



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2016 – 09:54 PM GMT

PDB ID : 5BXF
Title : Apo FcRn Structure at pH 4.5
Authors : Nam, H.-J.; Taha, M.
Deposited on : 2015-06-08
Resolution : 2.85 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 : unknown
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026982
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) : rb-20026982

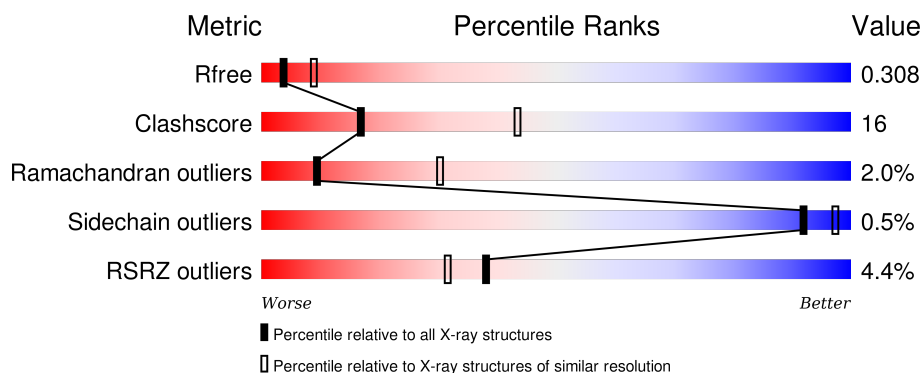
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.85 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	2228 (2.90-2.82)
Clashscore	102246	2499 (2.90-2.82)
Ramachandran outliers	100387	2439 (2.90-2.82)
Sidechain outliers	100360	2442 (2.90-2.82)
RSRZ outliers	91569	2236 (2.90-2.82)

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	300	<div> <div>2%</div> <div>67%19%12%</div> </div>
1	C	300	<div> <div>6%</div> <div>61%24%12%</div> </div>
2	B	119	<div> <div>66%17%17%</div> </div>
2	D	119	<div> <div>7%</div> <div>50%32%17%</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5797 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 IgG receptor FcRn large subunit p51.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	263	Total	C	N	O	S	0	0	0
			2069	1324	357	380	8			
1	C	263	Total	C	N	O	S	0	0	0
			2069	1324	357	380	8			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	268	VAL	-	expression tag	UNP P55899
A	269	ASP	-	expression tag	UNP P55899
A	270	HIS	-	expression tag	UNP P55899
A	271	HIS	-	expression tag	UNP P55899
A	272	HIS	-	expression tag	UNP P55899
A	273	HIS	-	expression tag	UNP P55899
A	274	HIS	-	expression tag	UNP P55899
A	275	HIS	-	expression tag	UNP P55899
A	276	VAL	-	expression tag	UNP P55899
A	277	ASP	-	expression tag	UNP P55899
C	268	VAL	-	expression tag	UNP P55899
C	269	ASP	-	expression tag	UNP P55899
C	270	HIS	-	expression tag	UNP P55899
C	271	HIS	-	expression tag	UNP P55899
C	272	HIS	-	expression tag	UNP P55899
C	273	HIS	-	expression tag	UNP P55899
C	274	HIS	-	expression tag	UNP P55899
C	275	HIS	-	expression tag	UNP P55899
C	276	VAL	-	expression tag	UNP P55899
C	277	ASP	-	expression tag	UNP P55899

- Molecule 2 is a protein called Beta-2-microglobulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	99	Total 829	C 528	N 140	O 158	S 3	0	0	0
2	D	99	Total 829	C 528	N 140	O 158	S 3	0	0	0

