Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 04:35 PM GMT

PDB ID	:	4FFW
Title	:	Crystal Structure of Dipeptidyl Peptidase IV (DPP4, DPP-IV, CD26) in Complex with Fab + sitagliptin
Authors	:	Wang, Z.; Sudom, A.; Walker, N.P.; Min, X.
Deposited on	:	2012-06-01
Resolution	:	2.90 Å(reported)

The following versions of software and data (see references (i)) 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 2.90 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		0.311
Clashscore		1
Ramachandran outliers		1.0%
Sidechain outliers		3.3%
RSRZ outliers		14.3%

Worse   *Better*

▮ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution
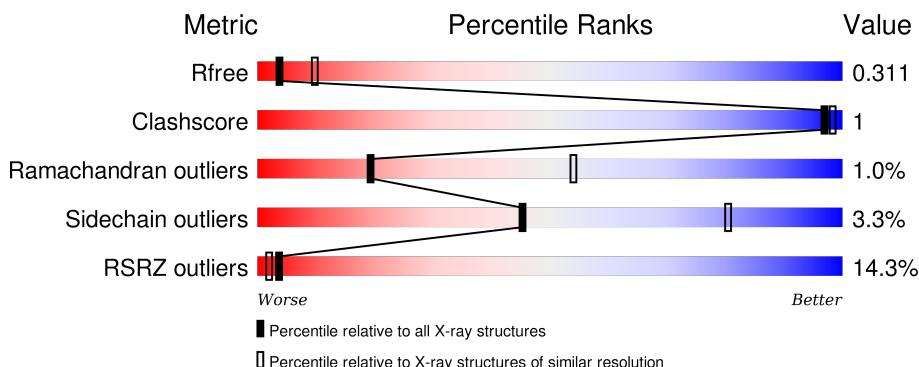
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	91344	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)

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	% 95% 5% ·
1	B	730	2% 94% 5%
2	C	210	44% 91% 7% ·
2	L	210	43% 91% 5% ·
3	D	217	31% 85% 10% · ·
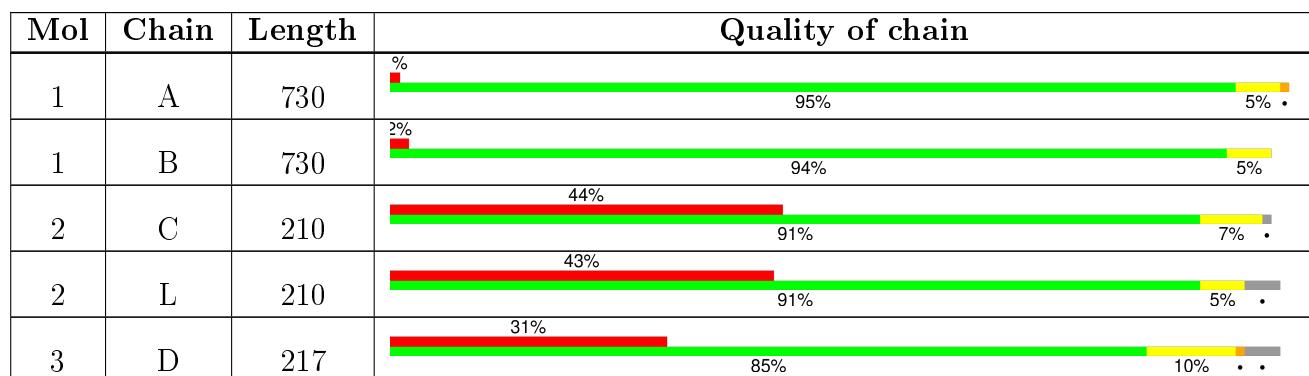
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Mol	Chain	Length	Quality of chain
3	H	217	24% 87% 8%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 18266 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 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	207	Total 1588	C 987	N 272	O 322	S 7	0	0	0
2	L	202	Total 1535	C 956	N 260	O 312	S 7	0	0	0

- Molecule 3 is a protein called Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	209	Total 1597	C 1019	N 259	O 314	S 5	0	0	0
3	H	208	Total 1590	C 1014	N 258	O 313	S 5	0	0	0

