Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:36 PM GMT

PDB ID	:	4YFC
Title	:	Crystal structure of PTP delta Ig1-Ig2 in complex with IL1RAPL1
Authors	:	Yamagata, A.; Fukai, S.
Deposited on	:	2015-02-25
Resolution	:	2.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

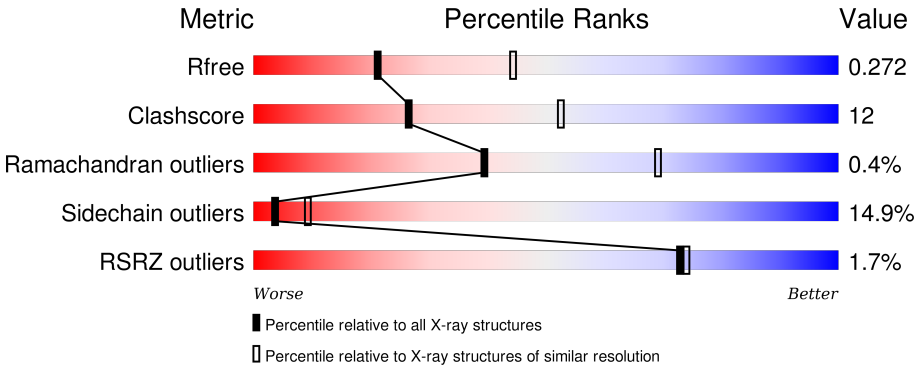
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.70 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	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)

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	B	348	% 62% 24% 6% 7%
2	A	305	% 44% 20% · 31%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 4428 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 Interleukin-1 receptor accessory protein-like 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	322	Total	C	N	O	S	0	0	0
			2591	1649	429	497	16			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	12	ALA	-	expression tag	UNP P59823
B	13	GLN	-	expression tag	UNP P59823
B	14	PRO	-	expression tag	UNP P59823
B	15	ALA	-	expression tag	UNP P59823
B	16	ALA	-	expression tag	UNP P59823
B	17	ARG	-	expression tag	UNP P59823
B	18	ASP	-	expression tag	UNP P59823
B	353	LYS	-	expression tag	UNP P59823
B	354	HIS	-	expression tag	UNP P59823
B	355	HIS	-	expression tag	UNP P59823
B	356	HIS	-	expression tag	UNP P59823
B	357	HIS	-	expression tag	UNP P59823
B	358	HIS	-	expression tag	UNP P59823
B	359	HIS	-	expression tag	UNP P59823

- Molecule 2 is a protein called Receptor-type tyrosine-protein phosphatase delta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	209	Total	C	N	O	S	0	0	0
			1617	999	294	318	6			

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	326	LYS	-	expression tag	UNP Q64487
A	327	HIS	-	expression tag	UNP Q64487

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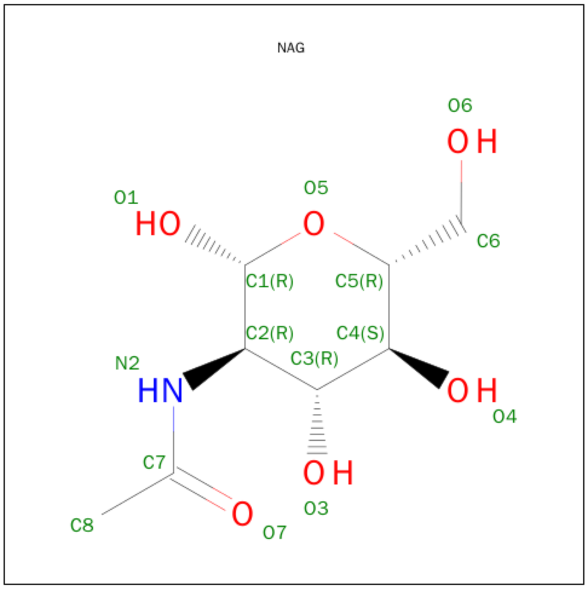
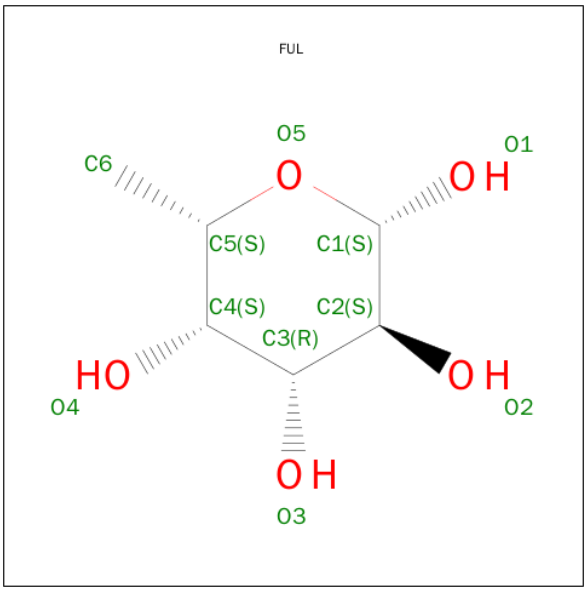
Chain	Residue	Modelled	Actual	Comment	Reference
A	328	HIS	-	expression tag	UNP Q64487
A	329	HIS	-	expression tag	UNP Q64487
A	330	HIS	-	expression tag	UNP Q64487
A	331	HIS	-	expression tag	UNP Q64487
A	332	HIS	-	expression tag	UNP Q64487

