



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:31 AM UTC

PDB ID : 4YFD / pdb_00004yfd
Title : Crystal structure PTP delta Ig1-Fn2 in complex with IL-1RAcP
Authors : Yamagata, A.; Fukai, S.
Deposited on : 2015-02-25
Resolution : 3.25 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

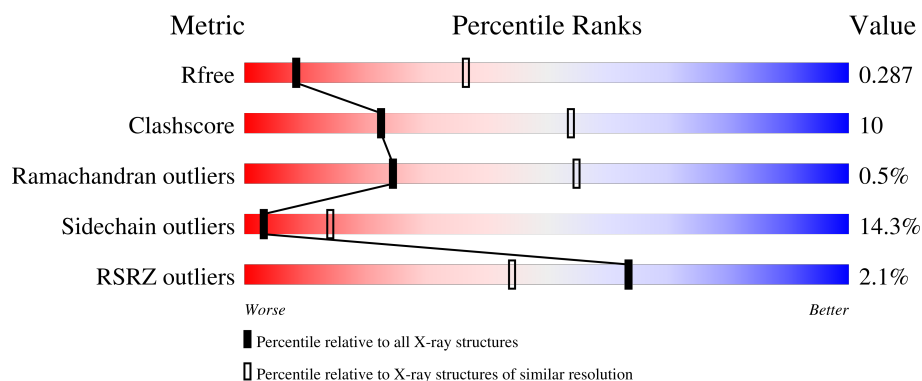
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.25 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}	180053	1605 (3.30-3.22)
Clashscore	190562	1660 (3.30-3.22)
Ramachandran outliers	187476	1630 (3.30-3.22)
Sidechain outliers	187428	1629 (3.30-3.22)
RSRZ outliers	180081	1605 (3.30-3.22)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	B	339	
2	A	491	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6505 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	322	Total	C	N	O	S	0	0	0
			2623	1672	440	495	16			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	352	ALA	-	expression tag	UNP Q61730
B	353	ALA	-	expression tag	UNP Q61730
B	354	HIS	-	expression tag	UNP Q61730
B	355	HIS	-	expression tag	UNP Q61730
B	356	HIS	-	expression tag	UNP Q61730
B	357	HIS	-	expression tag	UNP Q61730
B	358	HIS	-	expression tag	UNP Q61730
B	359	HIS	-	expression tag	UNP Q61730

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	491	Total	C	N	O	S	0	0	0
			3784	2364	658	746	16			

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	77.50Å 63.31Å 169.35Å 90.00° 94.23° 90.00°	Depositor
Resolution (Å)	48.97 – 3.25 48.97 – 3.25	Depositor EDS
% Data completeness (in resolution range)	97.0 (48.97-3.25) 97.1 (48.97-3.25)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.91 (at 3.25Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.256 , 0.287 0.258 , 0.287	Depositor DCC
R_{free} test set	1293 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	76.0	Xtriage
Anisotropy	0.356	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 84.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	6505	wwPDB-VP
Average B, all atoms (Å ²)	108.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.57% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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: 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	0.35	0/2696	0.85	6/3672 (0.2%)
2	A	0.37	0/3867	0.86	7/5278 (0.1%)
All	All	0.36	0/6563	0.85	13/8950 (0.1%)

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	128	ILE	CA-C-N	-6.70	113.40	120.03
2	A	128	ILE	C-N-CA	-6.70	113.40	120.03
1	B	322	THR	CA-C-N	6.34	126.03	119.56
1	B	322	THR	C-N-CA	6.34	126.03	119.56
1	B	117	ARG	N-CA-C	5.76	118.85	108.48
2	A	29	THR	CA-C-N	5.58	126.13	120.38
2	A	29	THR	C-N-CA	5.58	126.13	120.38
1	B	96	LYS	CB-CA-C	-5.42	109.86	117.23
1	B	241	LEU	CA-C-N	5.34	125.88	120.38
1	B	241	LEU	C-N-CA	5.34	125.88	120.38
2	A	490	VAL	CA-C-N	5.23	125.52	119.92
2	A	490	VAL	C-N-CA	5.23	125.52	119.92
2	A	72	SER	N-CA-C	-5.20	98.54	107.23