- Molecule 4 is (2R)-4-OXO-4-[3-(TRIFLUOROMETHYL)-5,6-DIHYDRO[1,2,4]TRIAZ OLO[4,3-A]PYRAZIN-7(8H)-YL]-1-(2,4,5-TRIFLUOROPHENYL)BUTAN-2-AMINE (three-letter code: 715) (formula: $C_{16}H_{15}F_6N_5O$).
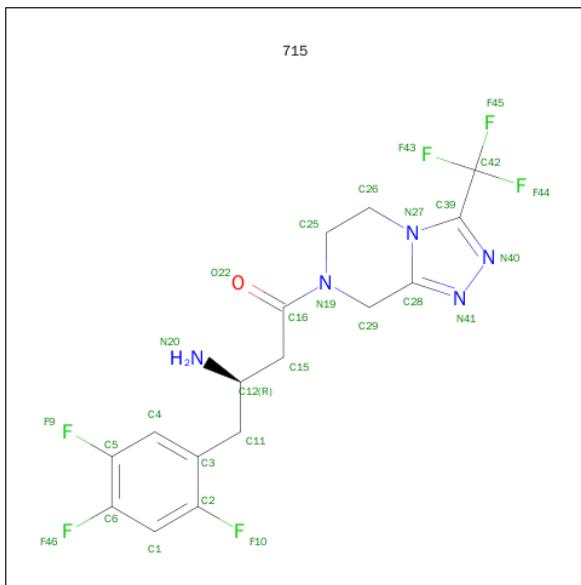
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	F	N	O	0	0
			28	16	6	5	1		
4	B	1	Total	C	F	N	O	0	0
			28	16	6	5	1		

• Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	27	Total	O	0	0
			27	27		
5	B	11	Total	O	0	0
			11	11		
5	C	1	Total	O	0	0
			1	1		

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
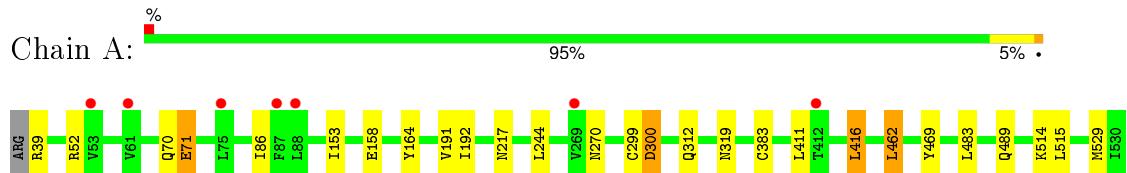
- Molecule 1: Dipeptidyl peptidase 4
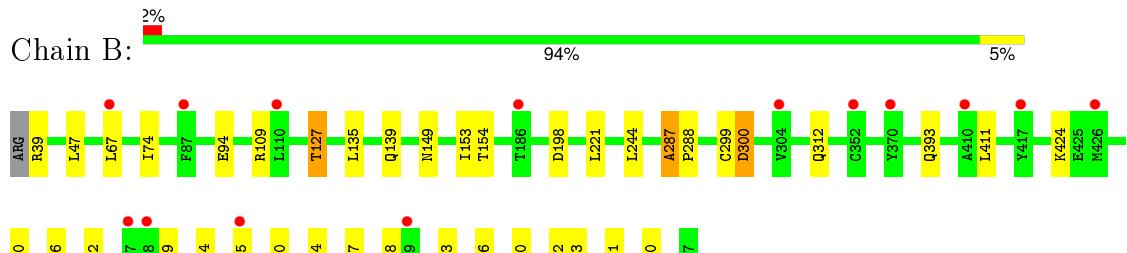
- Molecule 2: Fab light chain

- Molecule 2: Fab light chain

Q1 S7 P8 A9 I10 L11 S12 A13 K18 V19 T20 M21 T22 C23 V29 S40 W46 S55 G56 F61 S62 I74 S75 E78 A79 E80 D81 A82 Y85 F86 Q89 G98 G99 G100 T101 K102 L103 D106 R107 A108 D109 A110 A111 P112 T113 V114 S115