- Molecule 3 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



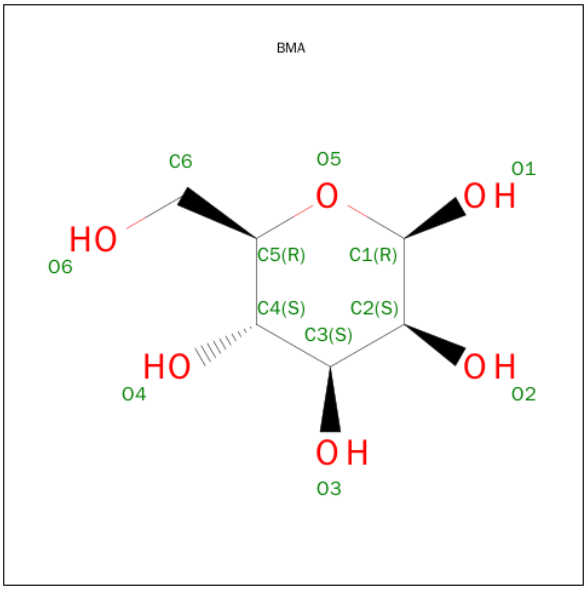
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total C N O 14 8 1 5	0	0
3	B	1	Total C N O 14 8 1 5	0	0
3	B	1	Total C N O 14 8 1 5	0	0
3	B	1	Total C N O 14 8 1 5	0	0
3	B	1	Total C N O 14 8 1 5	0	0
3	B	1	Total C N O 14 8 1 5	0	0
3	B	1	Total C N O 14 8 1 5	0	0
3	B	1	Total C N O 14 8 1 5	0	0

- Molecule 4 is BETA-L-FUCOSE (three-letter code: FUL) (formula: $C_6H_{12}O_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C O 10 6 4	0	0
4	B	1	Total C O 10 6 4	0	0

- Molecule 5 is BETA-D-MANNOSE (three-letter code: BMA) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total C O 11 6 5	0	0

- Molecule 6 is water.

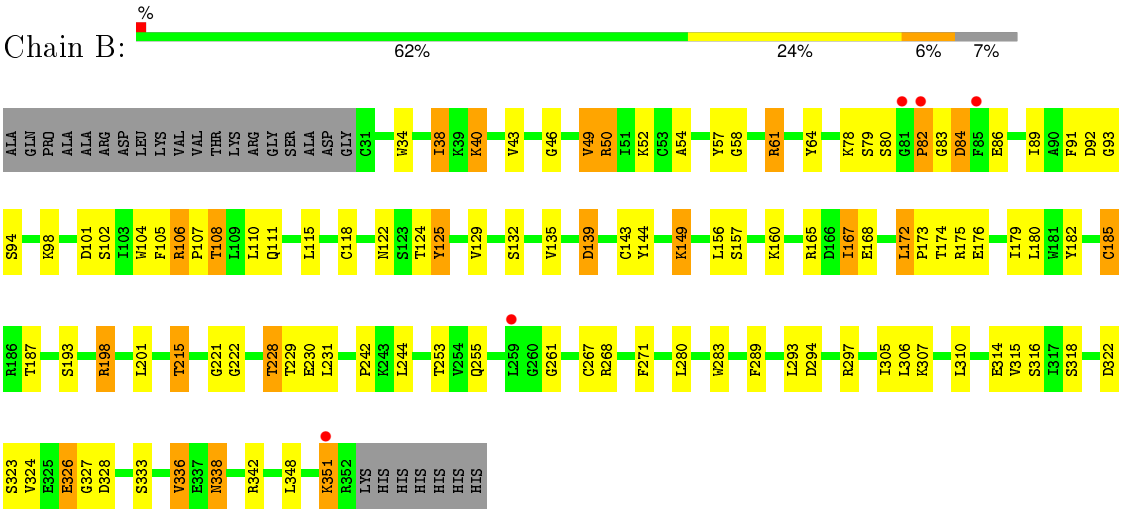
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	38	Total O 38 38	0	0
6	A	39	Total O 39 39	0	0

