WORLDWIDE PDB
PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:35 PM GMT

PDB ID	:	4FFV
Title	:	Crystal Structure of Dipeptidyl Peptidase IV (DPP4, DPP-IV, CD26) in Complex with 11A19 Fab
Authors	:	Wang, Z.; Sudom, A.; Walker, N.P.; Min, X.
Deposited on	:	2012-06-01
Resolution	:	2.40 Å(reported)

The following versions of software and data (see references ⓘ) were used in the production of this report:

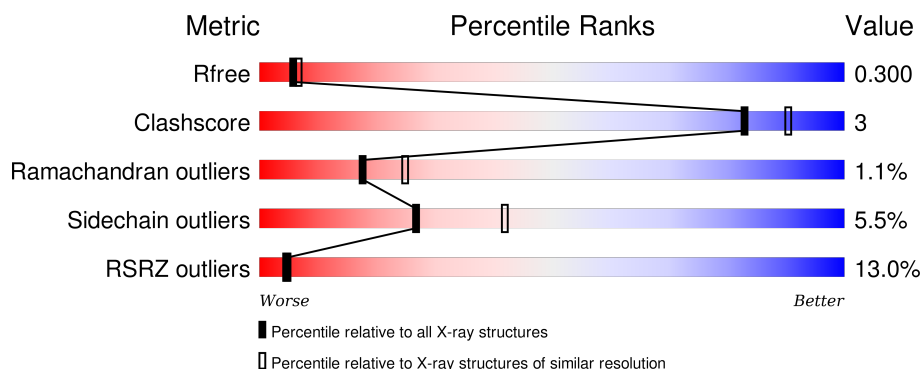|		
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
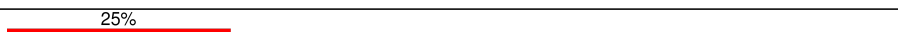*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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	Percentile Ranks	Value
Rfree		0.300
Clashscore		3
Ramachandran outliers		1.1%
Sidechain outliers		5.5%
RSRZ outliers		13.0%

Worse   *Better*

■ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	91344	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (2.40-2.40)

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 <=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	730	91% 8% •
1	B	730	88% 9% •
2	C	210	45% / 87% 10% ••
2	L	210	47% / 83% 14% ••
3	D	217	25% / 81% 12% • •

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Mol	Chain	Length	Quality of chain
3	H	217	

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 18423 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 Dipeptidyl peptidase 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	727	Total 5921	C 3792	N 980	O 1123	S 26	0	0	0
1	B	729	Total 5940	C 3804	N 985	O 1125	S 26	0	0	0

- Molecule 2 is a protein called 11A19 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	207	Total 1579	C 982	N 269	O 321	S 7	0	0	0
2	L	207	Total 1579	C 982	N 269	O 321	S 7	0	0	0

- Molecule 3 is a protein called 11A19 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	209	Total 1596	C 1017	N 259	O 315	S 5	0	0	0
3	H	209	Total 1595	C 1016	N 259	O 315	S 5	0	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	106	Total 106	O 106	0	0
4	B	100	Total 100	O 100	0	0
4	C	4	Total 4	O 4	0	0
4	D	3	Total 3	O 3	0	0

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: Dipeptidyl peptidase 4

Chain A:

- Molecule 1: Dipeptidyl peptidase 4

Chain B:

- Molecule 2: 11A19 Fab light chain

Chain C:

- Molecule 2: 11A19 Fab light chain

Chain L:

47%

83%

14%

Q1 I2 V3 Q6 S7 P8 L11 S12 A13 G16 E17 K18 V19 T20 M21 T22 C23 K44 P45 W46 L47 H48 N52 L53 A54 S55 G56 V57 F61 S62 G63 S64 G65 S66 G67 F70 S75 R76 V77 E78 A79 A82 Y85 Q89 W90 P95 G100

T101 K102 L103 E104 I105 D106 A110 A111 P112 T113 V114 S115 I116 P119 S120 S121 E122 T125 S126 G127 A128 A129 S130 V131 V132 C133 F134 L135 N136 N137 F138 Y139 P140 K141 D142 I143 N144 V145 K146 W147 K148 I149 D150 G151 S152 E153 ARG GLN ASN G157 V158 L159 N160 S161 W162 T163 D164