I116 F117 P118 P119 Q123 L124 T125 S126 G127 G128 A129 S130 V131 V132 C133 F134 L135 N136 N137 F138 Y139 P140 K141 D142 I143 N144 V145 K146 W147 K148 I149 D150 G151 S152 GLU ARG GLN ASN G157 V158 L159 W162 T163 D164 Q165 S173 M174 S175 S176 T177 L178 T179 K182 D183 E184 Y185

E186 N189 S190 Y191 T192 C193 E194 A195 T196 H197 K198 T199 S200 T201 S202 P203 I204 V205 K206 SER PHE ASN ARG

• Molecule 3: Fab heavy chain

Chain D:

31%

85% 10%

E1 F2 Q3 L4 I11 V12 V18 S25 G26 F29 T30 D31 Y32 N33 I34 N35 W36 M37 I52 P53 K54 Y55 G56 T57 V72 S75 L86 D90 C96 R100 D101 V102 F103 D104 D105 V106 T111 K119 Y126 P127 L128 A129 P130 V131 CYS GLY

GLY THR THR GLY SER SER V140 T141 L142 G143 C144 L145 V146 K147 F150 P151 E152 P153 V154 T155 L156 T157 G161 S162 L163 S164 S165 G166 V167 H168 L174 Y179 T180 L181 S183 S184 V185 T186 V187 W192 P193 S194 Q195 T196 I197 T198 C199 N200 V201 A202 A205 K209

V210 D211 K212 K213 I214 V215 P216 R217

• Molecule 3: Fab heavy chain

Chain H:

24%

87% 8%

E1 F2 Q3 L4 V12 V18 K19 I20 S25 F29 Q39 L45 E46 W47 I52 Q62 V72 C96 R100 D101 V102 F103 V106 S117 A118 K119 A122 V125 Y126 P127 L128 A129 P130 VAL CYS GLY GLY THR THR GLY SER SER V140 T141 L142

G143 C144 L145 V146 K147 G148 Y149 F150 P151 E152 T157 S160 G161 S162 L163 S164 S165 G166 L174 G177 L178 Y179 T180 L181 S184 V185 W192 P193 T196 N200 V201 A202 A205 D211 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	97.77Å 200.86Å 97.93Å 90.00° 93.64° 90.00°	Depositor
Resolution (Å)	29.99 – 2.90 29.99 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.1 (29.99-2.90) 98.7 (29.99-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	2.58 (at 2.90Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.287 , 0.311 0.286 , 0.311	Depositor DCC
R_{free} test set	4156 reflections (5.30%)	DCC
Wilson B-factor (Å^2)	68.8	Xtriage
Anisotropy	0.172	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 32.3	EDS
Estimated twinning fraction	0.450 for l,-k,h	Xtriage
L-test for twinning[2]	$< |L| > = 0.50, < L^2 > = 0.33$	Xtriage
Outliers	0 of 82544 reflections	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	18266	wwPDB-VP
Average B, all atoms (Å^2)	94.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.27% 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.

5   Model quality (i)

5.1   Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 715

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	0.26	0/6090	0.44	0/8280
1	B	0.26	0/6109	0.44	0/8305
2	C	0.27	0/1628	0.41	0/2213
2	L	0.26	0/1574	0.42	0/2143
3	D	0.27	0/1637	0.43	0/2236
3	H	0.27	0/1630	0.43	0/2226
All	All	0.26	0/18668	0.43	0/25403

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	5921	0	5658	10	0
1	B	5940	0	5682	12	0
2	C	1588	0	1515	4	0
2	L	1535	0	1466	2	0
3	D	1597	0	1575	11	0
3	H	1590	0	1566	9	0
4	A	28	0	15	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	28	0	15	0	0
5	A	27	0	0	0	0
5	B	11	0	0	0	0
5	C	1	0	0	0	0
All	All	18266	0	17492	45	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 1.