3 Residue-property plots (i)

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.

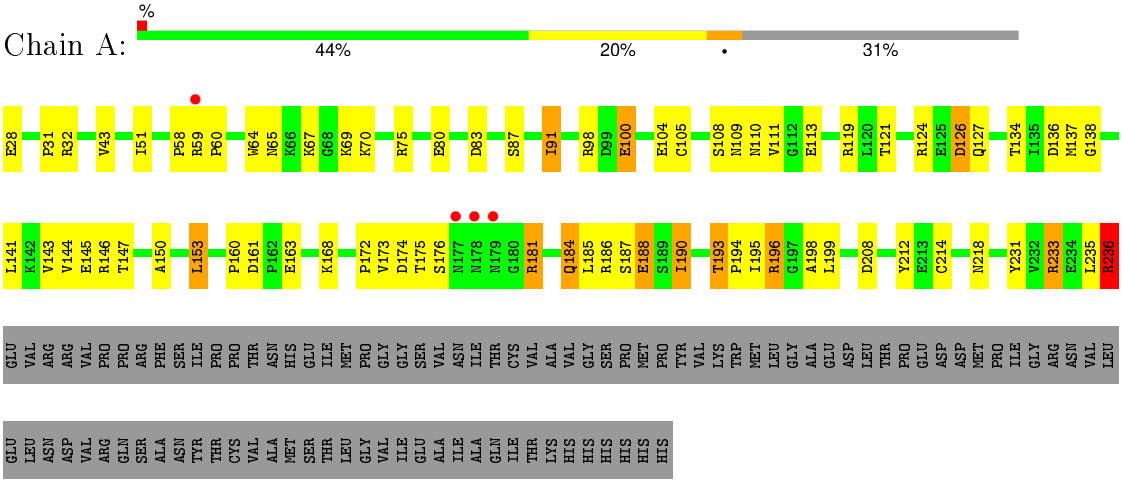
- Molecule 1: Interleukin-1 receptor accessory protein-like 1

Chain B:



- Molecule 2: Receptor-type tyrosine-protein phosphatase delta

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	162.97Å 81.17Å 91.48Å 90.00° 91.27° 90.00°	Depositor
Resolution (Å)	45.73 – 2.70 45.73 – 2.70	Depositor EDS
% Data completeness (in resolution range)	97.9 (45.73-2.70) 97.9 (45.73-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$< I/\sigma(I) >$ [1]	2.42 (at 2.69Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.226 , 0.263 0.242 , 0.272	Depositor DCC
R_{free} test set	1639 reflections (5.35%)	DCC
Wilson B-factor (Å^2)	40.2	Xtriage
Anisotropy	0.556	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 45.6	EDS
Estimated twinning fraction	0.003 for -h,-k,l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Outliers	0 of 32256 reflections	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	4428	wwPDB-VP
Average B, all atoms (Å^2)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.80% of the height of the origin peak. No significant pseudotranslation is detected.*

[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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FUL, BMA, NAG

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	B	0.27	0/2647	0.56	1/3576 (0.0%)
2	A	0.32	0/1646	0.67	2/2232 (0.1%)
All	All	0.29	0/4293	0.61	3/5808 (0.1%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	91	ILE	CG1-CB-CG2	5.58	123.68	111.40
2	A	236	ARG	NE-CZ-NH1	5.30	122.95	120.30
1	B	310	LEU	CA-CB-CG	5.28	127.45	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2591	0	2546	59	0
2	A	1617	0	1600	47	0
3	B	112	0	98	4	0
4	B	20	0	20	0	0
5	B	11	0	10	0	0
6	A	39	0	0	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	38	0	0	7	0
All	All	4428	0	4274	105	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 12.