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	2623	0	2525	72	0
2	A	3784	0	3738	70	1
3	A	28	0	26	0	0
3	B	70	0	65	0	0
All	All	6505	0	6354	135	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (135) 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:37:VAL:HG21	1:B:43:ALA:HB2	1.56	0.86
1:B:215:THR:HG1	1:B:224:HIS:HD1	1.26	0.81
1:B:288:LYS:O	1:B:290:ASP:N	2.20	0.74
2:A:438:SER:HB2	2:A:491:PRO:HB3	1.69	0.73
1:B:49:LEU:HA	1:B:53:PHE:HD2	1.56	0.70
1:B:254:TYR:HB3	1:B:262:LEU:HD21	1.75	0.69
1:B:245:ILE:HG23	1:B:248:PRO:HD2	1.77	0.67
1:B:248:PRO:HB3	1:B:343:GLN:C	2.20	0.67
1:B:100:TRP:HH2	1:B:166:TYR:HA	1.59	0.66
1:B:203:LEU:O	1:B:206:ASN:ND2	2.29	0.65
1:B:189:ASN:ND2	1:B:200:PHE:O	2.29	0.65
1:B:295:ASP:HB2	1:B:319:LYS:HB2	1.78	0.65
2:A:146:ARG:O	2:A:147:THR:OG1	2.15	0.63
2:A:271:MET:HE3	2:A:292:GLY:HA3	1.80	0.63
1:B:145:PRO:HG2	1:B:229:VAL:HG12	1.81	0.62
2:A:152:MET:HE2	2:A:230:LEU:HB2	1.81	0.62
2:A:240:ARG:HB3	2:A:315:LEU:HD11	1.79	0.62
1:B:179:LYS:NZ	1:B:207:ASN:O	2.32	0.61
1:B:298:ILE:HD12	1:B:316:LEU:HD11	1.82	0.61
1:B:58:TYR:OH	2:A:286:GLU:OE1	2.18	0.61
2:A:312:MET:HB3	2:A:317:VAL:HG22	1.82	0.61
2:A:160:PRO:HG2	2:A:218:ASN:HB2	1.83	0.61
1:B:48:PRO:HB2	1:B:125:VAL:HG11	1.83	0.60
1:B:214:VAL:HG13	1:B:225:LEU:HB2	1.84	0.60
2:A:125:GLU:HA	2:A:128:ILE:HG13	1.85	0.59
2:A:340:GLU:HB2	2:A:347:THR:HB	1.85	0.59
2:A:265:VAL:HG22	2:A:293:ARG:HG3	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:288:LYS:N	1:B:289:PRO:HD2	2.20	0.57
1:B:162:ASN:O	1:B:162:ASN:ND2	2.35	0.56
1:B:260:GLU:HB2	1:B:321:VAL:HG11	1.88	0.56
2:A:47:VAL:HG13	2:A:92:GLN:HB2	1.88	0.55
1:B:33:ARG:HH21	1:B:48:PRO:HG3	1.72	0.55
2:A:75:ARG:CZ	2:A:75:ARG:HB2	2.33	0.55
2:A:99:ASP:O	2:A:103:TYR:OH	2.18	0.55
1:B:343:GLN:N	1:B:343:GLN:OE1	2.39	0.55
1:B:254:TYR:HB3	1:B:262:LEU:HD11	1.88	0.54
1:B:294:VAL:HG23	1:B:296:ILE:HD11	1.88	0.54
1:B:57:ASN:OD1	1:B:57:ASN:N	2.39	0.54
2:A:177:ASN:O	2:A:177:ASN:ND2	2.40	0.53
2:A:256:PRO:HG3	2:A:326:VAL:HG11	1.90	0.53
1:B:209:ASN:HA	1:B:230:THR:HA	1.90	0.53