All (45) 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:287:ALA:HB1	1:B:288:PRO:HA	1.66	0.76
1:B:67:LEU:HB3	1:B:74:ILE:HD11	1.83	0.59
1:B:287:ALA:HB1	1:B:288:PRO:CA	2.31	0.58
3:H:12:VAL:HG11	3:H:18:VAL:HG13	1.86	0.57
1:A:547:VAL:HG21	1:A:636:VAL:HG11	1.88	0.56
3:D:163:LEU:HD23	3:D:185:VAL:HG21	1.87	0.56
3:H:150:PHE:HB3	3:H:151:PRO:HD3	1.88	0.54
3:H:163:LEU:HD23	3:H:185:VAL:HG21	1.90	0.53
1:B:547:VAL:HG21	1:B:636:VAL:HG11	1.92	0.52
1:A:191:VAL:HG12	1:A:192:ILE:HD12	1.91	0.51
1:B:299:CYS:O	1:B:300:ASP:HB2	2.10	0.51
1:B:462:LEU:HD23	1:B:469:TYR:HB3	1.92	0.50
1:B:299:CYS:O	1:B:300:ASP:CB	2.61	0.49
1:B:127:THR:HG23	1:B:149:ASN:HA	1.94	0.49
1:A:153:ILE:HG22	1:A:164:TYR:HB3	1.94	0.49
1:A:299:CYS:O	1:A:300:ASP:CB	2.60	0.48
1:B:139:GLN:HA	3:D:57:THR:HG23	1.96	0.48
3:D:150:PHE:HB3	3:D:151:PRO:HD3	1.95	0.48
1:A:462:LEU:HD23	1:A:469:TYR:HB3	1.95	0.47
3:D:52:ILE:HD11	3:D:55:TYR:CD1	2.50	0.46
1:A:529:MET:HE2	1:A:531:LEU:HD21	1.97	0.46
3:H:151:PRO:O	3:H:152:GLU:HB2	2.17	0.45
3:H:151:PRO:O	3:H:152:GLU:CB	2.65	0.45
3:H:4:LEU:HD13	3:H:106:VAL:HG11	1.99	0.45
3:D:154:VAL:O	3:D:154:VAL:HG13	2.17	0.45
1:A:411:LEU:HD13	1:A:416:LEU:CD2	2.48	0.44
2:C:19:VAL:HG21	2:C:77:VAL:HG21	2.00	0.44
1:A:70:GLN:O	1:A:71:GLU:HB2	2.18	0.44
1:B:94:GLU:OE1	3:D:33:ASN:ND2	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:161:GLY:O	3:D:163:LEU:N	2.52	0.43
3:D:4:LEU:HD13	3:D:106:VAL:HG11	2.01	0.42
3:H:39:GLN:HB2	3:H:45:LEU:HD23	2.02	0.42
3:H:150:PHE:O	3:H:151:PRO:C	2.57	0.42
2:L:61:PHE:CE1	2:L:74:ILE:HG23	2.55	0.42
1:B:47:LEU:HD22	1:B:750:GLN:HA	2.02	0.41
2:L:7:SER:HA	2:L:8:PRO:HA	1.95	0.41
3:H:174:LEU:HD11	3:H:177:GLY:HA2	2.03	0.41
1:A:70:GLN:O	1:A:71:GLU:CB	2.68	0.41
2:C:47:LEU:HD12	2:C:72:LEU:CD1	2.50	0.41
2:C:117:PHE:CD2	3:D:128:LEU:HB3	2.55	0.40
3:D:18:VAL:HG22	3:D:86:LEU:HD11	2.02	0.40
2:C:192:THR:HG22	2:C:194:GLU:HG3	2.02	0.40
3:D:156:LEU:HD13	3:D:201:VAL:HG22	2.02	0.40
1:A:411:LEU:HD13	1:A:416:LEU:HD23	2.03	0.40
1:B:530:ILE:HD12	1:B:530:ILE:N	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%)	680 (94%)	43 (6%)	2 (0%)	46	79
1	B	727/730 (100%)	683 (94%)	40 (6%)	4 (1%)	30	67
2	C	203/210 (97%)	177 (87%)	22 (11%)	4 (2%)	9	33
2	L	198/210 (94%)	173 (87%)	21 (11%)	4 (2%)	9	33
3	D	205/217 (94%)	179 (87%)	20 (10%)	6 (3%)	6	23
3	H	204/217 (94%)	186 (91%)	15 (7%)	3 (2%)	13	42
All	All	2262/2314 (98%)	2078 (92%)	161 (7%)	23 (1%)	19	54