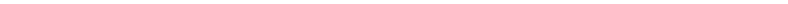

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	1	Total 1	O 1	0	0

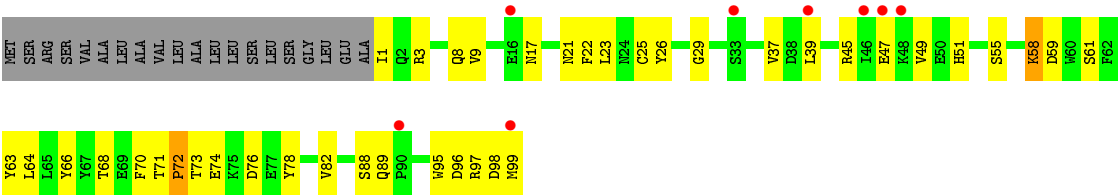
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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 ($\text{RSRZ} > 2$). 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.

- Chain A:
-
- 2% 67% 19% 12%
- MET GLY VAL PRO ARG PRO GLN TRP ALA LEU GLY LEU PHE LEU LEU SER HIS L5 S6 L11 S16 P17 A18 T21 V26 Y35 L36 C48 W51 W52 W53 W54 N55 Q56 W59 Y60 W61 E64 I70
- E77 K30 A81 L98 M102 F110 G114 M118 T126 R140 W141 Q142 Q143 Q144 D145 K146 K150 F154 S158 L163 H166 W176 P180 S181 K185 S190 P191 G192 F193 F203 Y204 P205 P206 E207 L208 Q209 L210 R211 N215 G216
- F234 L240 T241 V242 K243 S244 G245 V254 Q255 H256 A260 L267 VAL ASP HIS HIS HIS HIS HIS VAL ASP

- Chain C:
-
- 6% 61% 24% 12%
- Met GLY VAL PRO ARG PRO GLN GLY LEU LEU PHE LEU LEU PRO GLY SER LEU LEU GLY LEU GLU SER HIS L5 S6 L7 A18 T21 P22 V26 S27 G28 V29 L36 S37 Y38 L41 W33 V37 S38 W39 V57 S58 S59 R71 E77 A78 A81 G84 K85 T89 G89 P100 T103 L112 N113 G114 F117 D121 L122 K123 G125 G128 G129 D130 I137 S138 Q139 R140 Q141 Q142 Q144 Q145 K146 K147 A148 E151 L152 L156 C159 P160 L163 R164 S181 K185 S189 S190 G192 T197

- Chain B: 
- 

- Chain D: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	42.18Å 77.58Å 140.55Å 90.00° 93.60° 90.00°	Depositor
Resolution (Å)	46.76 – 2.85 46.76 – 2.85	Depositor EDS
% Data completeness (in resolution range)	99.3 (46.76-2.85) 79.8 (46.76-2.85)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.48 (at 2.86Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.237 , 0.314 0.238 , 0.308	Depositor DCC
R_{free} test set	1046 reflections (5.15%)	DCC
Wilson B-factor (Å ²)	45.9	Xtriage
Anisotropy	0.601	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 29.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 21222 reflections	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	5797	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 16.57% 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, 0.375 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	0.52	0/2134	0.72	2/2900 (0.1%)
1	C	0.52	0/2134	0.78	3/2900 (0.1%)
2	B	0.53	0/852	0.67	0/1152
2	D	0.46	0/852	0.65	0/1152
All	All	0.51	0/5972	0.72	5/8104 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	C	0	4
All	All	0	6

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	5	LEU	CA-CB-CG	6.76	130.85	115.30
1	C	217	LEU	CA-CB-CG	6.42	130.06	115.30
1	A	216	GLY	N-CA-C	-5.59	99.12	113.10
1	C	215	ASN	N-CA-C	-5.17	97.04	111.00
1	C	85	LYS	CD-CE-NZ	5.10	123.44	111.70

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	144	GLN	Peptide
1	A	243	LYS	Peptide

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Mol	Chain	Res	Type	Group
1	C	112	LEU	Peptide
1	C	123	LYS	Peptide
1	C	248	HIS	Peptide
1	C	249	HIS	Peptide