Q165 D166 S167 K168 D169 S170 M174 S175 S176 T177 L178 T179 L180 T181 K182 D183 E184 Y185 E186 R187 H188 N189 S190 Y191 T192 C193 E194 A195 T196 H197 K198 T199 S200 T201 S202 P203 I204 V205 K206 S207 F208 N209 R210

● Molecule 3: 11A19 Fab heavy chain

Chain D:

25%

81%

12%

E1 F2 L11 V12 V18 K19 I20 S25 G26 Y27 S28 F29 T30 N33 N41 I52 K67 S75 A79 C96 T97 R98 F99 R100 D101 V102 F103 F104 D105 V106 T111 K119 Y126 P127 L128 A129 P130 VAL CYS GLY GLY THR THR GLY SER S139 V140

T141 L142 G143 C144 L145 V146 Y149 F150 P151 E152 P153 V154 T157 G161 S162 L163 S164 S165 G166 V167 H168 L173 L174 G177 L178 Y179 S182 V185 T186 V187 T188 S189 W192 P193 S194 I197 N200 P204 A205 S206 S207 T208 K209 V210 K213 I214 V215 P216

R217

● Molecule 3: 11A19 Fab heavy chain

Chain H:

23%

82%

11%

E1 F2 V12 K13 V18 K19 I20 S25 G26 Y27 S28 F29 T30 D31 Y32 V51 T58 K67 C96 T97 R98 F99 R100 D101 V102 F103 F104 D105 V106 T111 K119 Y126 P127 L128 A129 P130 V131 CYS GLY GLY THR THR GLY SER S139 V140 T141 L142 G143 C144

L145 V146 F150 P151 E152 P153 V154 T157 G161 S162 LEU S164 S165 G166 V167 H168 T169 L173 L174 Q175 S176 G177 L178 Y179 T180 L181 S184 V185 T186 S189 W192 P193 S194 Q195 T196 I197 N200 V201 A202 T208 K209 V210 K213 I214 V215 P216 R217

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	97.26Å 201.72Å 97.28Å 90.00° 93.71° 90.00°	Depositor
Resolution (Å)	30.00 – 2.40 30.01 – 2.40	Depositor EDS
% Data completeness (in resolution range)	98.5 (30.00-2.40) 98.5 (30.01-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	2.18 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.271 , 0.301 0.272 , 0.300	Depositor DCC
R_{free} test set	7289 reflections (5.35%)	DCC
Wilson B-factor (Å^2)	36.4	Xtriage
Anisotropy	0.141	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 10.4	EDS
Estimated twinning fraction	0.477 for l,-k,h	Xtriage
L-test for twinning[2]	$< |L| > = 0.48, < L^2 > = 0.31$	Xtriage
Outliers	0 of 143426 reflections	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	18423	wwPDB-VP
Average B, all atoms (Å^2)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.15% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

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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	0.30	0/6090	0.53	0/8280
1	B	0.30	0/6109	0.54	0/8305
2	C	0.30	0/1619	0.48	0/2201
2	L	0.31	0/1619	0.48	0/2201
3	D	0.30	0/1636	0.49	0/2234
3	H	0.30	0/1634	0.47	0/2230
All	All	0.30	0/18707	0.52	0/25451

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
2	C	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	99	GLY	Peptide

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	5921	0	5658	22	0
1	B	5940	0	5682	43	0
2	C	1579	0	1503	6	0
2	L	1579	0	1503	11	0
3	D	1596	0	1571	14	0
3	H	1595	0	1568	16	0
4	A	106	0	0	1	0
4	B	100	0	0	4	0
4	C	4	0	0	0	0
4	D	3	0	0	0	0
All	All	18423	0	17485	110	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 3.