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	300	ASP
1	B	300	ASP
3	D	152	GLU
3	D	162	SER
3	H	152	GLU
1	A	71	GLU
3	D	150	PHE
3	H	150	PHE
2	L	75	SER
1	B	198	ASP
1	B	393	GLN
2	C	82	ALA
1	B	287	ALA
2	C	137	ASN
2	C	76	ARG
2	L	137	ASN
2	C	99	GLY
2	L	98	GLY
3	D	102	VAL
2	L	99	GLY
3	D	151	PRO
3	D	187	VAL
3	H	102	VAL

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%)	625 (96%)	23 (4%)	43	78
1	B	650/651 (100%)	628 (97%)	22 (3%)	44	79
2	C	183/185 (99%)	177 (97%)	6 (3%)	45	80
2	L	177/185 (96%)	174 (98%)	3 (2%)	68	91
3	D	184/189 (97%)	179 (97%)	5 (3%)	52	84
3	H	183/189 (97%)	176 (96%)	7 (4%)	40	76

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2025/2050 (99%)	1959 (97%)	66 (3%)	45 80

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	ARG
1	A	52	ARG
1	A	86	ILE
1	A	158	GLU
1	A	217	ASN
1	A	244	LEU
1	A	270	ASN
1	A	312	GLN
1	A	319	ASN
1	A	383	CYS
1	A	416	LEU
1	A	462	LEU
1	A	483	LEU
1	A	489	GLN
1	A	514	LYS
1	A	515	LEU
1	A	543	LEU
1	A	544	LEU
1	A	628	TRP
1	A	698	GLN
1	A	702	LEU
1	A	703	LEU
1	A	711	ASN
1	B	39	ARG
1	B	109	ARG
1	B	127	THR
1	B	135	LEU
1	B	153	ILE
1	B	154	THR
1	B	221	LEU
1	B	244	LEU
1	B	312	GLN
1	B	411	LEU
1	B	424	LYS
1	B	430	ARG
1	B	446	LEU
1	B	474	ARG

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Mol	Chain	Res	Type
1	B	515	LEU
1	B	544	LEU
1	B	598	ARG
1	B	603	GLU
1	B	690	MET
1	B	702	LEU
1	B	703	LEU
1	B	711	ASN
2	C	18	LYS
2	C	76	ARG
2	C	89	GLN
2	C	125	THR
2	C	144	ASN
2	C	198	LYS
3	D	12	VAL
3	D	52	ILE
3	D	90	ASP
3	D	103	PHE
3	D	119	LYS
3	H	12	VAL
3	H	20	ILE
3	H	52	ILE
3	H	62	GLN
3	H	100	ARG
3	H	103	PHE
3	H	119	LYS
2	L	18	LYS
2	L	29	VAL
2	L	89	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	139	GLN
1	A	149	ASN
1	A	217	ASN
1	A	227	ASN
1	A	261	ASN
1	A	270	ASN
1	A	319	ASN
1	A	436	GLN
1	A	440	HIS

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Mol	Chain	Res	Type
1	A	442	ASN
1	A	456	GLN
1	A	484	HIS
1	A	489	GLN
1	A	711	ASN
1	B	124	HIS
1	B	261	ASN
1	B	341	GLN
1	B	440	HIS
1	B	711	ASN
2	C	6	GLN
2	C	36	GLN
3	H	62	GLN
3	H	84	ASN
2	L	136	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)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$\|Z\| > 2$	Counts	RMSZ	#$\|Z\| > 2$
4	715	A	801	-	28,30,30	0.68	0	28,45,45	1.75	4 (14%)
4	715	B	801	-	28,30,30	0.69	0	28,45,45	1.70	5 (17%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	715	A	801	-	-	0/18/27/27	0/2/3/3
4	715	B	801	-	-	0/18/27/27	0/2/3/3

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	801	715	C26-C25-N19	-3.92	106.04	110.48
4	B	801	715	C1-C2-C3	-3.42	119.78	124.13
4	A	801	715	C1-C2-C3	-3.34	119.88	124.13
4	B	801	715	C26-C25-N19	-2.90	107.19	110.48
4	B	801	715	F43-C42-C39	-2.31	108.84	111.32
4	A	801	715	C26-N27-C39	3.70	130.49	125.73
4	B	801	715	C26-N27-C39	3.86	130.69	125.73
4	A	801	715	C4-C3-C2	4.09	119.70	116.52
4	B	801	715	C4-C3-C2	4.42	119.96	116.52