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	2069	0	1983	52	0
1	C	2069	0	1983	101	1
2	B	829	0	794	14	0
2	D	829	0	794	34	0
3	C	1	0	0	0	0
All	All	5797	0	5554	186	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 (186) 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:C:217:LEU:HD21	1:C:219:ALA:CB	1.40	1.50
1:C:208:LEU:HD12	1:C:255:GLN:O	1.40	1.15
1:C:249:HIS:NE2	1:C:251:CYS:SG	2.19	1.15
1:C:217:LEU:HG	1:C:219:ALA:N	1.64	1.12
1:C:217:LEU:CD2	1:C:219:ALA:CB	2.29	1.10
1:C:249:HIS:CD2	1:C:251:CYS:SG	2.52	1.02
1:C:217:LEU:CD2	1:C:219:ALA:HB2	1.88	1.01
1:A:208:LEU:HD13	1:A:256:HIS:HB2	1.42	0.98
1:C:217:LEU:HD21	1:C:219:ALA:HB2	0.93	0.92
1:C:251:CYS:SG	1:C:266:GLU:OE1	2.28	0.92
2:D:88:SER:OG	2:D:89:GLN:OE1	1.86	0.92
1:C:214:ARG:HH22	1:C:249:HIS:HD2	1.14	0.91
1:C:217:LEU:HD21	1:C:219:ALA:HB3	1.48	0.91
1:A:11:LEU:HG	1:A:26:VAL:HG22	1.53	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:11:LEU:HG	1:A:26:VAL:CG2	2.01	0.89
1:C:208:LEU:HD13	1:C:256:HIS:HB2	1.50	0.89
1:C:217:LEU:HG	1:C:218:ALA:C	1.94	0.87
1:C:217:LEU:CG	1:C:219:ALA:N	2.37	0.86
1:C:123:LYS:CG	1:C:124:GLN:H	1.85	0.86
1:A:208:LEU:CD1	1:A:256:HIS:HB2	2.06	0.84
1:C:217:LEU:HG	1:C:219:ALA:H	1.42	0.84
1:C:214:ARG:HH22	1:C:249:HIS:CD2	1.95	0.84
1:C:208:LEU:CD1	1:C:255:GLN:O	2.25	0.83
1:C:123:LYS:HG2	1:C:124:GLN:H	1.42	0.83
1:C:217:LEU:CD2	1:C:219:ALA:HB3	2.06	0.83
1:C:208:LEU:CD1	1:C:256:HIS:HB2	2.09	0.82
1:C:217:LEU:HG	1:C:218:ALA:N	1.96	0.81
1:C:160:PRO:HB2	1:C:164:ARG:HH12	1.47	0.80
1:C:214:ARG:HD2	1:C:250:TYR:HA	1.63	0.78
1:C:208:LEU:HD11	1:C:254:VAL:CG2	2.14	0.77
1:A:98:LEU:HD13	1:A:163:LEU:HD23	1.69	0.75
1:C:213:LEU:HD21	1:C:264:ARG:HH21	1.53	0.74
1:A:215:ASN:OD1	1:A:216:GLY:N	2.21	0.73
1:A:114:GLY:HA3	2:B:1:ILE:HD11	1.69	0.73
1:C:221:THR:O	1:C:238:SER:OG	2.08	0.72
1:C:185:LYS:NZ	2:D:98:ASP:HB3	2.06	0.71
1:A:55:ASN:HD21	1:C:181:SER:HA	1.56	0.71
1:C:217:LEU:CD2	1:C:219:ALA:N	2.54	0.70
2:D:17:ASN:HD21	2:D:74:GLU:HG3	1.56	0.70
1:C:217:LEU:HD21	1:C:219:ALA:CA	2.18	0.70
1:C:123:LYS:HG2	1:C:124:GLN:N	2.06	0.70
1:C:217:LEU:CG	1:C:218:ALA:N	2.54	0.70
