W O R L D W I D E
wwPDB
P R O T E I N   D A T A   B A N K

Full wwPDB X-ray Structure Validation Report (i)

Oct 3, 2016 – 08:44 PM EDT

PDB ID	:	5E4L
Title	:	Structure of ligand binding region of uPARAP at pH 5.3
Authors	:	Yuan, C.; Huang, M.
Deposited on	:	2015-10-06
Resolution	:	2.44 Å(reported)

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

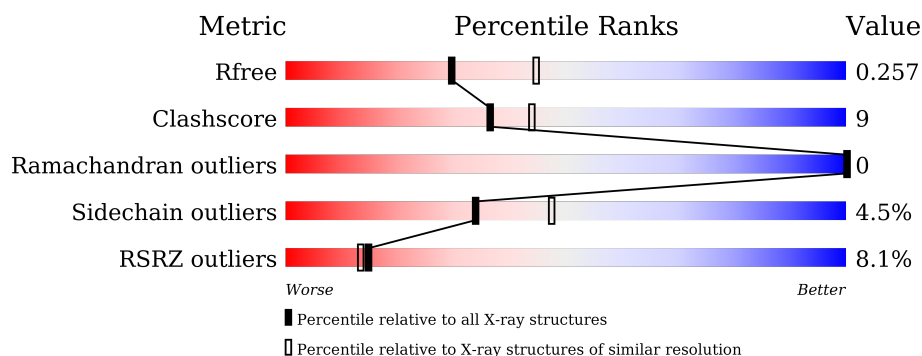|		
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027939
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027939

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 2.44 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		0.257
Clashscore		9
Ramachandran outliers		0
Sidechain outliers		4.5%
RSRZ outliers		8.1%

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	1003 (2.46-2.42)
Clashscore	102246	1071 (2.46-2.42)
Ramachandran outliers	100387	1065 (2.46-2.42)
Sidechain outliers	100360	1065 (2.46-2.42)
RSRZ outliers	91569	1005 (2.46-2.42)

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	492	3% / 67% / 17% · 13%
1	B	492	10% / 60% / 17% · 22%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 6747 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 C-type mannose receptor 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	428	Total 3426	C 2146	N 596	O 660	S 24	0	0	0
1	B	386	Total 3085	C 1930	N 535	O 598	S 22	0	0	0

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	29	ARG	-	expression tag	UNP Q9UBG0
A	30	SER	-	expression tag	UNP Q9UBG0
A	43	ILE	VAL	variant	UNP Q9UBG0
A	511	THR	-	expression tag	UNP Q9UBG0
A	512	ARG	-	expression tag	UNP Q9UBG0
A	513	THR	-	expression tag	UNP Q9UBG0
A	514	GLY	-	expression tag	UNP Q9UBG0
A	515	HIS	-	expression tag	UNP Q9UBG0
A	516	HIS	-	expression tag	UNP Q9UBG0
A	517	HIS	-	expression tag	UNP Q9UBG0
A	518	HIS	-	expression tag	UNP Q9UBG0
A	519	HIS	-	expression tag	UNP Q9UBG0
A	520	HIS	-	expression tag	UNP Q9UBG0
B	29	ARG	-	expression tag	UNP Q9UBG0
B	30	SER	-	expression tag	UNP Q9UBG0
B	43	ILE	VAL	variant	UNP Q9UBG0
B	511	THR	-	expression tag	UNP Q9UBG0
B	512	ARG	-	expression tag	UNP Q9UBG0
B	513	THR	-	expression tag	UNP Q9UBG0
B	514	GLY	-	expression tag	UNP Q9UBG0
B	515	HIS	-	expression tag	UNP Q9UBG0
B	516	HIS	-	expression tag	UNP Q9UBG0
B	517	HIS	-	expression tag	UNP Q9UBG0
B	518	HIS	-	expression tag	UNP Q9UBG0
B	519	HIS	-	expression tag	UNP Q9UBG0

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Chain	Residue	Modelled	Actual	Comment	Reference
B	520	HIS	-	expression tag	UNP Q9UBG0

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	3	Total 3	Ca 3	0	0
2	A	3	Total 3	Ca 3	0	0