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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(Å^2)	Q<0.9
1	A	727/730 (99%)	0.33	8 (1%)	82	80	36, 73, 104, 123	0
1	B	729/730 (99%)	0.33	14 (1%)	70	66	34, 74, 104, 123	0
2	C	207/210 (98%)	2.11	93 (44%)	0	0	89, 145, 190, 196	0
2	L	202/210 (96%)	2.10	90 (44%)	0	0	86, 138, 192, 200	0
3	D	209/217 (96%)	1.56	68 (32%)	1	0	83, 126, 163, 168	0
3	H	208/217 (95%)	1.33	53 (25%)	1	0	79, 124, 158, 167	0
All	All	2282/2314 (98%)	0.85	326 (14%)	4	2	34, 89, 169, 200	0

All (326) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	181	LEU	10.7
3	D	101	ASP	10.3
2	L	110	ALA	10.1
2	C	140	PRO	10.1
2	L	196	THR	8.8
2	C	115	SER	8.6
2	L	191	TYR	8.1
2	C	114	VAL	8.1
3	H	161	GLY	8.0
2	C	195	ALA	7.7
2	L	183	ASP	7.7
2	C	11	LEU	7.6
2	L	146	LYS	7.5
2	C	188	HIS	7.4
2	L	174	MET	7.4
2	C	79	ALA	7.4
3	D	146	VAL	7.3
2	C	23	CYS	7.2
2	L	203	PRO	7.2

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Mol	Chain	Res	Type	RSRZ
3	H	2	PHE	7.1
2	C	81	ASP	6.9
2	L	195	ALA	6.9
2	L	145	VAL	6.8
3	D	162	SER	6.8
2	L	131	VAL	6.8
2	L	133	CYS	6.6
3	D	163	LEU	6.5
3	H	150	PHE	6.4
2	C	110	ALA	6.4
2	L	116	ILE	6.3
2	L	147	TRP	6.2
2	C	149	ILE	6.1
2	L	140	PRO	6.0
2	C	177	THR	6.0
2	C	189	ASN	5.9
3	D	157	THR	5.8
2	C	139	TYR	5.8
3	H	163	LEU	5.7
3	H	192	TRP	5.7
2	C	62	SER	5.7
2	C	165	GLN	5.6
2	L	22	THR	5.6
3	D	131	VAL	5.5
2	C	164	ASP	5.5
3	D	213	LYS	5.5
3	D	151	PRO	5.4
2	C	133	CYS	5.3
3	H	140	VAL	5.3
2	C	196	THR	5.2
2	C	201	THR	5.1
2	C	184	GLU	5.1
3	D	196	THR	5.0
2	C	13	ALA	5.0
2	L	114	VAL	5.0
2	L	11	LEU	4.9
2	L	55	SER	4.9
2	C	145	VAL	4.9
2	L	192	THR	4.9
2	L	108	ALA	4.8
2	C	109	ASP	4.8
2	L	142	ASP	4.8

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Mol	Chain	Res	Type	RSRZ
2	C	12	SER	4.8
3	H	126	TYR	4.8
3	D	150	PHE	4.7
2	L	189	ASN	4.7
2	L	23	CYS	4.7
2	L	139	TYR	4.7
2	C	72	LEU	4.6
2	C	192	THR	4.5
2	L	165	GLN	4.5
3	H	151	PRO	4.5
2	C	191	TYR	4.5
2	C	179	THR	4.5
3	H	181	LEU	4.5
2	C	144	ASN	4.4
2	C	132	VAL	4.4
3	H	165	SER	4.3
2	L	141	LYS	4.3
2	L	62	SER	4.3
3	H	101	ASP	4.3
2	C	158	VAL	4.2
2	L	130	SER	4.2
2	L	202	SER	4.2
2	C	113	THR	4.2
3	H	142	LEU	4.1
3	D	185	VAL	4.1
2	L	176	SER	4.1
2	L	13	ALA	4.1
2	L	149	ILE	4.0
2	L	132	VAL	4.0
2	C	103	LEU	3.9
2	L	111	ALA	3.9
3	H	148	GLY	3.9
2	C	197	HIS	3.9
2	C	209	ASN	3.9
2	L	199	THR	3.8
3	H	164	SER	3.8
3	D	29	PHE	3.8
2	C	46	TRP	3.8
3	D	161	GLY	3.8
2	L	186	GLU	3.7
2	L	177	THR	3.7
3	H	185	VAL	3.7