1:C:208:LEU:HD11	1:C:254:VAL:HG23	1.73	0.69
1:C:214:ARG:O	1:C:217:LEU:N	2.26	0.69
2:D:64:LEU:HD21	2:D:66:TYR:CE1	2.29	0.68
1:A:208:LEU:HD12	1:A:255:GLN:O	1.94	0.68
1:C:222:GLY:HA2	1:C:240:LEU:HD13	1.77	0.66
1:C:81:ALA:HB2	1:C:140:ARG:HD2	1.77	0.66
1:C:77:GLU:OE1	1:C:144:GLN:NE2	2.28	0.65
1:C:121:ASP:OD1	1:C:122:LEU:N	2.28	0.65
1:A:208:LEU:HD11	1:A:254:VAL:CG2	2.29	0.63
1:C:217:LEU:HG	1:C:218:ALA:CA	2.29	0.62
1:A:11:LEU:HG	1:A:26:VAL:HG21	1.80	0.62
1:C:146:LYS:O	1:C:148:ALA:N	2.32	0.62
1:C:217:LEU:CD2	1:C:219:ALA:H	2.12	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:49:VAL:HG22	2:B:68:THR:HB	1.82	0.61
1:C:138:SER:O	1:C:142:GLN:HG3	2.00	0.60
1:C:214:ARG:NH2	1:C:214:ARG:HA	2.17	0.60
1:A:18:ALA:O	1:A:21:THR:HB	2.02	0.59
1:A:5:LEU:N	1:A:6:SER:HA	2.18	0.59
1:C:208:LEU:HD13	1:C:256:HIS:CB	2.28	0.59
2:B:77:GLU:HB3	2:B:94:LYS:HE3	1.83	0.59
1:C:84:GLY:HA2	1:C:85:LYS:HB2	1.85	0.59
1:C:247:GLU:O	1:C:250:TYR:N	2.37	0.58
1:C:160:PRO:HB2	1:C:164:ARG:NH1	2.19	0.58
1:C:211:ARG:NH2	1:C:221:THR:HG22	2.19	0.58
1:C:249:HIS:CE1	1:C:251:CYS:SG	2.97	0.58
1:C:217:LEU:CG	1:C:219:ALA:H	2.09	0.57
1:C:124:GLN:CG	1:C:125:GLY:H	2.17	0.57
1:A:185:LYS:NZ	2:B:98:ASP:OD2	2.25	0.57
1:C:213:LEU:HA	1:C:217:LEU:HB3	1.87	0.57
1:A:53:TRP:HB3	1:C:181:SER:OG	2.05	0.56
1:C:214:ARG:NH2	1:C:249:HIS:CD2	2.71	0.56
1:C:185:LYS:CE	2:D:98:ASP:HB3	2.36	0.56
1:A:81:ALA:HB2	1:A:140:ARG:HD3	1.88	0.56
1:A:11:LEU:CG	1:A:26:VAL:HG22	2.32	0.55
1:C:213:LEU:CD2	1:C:264:ARG:HH21	2.19	0.55
1:A:209:GLN:NE2	1:A:255:GLN:HE21	2.05	0.55
1:C:124:GLN:HG2	1:C:125:GLY:H	1.71	0.54
1:A:110:PHE:HB2	1:A:118:MET:HB3	1.88	0.54
2:D:58:LYS:N	2:D:58:LYS:HD2	2.23	0.54
2:D:59:ASP:OD1	2:D:61:SER:OG	2.22	0.54
1:C:28:GLY:HA3	1:C:36:LEU:HB3	1.88	0.54
1:C:217:LEU:HD12	1:C:218:ALA:H	1.73	0.54
2:D:29:GLY:HA2	2:D:61:SER:HB2	1.90	0.54
1:C:114:GLY:HA3	2:D:1:ILE:HG13	1.90	0.54
1:C:214:ARG:H	1:C:217:LEU:CB	2.22	0.53
1:A:77:GLU:OE2	1:A:144:GLN:NE2	2.42	0.53
1:C:189:SER:OG	1:C:190:SER:N	2.41	0.53
2:B:31:HIS:ND1	2:B:32:PRO:HA	2.24	0.52
1:A:208:LEU:HD13	1:A:256:HIS:CB	2.30	0.52