All (105) 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:122:ASN:HB2	1:B:125:TYR:HB3	1.57	0.87
2:A:190:ILE:O	6:A:423:HOH:O	1.96	0.82
1:B:64:TYR:OH	6:B:501:HOH:O	1.94	0.82
1:B:144:TYR:HB3	1:B:228:THR:HG21	1.59	0.82
1:B:38:ILE:HD11	2:A:137:MET:HG2	1.59	0.81
1:B:101:ASP:OD1	6:B:532:HOH:O	1.98	0.81
1:B:306:LEU:HD11	1:B:316:SER:HB2	1.62	0.80
1:B:333:SER:OG	6:B:521:HOH:O	1.99	0.80
1:B:46:GLY:H	1:B:108:THR:HG22	1.49	0.78
2:A:236:ARG:HG3	2:A:236:ARG:HH11	1.47	0.77
1:B:122:ASN:HB3	1:B:124:THR:H	1.50	0.76
2:A:126:ASP:OD1	2:A:126:ASP:N	2.18	0.74
1:B:174:THR:O	6:B:533:HOH:O	2.06	0.72
1:B:84:ASP:OD1	1:B:84:ASP:N	2.25	0.70
3:B:405:NAG:H83	3:B:405:NAG:H3	1.72	0.69
1:B:297:ARG:NH2	1:B:328:ASP:OD1	2.27	0.68
2:A:184:GLN:OE1	6:A:417:HOH:O	2.14	0.66
2:A:98:ARG:NH1	6:A:436:HOH:O	2.29	0.65
1:B:326:GLU:N	1:B:327:GLY:HA3	2.12	0.65
2:A:80:GLU:OE2	6:A:414:HOH:O	2.13	0.65
1:B:49:VAL:HG23	1:B:105:PHE:HB2	1.81	0.62
1:B:78:LYS:HB2	1:B:89:ILE:HD11	1.83	0.61
2:A:190:ILE:HD11	2:A:193:THR:OG1	2.01	0.60
2:A:64:TRP:NE1	2:A:87:SER:OG	2.35	0.60
1:B:149:LYS:HD2	1:B:230:GLU:HB2	1.84	0.59
1:B:143:CYS:N	1:B:185:CYS:SG	2.75	0.59
1:B:326:GLU:H	1:B:327:GLY:HA3	1.67	0.59
1:B:92:ASP:OD1	1:B:94:SER:N	2.27	0.58
1:B:106:ARG:NH2	6:B:503:HOH:O	2.38	0.56
2:A:65:ASN:HB2	2:A:104:GLU:HG3	1.87	0.56
2:A:69:LYS:NZ	6:A:439:HOH:O	2.39	0.56
2:A:58:PRO:HG2	2:A:109:ASN:HB2	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:100:GLU:HG3	2:A:121:THR:HA	1.88	0.55
3:B:404:NAG:O4	6:B:518:HOH:O	2.18	0.55
1:B:297:ARG:NH1	6:B:513:HOH:O	2.41	0.54
2:A:193:THR:HG22	2:A:194:PRO:HD2	1.88	0.54
1:B:221:GLY:N	1:B:222:GLY:HA2	2.24	0.52
2:A:108:SER:HB3	2:A:113:GLU:HG3	1.92	0.51
1:B:38:ILE:HD11	2:A:137:MET:CG	2.36	0.50
1:B:50:ARG:HG3	1:B:104:TRP:CE2	2.47	0.50
1:B:54:ALA:HB3	1:B:129:VAL:HG11	1.94	0.49
1:B:242:PRO:HD3	1:B:338:ASN:HB3	1.94	0.49
2:A:28:GLU:HB3	2:A:111:VAL:HG21	1.95	0.49
1:B:139:ASP:HB2	1:B:144:TYR:O	2.12	0.49
1:B:182:TYR:HB2	1:B:215:THR:HG23	1.96	0.48
1:B:40:LYS:HG3	1:B:132:SER:HB3	1.94	0.48
2:A:187:SER:HB2	2:A:196:ARG:HB2	1.95	0.48
3:B:405:NAG:C8	3:B:405:NAG:H3	2.42	0.48
1:B:307:LYS:HB2	1:B:314:GLU:HB2	1.97	0.47
2:A:185:LEU:HD12	2:A:198:ALA:HB3	1.96	0.47
2:A:51:ILE:HD13	2:A:172:PRO:HG3	1.97	0.47
2:A:168:LYS:HD3	2:A:212:TYR:CZ	2.50	0.46
2:A:175:THR:HG21	2:A:184:GLN:HG3	1.97	0.46
2:A:146:ARG:O	2:A:147:THR:OG1	2.27	0.46