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Mol	Chain	Res	Type	RSRZ
2	L	115	SER	3.7
3	H	127	PRO	3.7
3	H	193	PRO	3.7
3	D	105	ASP	3.6
2	C	198	LYS	3.6
2	C	138	PHE	3.6
2	C	190	SER	3.6
2	C	80	GLU	3.6
2	L	198	LYS	3.6
2	L	103	LEU	3.6
2	C	101	THR	3.5
3	D	1	GLU	3.5
3	H	72	VAL	3.5
2	C	128	GLY	3.5
2	C	159	LEU	3.5
3	D	106	VAL	3.5
2	L	182	LYS	3.5
2	C	82	ALA	3.5
3	H	200	ASN	3.5
3	D	182	SER	3.5
3	D	174	LEU	3.4
3	D	100	ARG	3.4
2	L	200	SER	3.4
3	D	144	CYS	3.4
2	L	194	GLU	3.4
2	L	12	SER	3.4
2	C	111	ALA	3.4
3	H	1	GLU	3.4
3	H	178	LEU	3.4
2	L	109	ASP	3.3
3	H	202	ALA	3.3
2	L	197	HIS	3.3
2	C	204	ILE	3.3
3	D	184	SER	3.3
2	C	194	GLU	3.3
2	L	143	ILE	3.3
3	D	34	ILE	3.3
2	C	130	SER	3.3
2	L	190	SER	3.3
3	H	128	LEU	3.3
2	C	163	THR	3.3
2	L	201	THR	3.3

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Mol	Chain	Res	Type	RSRZ
3	D	30	THR	3.3
3	H	184	SER	3.3
3	D	217	ARG	3.3
2	L	78	GLU	3.2
3	D	156	LEU	3.2
2	C	78	GLU	3.2
3	D	200	ASN	3.2
3	H	201	VAL	3.2
3	D	145	LEU	3.2
2	C	205	VAL	3.2
3	H	106	VAL	3.2
3	D	179	TYR	3.2
3	H	157	THR	3.2
3	D	215	VAL	3.1
3	H	146	VAL	3.1
2	L	164	ASP	3.1
2	L	135	LEU	3.1
3	D	25	SER	3.1
3	D	194	SER	3.1
2	L	21	MET	3.1
2	C	127	GLY	3.1
2	L	119	PRO	3.1
3	H	145	LEU	3.1
2	C	83	ALA	3.0
3	H	152	GLU	3.0
2	C	193	CYS	3.0
2	C	174	MET	3.0
2	C	22	THR	3.0
2	L	162	TRP	3.0
3	D	209	LYS	3.0
3	H	215	VAL	3.0
2	L	46	TRP	3.0
1	A	601	THR	3.0
3	H	130	PRO	3.0
3	D	36	TRP	3.0
2	L	101	THR	3.0
2	L	1	GLN	3.0
3	H	174	LEU	3.0
3	D	183	SER	2.9
2	C	16	GLY	2.9
3	D	2	PHE	2.9
3	H	96	CYS	2.9

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Mol	Chain	Res	Type	RSRZ
2	C	148	LYS	2.9
3	D	187	VAL	2.9
3	H	25	SER	2.9
2	L	179	THR	2.9
3	D	130	PRO	2.9
2	C	129	ALA	2.9
1	A	53	VAL	2.8
3	D	126	TYR	2.8
2	L	152	SER	2.8
2	C	168	LYS	2.8
3	H	162	SER	2.8
2	C	48	HIS	2.8
2	C	134	PHE	2.8
3	D	37	MET	2.8
2	L	204	ILE	2.7
2	L	86	PHE	2.7
3	D	53	PRO	2.7
2	C	104	GLU	2.7
2	C	49	GLY	2.7
2	L	128	GLY	2.7
2	C	162	TRP	2.7
2	L	81	ASP	2.7
2	L	40	SER	2.7
2	L	56	GLY	2.7
2	C	199	THR	2.7
2	L	151	GLY	2.6
3	H	141	THR	2.6
2	L	7	SER	2.6
3	D	192	TRP	2.6
3	H	18	VAL	2.6
2	C	208	PHE	2.6
3	H	196	THR	2.6
3	D	72	VAL	2.6
1	B	417	TYR	2.6
2	C	116	ILE	2.6
2	C	143	ILE	2.6
2	L	185	TYR	2.6
3	H	149	TYR	2.6
2	L	20	THR	2.6
2	L	163	THR	2.6
2	L	80	GLU	2.6
1	A	87	PHE	2.6