2:D:51:HIS:HB3	2:D:66:TYR:CD2	2.44	0.52
1:C:214:ARG:NH1	1:C:249:HIS:HB3	2.24	0.51
2:D:96:ASP:O	2:D:98:ASP:N	2.43	0.51
2:D:37:VAL:HG22	2:D:82:VAL:HG22	1.92	0.51
1:A:190:SER:OG	1:A:193:PHE:HB2	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:73:THR:HG23	2:D:76:ASP:H	1.75	0.50
1:A:36:LEU:HD12	1:A:61:TRP:HZ3	1.75	0.50
1:A:209:GLN:OE1	1:A:211:ARG:HD3	2.11	0.50
1:C:253:ILE:HD13	1:C:264:ARG:HA	1.94	0.50
1:C:21:THR:HG23	1:C:22:PRO:HD2	1.94	0.49
2:D:58:LYS:H	2:D:58:LYS:HD2	1.76	0.49
2:B:73:THR:HG22	2:B:75:LYS:H	1.77	0.49
1:A:11:LEU:HD12	1:A:26:VAL:HG13	1.94	0.49
1:A:209:GLN:HB3	1:A:255:GLN:HG2	1.94	0.49
2:D:70:PHE:CE1	2:D:78:TYR:CZ	3.01	0.49
1:C:197:THR:HG21	2:D:99:MET:HG2	1.94	0.49
2:D:49:VAL:HG22	2:D:68:THR:HB	1.95	0.48
2:D:17:ASN:ND2	2:D:74:GLU:HG3	2.25	0.48
1:A:5:LEU:O	1:A:5:LEU:HD23	2.12	0.48
1:A:192:GLY:O	1:A:244:SER:N	2.45	0.48
1:A:55:ASN:ND2	1:C:181:SER:HA	2.26	0.48
1:A:154:PHE:HA	1:A:158:SER:HB2	1.96	0.48
1:C:214:ARG:HD3	1:C:250:TYR:CD1	2.49	0.48
1:A:36:LEU:HD12	1:A:61:TRP:CZ3	2.48	0.48
1:A:206:PRO:HG3	1:A:234:PHE:CE1	2.49	0.48
1:A:35:TYR:OH	1:A:64:GLU:OE2	2.21	0.48
2:B:79:ALA:HB2	2:B:94:LYS:HD2	1.95	0.47
1:C:18:ALA:O	1:C:21:THR:HB	2.15	0.47
1:A:190:SER:OG	1:A:193:PHE:CD1	2.67	0.47
1:A:16:SER:O	1:A:16:SER:OG	2.24	0.47
1:C:226:PHE:O	2:D:8:GLN:NE2	2.41	0.46
1:C:214:ARG:H	1:C:217:LEU:HB3	1.79	0.46
2:D:21:ASN:OD1	2:D:22:PHE:N	2.44	0.46
2:D:71:THR:HA	2:D:72:PRO:HD2	1.73	0.46
1:C:245:GLY:N	1:C:247:GLU:OE1	2.38	0.46
1:C:214:ARG:NH2	1:C:249:HIS:HD2	1.95	0.46
1:C:211:ARG:HH22	1:C:221:THR:HG22	1.80	0.46
1:C:26:VAL:HB	1:C:38:TYR:HB3	1.97	0.46
1:A:241:THR:O	1:A:241:THR:HG23	2.14	0.46
1:C:57:VAL:HG11	1:C:59:TRP:CH2	2.51	0.45
1:A:143:GLN:O	1:A:145:ASP:N	2.49	0.45
1:A:181:SER:OG	1:C:53:TRP:HB3	2.16	0.45
1:C:223:GLN:HA	1:C:223:GLN:NE2	2.31	0.45
1:A:11:LEU:HA	1:A:26:VAL:HG22	1.98	0.45
1:A:80:LYS:HE3	1:A:140:ARG:HH22	1.81	0.45
1:C:7:LEU:HB2	1:C:163:LEU:HD13	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:55:SER:HB3	2:D:63:TYR:CE1	2.52	0.44
2:D:23:LEU:HA	2:D:23:LEU:HD12	1.84	0.44