All (110) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:112:VAL:HG23	1:B:135:LEU:HD21	1.69	0.75
3:H:150:PHE:HB3	3:H:151:PRO:HD3	1.74	0.69
1:A:191:VAL:HG12	1:A:192:ILE:HD12	1.73	0.69
1:A:607:GLN:NE2	4:A:849:HOH:O	2.29	0.64
1:B:607:GLN:NE2	4:B:838:HOH:O	2.28	0.62
1:A:182:ARG:NH1	1:A:184:THR:O	2.33	0.61
1:A:170:ILE:H	1:A:184:THR:HG22	1.67	0.60
1:B:130:TYR:CZ	1:B:153:ILE:HD11	2.36	0.60
3:H:51:VAL:HG22	3:H:58:THR:HG22	1.83	0.59
3:H:98:ARG:O	3:H:104:PHE:HA	2.03	0.59
1:B:67:LEU:HB3	1:B:74:ILE:HD11	1.84	0.59
1:B:503:LYS:O	1:B:504:MET:HB2	2.03	0.59
1:B:47:LEU:HD22	1:B:750:GLN:HA	1.86	0.57
1:B:518:ILE:HD12	1:B:613:GLN:HG3	1.87	0.56
1:B:94:GLU:OE1	3:D:33:ASN:ND2	2.38	0.56
2:C:35:TYR:HE1	2:C:88:GLN:HE21	1.52	0.56
3:H:154:VAL:HG13	3:H:154:VAL:O	2.06	0.56
1:B:121:GLN:NE2	4:B:897:HOH:O	2.38	0.56
1:A:47:LEU:HD22	1:A:750:GLN:HA	1.87	0.55
1:B:383:CYS:HB3	1:B:397:PHE:CD1	2.41	0.55
3:H:192:TRP:O	3:H:195:GLN:N	2.39	0.54
1:A:169:ASP:OD1	1:A:184:THR:HG23	2.07	0.54
1:B:601:THR:HG23	1:B:602:LEU:N	2.24	0.53
1:B:74:ILE:CG2	1:B:88:LEU:HB3	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:12:VAL:HG11	3:D:18:VAL:HG22	1.91	0.53
1:B:127:THR:HG23	1:B:149:ASN:HA	1.91	0.52
1:B:503:LYS:O	1:B:504:MET:CB	2.57	0.52
1:B:544:LEU:HD12	1:B:568:LEU:HD13	1.90	0.52
2:L:46:TRP:CZ3	2:L:57:VAL:HG13	2.45	0.52
3:H:169:THR:CG2	3:H:169:THR:O	2.59	0.51
3:D:20:ILE:HD12	3:D:111:THR:HB	1.93	0.51
1:B:427:PRO:O	1:B:430:ARG:NH2	2.44	0.50
1:B:148:ASN:HB3	1:B:149:ASN:HD22	1.76	0.50
3:H:12:VAL:HG11	3:H:18:VAL:HG13	1.94	0.49
1:B:711:ASN:C	1:B:711:ASN:HD22	2.16	0.49
1:B:130:TYR:OH	1:B:153:ILE:HD11	2.12	0.49
1:A:409:GLU:HG3	1:A:462:LEU:HD12	1.95	0.49
1:B:233:LEU:HD13	1:B:251:TRP:CD1	2.48	0.49
3:D:12:VAL:HG21	3:D:18:VAL:CG2	2.43	0.49
3:H:130:PRO:O	3:H:131:VAL:HB	2.13	0.49
1:A:544:LEU:HD12	1:A:568:LEU:HD13	1.94	0.49
3:D:151:PRO:O	3:D:152:GLU:HB2	2.13	0.49
3:D:149:TYR:CE2	3:D:154:VAL:HG21	2.48	0.49
1:B:58:LEU:O	1:B:58:LEU:HD23	2.13	0.49
1:B:153:ILE:HG23	1:B:164:TYR:HB3	1.94	0.48
1:B:601:THR:HG23	1:B:602:LEU:HG	1.95	0.48
3:H:194:SER:C	3:H:195:GLN:HE21	2.18	0.47
2:L:165:GLN:HG2	2:L:170:SER:HA	1.96	0.47
1:B:141:ILE:HD13	1:B:176:PRO:HB2	1.95	0.47
1:A:182:ARG:NH1	1:A:185:SER:HA	2.30	0.47
1:B:112:VAL:HG23	1:B:135:LEU:CD2	2.40	0.46
3:D:163:LEU:HD23	3:D:185:VAL:HG21	1.97	0.46
1:B:462:LEU:HD23	1:B:469:TYR:HB3	1.98	0.46
2:C:33:HIS:HB2	2:C:88:GLN:HB3	1.99	0.45
3:D:27:TYR:CE2	3:D:29:PHE:HA	2.51	0.45
1:A:235:GLU:HG2	1:A:251:TRP:HB3	1.98	0.45
1:B:213:TRP:CE2	1:B:301:VAL:HG13	2.52	0.44
3:D:153:PRO:HA	3:D:154:VAL:HB	1.99	0.44
2:L:47:LEU:CD2	2:L:53:LEU:HD23	2.48	0.44