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Mol	Chain	Res	Type	RSRZ
2	C	131	VAL	2.6
2	L	125	THR	2.6
2	L	113	THR	2.6
3	D	11	LEU	2.6
2	L	117	PHE	2.5
3	D	199	CYS	2.5
2	C	55	SER	2.5
3	H	179	TYR	2.5
3	D	168	HIS	2.5
2	C	207	SER	2.5
1	B	467	LYS	2.5
3	H	102	VAL	2.5
3	H	166	GLY	2.5
3	D	152	GLU	2.5
3	D	142	LEU	2.5
3	H	205	ALA	2.5
1	B	87	PHE	2.5
3	D	102	VAL	2.5
2	L	85	TYR	2.5
3	D	211	ASP	2.5
3	H	117	SER	2.5
3	D	201	VAL	2.5
3	D	180	THR	2.4
2	L	136	ASN	2.4
2	C	61	PHE	2.4
3	H	29	PHE	2.4
3	D	193	PRO	2.4
1	B	426	MET	2.4
3	D	75	SER	2.4
2	L	205	VAL	2.4
3	D	4	LEU	2.4
2	C	15	PRO	2.4
2	C	44	LYS	2.4
3	D	167	VAL	2.4
2	L	173	SER	2.4
3	H	122	ALA	2.4
1	B	370	TYR	2.4
2	C	135	LEU	2.4
2	L	79	ALA	2.3
3	D	26	GLY	2.3
3	H	143	GLY	2.3
2	L	123	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
2	L	134	PHE	2.3
3	D	143	GLY	2.3
3	D	197	ILE	2.3
1	A	88	LEU	2.3
2	C	65	GLY	2.3
2	C	85	TYR	2.3
3	D	96	CYS	2.3
3	H	45	LEU	2.3
1	A	412	THR	2.3
1	B	352	CYS	2.2
1	B	186	THR	2.2
2	C	125	THR	2.2
3	D	155	THR	2.2
2	C	172	TYR	2.2
3	D	165	SER	2.2
1	B	110	LEU	2.2
2	L	10	ILE	2.2
1	B	67	LEU	2.2
2	L	82	ALA	2.2
1	A	75	LEU	2.2
1	B	468	TYR	2.2
2	C	147	TRP	2.2
1	B	410	ALA	2.2
2	L	106	ASP	2.1
3	D	31	ASP	2.1
1	A	269	VAL	2.1
3	H	125	VAL	2.1
2	C	38	LYS	2.1
2	L	193	CYS	2.1
2	C	154	ARG	2.1
2	C	203	PRO	2.1
2	L	124	LEU	2.1
2	C	136	ASN	2.1
2	C	54	ALA	2.1
2	C	108	ALA	2.1
3	D	111	THR	2.1
2	C	182	LYS	2.1
1	B	304	VAL	2.1
1	B	599	LEU	2.1
2	L	127	GLY	2.1
3	H	211	ASP	2.1
1	A	61	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
3	D	202	ALA	2.1
3	D	205	ALA	2.1
3	H	47	TRP	2.1
3	D	147	LYS	2.0
1	B	515	LEU	2.0
3	H	160	SER	2.0
2	L	129	ALA	2.0
2	C	58	PRO	2.0
2	C	176	SER	2.0
2	L	159	LEU	2.0
3	D	210	VAL	2.0
2	C	122	GLU	2.0
2	C	126	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 ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
4	715	A	801	28/28	0.89	0.22	-0.04	69,78,91,92	0
4	715	B	801	28/28	0.91	0.21	-0.07	68,76,89,89	0

6.5 Other polymers ⓘ

There are no such residues in this entry.