2:A:374:TYR:OH	2:A:397:GLU:OE1	2.15	0.52
2:A:185:LEU:HB2	2:A:198:ALA:HB3	1.91	0.52
2:A:146:ARG:NH2	2:A:206:GLU:OE1	2.43	0.52
1:B:149:MET:HG2	1:B:156:HIS:ND1	2.25	0.52
1:B:265:PRO:HA	1:B:315:ILE:HG12	1.92	0.51
2:A:143:VAL:HG22	2:A:231:TYR:HB2	1.92	0.51
2:A:167:PHE:HB2	2:A:213:GLU:HG3	1.92	0.51
1:B:91:ARG:NH2	1:B:108:ASP:OD2	2.44	0.51
1:B:55:LYS:HZ2	2:A:188:GLU:HG3	1.76	0.51
1:B:280:VAL:O	1:B:314:GLN:NE2	2.42	0.51
2:A:413:GLU:HG3	2:A:414:PRO:HD2	1.91	0.50
2:A:144:VAL:HG11	2:A:150:ALA:HB2	1.92	0.50
2:A:257:GLY:N	2:A:258:GLY:HA3	2.26	0.50
2:A:175:THR:HG21	2:A:184:GLN:HG3	1.94	0.49
1:B:53:PHE:HE1	2:A:196:ARG:HG2	1.78	0.49
1:B:333:HIS:HD1	1:B:341:ALA:HB1	1.77	0.49
1:B:109:THR:HG23	1:B:130:GLU:HA	1.94	0.49
1:B:280:VAL:HG13	1:B:334:ALA:HB2	1.95	0.49
1:B:336:ASN:C	1:B:338:LYS:H	2.21	0.48
1:B:294:VAL:HB	1:B:318:ILE:HG23	1.96	0.48
1:B:331:VAL:HG13	1:B:343:GLN:HB3	1.95	0.48
2:A:211:LYS:HE3	2:A:211:LYS:HB2	1.62	0.48
2:A:126:ASP:OD1	2:A:126:ASP:N	2.47	0.48
1:B:284:ILE:HG23	1:B:285:ASP:H	1.79	0.47
1:B:248:PRO:HA	1:B:344:ALA:HA	1.95	0.47
2:A:239:ARG:HB2	2:A:239:ARG:HH11	1.80	0.47
2:A:186:ARG:HG2	2:A:187:SER:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:299:ASN:HB3	1:B:315:ILE:O	2.15	0.47
2:A:145:GLU:HA	2:A:233:ARG:O	2.14	0.47
1:B:258:PRO:HA	1:B:259:GLY:C	2.40	0.47
2:A:247:ILE:HB	2:A:265:VAL:HB	1.97	0.47
1:B:256:LYS:HA	1:B:256:LYS:HE2	1.96	0.47
2:A:181:ARG:HG2	2:A:202:GLU:O	2.14	0.46
1:B:55:LYS:NZ	2:A:188:GLU:HG3	2.31	0.46
1:B:107:ASN:OD1	1:B:107:ASN:N	2.47	0.46
2:A:276:TRP:CD1	2:A:296:LEU:HB2	2.51	0.46
2:A:95:ARG:HB3	2:A:98:ARG:HD3	1.97	0.45
2:A:206:GLU:O	2:A:209:GLN:HB2	2.16	0.45
2:A:239:ARG:HD3	2:A:239:ARG:HA	1.73	0.45
1:B:307:THR:HG23	1:B:309:ASP:OD2	2.17	0.45
2:A:490:VAL:HG22	2:A:493:LYS:HG3	1.97	0.45
1:B:87:LEU:HD12	1:B:87:LEU:HA	1.86	0.45
1:B:33:ARG:NH2	1:B:48:PRO:HG3	2.32	0.45
1:B:264:ILE:HD12	1:B:265:PRO:O	2.16	0.45
1:B:167:PHE:HB2	1:B:171:VAL:HG11	1.97	0.45
2:A:59:ARG:HA	2:A:60:PRO:HD3	1.77	0.44
2:A:65:ASN:HB2	2:A:104:GLU:HG3	1.98	0.44
1:B:215:THR:OG1	1:B:224:HIS:ND1	2.33	0.44