3:D:98:ARG:O	3:D:104:PHE:HA	2.17	0.44
1:B:595:ILE:HG21	1:B:603:GLU:HG3	2.00	0.44
1:A:184:THR:HG21	1:A:194:ASN:CB	2.46	0.44
3:H:20:ILE:HD12	3:H:111:THR:CB	2.48	0.44
2:C:31:ASN:HA	2:C:31:ASN:HD22	1.61	0.44
3:H:142:LEU:HD11	3:H:185:VAL:CG1	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:39:ARG:HD2	1:B:508:VAL:HG12	1.99	0.43
3:D:150:PHE:HB3	3:D:151:PRO:HD3	1.99	0.43
1:B:488:ASP:O	1:B:489:GLN:HB2	2.18	0.43
1:A:409:GLU:HG2	1:A:460:VAL:HG13	2.00	0.43
1:A:319:ASN:C	1:A:319:ASN:HD22	2.22	0.43
1:B:754:SER:O	1:B:758:HIS:ND1	2.51	0.43
1:B:318:GLN:OE1	1:B:670:ARG:HD3	2.19	0.43
2:L:7:SER:HA	2:L:8:PRO:HA	1.93	0.43
1:A:303:TRP:CE2	1:A:309:ILE:HD12	2.54	0.42
3:H:152:GLU:N	3:H:153:PRO:CD	2.82	0.42
2:L:19:VAL:HG21	2:L:77:VAL:HG21	2.01	0.42
1:B:74:ILE:HG23	1:B:88:LEU:HB3	2.00	0.42
2:L:47:LEU:HD22	2:L:53:LEU:HD23	2.01	0.42
1:A:409:GLU:CG	1:A:462:LEU:HD12	2.49	0.42
1:B:241:ASP:HB3	4:B:820:HOH:O	2.20	0.42
1:A:449:ASP:O	1:A:450:LEU:C	2.58	0.42
1:A:318:GLN:OE1	1:A:670:ARG:HD3	2.20	0.42
1:B:392:GLU:O	1:B:394:VAL:HG23	2.19	0.42
3:D:33:ASN:ND2	3:D:52:ILE:HG22	2.35	0.42
2:L:65:GLY:HA3	2:L:70:PHE:HA	2.01	0.42
2:L:48:HIS:O	2:L:52:ASN:HB2	2.20	0.42
3:H:20:ILE:HD12	3:H:111:THR:HB	2.02	0.41
2:L:21:MET:HG3	2:L:101:THR:HG21	2.02	0.41
1:B:280:THR:HG22	4:B:821:HOH:O	2.20	0.41
2:C:181:THR:O	2:C:185:TYR:N	2.51	0.41
2:L:159:LEU:HD23	2:L:160:ASN:N	2.35	0.41
2:C:7:SER:HA	2:C:8:PRO:HA	1.92	0.41
2:L:90:TRP:CG	2:L:95:PRO:HB3	2.56	0.41
3:H:169:THR:HG22	3:H:169:THR:O	2.21	0.41
2:C:159:LEU:HD23	2:C:160:ASN:N	2.35	0.41
1:B:599:LEU:HD13	1:B:671:TYR:HB3	2.01	0.41
1:B:316:ARG:HD3	1:B:669:GLU:OE1	2.20	0.41
1:B:74:ILE:HG23	1:B:88:LEU:CB	2.51	0.41
3:D:142:LEU:HB2	3:D:214:ILE:HD13	2.03	0.41
1:A:547:VAL:HG21	1:A:636:VAL:HG11	2.02	0.41
1:B:598:ARG:HA	1:B:683:HIS:CD2	2.56	0.41
1:A:652:ILE:HG23	1:A:702:LEU:HB3	2.03	0.41
1:A:43:LEU:HD21	1:A:754:SER:HA	2.02	0.41
3:H:154:VAL:O	3:H:154:VAL:CG1	2.68	0.41
3:H:27:TYR:CE2	3:H:29:PHE:HA	2.57	0.40
3:D:129:ALA:O	3:D:217:ARG:NH2	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:153:ILE:CG2	1:B:164:TYR:HB3	2.52	0.40
1:B:601:THR:CG2	1:B:602:LEU:N	2.85	0.40
1:A:232:PRO:HB2	1:B:246:TYR:CZ	2.56	0.40
1:A:344:ILE:N	1:A:344:ILE:HD12	2.37	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	725/730 (99%)	693 (96%)	32 (4%)	0	100	100
1	B	727/730 (100%)	691 (95%)	31 (4%)	5 (1%)	26	38
2	C	203/210 (97%)	186 (92%)	14 (7%)	3 (2%)	13	17
2	L	203/210 (97%)	179 (88%)	20 (10%)	4 (2%)	9	11
3	D	205/217 (94%)	183 (89%)	12 (6%)	10 (5%)	3	1
3	H	203/217 (94%)	187 (92%)	12 (6%)	4 (2%)	9	11
All	All	2266/2314 (98%)	2119 (94%)	121 (5%)	26 (1%)	17	25