- Molecule 3 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).
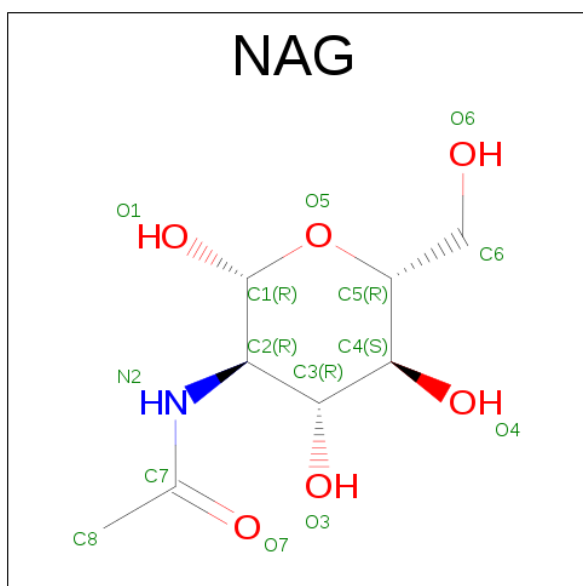
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total 14	C 8	N 1	O 5	0	0
3	B	1	Total 14	C 8	N 1	O 5	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	121	Total 121	O 121	0	0
4	B	81	Total 81	O 81	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: C-type mannose receptor 2

- Molecule 1: C-type mannose receptor 2

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	74.27Å 102.70Å 87.76Å 90.00° 94.54° 90.00°	Depositor
Resolution (Å)	54.43 – 2.44 66.60 – 2.44	Depositor EDS
% Data completeness (in resolution range)	99.9 (54.43-2.44) 96.1 (66.60-2.44)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	3.25 (at 2.45Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.217 , 0.259 0.213 , 0.257	Depositor DCC
R_{free} test set	2362 reflections (5.02%)	DCC
Wilson B-factor (Å^2)	41.9	Xtriage
Anisotropy	0.343	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 48.5	EDS
L-test for twinning[2]	$<|L|> = 0.48$, $<L^2> = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	6747	wwPDB-VP
Average B, all atoms (Å^2)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.67% 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, 0.333 respectively for untwinned datasets, and 0.375, 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: CA, 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	A	0.45	1/3520 (0.0%)	0.62	2/4779 (0.0%)
1	B	0.41	0/3173	0.59	1/4317 (0.0%)
All	All	0.43	1/6693 (0.0%)	0.61	3/9096 (0.0%)

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	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	466	TRP	C-N	-5.63	1.21	1.34

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	137	ARG	NE-CZ-NH2	-5.74	117.43	120.30
1	A	235	CYS	CA-CB-SG	-5.54	104.02	114.00
1	B	179	GLN	C-N-CA	-5.53	110.70	122.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	405	GLU	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	3426	0	3185	63	0
1	B	3085	0	2839	58	0
2	A	3	0	0	0	0
2	B	3	0	0	0	0
3	A	14	0	13	0	0
3	B	14	0	13	0	0
4	A	121	0	0	4	0
4	B	81	0	0	2	0
All	All	6747	0	6050	119	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 9.