1:B:184:ILE:HG23	1:B:187:PHE:CD1	2.53	0.44
2:A:75:ARG:C	2:A:76:PHE:HD1	2.25	0.44
2:A:277:MET:HE2	2:A:310:VAL:HG21	1.99	0.44
1:B:75:GLN:O	1:B:76:ASP:HB2	2.17	0.44
1:B:144:PHE:CD1	1:B:228:THR:HB	2.52	0.44
1:B:244:GLN:O	1:B:268:VAL:HA	2.17	0.44
2:A:47:VAL:HG22	2:A:92:GLN:HG3	1.99	0.44
2:A:181:ARG:HH22	2:A:208:ASP:CG	2.26	0.43
2:A:133:PRO:HA	2:A:157:SER:O	2.18	0.43
1:B:27:TRP:O	2:A:153:LEU:HD11	2.18	0.43
2:A:28:GLU:N	2:A:28:GLU:OE1	2.51	0.43
1:B:195:MET:HE3	1:B:195:MET:HB3	1.90	0.43
1:B:167:PHE:HB2	1:B:171:VAL:CG1	2.49	0.42
2:A:186:ARG:HG3	2:A:195:ILE:HD11	2.01	0.42
2:A:75:ARG:HG2	2:A:93:PRO:HD2	2.01	0.42
2:A:257:GLY:HA2	2:A:300:ASP:HA	2.01	0.42
2:A:429:ARG:NH1	2:A:449:GLU:OE2	2.52	0.42
2:A:75:ARG:HH12	2:A:99:ASP:CG	2.27	0.42
1:B:185:VAL:HG23	1:B:186:ASP:H	1.83	0.42
2:A:278:LEU:HD13	2:A:307:TYR:CE2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:429:ARG:HD3	2:A:449:GLU:HG2	2.02	0.42
1:B:79:LEU:H	1:B:79:LEU:HG	1.65	0.41
1:B:179:LYS:HG3	1:B:210:TYR:CZ	2.55	0.41
2:A:364:GLN:HG2	2:A:376:GLU:HG2	2.02	0.41
1:B:155:ILE:HA	1:B:199:PHE:O	2.19	0.41
1:B:82:PRO:HG2	2:A:291:ILE:HD13	2.00	0.41
1:B:138:PHE:HE2	1:B:178:TYR:CG	2.39	0.41
1:B:168:PRO:HD2	1:B:171:VAL:HG12	2.01	0.41
2:A:271:MET:HA	2:A:272:PRO:HD3	1.89	0.41
1:B:257:GLU:OE1	1:B:257:GLU:N	2.52	0.41
2:A:173:VAL:HG11	2:A:199:LEU:HD11	2.03	0.41
1:B:250:ASP:CG	1:B:345:ALA:HB3	2.46	0.41
2:A:364:GLN:HB2	2:A:399:ARG:HB2	2.03	0.41
2:A:470:VAL:HA	2:A:473:TRP:CD1	2.56	0.41
1:B:142:MET:HE2	1:B:142:MET:HB3	1.85	0.41
1:B:25:ASP:OD1	2:A:183:LYS:NZ	2.31	0.41
1:B:150:TYR:OH	1:B:274:MET:HG3	2.20	0.41
2:A:251:ASN:OD1	2:A:323:GLN:HB2	2.21	0.41
2:A:462:TYR:HA	2:A:496:SER:O	2.21	0.41
1:B:294:VAL:HG12	1:B:320:LYS:O	2.21	0.40
2:A:233:ARG:HD3	2:A:233:ARG:HA	1.94	0.40
2:A:442:LEU:HD21	2:A:483:ILE:HD11	2.02	0.40
2:A:61:LYS:O	2:A:107:ALA:HA	2.21	0.40
2:A:209:GLN:HG3	2:A:231:TYR:HA	2.03	0.40
1:B:191:LEU:HD12	1:B:192:PRO:HD2	2.03	0.40
2:A:310:VAL:HG22	2:A:319:GLU:HG2	2.03	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:104:GLU:OE2	2:A:485:THR:OG1[2_655]	2.19	0.01