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	136	ASN
3	D	152	GLU
3	D	162	SER
1	B	393	GLN
1	B	504	MET
2	C	139	TYR
3	D	41	ASN
1	B	189	GLU

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Mol	Chain	Res	Type
3	D	150	PHE
3	D	153	PRO
2	L	53	LEU
2	L	75	SER
2	L	199	THR
3	H	130	PRO
3	H	150	PHE
1	B	391	PRO
2	C	82	ALA
2	L	76	ARG
1	B	148	ASN
3	D	127	PRO
3	D	161	GLY
3	H	153	PRO
3	D	102	VAL
3	D	154	VAL
3	D	185	VAL
3	H	192	TRP

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	648/651 (100%)	617 (95%)	31 (5%)	31	49
1	B	650/651 (100%)	613 (94%)	37 (6%)	25	40
2	C	181/184 (98%)	167 (92%)	14 (8%)	16	24
2	L	181/184 (98%)	170 (94%)	11 (6%)	23	36
3	D	184/189 (97%)	176 (96%)	8 (4%)	35	55
3	H	184/189 (97%)	174 (95%)	10 (5%)	27	43
All	All	2028/2048 (99%)	1917 (94%)	111 (6%)	27	42

All (111) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	54	LYS
1	A	86	ILE
1	A	88	LEU
1	A	139	GLN
1	A	148	ASN
1	A	174	ILE
1	A	227	ASN
1	A	244	LEU
1	A	248	LYS
1	A	270	ASN
1	A	291	VAL
1	A	319	ASN
1	A	332	THR
1	A	383	CYS
1	A	389	ARG
1	A	416	LEU
1	A	462	LEU
1	A	483	LEU
1	A	489	GLN
1	A	503	LYS
1	A	508	VAL
1	A	515	LEU
1	A	543	LEU
1	A	544	LEU
1	A	567	TYR
1	A	598	ARG
1	A	604	VAL
1	A	702	LEU
1	A	703	LEU
1	A	705	HIS
1	A	711	ASN
1	B	39	ARG
1	B	58	LEU
1	B	81	HIS
1	B	88	LEU
1	B	109	ARG
1	B	127	THR
1	B	140	LEU
1	B	153	ILE
1	B	154	THR
1	B	221	LEU
1	B	244	LEU
1	B	251	TRP

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Mol	Chain	Res	Type
1	B	280	THR
1	B	283	MET
1	B	301	VAL
1	B	316	ARG
1	B	376	LYS
1	B	411	LEU
1	B	414	ASP
1	B	424	LYS
1	B	430	ARG
1	B	437	LEU
1	B	446	LEU
1	B	453	GLU
1	B	474	ARG
1	B	508	VAL
1	B	515	LEU
1	B	523	THR
1	B	544	LEU
1	B	567	TYR
1	B	598	ARG
1	B	603	GLU
1	B	702	LEU
1	B	703	LEU
1	B	705	HIS
1	B	711	ASN
1	B	729	VAL
2	C	6	GLN
2	C	31	ASN
2	C	47	LEU
2	C	59	VAL
2	C	60	ARG
2	C	88	GLN
2	C	89	GLN
2	C	107	ARG
2	C	138	PHE
2	C	144	ASN
2	C	168	LYS
2	C	185	TYR
2	C	187	ARG
2	C	198	LYS
3	D	20	ILE
3	D	52	ILE
3	D	67	LYS