2:A:161:ASP:HB3	2:A:195:ILE:HD11	1.98	0.46
2:A:236:ARG:CG	2:A:236:ARG:HH11	2.23	0.46
2:A:31:PRO:O	2:A:32:ARG:NH1	2.41	0.46
1:B:261:GLY:O	1:B:324:VAL:HG23	2.15	0.46
2:A:136:ASP:OD2	2:A:194:PRO:HB3	2.16	0.46
1:B:82:PRO:HA	1:B:83:GLY:HA2	1.53	0.45
1:B:167:ILE:HD12	1:B:167:ILE:HA	1.77	0.45
2:A:236:ARG:HG3	2:A:236:ARG:NH1	2.26	0.45
2:A:144:VAL:HG11	2:A:150:ALA:HB2	1.99	0.45
2:A:67:LYS:HD3	2:A:67:LYS:HA	1.77	0.45
1:B:305:ILE:HA	1:B:315:VAL:HG12	1.99	0.45
2:A:143:VAL:HG22	2:A:231:TYR:HB2	1.98	0.45
2:A:124:ARG:HB2	2:A:127:GLN:HG3	1.99	0.44
2:A:174:ASP:OD1	2:A:176:SER:OG	2.33	0.44
2:A:181:ARG:NH1	2:A:208:ASP:OD2	2.25	0.44
1:B:271:PHE:CZ	1:B:336:VAL:HG22	2.51	0.44
1:B:110:LEU:HD23	1:B:110:LEU:HA	1.79	0.44
2:A:59:ARG:HA	2:A:60:PRO:HD3	1.81	0.44
2:A:199:LEU:HA	2:A:199:LEU:HD12	1.88	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:119:ARG:NH1	6:A:431:HOH:O	2.50	0.44
1:B:172:LEU:HA	1:B:172:LEU:HD12	1.83	0.44
2:A:173:VAL:HG11	2:A:199:LEU:HD21	2.00	0.44
3:B:410:NAG:O3	3:B:410:NAG:O7	2.29	0.44
1:B:242:PRO:HG2	1:B:336:VAL:HG13	2.00	0.43
1:B:173:PRO:HA	1:B:198:ARG:HH22	1.83	0.43
1:B:156:LEU:O	1:B:157:SER:HB3	2.19	0.43
1:B:38:ILE:HD12	1:B:38:ILE:HA	1.51	0.43
2:A:137:MET:HG3	2:A:138:GLY:N	2.34	0.43
1:B:78:LYS:HB2	1:B:89:ILE:CD1	2.49	0.42
1:B:173:PRO:HA	1:B:198:ARG:NH2	2.34	0.42
1:B:61:ARG:HB2	2:A:188:GLU:HG2	2.01	0.42
1:B:106:ARG:HA	1:B:107:PRO:HA	1.79	0.42
1:B:297:ARG:HH22	1:B:328:ASP:CG	2.23	0.42
1:B:52:LYS:HB3	1:B:57:TYR:HE2	1.83	0.42
1:B:34:TRP:O	2:A:153:LEU:HD11	2.19	0.42
2:A:160:PRO:HG2	2:A:218:ASN:HB2	2.02	0.41
1:B:267:CYS:HB2	1:B:283:TRP:CZ2	2.55	0.41
1:B:268:ARG:NH1	1:B:306:LEU:HD13	2.34	0.41
1:B:50:ARG:HG3	1:B:104:TRP:NE1	2.36	0.41
1:B:115:LEU:HD23	1:B:132:SER:HA	2.02	0.41
1:B:297:ARG:NH1	1:B:323:SER:O	2.49	0.41
2:A:64:TRP:CZ3	2:A:105:CYS:HB2	2.56	0.41
2:A:75:ARG:O	2:A:91:ILE:HA	2.21	0.41
1:B:289:PHE:CZ	2:A:98:ARG:HD2	2.56	0.41
1:B:351:LYS:HB2	1:B:351:LYS:HE3	1.83	0.41
1:B:92:ASP:OD1	1:B:93:GLY:N	2.53	0.40
2:A:145:GLU:HA	2:A:233:ARG:O	2.22	0.40
1:B:110:LEU:HD23	1:B:135:VAL:HG12	2.03	0.40
1:B:91:PHE:CE2	1:B:98:LYS:HG3	2.56	0.40
2:A:124:ARG:HD3	2:A:127:GLN:NE2	2.36	0.40
1:B:160:LYS:HA	1:B:160:LYS:HD2	1.84	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	B	320/348 (92%)	287 (90%)	31 (10%)	2 (1%)	30 59
2	A	207/305 (68%)	203 (98%)	4 (2%)	0	100 100
All	All	527/653 (81%)	490 (93%)	35 (7%)	2 (0%)	39 69