2:B:77:GLU:HB3	2:B:94:LYS:CE	2.46	0.44
1:A:180:PRO:HB3	1:A:203:PHE:HB3	1.98	0.44
1:A:243:LYS:O	1:A:245:GLY:O	2.36	0.44
1:C:139:GLN:HA	1:C:142:GLN:HG3	1.99	0.44
2:D:45:ARG:HG2	2:D:47:GLU:HG3	1.98	0.44
2:B:38:ASP:OD1	2:B:45:ARG:NH1	2.51	0.44
1:C:122:LEU:HD23	1:C:152:LEU:HD23	2.00	0.44
2:D:9:VAL:HG12	2:D:95:TRP:CD1	2.53	0.44
1:C:122:LEU:HD22	1:C:156:LEU:HD21	1.99	0.43
2:B:73:THR:HB	2:B:76:ASP:HB2	2.00	0.43
1:A:126:THR:HG23	1:A:142:GLN:OE1	2.17	0.43
1:C:217:LEU:HD23	1:C:219:ALA:HB3	1.94	0.43
1:C:185:LYS:CE	2:D:98:ASP:CB	2.97	0.43
1:C:89:THR:N	1:C:113:ASN:OD1	2.52	0.43
1:C:114:GLY:HA3	2:D:1:ILE:CD1	2.48	0.42
1:A:56:GLN:OE1	1:A:56:GLN:HA	2.19	0.42
1:C:217:LEU:CD2	1:C:219:ALA:CA	2.89	0.42
2:D:51:HIS:HB3	2:D:66:TYR:CE2	2.54	0.42
1:A:209:GLN:O	1:A:210:LEU:HD23	2.19	0.42
1:A:60:TYR:OH	1:A:166:HIS:NE2	2.26	0.42
1:A:48:CYS:O	1:A:51:TRP:HB2	2.19	0.42
2:B:96:ASP:O	2:B:98:ASP:N	2.53	0.42
1:A:190:SER:HG	1:A:193:PHE:HD1	1.60	0.42
1:A:240:LEU:HD12	1:A:240:LEU:HA	1.96	0.42
2:D:70:PHE:HE1	2:D:78:TYR:CZ	2.37	0.41
1:C:185:LYS:HE2	2:D:98:ASP:CB	2.51	0.41
1:C:214:ARG:H	1:C:217:LEU:HB2	1.84	0.41
2:D:1:ILE:HD13	2:D:3:ARG:HG3	2.02	0.41
2:B:12:ARG:HG2	2:B:12:ARG:O	2.20	0.41
1:C:185:LYS:HZ1	2:D:98:ASP:HB3	1.85	0.41
2:B:12:ARG:HD2	2:B:13:HIS:CD2	2.56	0.41
2:D:25:CYS:HB2	2:D:39:LEU:HD21	2.02	0.41
1:C:217:LEU:CD1	1:C:218:ALA:H	2.34	0.41
1:C:208:LEU:HD13	1:C:256:HIS:CG	2.56	0.41
1:C:214:ARG:O	1:C:215:ASN:HB3	2.21	0.41
1:C:117:PHE:CD2	1:C:117:PHE:N	2.88	0.41
1:A:204:TYR:O	1:A:256:HIS:HE1	2.03	0.41
1:A:209:GLN:O	1:A:254:VAL:HA	2.21	0.41
1:C:214:ARG:HH21	1:C:214:ARG:HD2	1.65	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:8:GLN:NE2	2:D:26:TYR:HD2	2.18	0.40
1:A:146:LYS:HB3	1:A:150:LYS:HZ3	1.87	0.40
1:C:78:ALA:HB1	1:C:137:ILE:HG12	2.04	0.40
2:B:50:GLU:HB2	2:B:67:TYR:CE2	2.55	0.40
1:C:217:LEU:CG	1:C:218:ALA:H	2.30	0.40
1:C:71:LYS:HE3	1:C:151:GLU:OE2	2.21	0.40
1:C:214:ARG:CZ	1:C:249:HIS:HB3	2.51	0.40
1:C:27:SER:OG	1:C:29:TRP:NE1	2.45	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)
1:C:130:ASP:OD2	1:C:189:SER:OG[2_655]	2.06	0.14