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Mol	Chain	Res	Type
3	D	100	ARG
3	D	103	PHE
3	D	119	LYS
3	D	128	LEU
3	D	208	THR
2	L	1	GLN
2	L	6	GLN
2	L	18	LYS
2	L	44	LYS
2	L	47	LEU
2	L	89	GLN
2	L	125	THR
2	L	137	ASN
2	L	168	LYS
2	L	189	ASN
2	L	199	THR
3	H	13	LYS
3	H	18	VAL
3	H	20	ILE
3	H	67	LYS
3	H	100	ARG
3	H	103	PHE
3	H	119	LYS
3	H	157	THR
3	H	195	GLN
3	H	208	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	ASN
1	A	81	HIS
1	A	177	HIS
1	A	227	ASN
1	A	270	ASN
1	A	319	ASN
1	A	436	GLN
1	A	442	ASN
1	A	456	GLN
1	A	484	HIS
1	A	573	ASN
1	A	711	ASN

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Mol	Chain	Res	Type
1	B	121	GLN
1	B	149	ASN
1	B	261	ASN
1	B	484	HIS
1	B	489	GLN
1	B	528	GLN
1	B	686	ASN
1	B	711	ASN
2	C	31	ASN
2	C	136	ASN
2	C	144	ASN
3	D	175	GLN
2	L	136	ASN
2	L	189	ASN
3	H	5	GLN
3	H	6	GLN
3	H	175	GLN
3	H	195	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no 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 (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å²)	Q<0.9
1	A	727/730 (99%)	-0.16	1 (0%)	95	95	14, 34, 58, 77	0
1	B	729/730 (99%)	-0.15	2 (0%)	94	94	14, 34, 57, 80	1 (0%)
2	C	207/210 (98%)	2.24	94 (45%)	0	0	41, 90, 146, 162	0
2	L	207/210 (98%)	2.27	98 (47%)	0	0	38, 95, 146, 156	0
3	D	209/217 (96%)	1.33	54 (25%)	1	1	36, 80, 118, 132	0
3	H	209/217 (96%)	1.24	49 (23%)	1	1	38, 77, 117, 124	0
All	All	2288/2314 (98%)	0.55	298 (13%)	5	4	14, 43, 124, 162	1 (0%)

All (298) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	195	ALA	14.5
2	C	201	THR	12.5
2	L	195	ALA	11.4
2	C	191	TYR	9.1
2	L	145	VAL	8.8
2	L	23	CYS	8.0
3	D	101	ASP	7.9
2	L	201	THR	7.7
2	L	110	ALA	7.6
3	D	194	SER	7.6
2	C	56	GLY	7.5
2	C	147	TRP	7.5
2	C	110	ALA	7.5
3	D	140	VAL	7.4
2	L	205	VAL	7.4
2	C	149	ILE	7.3
2	C	111	ALA	7.0
2	C	196	THR	7.0
2	L	56	GLY	6.2

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Mol	Chain	Res	Type	RSRZ
3	H	184	SER	6.2
3	D	200	ASN	6.1
2	C	131	VAL	5.9
2	C	13	ALA	5.9
2	L	179	THR	5.8
2	C	179	THR	5.8
2	L	147	TRP	5.8
3	H	140	VAL	5.7
2	L	103	LEU	5.6
2	C	139	TYR	5.6
2	L	208	PHE	5.6
2	C	205	VAL	5.5
3	H	101	ASP	5.4
3	H	164	SER	5.4
2	L	193	CYS	5.3
2	L	192	THR	5.3
2	C	189	ASN	5.2
2	L	13	ALA	5.2
2	L	111	ALA	5.2
3	H	177	GLY	5.2
2	L	194	GLU	5.2
3	H	106	VAL	5.1
3	H	126	TYR	5.0
2	C	55	SER	5.0
2	L	22	THR	5.0
3	D	192	TRP	5.0
2	L	131	VAL	4.9
2	C	183	ASP	4.9
2	C	145	VAL	4.9
2	L	128	GLY	4.9
2	L	140	PRO	4.9
2	L	209	ASN	4.8
3	D	162	SER	4.8
2	L	207	SER	4.7
2	L	196	THR	4.7
2	L	127	GLY	4.7
2	C	22	THR	4.7
2	L	149	ILE	4.7
2	C	11	LEU	4.6
3	H	166	GLY	4.6
2	L	11	LEU	4.6
3	D	2	PHE	4.6