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	82	PRO
1	B	58	GLY

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	B	289/309 (94%)	240 (83%)	49 (17%)	2 6
2	A	180/264 (68%)	159 (88%)	21 (12%)	7 15
All	All	469/573 (82%)	399 (85%)	70 (15%)	4 9

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	38	ILE
1	B	40	LYS
1	B	43	VAL
1	B	49	VAL
1	B	50	ARG
1	B	61	ARG
1	B	79	SER
1	B	80	SER
1	B	84	ASP
1	B	86	GLU

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Mol	Chain	Res	Type
1	B	102	SER
1	B	106	ARG
1	B	108	THR
1	B	111	GLN
1	B	118	CYS
1	B	125	TYR
1	B	139	ASP
1	B	149	LYS
1	B	165	ARG
1	B	167	ILE
1	B	168	GLU
1	B	172	LEU
1	B	175	ARG
1	B	176	GLU
1	B	179	ILE
1	B	180	LEU
1	B	185	CYS
1	B	187	THR
1	B	193	SER
1	B	198	ARG
1	B	201	LEU
1	B	215	THR
1	B	228	THR
1	B	229	THR
1	B	231	LEU
1	B	244	LEU
1	B	253	THR
1	B	255	GLN
1	B	280	LEU
1	B	293	LEU
1	B	294	ASP
1	B	318	SER
1	B	322	ASP
1	B	326	GLU
1	B	336	VAL
1	B	338	ASN
1	B	342	ARG
1	B	348	LEU
1	B	351	LYS
2	A	43	VAL
2	A	70	LYS
2	A	83	ASP

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Mol	Chain	Res	Type
2	A	100	GLU
2	A	110	ASN
2	A	126	ASP
2	A	134	THR
2	A	141	LEU
2	A	153	LEU
2	A	163	GLU
2	A	181	ARG
2	A	184	GLN
2	A	186	ARG
2	A	188	GLU
2	A	190	ILE
2	A	193	THR
2	A	196	ARG
2	A	214	CYS
2	A	233	ARG
2	A	235	LEU
2	A	236	ARG

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

Mol	Chain	Res	Type
1	B	68	GLN
1	B	258	GLN
2	A	74	GLN
2	A	110	ASN
2	A	184	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)

11 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	$\#\|Z\| > 2$
3	NAG	B	400	1,3,4	14,14,15	0.83	1 (7%)	15,19,21	1.10	1 (6%)
3	NAG	B	401	3	14,14,15	0.26	0	15,19,21	0.21	0
4	FUL	B	402	3	10,10,11	0.85	0	14,14,16	1.77	3 (21%)
3	NAG	B	403	1,3	14,14,15	0.57	1 (7%)	15,19,21	0.33	0
3	NAG	B	404	3	14,14,15	0.18	0	15,19,21	0.38	0
3	NAG	B	405	1,3,4	14,14,15	0.58	0	15,19,21	1.59	2 (13%)
3	NAG	B	406	3,5	14,14,15	0.45	0	15,19,21	0.62	0
5	BMA	B	407	3	11,11,12	0.76	0	14,15,17	0.98	1 (7%)
4	FUL	B	408	3	10,10,11	0.83	1 (10%)	14,14,16	1.98	3 (21%)
3	NAG	B	409	1	14,14,15	0.16	0	15,19,21	0.30	0
3	NAG	B	410	1	14,14,15	0.94	1 (7%)	15,19,21	0.75	1 (6%)