All (119) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:245:THR:HG23	1:A:247:SER:H	1.42	0.84
1:A:221:LYS:NZ	4:A:701:HOH:O	2.23	0.70
1:B:488:GLU:O	1:B:490:ARG:N	2.25	0.70
1:A:339:ARG:HD3	1:A:341:GLU:HB3	1.72	0.69
1:B:49:HIS:NE2	1:B:164:GLU:OE2	2.24	0.69
1:A:399:GLU:OE2	1:A:401:ARG:NH1	2.19	0.66
1:A:397:GLN:NE2	1:A:502:SER:OG	2.28	0.65
1:A:236:GLU:HG2	1:A:237:THR:HG23	1.79	0.64
1:A:343:SER:HB3	1:B:243:GLN:HG3	1.80	0.64
1:A:408:LYS:NZ	4:A:708:HOH:O	2.30	0.64
1:A:472:ASN:OD1	1:A:473:ASN:N	2.34	0.61
1:B:87:ASN:HB3	1:B:90:THR:HG22	1.82	0.61
1:A:87:ASN:HB3	1:A:90:THR:HG22	1.81	0.61
1:A:450:GLN:NE2	1:A:480:ASP:OD1	2.35	0.60
1:B:444:LEU:HB3	1:B:482:VAL:HB	1.83	0.59
1:B:485:TRP:HE3	1:B:490:ARG:HE	1.50	0.59
1:A:83:ASN:HB2	1:A:120:ARG:HG3	1.83	0.59
1:A:287:GLY:O	1:A:290:THR:OG1	2.22	0.57
1:A:339:ARG:HE	1:A:347:GLN:NE2	2.01	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:467:HIS:HB3	1:A:470:GLU:HG3	1.88	0.56
1:B:483:THR:O	1:B:491:TRP:HA	2.07	0.55
1:A:347:GLN:OE1	1:A:349:ARG:NH1	2.40	0.55
1:A:466:TRP:CH2	1:A:471:PRO:HG3	2.43	0.54
1:A:281:GLU:O	1:A:285:ILE:HG12	2.08	0.54
1:A:405:GLU:HB3	1:A:408:LYS:HB2	1.90	0.53
1:B:326:GLN:HG3	1:B:347:GLN:HG2	1.90	0.53
1:A:90:THR:HG21	1:A:109:MET:HE2	1.91	0.53
1:A:329:ASN:HB3	1:A:332:GLU:HB2	1.90	0.52
1:A:177:THR:HB	1:A:226:GLY:HA3	1.90	0.52
1:A:318:LYS:HD2	1:A:461:VAL:HB	1.89	0.52
1:B:297:TRP:CE2	1:B:355:LEU:HD12	2.45	0.52
1:B:449:LEU:HG	1:B:452:ASN:HB3	1.91	0.52
1:B:90:THR:HG21	1:B:109:MET:HE2	1.92	0.52
1:A:397:GLN:NE2	1:A:502:SER:HG	2.06	0.52
1:B:148:GLU:HG2	1:B:149:ARG:N	2.23	0.51
1:B:467:HIS:HB2	1:B:490:ARG:HA	1.92	0.51
1:A:484:ILE:HG22	1:A:484:ILE:O	2.11	0.51
1:B:281:GLU:O	1:B:285:ILE:HG12	2.11	0.51
1:B:472:ASN:OD1	1:B:473:ASN:N	2.44	0.51
1:A:296:LEU:HD23	1:A:356:PRO:HB2	1.93	0.51
1:B:503:ILE:HG22	1:B:504:CYS:H	1.76	0.50
1:B:320:LEU:HD23	1:B:322:TRP:CD1	2.46	0.50
1:B:467:HIS:HB3	1:B:470:GLU:HG3	1.94	0.50
1:A:343:SER:CB	1:B:243:GLN:HG3	2.41	0.49
1:B:147:LEU:H	1:B:147:LEU:HD23	1.77	0.49
1:B:467:HIS:CG	1:B:490:ARG:HD3	2.48	0.49
1:A:405:GLU:HA	1:A:408:LYS:H	1.78	0.49
1:B:148:GLU:O	1:B:149:ARG:NE	2.41	0.49
1:B:485:TRP:H	1:B:490:ARG:HB2	1.77	0.49
1:A:442:ILE:HG21	1:A:484:ILE:HD11	1.94	0.48
1:A:411:LEU:HB2	4:A:712:HOH:O	2.13	0.48
1:A:439:GLU:HG2	1:A:485:TRP:HB2	1.95	0.48
1:B:498:GLN:HG2	1:B:500:LEU:HG	1.96	0.47
1:B:296:LEU:HD23	1:B:356:PRO:HB2	1.97	0.47
1:B:90:THR:HG23	1:B:92:GLN:HB2	1.97	0.46
1:B:322:TRP:CE2	1:B:327:PRO:HG3	2.50	0.46
1:A:399:GLU:HB2	1:A:401:ARG:NH1	2.31	0.46
1:A:485:TRP:CD1	1:A:485:TRP:C	2.89	0.46
1:A:83:ASN:OD1	1:A:120:ARG:NH1	2.47	0.46
1:A:165:GLU:HG2	1:A:169:ALA:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:320:LEU:HD23	1:B:322:TRP:NE1	2.31	0.46
1:B:350:ASP:OD2	1:B:352:SER:OG	2.32	0.46