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Mol	Chain	Res	Type	RSRZ
3	H	131	VAL	4.6
2	L	136	ASN	4.6
2	L	183	ASP	4.4
2	C	202	SER	4.4
2	C	152	SER	4.4
2	C	192	THR	4.4
2	L	189	ASN	4.4
2	L	139	TYR	4.4
2	L	146	LYS	4.3
2	C	23	CYS	4.3
2	L	191	TYR	4.3
2	L	168	LYS	4.2
3	D	187	VAL	4.2
2	L	204	ILE	4.2
3	H	179	TYR	4.2
2	L	133	CYS	4.2
2	C	208	PHE	4.2
2	C	62	SER	4.1
2	L	210	ARG	4.1
2	L	55	SER	4.1
2	L	148	LYS	4.1
3	D	145	LEU	4.1
2	L	143	ILE	4.0
2	C	182	LYS	4.0
2	C	204	ILE	4.0
2	L	100	GLY	4.0
3	H	168	HIS	4.0
3	H	174	LEU	4.0
3	D	106	VAL	4.0
2	C	203	PRO	3.9
2	C	194	GLU	3.9
3	D	163	LEU	3.9
3	H	96	CYS	3.9
2	C	210	ARG	3.8
2	C	188	HIS	3.8
2	C	103	LEU	3.8
2	L	16	GLY	3.8
2	C	132	VAL	3.8
3	H	213	LYS	3.8
2	C	136	ASN	3.8
2	C	82	ALA	3.7
2	L	79	ALA	3.7

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Mol	Chain	Res	Type	RSRZ
2	L	115	SER	3.7
3	H	25	SER	3.7
2	C	128	GLY	3.7
2	C	137	ASN	3.7
2	L	135	LEU	3.7
3	D	168	HIS	3.7
3	D	185	VAL	3.6
3	H	2	PHE	3.6
2	L	165	GLN	3.6
3	H	165	SER	3.6
2	C	117	PHE	3.6
3	D	173	LEU	3.6
3	D	151	PRO	3.6
2	C	8	PRO	3.5
3	H	210	VAL	3.5
3	D	193	PRO	3.5
2	L	12	SER	3.5
2	C	144	ASN	3.5
2	C	163	THR	3.5
2	L	159	LEU	3.5
2	L	151	GLY	3.4
2	C	199	THR	3.4
3	D	25	SER	3.4
2	L	62	SER	3.4
2	L	144	ASN	3.4
3	H	215	VAL	3.4
2	C	143	ILE	3.4
3	D	197	ILE	3.4
3	H	162	SER	3.4
3	H	197	ILE	3.4
2	C	159	LEU	3.3
3	D	153	PRO	3.3
3	D	179	TYR	3.3
2	L	203	PRO	3.3
3	D	150	PHE	3.3
2	C	187	ARG	3.3
2	C	64	SER	3.3
2	L	142	ASP	3.3
2	L	153	GLU	3.3
2	C	177	THR	3.2
2	C	193	CYS	3.2
2	C	165	GLN	3.2