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
3	NAG	B	400	1,3,4	-	0/6/23/26	0/1/1/1
3	NAG	B	401	3	-	0/6/23/26	0/1/1/1
4	FUL	B	402	3	-	0/0/17/20	0/1/1/1
3	NAG	B	403	1,3	-	0/6/23/26	0/1/1/1
3	NAG	B	404	3	-	0/6/23/26	0/1/1/1
3	NAG	B	405	1,3,4	-	0/6/23/26	0/1/1/1
3	NAG	B	406	3,5	-	0/6/23/26	0/1/1/1
5	BMA	B	407	3	-	0/2/19/22	0/1/1/1
4	FUL	B	408	3	-	0/0/17/20	0/1/1/1
3	NAG	B	409	1	-	0/6/23/26	0/1/1/1
3	NAG	B	410	1	-	0/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	410	NAG	O5-C1	-2.96	1.38	1.43
3	B	400	NAG	O5-C1	-2.51	1.39	1.43
3	B	403	NAG	O5-C1	-2.00	1.40	1.43
4	B	408	FUL	C1-C2	2.04	1.57	1.52

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	407	BMA	O2-C2-C3	-2.60	104.90	110.12
3	B	410	NAG	C1-O5-C5	-2.16	109.51	112.25
4	B	402	FUL	O5-C1-C2	2.47	114.86	110.86
4	B	402	FUL	O2-C2-C1	2.48	114.18	109.21
3	B	405	NAG	C1-O5-C5	3.04	116.11	112.25
4	B	408	FUL	O5-C1-C2	3.36	116.31	110.86
3	B	400	NAG	C3-C4-C5	3.55	116.38	110.20
4	B	408	FUL	C1-C2-C3	3.91	114.17	109.54
3	B	405	NAG	C2-N2-C7	4.61	128.96	123.04
4	B	402	FUL	C1-O5-C5	4.68	119.61	112.38
4	B	408	FUL	C1-O5-C5	4.70	119.64	112.38

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	404	NAG	1	0
3	B	405	NAG	2	0
3	B	410	NAG	1	0

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, 95^{th} 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	B	322/348 (92%)	0.02	5 (1%)	74	75	22, 50, 83, 111	0
2	A	209/305 (68%)	-0.02	4 (1%)	70	70	17, 37, 80, 127	0
All	All	531/653 (81%)	0.01	9 (1%)	73	74	17, 46, 82, 127	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	A	179	ASN	4.8
2	A	178	ASN	3.9
1	B	85	PHE	3.1
1	B	82	PRO	3.0
1	B	81	GLY	2.9
1	B	351	LYS	2.3
1	B	259	LEU	2.3
2	A	59	ARG	2.1
2	A	177	ASN	2.1

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, 95^{th} 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	FUL	B	402	10/11	0.90	0.28	1.59	65,74,90,99	0
3	NAG	B	409	14/15	0.63	0.26	1.42	105,119,124,124	0
3	NAG	B	403	14/15	0.95	0.17	0.21	48,61,76,86	0
3	NAG	B	406	14/15	0.90	0.20	0.07	42,68,89,91	0
3	NAG	B	405	14/15	0.93	0.13	-0.83	51,55,61,63	0
3	NAG	B	400	14/15	0.93	0.12	-	49,69,79,86	0
3	NAG	B	410	14/15	0.84	0.14	-	80,91,99,102	0
3	NAG	B	401	14/15	0.88	0.20	-	44,98,106,107	0
3	NAG	B	404	14/15	0.88	0.25	-	75,101,109,109	0
5	BMA	B	407	11/12	0.74	0.29	-	88,100,110,113	0
4	FUL	B	408	10/11	0.86	0.21	-	64,81,101,104	0

6.5 Other polymers (i)

There are no such residues in this entry.