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	320/339 (94%)	288 (90%)	29 (9%)	3 (1%)	14	42
2	A	489/491 (100%)	476 (97%)	12 (2%)	1 (0%)	43	70
All	All	809/830 (98%)	764 (94%)	41 (5%)	4 (0%)	24	55

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	289	PRO
2	A	191	GLY
1	B	242	PRO
1	B	258	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	300/315 (95%)	242 (81%)	58 (19%)	1	6
2	A	428/428 (100%)	382 (89%)	46 (11%)	6	24
All	All	728/743 (98%)	624 (86%)	104 (14%)	3	14

All (104) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	34	GLN
1	B	35	ILE
1	B	37	VAL
1	B	44	ARG
1	B	49	LEU
1	B	51	GLU
1	B	52	HIS
1	B	57	ASN
1	B	66	LEU

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Mol	Chain	Res	Type
1	B	67	THR
1	B	69	ILE
1	B	79	LEU
1	B	80	GLU
1	B	83	ILE
1	B	87	LEU
1	B	91	ARG
1	B	93	SER
1	B	99	LEU
1	B	107	ASN
1	B	113	THR
1	B	116	LEU
1	B	119	THR
1	B	123	SER
1	B	129	LEU
1	B	132	VAL
1	B	135	ASP
1	B	155	ILE
1	B	159	THR
1	B	162	ASN
1	B	179	LYS
1	B	182	THR
1	B	185	VAL
1	B	186	ASP
1	B	206	ASN
1	B	209	ASN
1	B	214	VAL
1	B	215	THR
1	B	225	LEU
1	B	238	LYS
1	B	245	ILE
1	B	247	SER
1	B	253	VAL
1	B	262	LEU
1	B	264	ILE
1	B	267	LYS
1	B	268	VAL
1	B	274	MET
1	B	277	HIS
1	B	281	TRP
1	B	284	ILE
1	B	288	LYS

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Mol	Chain	Res	Type
1	B	296	ILE
1	B	302	VAL
1	B	308	GLU
1	B	313	THR
1	B	322	THR
1	B	326	LEU
1	B	333	HIS
2	A	43	VAL
2	A	44	SER
2	A	47	VAL
2	A	51	ILE
2	A	61	LYS
2	A	67	LYS
2	A	70	LYS
2	A	75	ARG
2	A	82	ASP
2	A	95	ARG
2	A	104	GLU
2	A	117	SER
2	A	125	GLU
2	A	126	ASP
2	A	130	ARG
2	A	137	MET
2	A	141	LEU
2	A	145	GLU
2	A	148	ARG
2	A	163	GLU
2	A	164	ILE
2	A	165	THR
2	A	168	LYS
2	A	175	THR
2	A	177	ASN
2	A	181	ARG
2	A	184	GLN
2	A	187	SER
2	A	195	ILE
2	A	209	GLN
2	A	213	GLU
2	A	222	THR
2	A	234	GLU
2	A	235	LEU
2	A	236	ARG

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Mol	Chain	Res	Type
2	A	239	ARG
2	A	251	ASN
2	A	254	ILE
2	A	295	VAL
2	A	312	MET
2	A	321	ILE
2	A	323	GLN
2	A	327	LYS
2	A	348	LEU
2	A	435	MET
2	A	490	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	62	HIS
1	B	139	ASN
1	B	147	HIS
1	B	244	GLN
2	A	184	GLN
2	A	229	ASN
2	A	482	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