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Mol	Chain	Res	Type	RSRZ
2	L	164	ASP	3.2
2	L	190	SER	3.2
3	D	205	ALA	3.2
2	L	114	VAL	3.2
3	D	174	LEU	3.1
3	D	149	TYR	3.1
3	D	126	TYR	3.1
3	D	127	PRO	3.1
2	C	207	SER	3.1
2	C	140	PRO	3.0
2	C	176	SER	3.0
3	D	207	SER	3.0
2	L	177	THR	3.0
3	H	142	LEU	3.0
2	L	188	HIS	3.0
3	D	213	LYS	3.0
3	D	165	SER	3.0
2	C	151	GLY	2.9
3	H	150	PHE	2.9
2	L	137	ASN	2.9
3	D	96	CYS	2.9
3	H	128	LEU	2.9
3	D	186	THR	2.9
3	D	130	PRO	2.9
2	L	130	SER	2.9
3	H	167	VAL	2.9
3	D	177	GLY	2.9
2	C	181	THR	2.9
2	L	176	SER	2.8
3	H	152	GLU	2.8
3	H	192	TRP	2.8
2	C	198	LYS	2.8
2	C	25	ALA	2.8
3	D	215	VAL	2.8
2	C	115	SER	2.8
3	D	100	ARG	2.8
3	H	157	THR	2.8
2	L	166	ASP	2.8
3	D	157	THR	2.8
3	H	186	THR	2.8
3	H	173	LEU	2.7
2	L	82	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
2	C	114	VAL	2.7
3	D	210	VAL	2.7
2	L	163	THR	2.7
2	C	65	GLY	2.7
2	C	178	LEU	2.7
2	C	46	TRP	2.7
2	C	54	ALA	2.7
2	C	85	TYR	2.7
3	D	161	GLY	2.7
2	C	209	ASN	2.7
2	L	105	ILE	2.7
3	D	142	LEU	2.7
3	D	75	SER	2.7
3	H	151	PRO	2.6
2	L	158	VAL	2.6
2	L	112	PRO	2.6
2	L	152	SER	2.6
2	C	158	VAL	2.6
3	D	20	ILE	2.6
2	C	116	ILE	2.6
2	L	141	LYS	2.6
2	L	61	PHE	2.6
2	L	197	HIS	2.6
2	L	120	SER	2.5
3	H	127	PRO	2.5
2	C	135	LEU	2.5
2	L	198	LYS	2.5
3	D	139	SER	2.5
2	L	85	TYR	2.5
3	H	146	VAL	2.5
2	C	164	ASP	2.5
2	C	146	LYS	2.5
2	C	80	GLU	2.5
2	C	10	ILE	2.5
2	C	133	CYS	2.5
2	L	3	VAL	2.5
2	L	119	PRO	2.5
2	L	48	HIS	2.5
2	L	101	THR	2.5
2	L	132	VAL	2.4
2	L	54	ALA	2.4
3	H	29	PHE	2.4

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Mol	Chain	Res	Type	RSRZ
2	C	48	HIS	2.4
3	H	145	LEU	2.4
2	C	162	TRP	2.4
3	H	194	SER	2.4
2	L	185	TYR	2.4
2	L	64	SER	2.4
3	H	32	TYR	2.4
2	L	106	ASP	2.4
2	C	153	GLU	2.4
2	L	187	ARG	2.4
3	D	146	VAL	2.4
3	H	209	LYS	2.4
2	C	106	ASP	2.4
2	C	109	ASP	2.4
3	H	30	THR	2.4
2	C	160	ASN	2.3
3	D	217	ARG	2.3
2	C	166	ASP	2.3
2	L	121	SER	2.3
2	L	65	GLY	2.3
2	C	172	TYR	2.3
3	H	217	ARG	2.3
2	L	46	TRP	2.3
3	D	30	THR	2.3
3	H	143	GLY	2.3
2	L	182	LYS	2.3
3	D	204	PRO	2.3
2	C	174	MET	2.3
2	C	66	SER	2.3
3	D	164	SER	2.2
3	H	176	SER	2.2
2	L	122	GLU	2.2
3	D	143	GLY	2.2
2	C	130	SER	2.2
2	L	134	PHE	2.2
2	C	50	THR	2.2
2	C	5	SER	2.2
2	C	12	SER	2.2
3	H	189	SER	2.2
2	L	138	PHE	2.2
1	B	391	PRO	2.2
1	B	758	HIS	2.2

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Mol	Chain	Res	Type	RSRZ
3	D	189	SER	2.2
3	D	178	LEU	2.2
2	L	174	MET	2.2
2	L	116	ILE	2.2
3	H	185	VAL	2.1
2	C	36	GLN	2.1
2	L	202	SER	2.1
1	A	68	TYR	2.1
2	C	141	LYS	2.1
2	C	150	ASP	2.1
2	L	180	LEU	2.1
3	D	11	LEU	2.1
2	C	167	SER	2.1
3	H	139	SER	2.1
3	H	202	ALA	2.1
3	H	200	ASN	2.1
2	L	67	GLY	2.1
3	D	166	GLY	2.1
2	C	121	SER	2.1
2	L	186	GLU	2.0
2	L	162	TRP	2.0
3	H	161	GLY	2.0
3	D	79	ALA	2.0
2	C	124	LEU	2.0
3	H	181	LEU	2.0
2	C	180	LEU	2.0
3	D	182	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.