1:A:426:LEU:O	1:A:430:THR:HG23	2.16	0.45
1:B:195:ASN:N	4:B:702:HOH:O	2.29	0.45
1:A:86:PHE:CZ	1:A:91:MET:HA	2.51	0.45
1:A:84:ARG:NH1	1:A:112:CYS:O	2.50	0.45
1:B:466:TRP:CE2	1:B:471:PRO:HD3	2.52	0.45
1:A:162:GLY:O	1:A:164:GLU:HG2	2.17	0.44
1:B:233:ASN:HB3	1:B:365:ALA:HB3	1.99	0.44
1:B:48:SER:HB2	1:B:158:TRP:CD2	2.51	0.44
1:A:90:THR:HG23	1:A:92:GLN:N	2.32	0.44
1:B:473:ASN:HB3	1:B:477:SER:O	2.17	0.44
1:B:490:ARG:N	4:B:711:HOH:O	2.49	0.44
1:A:405:GLU:HA	1:A:405:GLU:OE1	2.17	0.44
1:B:73:PRO:HB2	1:B:89:GLY:HA2	1.99	0.44
1:B:86:PHE:CZ	1:B:91:MET:HA	2.53	0.44
1:B:234:ASP:OD1	1:B:236:GLU:N	2.50	0.44
1:B:73:PRO:HA	1:B:76:ARG:HD3	1.99	0.44
1:B:301:ASN:HB2	1:B:303:LEU:HD22	2.00	0.44
1:B:320:LEU:HD23	1:B:322:TRP:HE1	1.83	0.44
1:B:126:LEU:HD23	1:B:167:LEU:HD13	1.99	0.43
1:B:328:ASP:O	1:B:348:ASN:ND2	2.45	0.43
1:A:90:THR:HG23	1:A:92:GLN:HB2	1.98	0.43
1:B:323:GLU:OE2	1:B:339:ARG:NH1	2.51	0.43
1:A:302:ASP:HA	1:A:308:GLY:O	2.18	0.43
1:A:361:LYS:HG3	1:A:363:PRO:HD3	1.99	0.43
1:A:482:VAL:HA	1:A:492:ASN:O	2.17	0.43
1:A:83:ASN:HB3	1:A:121:TRP:O	2.18	0.43
1:B:242:ASP:HB2	1:B:284:TYR:CE2	2.54	0.43
1:B:165:GLU:HB3	1:B:169:ALA:HB2	1.99	0.43
1:B:453:PHE:CE1	1:B:471:PRO:HG3	2.54	0.43
1:A:306:SER:N	4:A:716:HOH:O	2.51	0.43
1:B:275:SER:HA	1:B:311:TRP:CE3	2.53	0.43
1:B:177:THR:HB	1:B:226:GLY:HA3	1.99	0.43
1:A:421:HIS:CE1	1:A:459:SER:HB2	2.54	0.42
1:A:405:GLU:CB	1:A:408:LYS:HB2	2.49	0.42
1:A:185:LYS:HG3	1:A:186:PRO:HD2	2.00	0.42
1:A:236:GLU:HG2	1:A:237:THR:N	2.34	0.42
1:A:49:HIS:NE2	1:A:164:GLU:OE1	2.51	0.42
1:B:467:HIS:ND1	1:B:490:ARG:HG2	2.34	0.42
1:A:339:ARG:NH2	1:A:349:ARG:HH12	2.17	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:48:SER:HB2	1:A:158:TRP:CZ3	2.55	0.42
1:A:479:GLU:HG2	1:A:495:PRO:HD3	2.02	0.42
1:A:431:LYS:HE3	1:A:435:GLN:HE22	1.85	0.42
1:A:403:TRP:CE3	1:A:404:GLN:HA	2.55	0.42
1:B:87:ASN:HB3	1:B:90:THR:CG2	2.49	0.42
1:A:126:LEU:HD23	1:A:167:LEU:HD13	2.01	0.41
1:B:162:GLY:O	1:B:164:GLU:N	2.53	0.41
1:B:491:TRP:CD1	1:B:491:TRP:N	2.88	0.41
1:A:403:TRP:HE3	1:A:404:GLN:HA	1.84	0.41
1:B:151:ASP:OD1	1:B:151:ASP:N	2.54	0.41
1:A:192:LYS:HD3	1:A:195:ASN:HA	2.02	0.41
1:B:326:GLN:HG2	1:B:326:GLN:H	1.54	0.41
1:B:361:LYS:HG3	1:B:363:PRO:HD3	2.01	0.41
1:A:474:PHE:HD1	1:A:475:ARG:H	1.69	0.41
1:B:80:VAL:HG21	1:B:190:PRO:HD3	2.02	0.40
1:A:82:ARG:NH2	1:A:115:GLU:OE1	2.54	0.40
1:A:492:ASN:OD1	1:A:493:ASP:N	2.53	0.40
1:B:463:PHE:CZ	1:B:465:HIS:HB2	2.56	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	420/492 (85%)	403 (96%)	17 (4%)	0	100	100
1	B	378/492 (77%)	364 (96%)	14 (4%)	0	100	100
All	All	798/984 (81%)	767 (96%)	31 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	375/427 (88%)	358 (96%)	17 (4%)	34	47
1	B	339/427 (79%)	324 (96%)	15 (4%)	35	49
All	All	714/854 (84%)	682 (96%)	32 (4%)	34	47