7 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	401	1	14,14,15	0.40	0	17,19,21	0.76	1 (5%)
3	NAG	B	405	1	14,14,15	1.10	2 (14%)	17,19,21	0.60	0
3	NAG	A	601	2	14,14,15	0.29	0	17,19,21	0.44	0
3	NAG	B	404	1	14,14,15	1.18	1 (7%)	17,19,21	0.86	1 (5%)
3	NAG	A	602	2	14,14,15	0.35	0	17,19,21	0.64	1 (5%)
3	NAG	B	403	1	14,14,15	0.59	0	17,19,21	0.65	0
3	NAG	B	402	1	14,14,15	0.93	1 (7%)	17,19,21	1.14	1 (5%)

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	401	1	-	1/6/23/26	0/1/1/1
3	NAG	B	405	1	-	1/6/23/26	0/1/1/1
3	NAG	A	601	2	-	1/6/23/26	0/1/1/1
3	NAG	B	404	1	-	2/6/23/26	0/1/1/1
3	NAG	A	602	2	-	2/6/23/26	0/1/1/1
3	NAG	B	403	1	-	0/6/23/26	0/1/1/1
3	NAG	B	402	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	404	NAG	O5-C1	-4.02	1.36	1.43
3	B	402	NAG	O5-C1	3.28	1.49	1.43
3	B	405	NAG	C1-C2	2.79	1.56	1.52
3	B	405	NAG	O5-C1	-2.70	1.39	1.43

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
3	B	402	NAG	C1-O5-C5	4.34	118.01	112.19
3	B	401	NAG	C1-O5-C5	2.70	115.80	112.19
3	B	404	NAG	C1-O5-C5	-2.52	108.81	112.19
3	A	602	NAG	C1-O5-C5	2.13	115.05	112.19

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	602	NAG	C4-C5-C6-O6
3	A	602	NAG	O5-C5-C6-O6
3	A	601	NAG	O5-C5-C6-O6
3	B	404	NAG	C4-C5-C6-O6
3	B	405	NAG	O5-C5-C6-O6
3	B	404	NAG	O5-C5-C6-O6
3	B	401	NAG	C4-C5-C6-O6

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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	B	322/339 (94%)	0.15	5 (1%)	70	52	42, 89, 220, 285	0
2	A	491/491 (100%)	0.10	12 (2%)	59	40	44, 101, 180, 246	0
All	All	813/830 (97%)	0.12	17 (2%)	63	44	42, 98, 208, 285	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	A	484	THR	3.0
2	A	483	ILE	2.6
1	B	264	ILE	2.6
2	A	443	VAL	2.5
1	B	154	GLY	2.4
2	A	406	ILE	2.3
2	A	470	VAL	2.2
2	A	492	GLN	2.2
1	B	79	LEU	2.1
1	B	56	TYR	2.1
2	A	373	PRO	2.1
2	A	474	MET	2.1
2	A	462	TYR	2.1
2	A	127	GLN	2.0
1	B	258	PRO	2.0
2	A	438	SER	2.0
2	A	495	TYR	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 [i](#)

There are no oligosaccharides 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. 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	B-factors($\text{\AA}^2$)	Q<0.9
3	NAG	B	402	14/15	0.74	0.11	113,128,132,135	0
3	NAG	A	602	14/15	0.75	0.11	124,138,141,144	0
3	NAG	B	401	14/15	0.76	0.15	112,122,126,127	0
3	NAG	B	405	14/15	0.79	0.13	105,108,130,141	0
3	NAG	B	403	14/15	0.80	0.11	72,88,96,102	0
3	NAG	A	601	14/15	0.82	0.14	136,145,157,163	0
3	NAG	B	404	14/15	0.82	0.10	98,102,128,131	0

6.5 Other polymers [i](#)

There are no such residues in this entry.