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	261/300 (87%)	240 (92%)	17 (6%)	4 (2%)	13	38
1	C	261/300 (87%)	233 (89%)	21 (8%)	7 (3%)	6	22
2	B	97/119 (82%)	91 (94%)	5 (5%)	1 (1%)	19	49
2	D	97/119 (82%)	86 (89%)	9 (9%)	2 (2%)	9	29
All	All	716/838 (85%)	650 (91%)	52 (7%)	14 (2%)	9	30

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	100	PRO
1	C	113	ASN

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Mol	Chain	Res	Type
1	C	123	LYS
1	C	147	ALA
2	B	97	ARG
1	C	145	ASP
1	C	217	LEU
2	D	97	ARG
1	A	176	TRP
1	A	216	GLY
1	A	144	GLN
1	A	158	SER
1	C	221	THR
2	D	72	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	217/248 (88%)	216 (100%)	1 (0%)	92	97
1	C	217/248 (88%)	216 (100%)	1 (0%)	92	97
2	B	94/109 (86%)	94 (100%)	0	100	100
2	D	94/109 (86%)	93 (99%)	1 (1%)	80	94
All	All	622/714 (87%)	619 (100%)	3 (0%)	92	97

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	70	ILE
1	C	243	LYS
2	D	58	LYS

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

Mol	Chain	Res	Type
1	A	144	GLN

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Mol	Chain	Res	Type
1	A	255	GLN
1	C	223	GLN
1	C	249	HIS
2	D	17	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 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	263/300 (87%)	0.15	5 (1%) 70 66	19, 36, 66, 75	0
1	C	263/300 (87%)	0.40	19 (7%) 18 12	29, 47, 81, 90	0
2	B	99/119 (83%)	-0.06	0 100 100	21, 31, 48, 63	0
2	D	99/119 (83%)	0.33	8 (8%) 15 9	29, 46, 70, 75	0
All	All	724/838 (86%)	0.23	32 (4%) 38 31	19, 41, 71, 90	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	99	MET	3.7
1	C	219	ALA	3.6
2	D	46	ILE	3.4
1	C	58	SER	3.4
1	A	145	ASP	3.3
1	C	218	ALA	3.1
1	C	129	GLY	3.0
1	C	264	ARG	2.7
1	C	85	LYS	2.7
1	C	213	LEU	2.6
1	C	250	TYR	2.6
1	A	59	TRP	2.5
1	C	128	GLY	2.5
1	C	215	ASN	2.5
1	C	103	THR	2.5
2	D	16	GLU	2.5
1	C	190	SER	2.4
1	C	246	ASP	2.4
2	D	90	PRO	2.4
1	A	102	ASN	2.3
1	A	260	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
2	D	48	LYS	2.3
1	C	130	ASP	2.3
2	D	47	GLU	2.3
1	C	220	GLY	2.3
1	C	192	GLY	2.2
2	D	39	LEU	2.2
1	C	41	LEU	2.1
1	C	159	CYS	2.1
1	C	99	GLY	2.0
1	A	215	ASN	2.0
2	D	33	SER	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 carbohydrates 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.