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	90	THR
1	A	115	GLU
1	A	234	ASP
1	A	236	GLU
1	A	318	LYS
1	A	325	ASP
1	A	339	ARG
1	A	395	ARG
1	A	399	GLU
1	A	404	GLN
1	A	428	PHE
1	A	449	LEU
1	A	474	PHE
1	A	476	ASP
1	A	484	ILE
1	A	485	TRP
1	A	490	ARG
1	B	43	ILE
1	B	61	GLN
1	B	147	LEU
1	B	149	ARG
1	B	151	ASP
1	B	303	LEU
1	B	442	ILE
1	B	445	ASN
1	B	450	GLN
1	B	463	PHE

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Mol	Chain	Res	Type
1	B	474	PHE
1	B	476	ASP
1	B	490	ARG
1	B	494	SER
1	B	504	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	397	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)

Of 8 ligands modelled in this entry, 6 are monoatomic - leaving 2 for Mogul analysis.

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	A	604	1	14,14,15	0.22	0	15,19,21	0.43	0
3	NAG	B	604	1	14,14,15	0.52	0	15,19,21	0.48	0

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	A	604	1	-	0/6/23/26	0/1/1/1
3	NAG	B	604	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

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	428/492 (86%)	0.45	16 (3%) 45	45	22, 51, 120, 211	0
1	B	386/492 (78%)	0.73	50 (12%) 5	3	26, 58, 144, 177	0
All	All	814/984 (82%)	0.58	66 (8%) 15	13	22, 54, 137, 211	0

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	454	GLU	5.6
1	B	447	LEU	5.3
1	B	442	ILE	5.2
1	B	469	PHE	5.1
1	B	456	SER	5.0
1	B	332	GLU	4.9
1	B	444	LEU	4.8
1	B	483	THR	4.4
1	B	460	LEU	4.3
1	A	413	GLY	4.3
1	B	485	TRP	4.2
1	A	469	PHE	4.2
1	B	459	SER	4.1
1	B	449	LEU	3.8
1	B	453	PHE	3.7
1	B	471	PRO	3.7
1	A	314	ASN	3.5
1	A	505	LYS	3.4
1	B	499	SER	3.4
1	B	466	TRP	3.4
1	B	467	HIS	3.3
1	B	463	PHE	3.3
1	B	461	VAL	3.3
1	B	330	PRO	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	448	LYS	3.2
1	A	467	HIS	3.2
1	B	465	HIS	3.1
1	A	396	LEU	3.0
1	B	482	VAL	3.0
1	B	455	TRP	2.9
1	B	468	PRO	2.9
1	B	317	LEU	2.9
1	B	475	ARG	2.9
1	B	464	THR	2.8
1	B	311	TRP	2.8
1	B	484	ILE	2.8
1	B	496	CYS	2.7
1	A	504	CYS	2.7
1	A	395	ARG	2.6
1	B	478	LEU	2.6
1	B	451	MET	2.6
1	B	276	ILE	2.6
1	B	470	GLU	2.6
1	A	405	GLU	2.6
1	A	440	LEU	2.6
1	B	310	GLN	2.5
1	B	503	ILE	2.5
1	A	420	ILE	2.5
1	B	341	GLU	2.5
1	B	486	GLY	2.5
1	A	438	GLU	2.4
1	B	480	ASP	2.3
1	B	150	GLY	2.3
1	B	474	PHE	2.2
1	A	506	LYS	2.2
1	B	487	PRO	2.2
1	B	488	GLU	2.2
1	B	151	ASP	2.1
1	B	342	SER	2.1
1	B	472	ASN	2.1
1	A	417	LEU	2.1
1	A	330	PRO	2.1
1	B	491	TRP	2.1
1	A	442	ILE	2.1
1	B	318	LYS	2.1
1	B	149	ARG	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)

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
2	CA	A	602	1/1	0.83	0.14	-1.01	110,110,110,110	0
2	CA	B	602	1/1	0.92	0.09	-2.75	150,150,150,150	0
2	CA	B	601	1/1	0.97	0.08	-3.33	115,115,115,115	0
2	CA	A	601	1/1	0.95	0.07	-4.11	61,61,61,61	0
2	CA	B	603	1/1	0.88	0.08	-4.58	103,103,103,103	0
2	CA	A	603	1/1	0.90	0.06	-5.40	83,83,83,83	0
3	NAG	A	604	14/15	0.79	0.16	-	94,94,94,94	0
3	NAG	B	604	14/15	0.59	0.23	-	115,115,115,115	0

6.5 Other polymers (i)

There are no such residues in this entry.