PRO:O	2.40	0.40
2:B:68:ILE:HG12	2:B:69:SER:H	1.87	0.40
2:B:79:PHE:N	2:B:79:PHE:CD1	2.88	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	215/217 (99%)	153 (71%)	43 (20%)	19 (9%)	1	4
2	B	216/218 (99%)	161 (74%)	34 (16%)	21 (10%)	1	3
All	All	431/435 (99%)	314 (73%)	77 (18%)	40 (9%)	1	3

All (40) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	82	VAL
1	A	97	GLU
1	A	172	LYS
1	A	174	SER
1	A	216	GLU
2	B	44	ASN
2	B	140	SER
2	B	194	TRP
1	A	61	GLY
1	A	187	ASP
2	B	32	ASP
2	B	103	SER
2	B	132	PRO
2	B	134	SER
2	B	139	ASN
1	A	11	LEU
1	A	32	SER
1	A	44	PRO
1	A	58	LEU
1	A	63	PRO
2	B	2	VAL
2	B	33	TYR
2	B	74	THR
2	B	125	PRO
2	B	141	MET
1	A	25	ALA
1	A	29	VAL
1	A	88	ALA
1	A	95	ILE
2	B	42	PRO
2	B	104	SER
2	B	105	HIS
2	B	153	PRO
1	A	48	PRO
1	A	55	VAL
2	B	43	GLY
2	B	133	GLY
1	A	147	ILE
2	B	99	GLY
2	B	195	PRO

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	190/190 (100%)	163 (86%)	27 (14%)	3	17
2	B	194/194 (100%)	177 (91%)	17 (9%)	11	39
All	All	384/384 (100%)	340 (88%)	44 (12%)	6	25

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	THR
1	A	17	GLN
1	A	20	THR
1	A	21	ILE
1	A	23	CYS
1	A	27	LYS
1	A	34	TYR
1	A	37	MET
1	A	40	ASN
1	A	41	GLN
1	A	65	ARG
1	A	79	ILE
1	A	89	THR
1	A	95	ILE
1	A	99	LEU
1	A	111	ARG
1	A	128	LEU
1	A	146	ASP
1	A	148	ASN
1	A	150	LYS
1	A	160	ASN
1	A	178	MET
1	A	181	THR
1	A	182	LEU
1	A	184	LEU
1	A	191	ARG
1	A	214	ARG

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Mol	Chain	Res	Type
2	B	4	LEU
2	B	6	GLU
2	B	18	LEU
2	B	20	LEU
2	B	36	ASN
2	B	38	ILE
2	B	42	PRO
2	B	58	THR
2	B	64	LEU
2	B	79	PHE
2	B	116	THR
2	B	119	SER
2	B	130	LEU
2	B	135	LEU
2	B	183	LEU
2	B	194	TRP
2	B	217	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	GLN
1	A	127	GLN
1	A	160	ASN
1	A	164	ASN
1	A	192	HIS
1	A	193	ASN
1	A	201	HIS
2	B	44	ASN
2	B	177	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.